Advanced Mathematical Programming

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Contents

I Setting the scene **11**

1 Introduction **13**

1.1 Some easy examples . . . 14

1.2 Real vs. didactical problems . . . 16

1.3 Solutions of the easy problems . . . 16

1.3.1 Investments . . . 17

1.3.1.1 Missing trivial constraints . . . 17

1.3.1.2 No numbers in formulations . . . 17

1.3.1.3 Formulation generality . . . 17

1.3.1.4 Technical constraints . . . 18

1.3.2 Blending . . . 18

1.3.2.1 Decision variables . . . 18

1.3.2.2 Parameters . . . 19

1.3.2.3 Objective function . . . 20

1.3.2.4 Constraints . . . 20

1.3.2.5 Ambiguities in the text description . . . 21

1.3.2.6 Unused textual elements . . . 21

1.3.3 Assignment . . . 21

1.3.3.1 Decision variables . . . 22

1.3.3.2 Objective function . . . 22

1.3.3.3 Constraints . . . 23

1.3.4 Demands . . . 23

1.3.5 Multi-period production . . . 24

1.3.6 Capacities . . . 25

1.3.7 Demands, again . . . 25
1.3.8 Rostering . . . 26
1.3.9 Covering, set-up costs and transportation . . . 26
1.3.10 Circle packing . . . 28
1.3.11 Distance geometry . . . 29

2 The language of optimization 31

2.1 MP as a language . . . 31
2.1.1 The arithmetic expression language . . . 32
2.1.1.1 Semantics . . . 33
2.1.2 MP entities . . . 33
2.1.2.1 Parameters . . . 33
2.1.2.2 Decision variables . . . 33
2.1.2.3 Objective functions . . . 34
2.1.2.4 Functional constraints . . . 34
2.1.2.5 Implicit constraints . . . 34
2.1.3 The MP formulation language . . . 34
2.1.3.1 Solvers as interpreters . . . 35
2.1.3.2 Imperative and declarative languages . . . 35
2.2 Definition of MP and basic notions . . . 36
2.2.1 Certifying feasibility and boundedness . . . 37
2.2.2 Cardinality of the $\overline{\mathbb{MP}}$ class . . . 37
2.2.3 Reformulations . . . 38
2.2.3.1 Minimization and maximization . . . 38
2.2.3.2 Equation and inequality constraints . . . 38
2.2.3.3 Right-hand side constants . . . 38
2.2.3.4 Symbolic transformations . . . 39
2.2.4 Coarse systematics . . . 39
2.2.5 Solvers state-of-the-art . . . 39
2.2.6 Flat versus structured formulations . . . 40
2.2.6.1 Modelling languages . . . 41
2.2.7 Some examples . . . 42

2.2.7.1 Diet problem . . . 42
2.2.7.2 Transportation problem . . . 42
2.2.7.3 Network flow . . . 43
2.2.7.4 Set covering problem . . . 43
2.2.7.5 Multiprocessor scheduling with communication delays . . . 43
2.2.7.5.1 The infamous "big M" . . . 45
2.2.7.6 Graph partitioning . . . 46
2.2.7.7 Haverly's Pooling Problem . . . 47
2.2.7.8 Pooling and Blending Problems . . . 48
2.2.7.9 Euclidean Location Problems . . . 48
2.2.7.10 Kissing Number Problem . . . 49

3 The AMPL language 51

3.1 The workflow . . . 51
3.2 Input files . . . 52
3.3 Basic syntax . . . 52
3.4 LP example . . . 53
3.4.1 The `.mod` file . . . 53
3.4.2 The `.dat` file . . . 55
3.4.3 The `.run` file . . . 56
3.5 The imperative sublanguage . . . 57

II Computability and complexity 59

4 Computability 61

4.1 A short summary . . . 61
4.1.1 Models of computation . . . 61
4.1.2 Decidability . . . 62
4.2 Solution representability . . . 62
4.2.1 The real RAM model . . . 62
4.2.2 Approximation of the optimal objective function value . . . 62
4.2.3 Approximation of the optimal solution . . . 63
4.2.4 Representability of algebraic numbers . . . 63

4.2.4.1 Solving polynomial systems of equations 63
4.2.4.2 Optimization using Gröbner bases 64
4.3 Computability in MP 64
4.3.1 Polynomial feasibility in continuous variables 64
4.3.1.1 Quantifier elimination 65
4.3.1.2 Cylindrical decomposition 65
4.3.2 Polynomial feasibility in integer variables 66
4.3.2.1 Undecidability versus incompleteness 66
4.3.2.2 Hilbert's 10th problem 67
4.3.3 Universality 68
4.3.4 What is the cause of MINLP undecidability? 68
4.3.5 Undecidability in MP 69

5 Complexity **73**
5.1 Some introductory remarks 73
5.1.1 Problem classes 73
5.1.1.1 The class **P** 73
5.1.1.2 The class **NP** 74
5.1.2 Reductions 74
5.1.2.1 The hardest problem in the class 75
5.1.2.2 The reduction digraph 77
5.1.2.3 Decision vs. optimization 77
5.1.2.4 When the input is numeric 77
5.2 Complexity of solving general MINLP 78
5.3 Quadratic programming 79
5.3.1 **NP**-hardness 79
5.3.1.1 Strong **NP**-hardness 79
5.3.2 **NP**-completeness 80
5.3.3 Box constraints 80
5.3.4 Trust region subproblems 81
5.3.5 Continuous Quadratic Knapsack 81
5.3.5.1 Convex QKP 82

5.3.6 The Motzkin-Straus formulation . . . 82
5.3.6.1 QP on a simplex . . . 83
5.3.7 QP with one negative eigenvalue . . . 83
5.3.8 Bilinear programming . . . 84
5.3.8.1 Products of two linear forms . . . 84
5.3.9 Establishing local minimality . . . 85
5.4 General Nonlinear Programming . . . 86
5.4.1 Verifying convexity . . . 87
5.4.1.1 The copositive cone . . . 87

III Basic notions 91

6 Fundamentals of convex analysis 93
6.1 Convex analysis . . . 93
6.2 Conditions for local optimality . . . 95
6.2.1 Equality constraints . . . 96
6.2.2 Inequality constraints . . . 97
6.2.3 General NLPs . . . 101
6.3 Duality . . . 102
6.3.1 The Lagrangian function . . . 102
6.3.2 The dual of an LP . . . 102
6.3.2.1 Alternative derivation of LP duality . . . 103
6.3.2.2 Economic interpretation of LP duality . . . 103
6.3.3 Strong duality . . . 103

7 Fundamentals of Linear Programming 105
7.1 The Simplex method . . . 105
7.1.1 Geometry of Linear Programming . . . 106
7.1.2 Moving from vertex to vertex . . . 108
7.1.3 Decrease direction . . . 109
7.1.4 Bland's rule . . . 109
7.1.5 Simplex method in matrix form . . . 110
7.1.6 Sensitivity analysis . . . 111

7.1.7 Simplex variants 111
7.1.7.1 Revised Simplex method 111
7.1.7.2 Two-phase Simplex method 111
7.1.7.3 Dual Simplex method 111
7.1.8 Column generation 112
7.2 Polytime algorithms for LP 112
7.3 The ellipsoid algorithm 112
7.3.1 Equivalence of LP and LSI 113
7.3.1.1 Reducing LOP to LI 113
7.3.1.1.1 Addressing feasibility 113
7.3.1.1.2 Instance size 113
7.3.1.1.3 Bounds on bfs components 113
7.3.1.1.4 Addressing unboundedness 114
7.3.1.1.5 Approximating the optimal bfs 114
7.3.1.1.6 Approximation precision 114
7.3.1.1.7 Approximation rounding 114
7.3.1.2 Reducing LI to LSI 115
7.3.2 Solving LSIs in polytime 115
7.4 Karmarkar's algorithm 116
7.5 Interior point methods 117
7.5.1 Primal-Dual feasible points 118
7.5.2 Optimal partitions 119
7.5.3 A simple IPM for LP 120
7.5.4 The Newton step 120

8 Fundamentals of Mixed-Integer Linear Programming 121
8.1 Total unimodularity 121
8.2 Cutting planes 123
8.2.1 Separation Theory 124
8.2.2 Chvátal Cut Hierarchy 124
8.2.3 Gomory Cuts 125
8.2.3.1 Cutting plane algorithm 125

8.2.4 Disjunctive cuts . . . 129
8.2.5 Lifting . . . 130
8.2.6 RLT cuts . . . 130
8.3 Branch-and-Bound . . . 131
8.3.1 Example . . . 132
8.3.2 Branch-and-Cut . . . 133
8.3.3 Branch-and-Price . . . 133
8.4 Lagrangean relaxation . . . 133

9 Fundamentals of Nonlinear Programming 137
9.1 Sequential quadratic programming . . . 137
9.2 The structure of GO algorithms . . . 138
9.2.1 Deterministic vs. stochastic . . . 138
9.2.2 Algorithmic reliability . . . 139
9.2.3 Stochastic global phase . . . 139
9.2.3.1 Sampling approaches . . . 139
9.2.3.2 Escaping approaches . . . 140
9.2.3.3 Mixing sampling and escaping . . . 140
9.2.3.4 Clustering starting points . . . 140
9.2.4 Deterministic global phase . . . 141
9.2.4.1 Fathoming . . . 143
9.2.5 Example of solution by B&S . . . 144
9.3 Variable Neighbourhood Search . . . 146
9.4 Spatial Branch-and-Bound . . . 147
9.4.1 Bounds tightening . . . 148
9.4.1.1 Optimization-based bounds tightening . . . 148
9.4.1.2 Feasibility-based bounds tightening . . . 149
9.4.2 Choice of region . . . 149
9.4.3 Convex relaxation . . . 150
9.4.3.1 Reformulation to standard form . . . 150
9.4.3.2 Convexification . . . 152
9.4.4 Local solution of the original problem . . . 153

9.4.4.1 Branching on additional variables 153

9.4.4.2 Branching on original variables 153

9.4.5 Branching 154

IV Advanced Mathematical Programming 155

Part I

Setting the scene

Chapter 1

Introduction

The Dean, in his office, is receiving a delegation from a prominent firm, with the aim of promoting a partnership between the two institutions. The goal is to pair a technical contact from the firm with a faculty member from the university. The hope is that the two will talk and find something interesting to do together. This might induce the firm to give some money to the university. It's a well-tested endeavour, which invariably ends up generating a "framework contract" (which mentions no money whatsoever), followed, sometimes, by more substantial contracts.

There's a physics professor who extols the virtues of a new revolutionary battery for storing energy. There's a mathematics professor who entered the now burgeoning field of "data science" and talks about how it took them two years to "clean" a certain vendor database, after which they could apparently forecast all future sales to a 1% precision. Another professor from the computer science department says "me too". When it's my turn, as usual, I mentally groan, and brace for impact.

— And now we come to Prof. Liberti, says the Dean with his usual sneer, for he's heard the communication failure of my trade too many times for him to be optimistic about it.

— We are listening, Prof. Liberti, says the CTO of the firm, tell us what you do. We're sure your research will be very useful to our firm.

— Well, ehm. OK. What I do is called "mathematical programming". It is a language for describing and then solving optimization problems.

— Interesting. And tell me, Prof. Liberti: what type of problems do you work on?

— All, really. Any optimization problem can be modelled as a mathematical program.

— Yes, yes of course. But could you tell us exactly *what* this mathematical thingy can be applied to?

— But this is exactly what I'm trying to say: it is a language, you can use it to describe *any* problem! So the application field really does not matter!

This can go on and on, with the industry leader who tries to extract an application field name out of me (optimal power flow in electrical grids, vehicle routing on road/rail networks, economic planning, shortest paths in urban settings, facility location in view of minimizing costs, crew rostering in the airline business, pricing of goods and services based on market demand, mixing and transforming materials, scheduling of tasks on processors, packing of crates/boxes in variously shaped containers, packing of said containers in a ship, docking the damn ships in the port, strategic decisions to address market segmentation, retrieving a clean signal from a noisy one, assigning personnel to different jobs, analysing data by clustering points, finding the shape of proteins and other molecules, aligning strands of RNA or DNA so that they match as closely as possible, and many, many more), while I attempt to wiggle out of

having an application label slapped on my work.

Once, when I was younger and more naive, I figured I might as well make the industrialist happy. During one of these meetings, after a couple of iterations of "what application field do you work on?" followed by "this is really the wrong question", I had decided to break the monotony and hopelessness of the exchange by stating I work on shortest paths in road networks.

— Ah, this is fantastic! came the reply, but unfortunately we don't do any of that.

This had two adverse effects: the first, and less serious, was that the industrialist did not wish to work with me. The second, much more damaging, was that I had inadvertently convinced the Dean that I worked on shortest paths. So he never invited me to any further industry meeting unless the words "shortest paths" appeared prominently in the firm's product descriptions.

On the other hand, the "stalling choice" I adopt today, while it keeps me invited to meetings with the Dean, is no less disastrous with industry leaders. At one point I thought to myself, I'll try and collaborate with firms which already employ an operations research team, who'll be obviously familiar with mathematical programming. So, additionally to the "Dean scenario", I sometimes also went to visit operations research teams in large firms directly. This approach elicited the polite answer "thank you, but we already know how to do that", followed by vague promises of future possible scientific collaborations, never actually pursued.

When the top boss of a large firm, which includes an operations research team internally, asks my Dean about mathematical programming or operations research, I immediately get called, and the meeting itself is usually successful. Unfortunately, however, the very need for hiring outside hands instead of relying on the internal team means that there is a disagreement between the latter and their top boss. I am henceforth tasked to working with the internal team, which means that I rely on their availability for data, explanations, and so on; and then I am supposed to deliver what they could not. Quite aside from the difficulty of producing better results than a whole team of specialists, the real issue is that the internal team have all the motivations to sabotage the outsider's work, so it takes fairly advanced diplomatic skills to actually produce something.

To recap: mathematical programming is a general framework for describing and solving optimization problems. It is not only theoretical: quite on the contrary, it applies to practically everything. Its methods are used in engineering, chemistry, biology, mathematics, economics, psychology and even some social and human sciences. As far as communication is concerned, this polyvalence is its worst weakness. The generalization and efficiency of some mathematical programming algorithms, on the other hand, boggle the mind: it seems they can solve every optimization problem under the sun — which is exactly what they are meant to do.

1.1 Some easy examples

Look at the list of problems below. We start from a bank and its investment strategy. There follows a refinery wishing to make fuels from a blend of crudes. We then look at pairing jobs to machines in a production environment. We continue with a firm deciding some expenses to satisfy demands. Then there is a firm planning production and storage to match sales forecasts. Then a network operator deciding its data routing on two possible backbone links. Then a firm confronted with hiring and training decisions in view of demands. Then a hospital rostering nurses. The ninth problem requires decision on three issues: how to cover a set of customers with facilities, how to deal with a one-time cost, and how to transport the goods from the built facilities to the customers. Then there is a beer crate packing operation. Lastly, we look at a protein structure problem.

1. *Investments.* A bank needs to invest C gazillion dollars, and focuses on two types of investments: one, imaginatively called (a), guarantees a 15% return, while the other, riskier and called, surprise

surprise, (b), is set to a 25%. At least one fourth of the budget C must be invested in (a), and the quantity invested in (b) cannot be more than double the quantity invested in (a). How do we choose how much to invest in (a) and (b) so that revenue is maximized?

2. *Blending.* A refinery produces two types of fuel by blending three types of crude. The first type of fuel requires at most 30% of crude 1 and at least 40% of crude 2, and retails at 5.5EUR per unit. The second type requires at most 50% of crude 1 and at least 10% of crude 2, and retails at 4.5EUR. The availability of crude 1 is 3000 units, at a unit cost of 3EUR; for crude 2 we have 2000 units and a unit cost of 6EUR; for crude 3, 4000 and 4EUR. How do we choose the amounts of crude to blend in the two fuels so as to maximize net profit?

3. *Assignment.* There are n jobs to be dispatched to m identical machines. The j-th job takes time p_j to complete. Jobs cannot be interrupted and resumed. Each machine can only process one job at a time. Assign jobs to machines so the whole set of jobs is completed in the shortest possible time.

4. *Demands.* A small firm needs to obtain a certain number of computational servers on loan. Their needs change every month: 9 in January, 5 in February, 7 in March, 9 in April. The loan cost depends on the length: 200EUR for one month, 350 for two, and 450 for three. Plan the needed loans in the cheapest possible way.

5. *Multi-period production.* A manufacturing firm needs to plan its activities on a 3-month horizon. It can produce 110 units at a cost of 300$ each; moreover, if it produces at all in a given month, it must produce at least 15 units per month. It can also subcontract production of 60 supplementary units at a cost of 330% each. Storage costs amount to 10$ per unit per month. Sales forecasts for the next three months are 100, 130, and 150 units. Satisfy the demand at minimum cost.

6. *Capacities.* A total of n data flows must be routed on one of two possible links between a source and a target node. The j-th data flow requires c_j Mbps to be routed. The capacity of the first link is 1Mbps; the capacity of the second is 2Mbps. Routing through the second link, however, is 30% more expensive than routing through the first. Minimize the routing cost while respecting link capacities.

7. *Demands, again.* A computer service firm estimates the need for service hours over the next five months as follows: 6000, 7000, 8000, 9500, 11000. Currently, the firm employs 50 consultants: each works at most 160 hours/month, and is paid 2000EUR/month. To satisfy demand peaks, the firm must recruit and train new consultants: training takes one month, and 50 hours of supervision work of an existing consultant. Trainees are paid 1000EUR/month. It was observed that 5% of the trainees leave the firm for the competition at the end of training. Plan the activites at minimum cost.

8. *Rostering.* A hospital needs to roster nurses: each can work 5 consecutive days followed by two days of rest. The demand for each day of the week (mon-sun) are: 11, 9, 7, 12, 13, 8, 5. Plan the roster in order to minimize the number of nurses.

9. *Covering, set-up costs and transportation.* A distribution firm has identified n candidate sites to build depots. The i-th candidate depot, having given capacity b_i, costs f_i to build (for $i \leq n$). There are m stores to be supplied, each having a minimum demand d_j (for $j \leq n$). The cost of transporting one unit of goods between depot i and store j is c_{ij}. Plan openings and transportation so as to minimize costs.

10. *Circle packing.* Maximize the number of cylindrical crates of beer (each having 20cm radius) which can be packed in the carrying area (6m long and 2.5m wide) of a pick-up truck.

11. *Molecular distance geometry.* A protein with n atoms is examined with a nuclear magnetic resonance experiment, which determines all and only the distances d_{ij} between the pairs of atoms closer than 5Å. Decide the atomic positions that best satisfy these distance data.

1.2 Real vs. didactical problems

What is the the most prominent common feature of the problems in Sect. 1.1? To a student, they possibly contribute to raise a state of mind between boredom and despair. To a professor, it is the fact that they can all be formulated by means of mathematical programming. To a practitioner, the fact that they are *all invented for the purpose of teaching.* No real world problem ever presents itself as clearly as the problems above.

Should any reader of this text ever become a mathematical programming consultant, let her or him be aware of this fact: on being assigned a task by your client, *you shall be given almost no explanation and a small*[1] *portion of incomprehensible data.* The sketch below is sadly much closer to the truth than one might imagine.

— Dr. Liberti, thank you for visiting the wonderful, magnificent firm I preside. I'll come straight to the point: we have a problem we want you to solve.

— Why, certainly sir; what is the problem?

— Exactly this thing we want you to solve.

— I understand you want me to solve the problem; but what *is* it?

— My dear fellow, if we knew what the problem was, we very possibly wouldn't need your help! Now off you go and do your mathemathingy trick or whatever it is that you do, and make us rich! Oh and by the way we'll try and withhold any payment for your services with any excuse we deem fit to use. And if forced by law to actually pay you (God forbid!), we'll at least delay the payment indefinitely. You won't mind, won't you?

Although it is usually not quite as bad, the "definition" of a problem, in an industrialist's view, is very often a partial set of database tables, with many essential columns missing for nondisclosure (or forgetfulness, or loss) purposes, accompanied by an email reading more or less as follows. *These 143 tables are all I found to get you going. I don't have any further time for you over the next three months. I don't know what the tables contain, nor what most of the column labels mean, but I'm almost sure that the column labeled* `t5y/3R` *denotes a complicated function – I forget which one – of the estimated contribution of the product indexed by the row to our fiscal imposition in 2005, scaled by a 2.2% inflation, well more or less. Oh, and we couldn't give you the unit costs or profits, since of course they are confidential. Your task is to optimize our revenues. You have three days. Best of luck.*

Coming back to the common features of the list of problems in Sect. 1.1, the majority concern industry. This is not by chance: most of the *direct* practical value provided by mathematical programming is to technological processes. In the last twenty years, however, the state-of-the-art has advanced enough so that mathematical programming methods now feature prominently as substeps of complex algorithmic frameworks designed to address systemic issues. This provides an indirect, though no less important, value to the real world.

1.3 Solutions of the easy problems

We now provide solutions for all of the problems listed in Sect. 1.1. Some of these solutions are heavily commented: I am hoping to address many of the issues raised by students when they learn how to model by mathematical programming.

[1] Or huge, the net effect is the same.

1.3.1 Investments

We start with a simplistic bank wishing to invest an unknown, but given, budget C in two types of investments, (a) and (b). Let x_a denote the part of the budget C invested in (a), and x_b the same for (b): their relation is $x_a + x_b = C$. The revenue is $1.15x_a + 1.25x_b$. The "technical constraints" require that $x_a \geq \frac{1}{4}C$ and $x_b \leq 2x_a$. This might appear to be all: written properly, it looks like the following formulation.

$$\left.\begin{array}{rrcl} \max\limits_{x_a,x_b} & 1.15x_a + 1.25x_b & & \\ & x_a + x_b & = & C \\ & x_a & \geq & \frac{1}{4}C \\ & 2x_a - x_b & \geq & 0. \end{array}\right\}$$

1.3.1.1 Missing trivial constraints

Now, it is easy to see that $x_a = C + 1$ and $x_b = -1$ satisfies all the constraints, but what is the meaning of a negative part of a budget? This should make readers realize we had left out an apparently trivial, but crucial piece of information: $x_a \geq 0$ and $x_b \geq 0$.

Like all programming, mathematical programming is also subject to bugs: in our brains, the "part of a budget" is obviously nonnegative, but this is a meaning corresponding only to the natural language description of the problem. When we switch to formal language, anything not explicitly stated is absent: everything must be laid out explicitly. So the correct formulation is

$$\left.\begin{array}{rrcl} \max\limits_{x_a,x_b} & 1.15x_a + 1.25x_b & & \\ & x_a + x_b & = & C \\ & x_a & \geq & \frac{1}{4}C \\ & 2x_a - x_b & \geq & 0 \\ & x_a, x_b & \geq & 0. \end{array}\right\}$$

We remark that writing $x_a, x_b \geq 0$ (which is formally wrong) is just a short-hand for its correct counterpart $x_a \geq 0 \wedge x_b \geq 0$. Variable restrictions can also be stated under the minimum operator:

$$\max_{x_a,x_b \geq 0} 1.15x_a + 1.25x_b.$$

1.3.1.2 No numbers in formulations

Something else we draw from computer programming is that good coding practices forbid the use of numerical constants within the code itself: they should instead appear at the beginning of the coding section where they are used. Correspondingly, we let $c_a = 1.15$, $c_b = 1.25$, $p = \frac{1}{4}$ and $d = 2$, and rewrite the formulation as follows:

$$\left.\begin{array}{rrcl} \max\limits_{x_a,x_b \geq 0} & c_a x_a + c_b x_b & & \\ & x_a + x_b & = & C \\ & x_a & \geq & pC \\ & dx_a - x_b & \geq & 0. \end{array}\right\} \quad (1.1)$$

1.3.1.3 Formulation generality

Most mathematical writing attempts to set the object of interest in the most general setting. What if we had n possible investments rather than only two? We should rename our variables $x_1, \ldots, x_n$, and our

returns $c_1, \ldots, c_n$, yielding:

$$\left.\begin{array}{rrcl} \max\limits_{x\ge 0} & \sum\limits_{j\le n} c_j x_j & & \\ & \sum\limits_{j\le n} x_j & = & C \\ & x_1 & \ge & pC \\ & dx_1 - x_2 & \ge & 0, \end{array}\right\} \quad (1.2)$$

a formulation which generalizes Eq. (1.1) since the latter is an instance of Eq. (1.2) where $n = 2$. In particular, Eq. (1.1) is the type of formulation that can be an input to a mathematical programming solver (once C is fixed to some value), since it involves a list of (scalar) variables, and a list of (single-row) constraints. Such formulations are called *flat*. On the other hand, Eq. (1.2) involves a variable vector x (of unspecified length n) with some components x_j: it needs to be *flattened* before it can be passed to a solver. This usually involves fixing a parameter (in this case n) to a given value (in this case, 2), with all the consequences this entails on the formulation (see Sect. 2.2.6). Formulations involving parameter symbols and quantifiers are called *structured*.

1.3.1.4 Technical constraints

Lastly, there are two reasons why I called the last two constraints “technical”. The first has to do with the application field: they provide a way to limit the risk of pledging too much money to the second investment. They would not be readily explained in a different field (whereas the objective maximizes revenue, something which is common to practically all fields). The second is that they cannot be generalized with the introduction of the parameter n: they still only concern the first two investments. Of course, had the problem been described as “the quantity invested in anything different from (a) cannot be more than double the quantity invested in (a)”, then the corresponding formulation would have been:

$$\left.\begin{array}{rrcl} \max\limits_{x\ge 0} & \sum\limits_{j\le n} c_j x_j & & \\ & \sum\limits_{j\le n} x_j & = & C \\ & x_1 & \ge & pC \\ \forall 2 \le j \le n & dx_1 - x_j & \ge & 0, \end{array}\right\}$$

an even “more structured” formulation than Eq. (1.2) since it also involves a constraint vector (the last line in the formulation above) including $n - 1$ single-row constraints.

How far is it reasonable to generalize formulations? It depends on the final goals: in the real world of production, one is usually confronted with the problem of improving an existing system, so some of the sizes (e.g. the number of machines) might be fixed, while others (e.g. the demands, which might vary by day or month) are not.

1.3.2 Blending

We come to the world of oil production: when we refuel our vehicles, we are actually buying a blend of different crudes with different qualities. In Sect. 2.2.7.7 we shall look at blending operations with a decision on based on the qualities. Here we look at a simple setting where we have prescriptions on the fraction of each crude to put in the blend for a particular fuel.

1.3.2.1 Decision variables

Although I did not stress this fact in Sect. 1.3.1, the first (and most critical) decision to make when modelling a problem is to define the *decision variables*. In Sect. 1.3.1 it was quite obvious we needed

to decide the parts of budget x_a, x_b, so there was no need to reflect on the concept. Here, however, the natural language description of this problem is sufficiently fuzzy for the issue to deserve some remarks.

- The process of turning a problem description from natural language to formal language is called *modelling*. It involves human intelligence. So far, no-one has ever produced a computer program that is able to automate this task. The difficulty of modelling is that natural language is ambiguous. The natural language description is usually interpreted in each stakeholder's cultural context. When working with a client in the real world, the modelling part might well take the largest part of the meeting time.

- For most problems arising in a didactical setting, my advice is: start modelling by deciding a semi-formal meaning for the decision variables; then try and express the objective function and constraints in terms of these variables. If you cannot, or you obtain impossibly nonlinear expressions, try adding new variables. If you still fail, go back and choose a different set of decision variables. One is generally better off modelling structured formulations rather than flat formulations: so, while you decide the variables, you also have to decide how they are indexed, in what sets these indices range, and what parameters appear in the formulation.

- For real world problems, where information is painstakingly collected during many meetings with the client, the first task is to understand what the client has in mind. Usually, the client tries to describe the whole system in which she works. Naturally, she will give more information about the parts of the system which, to her mind, are most problematic. On the other hand, it might well be that the problematic parts are only symptoms of an issue originating because poor decisions are being taken elsewhere in the system. When you think you have a sufficiently clear picture of the whole system (meaning the interactions between all the parts, and every entity on which decisions can be taken), then you can start modelling as sketched above (think of decision variables first).

In the present case, the hint about "what decision variables to consider" is given in the final question "how do we choose the amounts of crude to blend in the two fuels?" So each choice must refer to crudes and fuels: as such, we need variables indexed over crudes and over fuels. Let us define the set of C of crudes, and the set F of fuels, and then decision variables x_{ij} indicating the fraction of crude $i \in C$ in fuel $j \in F$. What else does the text of the problem tell us? We know that each fuel $j \in F$ has a retail price, which we shall call r_j, and that each crude $i \in C$ has an availability in terms of units, which we shall call a_i, and a unit cost, called c_i.

1.3.2.2 Parameters

The other numeric information given in the text concerns upper or lower bounds to the amount of crude in each fuel. Since we are employing decision variables x_{ij} to denote this amount, we can generalize these lower and upper bounds by a set of intervals $[x^L_{ij}, x^U_{ij}]$, which define the ranges $x^L_{ij} \leq x_{ij} \leq x^U_{ij}$ of each decision variable. Specifically, we have $x^U_{11} = 0.3$, $x^L_{21} = 0.4$, $x^U_{12} = 0.5$ and $x^L_{22} = 0.1$. Unspecified lower bounds must be set to 0 and unspecified upper bounds to 1, since x_{ij} denotes a fraction. We remark that x^L, x^U, r, a are vectors of parameters, which, together with the index sets C, F, will allow us to write a structured formulation.

1.3.2.3 Objective function

Let us see whether this choice of decision variables lets us easily express the objective function: the text says "maximize the net profit". A net profit is the difference between revenue and cost. We have:

$$\begin{aligned} \text{revenue} &= \sum_{j\in F} r_j \, \text{fuel}_j \\ \text{cost} &= \sum_{i\in C} c_i \, \text{crude}_i. \end{aligned}$$

We have not defined decision variables denoting the amounts of produced fuels and crudes used for production. But these can be written in terms of the decision variables x_{ij} as follows:

$$\begin{aligned} \forall j \in F \quad \text{fuel}_j &= \sum_{i\in C} a_i x_{ij} \\ \forall i \in C \quad \text{crude}_i &= a_i \sum_{j\in F} x_{ij}. \end{aligned}$$

So, now, the objective function is:

$$\max \left(\sum_{j\in F} r_j \sum_{i\in C} a_i x_{ij} - \sum_{i\in C} c_i a_i \sum_{j\in F} x_{ij} \right).$$

We can rewrite the objective more compactly as follows:

$$\begin{aligned} & \max \left(\sum_{j\in F} r_j \sum_{i\in C} a_i x_{ij} - \sum_{i\in C} c_i a_i \sum_{j\in F} x_{ij} \right) = \\ = \; & \max \left(\sum_{\substack{i\in C \\ j\in F}} a_i r_j x_{ij} - \sum_{\substack{i\in C \\ j\in F}} a_i c_i x_{ij} \right) = \\ = \; & \max \sum_{\substack{i\in C \\ j\in F}} a_i (r_j - c_i) x_{ij}. \end{aligned}$$

1.3.2.4 Constraints

What about the constraints? As mentioned already, we have range constraints, which we express in tensor form:

$$x \in [x^L, x^U].$$

(The scalar form would need a quantification: $\forall i \in C, j \in F \; x^L_{ij} \leq x_{ij} \leq x^U_{ij}$).

Any other constraint? As in Problem 1 of Sect. 1.1, there is a risk of a bug due to a forgotten trivial constraint: we know that x_{ij} are supposed to indicate a fraction of crude $i \in C$ over all $j \in F$. So, for all $i \in C$, the sum of the fractions cannot exceed 1:

$$\forall i \in C \quad \sum_{j\in F} x_{ij} \leq 1.$$

The complete formulation is as follows:

$$\left.\begin{array}{llrcl}\max\limits_{0\le x\le 1} & \sum\limits_{\substack{i\in C\\ j\in F}} a_i(r_j-c_i)x_{ij} & & & \\ \forall i\in C & & \sum\limits_{j\in F} x_{ij} & \le & 1 \\ & & x & \in & [x^L,x^U]. \end{array}\right\}$$

1.3.1 Exercise
Propose a formulation of this problem based on decision variables y_{ij} is the total amount (rather than the fraction) of crude i in fuel j.

1.3.2.5 Ambiguities in the text description

Unfortunately, whether the problem is didactical or from the real world, human communication is given in natural language, which is prone to ambiguities. Sometimes "almost the same text" yields important, or even dramatic differences in the formulation, as Exercise 1.3.2 shows. If you are working with a client, if in doubt ask — do not be afraid of being considered an idiot for asking multiple times: you will certainly be considered an idiot if you produce the wrong formulation. If the setting is didactical, perhaps the ambiguity is desired, and you have to deal with it as well as you can (you might be judged exactly for the way you dealt with a textual ambiguity).

1.3.2 Exercise
How would the formulation change if, instead of saying "fuel i requires at most/least a given fraction of crude i", the problem said "the amount of crude i must be at most/least a given fraction of fuel j"?

1.3.2.6 Unused textual elements

Recall that the text mentioned three crudes. Although our structured formulations are invariant to the actual number of crudes, the data are such that the third crude is completely irrelevant to the problem. This is a typical feature of modelling real world problems: some (much?) of the information given to the modeller turns out to be irrelevant. The issue is that one may only recognize irrelevance *a posteriori*. During the modelling process, irrelevant information gives a nagging sensation of failure, which a good modeller must learn to recognize and ignore.

In fact, recognizing data irrelevance often provides a valuable feedback to the client: they may use this information in order to simplify and rationalize the dynamics of their system processes. Mostly, the reason why some data are irrelevant, and yet given to the modeller, is that, historically, those data were once relevant. In the present case, perhaps the firm once used all three crude types to produce other types of fuels. Some fuel types may have been discontinued to various reasons, but the database system remained unchanged.

1.3.3 Assignment

When hearing talk of "jobs" and "machines" (or "tasks" and "processors"), a mathematical programmer's brain pathways immediately synthesize the concept of "scheduling". Scheduling problems consist of an assignment (of jobs to machines or tasks to processors) and of a linear order (on jobs on a given machine). But sometimes text descriptions can be misleading, and the problem is simpler than it might appear.

In this case we have identical machines, jobs cannot be interrupted/resumed, each machine can process at most one job at a time, and the requirement is to assign jobs to machines so that the set of jobs is completed "in the shortest possible time". The appearance of the word "shortest time" seems to require

an order of the jobs on each machine: after all completing a set of jobs requires the maximum completion time of the *last job* over all machines.

But now suppose someone already gave you the optimal assignment of jobs to machines: then the working time of each machine would simply be the sum of the completion times of all the jobs assigned to the machine. And the completion times for all jobs would involve minimizing the working time of the slowest machine. This does not involve an order of the jobs assigned to each machine. The problem can therefore be more simply formulated by means of an assignment.

1.3.3.1 Decision variables

Assignment problems are among the fundamental problems which we can solve efficiently. You should therefore learn to recognize and formulate them without even thinking about it.

The beginner's mistake is to define two sets of binary variables x_i (relating to job i) and y_j (relating to machine j) and stating that $x_i y_j$ denotes the assignment of job i to machine j, because "$x_i y_j = 1$ if and only if both are 1". This is a mistake for at least two reasons:

- the definition of a binary decision variable should reflect a boolean condition, whereas here the condition (the assignment of i to j) is related to the product of two variables;
- introducing a product of variables in the formulation introduces a nonlinearity, which yields more difficult formulations to solve. While sometimes nonlinearity is necessary, one should think twice (or more) before introducing it in a formulation.

Nonetheless, the first reason points us towards the correct formulation. Since the boolean condition is "whether job i is assigned to machine j", we need binary decision variables indexed on the pair i, j. So we introduce the index sets J of jobs and the set M of machines, and decision variables $x_{ji} \in \{0, 1\}$ for each $j \in J$ and $i \in M$. The only other formulation parameters are the completion times p_j for each job $j \in J$.

1.3.3.2 Objective function

We can write the working time μ_i of machine $i \in M$ as the sum of the completion times of the jobs assigned to it:

$$\forall i \in M \quad \mu_i = \sum_{j \in J} p_j x_{ji}. \tag{1.3}$$

Now the objective function minimizes the maximum μ_i:

$$\min_{\mu,x} \max_{i \in M} \mu_i.$$

Several remarks are in order.

- New decision variables μ_i (for $i \in M$) were "surreptitiously" introduced. This is a helpful trick in order to help us cope with increasing formulation complexity while modelling. It is clear that μ_i can be eliminated by the formulation by replacing it with the right-hand side (RHS) of Eq. (1.3), so they are inessential. They simply serve the purpose of writing the formulation more clearly.
- The function in Eq. (1.3.3.2) involves both a minimization and a maximization; at first sight, it might remind the reader of a a saddle point search. On closer inspection, the minimization operator occurs over decision variables, but the second only occurs over the indices of a given set: so the maximization does not involve an optimization procedure, but simply the choice of maximum value

amongs $|M|$. It simply means that the function being optimized is $\max_{i\in M}\mu_i$. Such a function is piecewise linear and concave.

- Eq. (1.3.3.2) can be reformulated to a purely linear form by means of an additional decision variable t, as follows:

$$\min_{\mu,x,t} \quad t \tag{1.4}$$

$$\forall i \in M \quad t \geq \mu_i. \tag{1.5}$$

It is clear that t will be at least as large as the maximum μ_i, and by minimizing it we shall select the "min max μ".

1.3.3.3 Constraints

The unmentioned constraint implicit in the term "assignment" is that each job j is assigned to exactly one machine i. This is written formally as follows:

$$\forall j \in J \quad \sum_{i\in M} x_{ji} = 1. \tag{1.6}$$

Eq. (1.6) is known as an *assignment constraint*. It does its work by stating that exactly one variable in the set $\{x_{ji} \mid i \in M\}$ will take value 1, while the rest will take value 0. All that is left to do is to state that the variables are binary:

$$\forall j \in J, i \in M \quad x_{ji} \in \{0,1\}. \tag{1.7}$$

Eq. (1.7), known as *boolean constraint*, are part of the wider class of *integrality constraints*.

The whole formulation can now be written as follows.

$$\left.\begin{array}{rrcl} \min\limits_{x,t} & t & & \\ \forall i \in M & \sum\limits_{j\in J} p_j x_{ji} & \leq & t \\ \forall j \in J & \sum\limits_{i\in M} x_{ji} & = & 1 \\ & x & \in & \{0,1\}^{|J||M|}. \end{array}\right\}$$

1.3.4 Demands

As there are no new difficulties with formulating this problem, I will simply present the formulation in a way I consider concise and clear.

1. **Index sets**
   (a) T: set of month indices ($\{1,2,3,4\}$)
   (b) L: loan lengths in months ($\{1,2,3\}$)
2. **Parameters**
   (a) $\forall t \in T$ let d_t = demand in month t
   (b) $\forall \ell \in L$ let c_ℓ = cost of loan length ℓ
3. **Decision variables**
   $\forall t \in T, \ell \in L$ let $x_{t\ell}$ = number of servers loaned for ℓ months in month t

4. **Objective function**: $\min \sum\limits_{\ell \in L} c_\ell \sum\limits_{t \in T} x_{t\ell}$
5. **Constraints**
demand satisfaction: $\forall t \in T \ \sum\limits_{\substack{\ell \in L \\ \ell < t}} x_{t-\ell,\ell} \geq d_\ell$.

We note that variables indexed by time might involve some index arithmetic (see $x_{t-\ell,\ell}$ in the demand satisfaction constraint).

1.3.5 Multi-period production

1. **Index sets**
   (a) T: set of month indices ($\{1, 2, 3\}$)
   (b) $T' = T \cup \{0\}$
2. **Parameters**
   (a) $\forall t \in T$ let f_t = sales forecasts in month t
   (b) let p = max normal monthly production
   (c) let r = max subcontracted monthly production
   (d) let d = min monthly production level in normal production
   (e) let c^{normal} = unit cost in normal production
   (f) let c^{sub} = unit cost in subcontracted production
   (g) let c^{store} = unit storage cost
3. **Decision variables**
   (a) $\forall t \in T$ let x_t = units produced in month t
   (b) $\forall t \in T$ let $w_t = 1$ iff normal production active in month t, 0 otherwise
   (c) $\forall t \in T$ let y_t = units subcontracted in month t
   (d) $\forall t \in T'$ let z_t = units stored in month t
4. **Objective function**: $\min c^{\text{normal}} \sum\limits_{t \in T} x_t + c^{\text{sub}} \sum\limits_{t \in T} y_t + c^{\text{store}} \sum\limits_{t \in T} z_t$
5. **Constraints**
   (a) demand satisfaction: $\forall t \in T \ x_t + y_t + z_{t-1} \geq f_t$
   (b) storage balance: $\forall t \in T \ x_t + y_t + z_{t-1} = z_t + f_t$
   (c) max production capacity: $\forall t \in T \ x_t \leq p$
   (d) max subcontracted capacity: $\forall t \in T \ x_t \leq r$
   (e) storage is empty when operation starts: $z_0 = 0$
   (f) minimum normal production level:

$$\begin{aligned} \forall t \in T \ x_t &\geq dw_t && (1.8) \\ \forall t \in T \ x_t &\leq pw_t. && (1.9) \end{aligned}$$

   (g) integrality constraints: $\forall t \in T \ w_t \in \{0, 1\}$
   (h) non-negativity constraints: $\forall t \in T \ x, y, z \geq 0$.

We remark that Eq. (1.8)-(1.9) ensure that $x_t \geq 0$ iff $w_t = 1$, and, conversely, $x_t = 0$ iff $w_t = 0$ (also see Sect. 2.2.7.5.1).

1.3.6 Capacities

Note that the text hints to an assignment of data flows to links, as well as to capacity constraints.

1. **Index sets**
   (a) F: set of data flow indices
   (b) L: set of links joining source an target
2. **Parameters**
   (a) $\forall j \in F$ let c_j = required capacity for flow j
   (b) $\forall i \in L$ let k_i = capacity of link i
   (c) $\forall i \in L$ let p_i = cost of routing 1Mbps through link i
3. **Decision variables**
   (a) $\forall i \in L, j \in F$ let $x_{ij} = 1$ iff flow j assigned to link i, 0 otherwise
4. **Objective function**: $\min \sum_{i \in L} p_i \sum_{j \in F} c_j x_{ij}$
5. **Constraints**
   (a) assignment: $\forall j \in F \ \sum_{i \in L} x_{ij} = 1$
   (b) link capacity: $\forall i \in L \ \sum_{j \in F} c_j x_{ij} \leq k_i$

1.3.7 Demands, again

1. **Index sets**
   (a) T: set of month indices
   (b) $T' = T \cup \{0\}$
2. **Parameters**
   (a) $\forall t \in T$ let d_t = service hour demands for month t
   (b) σ = starting number of consultants
   (c) ω = hours/month worked by each consultant
   (d) γ = monthly salary for each consultant
   (e) τ = number of hours needed for training a new consultant
   (f) δ = monthly salary for trainee
   (g) p = percentage of trainees who leave the firm after training
3. **Decision variables**
   (a) $\forall t \in T$ let x_t = number of trainees hired at month t
   (b) $\forall t \in T$ let y_t = number of consultants at month t
4. **Objective function**: $\min \gamma \sum_{t \in T} y_t + \tau \sum_{t \in T} x_t$
5. **Constraints**
   (a) demand satisfaction: $\forall t \in T \ \omega y_t - \tau x_t \geq d_t$

(b) active consultants: $\forall t \in T\ y_{t-1} + px_{t-1} = y_t$

(c) boundary conditions: $y_0 = \sigma$, $x_0 = 0$

(d) integrality and nonnegativity: $x, y \in \mathbb{Z}_+$.

We remark that nowhere does the text state that $x_0 = 0$. But this is a natural condition in view of the fact that hiring does not occur before the need arises, i.e. before the start of the planning horizon T.

1.3.8 Rostering

The text of this problem says nothing about the total number of nurses. In real life, the output of a rostering problem should be a timetable stating that, e.g., nurse John works from Monday to Friday, nurse Mary from Tuesday to Saturday, and so on. In this sense, the timetable assigns nurses to days in a similar way as scheduling assigns jobs to machines. But in this didactical setting the modeller is asked to work without the set of nurses. The trick is to define variables for the number of nurses starting on a certain day. This provides a neat way for decomposing the assignment problem from the resource allocation.

1. **Index sets**
   (a) $T = \{0, \ldots, |T| - 1\}$: set of days indices (periodic set)
2. **Parameters**
   (a) $\forall t \in T$ let d_t = demand for day t
   (b) let α = number of consecutive working days
3. **Decision variables**
   (a) $\forall t \in T$ let x_t = number of nurses starting on day t
4. **Objective function**: $\min \sum\limits_{t \in T} x_t$
5. **Constraints**
   (a) resource allocation: $\forall t \in T\ \sum\limits_{i=0}^{\alpha-1} x_{t+i} \geq d_t$

- Does it make sense to generalize the "days of the week" to a set T? After all, there will never be weeks composed of anything other than seven days. However, some day an administrator might plan the rostering over two weeks, or any other number of days. Moreover, this allows writing indexed variables (such as x_t for $t \in T$) rather than "flat" variables (e.g. a for Monday, b for Tuesday, and so on).
- The set T is interpreted as being a periodic set: it indexes $\{\text{Monday}, \text{Tuesday}, \ldots, \text{Sunday}\}$, where "Monday" obviously follows "Sunday": this is seen in the resource allocation constraints, where $t + i$ must be interpreted as modular arithmetic modulo $|T|$.

1.3.9 Covering, set-up costs and transportation

This problem embodies three important features seen in many real-world supply chain problems: covering a set of stores with facilities, set-up costs (already seen in Sect. 1.3.5, and modelled with the binary variables w), and transportation. While we shall look at covering in Sect. 2.2.7.4 and transportation in

Sect. 2.2.7.2, this problem is typical in that it mixes these aspects together. Most real-world problems I came across end up being modelled by combining variables and constraints from classic examples (covering, packing, network flow, transportation, assignment, ordering and so on) in a smart way.

1. **Index sets**
   (a) $N = \{1, \ldots, n\}$: index set for candidate sites
   (b) $M = \{1, \ldots, m\}$: index set for stores
2. **Parameters**
   (a) $\forall i \in N$ let b_i = capacity of candidate depot i
   (b) $\forall i \in N$ let f_i = cost of building depot i
   (c) $\forall j \in M$ let d_j = minimum demand for store j
   (d) $\forall i \in N, j \in M$ let c_{ij} = cost of transporting one unit from i to j
3. **Decision variables**
   (a) $\forall i \in N, j \in M$ let x_{ij} = units transported from i to j
   (b) $\forall i \in N$ let $y_i = 1$ iff depot i is transported, 0 otherwise
4. **Objective function**: $\min \sum\limits_{i \in N, j \in M} c_{ij} x_{ij} + \sum\limits_{i \in N} f_i y_i$
5. **Constraints**
   (a) facility capacity: $\forall i \in N \ \sum\limits_{j \in M} x_{ij} \leq b_i$
   (b) facility choice: $\forall i \in N, j \in M \ x_{ij} \leq b_i y_i$
   (also see Sect. 2.2.7.5.1)
   (c) demand satisfaction: $\forall j \in N \ \sum\limits_{i \in M} x_{ij} \geq d_j$
   (d) integrality: $\forall i \in M \ y_i \in \{0, 1\}$
   (e) nonnegativity: $\forall i \in M, jinN \ x_{ij} \geq 0$

A few remarks are in order.

- The facility choice constraint forces x_{ij} to be zero (for all $j \in M$) if facility i is not built (i.e. $y_i = 0$); this constraint is inactive if $y_i = 1$, since it reduces to $x_{ij} \leq b_i$, which is the obvious production limit for candidate facility i (for $i \in N$).
- Facility capacity and demand satisfaction constraints encode the transportation problem within the formulation. Set-up costs are modelled using the binary variables y_i. Note that we do not need to ensure an "only if" direction on the relationship between x and y, i.e. if $y_i = 1$ we still allow $x_{ij} = 0$ (in other words, if a facility is built, it might not produce anything), since it is enforced by the objective function direction (a built facility which does not produce anything contradicts minimality of the objective, since otherwise we could set the corresponding y_i to zero and obtain a lower value). The covering aspect of the problem (i.e. selecting a minimum cardinality subset of facilities that cover the stores) is somewhat hidden: it is partly encoded in the term $\sum_i y_i$ of the objective (minimality of the covering subset), by the facility choice constraints (which let the y variables control whether the x variables are zero), and by the demand satisfaction constraints, ensuring that ever store is covered.

- An alternative formulation, with fewer constraints, can be obtained by combining facility capacity and facility choice as follows:

$$\forall i \in N \quad \sum_{j \in M} x_{ij} \leq b_i y_i, \tag{1.10}$$

 and then removing the facility choice constraints entirely. The formulation was presented with explicit facility choice constraints because, in general, they are "solver-frendlier" (i.e. solvers work better with them). In this specific case, this may or may not be the case, depending on the instance. But suppose you knew the transportation capacity limits q_{ij} on each pair $i \in M, j \in N$. Then you could rewrite the facility choice constraints as:

$$\forall i \in N, j \in M \quad x_{ij} \leq q_{ij} y_i. \tag{1.11}$$

 Obviously, the transportation capacities from each facility cannot exceed the production capacity, so $\sum_j q_{ij} \leq b_i$. This implies that by summing Eq. (1.11) over $j \in M$, we obtain Eq. (1.10). By contrast, we cannot "disaggregate" Eq. (1.10) to retrieve Eq. (1.11), which shows that the formulation using Eq. (1.11) is somehow tighter (more precisely, it yields a better continuous relaxation — we shall see this in Part III). Again, while this may not be the case in the formulation above (since we do not have the q_{ij} parameters as given), using facility choice constraints is nonetheless a good coding habit.

1.3.10 Circle packing

In this problem we have to make an assumption: i.e. that we know at least an upper bound ν to the maximum number of crates of beer. We can compute it by e.g. dividing the carrying area of the pick-up truck by the area of a circular base of the cylinder representing a beer crate.

1. **Index sets**
   (a) $N = \{1, \ldots, \nu\}$
2. **Parameters**
   (a) let r = radius of the circular base of the crates
   (b) let a = length of the carrying area of the pick-up truck
   (c) let b = width of the carrying area of the pick-up truck
3. **Decision variables**
   (a) $\forall i \in N$ let x_i = abscissa of the center of circular base of the i-th crate
   (b) $\forall i \in N$ let y_i = coordinate of the center of circular base of the i-th crate
   (c) $\forall i \in N$ let $z_i = 1$ iff the i-th crate can be packed, and 0 otherwise
4. **Objective function**: $\max \sum_{i \in N} z_i$
5. **Constraints**
   (a) packing (abscissae): $\forall i \in N \; r z_i \leq x_i \leq (a - r) z_i$
   (b) packing (coordinates): $\forall i \in N \; r z_i \leq y_i \leq (b - r) z_i$
   (c) non-overlapping: $\forall i < j \in N \; (x_i - x_j)^2 + (y_i - y_j)^2 \geq (2r)^2 y_i y_j$
   (d) integrality: $\forall i \in N \; z_i \in \{0, 1\}$

This problem is also known in combinatorial geometry as packing of equal circles in a rectangle. Note that any packing is invariant by translations, rotations and reflections. We therefore arbitrarily choose the origin as the lower left corner of the rectangle, and align its sides with the Euclidean axes. Note that the packing constraints ensure that either a circle is active, in which case it stays within the boundaries of the rectangle, or it is inactive (and its center is set to the origin) — also see Sect. 2.2.7.5.1. The non-overlapping constraints state that the centers of two active circles must be at least $2r$ distance units apart.

1.3.11 Distance geometry

1. **Index sets**
   (a) V: set of atoms
   (b) E: set of unordered pairs of atoms at distance ≤ 5Å
2. **Parameters**
   (a) $\forall \{i,j\} \in E$ let d_{ij} = Euclidean distance between atoms i,j
   (b) let $K = 3$ be the number of dimensions of the Euclidean space we consider
3. **Decision variables**
   (a) $\forall i \in V, k \leq K$ let x_{ik} = value of the k-th component of the i-th atom position vector
4. **Objective function**: $\min \sum\limits_{\{i,j\} \in E} (\|x_i - x_j\|_2^2 - d_{ij}^2)^2$

A few remarks follow.

- Notationwise, we write x_i to mean the vector $(x_{i1}, \ldots, x_{iK})$. This allows us to write the Euclidean distance between two vectors more compactly.
- Although the distance measure 5Å was given in the text of the problem, it is not a formulation parameter. Rather, it simply states that E might not contain all the possible unordered pairs (it usually doesn't).
- The objective function appears to be a sum of squares, but this is deceiving: if you write it in function of each component x_{ik} you soon discover that it is a quartic multivariate polynomial of the x variables.
- The formulation is unconstrained. Like packings, a set of vectors identified by pairwise distances is invariant to congruences. One way to make it invariant to rotations is to fix the barycenter of the vector set to the origin, which corresponds to the constraint:

$$\sum_{i \in N} x_i = 0.$$

- Most solvers are happier if you provide bounds to the variables (there are some exceptions to this rule). The worst that can happen is that all vectors are on a segment as long as $D = \sum\limits_{\{i,j\} \in E} d_{ij}$.

  Since the barycenter is at the origin, you can impose the following variable bounds:

$$\forall i \in N, k \leq K \quad -\frac{D}{2} \leq x_{ik} \leq \frac{D}{2}.$$

Chapter 2

The language of optimization

Mathematical Programming (MP) is a formal language for describing and solving optimization problems.

In general, languages can be natural or formal. Natural languages are those spoken by people to communicate. Almost every sentence we utter is ambiguous, as it can be interpreted by different people in different ways. By contrast, its expressivity is incredibly rich, as it can be used to describe reality. Formal languages can be defined formally through recursive rules for interpreting their sentences within the confines of an abstract model of a tiny part of reality. If ambiguity occurs in formal languages, it is limited in scope, announced and controlled.

Optimization refers to the improvement of a process which an agent can modify through his/her/its decisions. For example, the airplane departure sequence is decided by controllers who usually try and reduce the average (or maximum) delay.

We use the word "problem" here in the semi-formal sense of computer science: a problem is a formal question relating some given input to a corresponding output: both input and output are encoded through a sequence of bits respecting some given formats and rules. For example, a decision problem might ask whether a given integer is even or odd: the input is an integer, and the output is a bit encoded by the mapping $1 \leftrightarrow \text{YES}$, $0 \leftrightarrow \text{NO}$. An optimization problem might ask the shortest sequence of consecutive vertices linking two given vertices in a graph (provided it exists).

2.1 MP as a language

In computer science, a (basic) *language* $\mathscr{L}$ is a collection of *strings*, each of which is a sequence of *characters* from a given *alphabet* $\mathscr{A}$. Composite languages can be formed as Cartesian products of basic languages. The fundamental problem, given a language and a string, is to determine whether or not the string belongs to the language. This is called *recognition problem*.

2.1.1 Exercise
Implement algorithms to recognize: (a) strings made entirely of digits; (b) strings consisting of a finite sequence of floating point numbers (in exponential notation) separated by any amount of spaces, tabs and commas; (c) strings consisting of multi-indexed symbols (use square brackets for indices, as in, e.g. $x[2,4]$*); (d) strings consisting of English words from a dictionary of your choice.*

2.1.2 Exercise
Implement an algorithm that recognizes a language consisting of strings in the union of (b) and (d) in Exercise 2.1.1 above.

2.1.1 The arithmetic expression language

The most basic language we use in this book includes all functions that can be expressed in "closed form" using a set of primitive operators, say $+, -, \times, \div, (\cdot)^{(\cdot)}, \log, \exp, \sin, \cos, \tan$. Some of these operators are binary, some are unary, and others, like $-$, can be both, depending on context: the number of arguments of an operator is its *arity*.

Operators recursively act on their arguments, which are either other operators, or symbols representing numerical quantities (which can also be considered as operators of zero arity). Ambiguous cases, such as $x_1 + x_2x_3$, are resolved by assigning to each operator a precedence: $\times$ trumps $+$, so the order of the operations is x_2x_3 first, and then x_1+the result. In cases of tie, the left-to-right scanning order is used.

Given a string such as $x_1 + \frac{x_1x_2}{\log x_2}$, the recognition problem can be solved by the following recognition algorithm, given here in pseudocode:

1. find the operator of leftmost lowest precedence in the string
2. identify its arguments and tag them by their arity, marking the characters of the string that compose them
3. recurse over all operators of positive arity

If all characters in the string have been marked at the end of this algorithm, the string is a valid sentence of the language. By representing each recursive call by a node, and the relation "parent-child" by an arrow, we obtain a directed tree (called *parsing tree*) associated with each execution of the recognition algorithm. If, moreover, we contract leaf nodes with equal labels, we obtain a *directed acyclic graph* (DAG) representation of the arithmetical expression (see Example 2.1.3). This representation is called *expression DAG* or *expression tree*.

2.1.3 Example
Consider the expression $x_1 + \frac{x_1x_2}{\log x_2}$. Precedences may be re-written using brackets and implicit operators are written explicitly: this yields $x_1 + (x_1 \times x_2)/\log(x_2)$. The corresponding parsing tree and DAG are shown in Fig. 2.1.

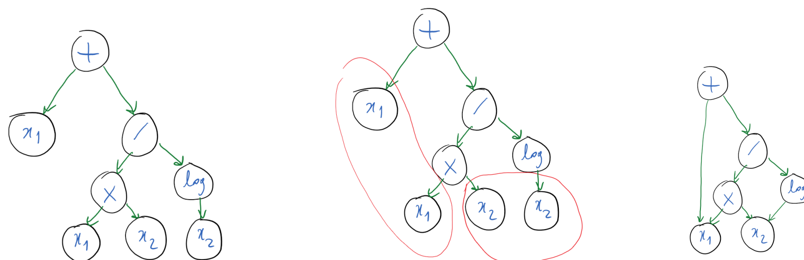


Figure 2.1: A parsing tree (left), the nodes being contracted (center), and the corresponding DAG (right).

Note that implementing this algorithm in code requires a nontrivial amount work, mostly necessary to accommodate operator precedence (using brackets) and scope within the string. On the other hand, easy modifications to the recognition algorithm sketched above yield more interesting behaviour. For example, a minor change allows the recursive recognition algorithm to compute the result of an arithmetical expression where all symbols representing numerical values are actually replaced by those values. This algorithm performs what is called *evaluation* of an arithmetic expression.

2.1.4 Exercise
Implement recognition and evaluation algorithms for an arithmetic expression language.

2.1.1.1 Semantics

By *semantics* of a sentence we mean a set of its interpretations. A possible semantics of an arithmetic expression language is the value of the function represented by the expression at a given point x. The algorithm for this semantics can be readily obtained by the evalution algorithm described in Sect. 2.1.1 above as follows:

- replace each symbol (operator of zero arity) with the value of the corresponding component of the vector x;
- evaluate the arithmetic expression.

Other semantics are possible, of course.

2.1.5 Exercise
Define a semantics for SAT *sentences, namely conjunctions of disjunctions of literals such as* $(x_1 \vee \bar{x}_2) \wedge (x_2 \vee x_3) \wedge (\bar{x}_1 \vee x_2 \vee x_3)$*, where* $\bar{x}_i$ *is equivalent to* $\neg x_i$*, i.e. the negation of the literal* x_i*.*

2.1.6 Exercise
How would you define a semantics for the English language?

2.1.2 MP entities

The sentences of the MP formal language consist of symbols belonging to five categories: parameters, decision variables, objective functions, functional constraints and implicit constraints. The parameters encode the problem input, the decision variables encode the problem output (the solution), an objective function defines a search direction of optimality, the functional constraints are expressed as equations ($=$) or (non-strict) inequalities ($\leq$, $\geq$) involving functions, and the implicit constraints express range constraints, integrality, membership in a cone, and so on.

The distinction between functional and implicit constraints need not be strict. For example, one can write $x \in \{0, 1\}$ (an implicit integrality constraint) as $x^2 = x$ (a functional constraint), and vice versa. In such cases, the choice often depends on the solution algorithm. For example, an algorithm that can accept nonlinear functions as part of its input, but is limited to continuous variables, will accept $x^2 = x$. Conversely, an algorithm that only accepts linear functions but can deal with integrality constraints directly will accept $x \in \{0, 1\}$.

2.1.2.1 Parameters

The input of the optimization problem that the MP describes is contained in various data structures, which can be vectors, matrices, arrays and so on. Each component of these data structures appears as a symbol in the MP formulation. These symbols are known as *parameters*. The parameter language must simply recognize an appropriately structured set of parameter symbols (which are initially declared as such) or numerical values.

2.1.2.2 Decision variables

The decisions that can be taken by the agent interested in solving the optimization problems are also contained in various data structures, each component of which appears as a symbol in the MP formulation. These symbols are known as *decision variables*. The decision variable language must simply recognize an appropriately structured set of decision variable symbols (which are initially declared as such). After the problem is solved, these symbols are assigned the values of the optimal solutions found.

2.1.2.3 Objective functions

An objective function string is an arithmetical expression having decision variables and (optionally) parameter symbols as operators of zero arity, together with an *optimization direction*, denoted by min or max. Depending on whether the optimization problem is feasibility-only, single-objective or multi-objective, there may be zero, one or a finite number of objective functions in the problem.

The single objective function language is a trivial extension of the arithmetical expression language: it must also recognize an optimization direction. The objective function language must be able to recognize a sequence of single objective function language sentences.

2.1.7 Exercise
Consider an optimization problem that aims at minimizing the objective function $f(x) = \sum_{j\le n} c_j x_j$. *Typically, people use the 'x' symbols to denote decision variables: thus each component of the vector* $x = (x_1, \ldots, x_n)$ *is a decision variable. Since we wrote* f *as a function of* x*, we implicitly mean that the symbol* $c = (c_1, \ldots, c_n)$ *is a parameter vector.*

2.1.2.4 Functional constraints

A constraint string is an arithmetical expression having decision variables and (optionally) parameter symbols as operators of zero arity, together with a relational sign, denoted by $=, \le, \ge$ and a numerical value. Depending on whether the problem is constrained or unconstrained, there may be multiple constraint strings in the MP formulation or none.

The single constraint function language is a trivial extension of the arithmetical expression language: it must also recognize the relational operator and the numerical value. The functional constraint function langauge must be able to recognize a sequence of single constraint function language sentences.

2.1.2.5 Implicit constraints

Constraints are *implicit* when their description does not include an arithmetical expression string. We shall consider two types:

- integrality constraints, which require that a certain subset of decision variables must attain integer values to be feasible;
- semidefinite programming (SDP) constraints, which require that a certain square symmetric matrix of decision variables must attain a positive semidefinite (PSD) matrix of values to be feasible.

An integrality constraint string simply consists of a tuple of indices denoting the decision variable symbols required to be integer. Equivalently, an SDP constraint indicates that the decision variable matrix is required to attain a PSD matrix value.

2.1.3 The MP formulation language

A MP *formulation* is a description of a MP problem. It consists of a tuple (P, V, O, F, I) where P is a parameter string, V a decision variable string, O an objective function string, F a functional constraint string, and I an implicit constraint string. An MP formulation indicates a optimization problem, if at least one parameter is a symbol, or an *instance* of this problem if all parameters have numerical values.

A problem is nontrivial if the parameter symbols can range over infinite sets of values. Each assignment of values to the parameter symbols yields an instance, so that problems can also be considered as sets of instances.

2.1.3.1 Solvers as interpreters

The semantics of an MP formulation are given by the assignment of optimal solution values to the decision variable symbols. The algorithms for computing optima of MP formulations are called *solvers*. There exist different solvers for MP, each targeting a particular MP restriction.

For example, if the objective and constraint functions are linear, several off-the-shelf solvers exist, most of which are commercial, e.g. CPLEX [73], XPress-MP [62]. Many of these solvers have lately endowed their products with algorithms for dealing also with nonlinear terms involving specific operators. There are also some free and open-source solvers, though: look at the COIN-OR project [97] page `www.coin-or.org`, as well as GLPK [100].

A solver establishes the semantics of an MP language sentence P. In this sense, it can be seen as a natural *interpreter* for the MP language. Its input is the set of parameter values, i.e. the instance, which suffices to reconstruct the formulation P. Its output (if the solver is successful) is usually the pair (f^*, x^*) where f^* is the optimal objective function value and x^* an optimum with value f^*. We denote this by $[\![P]\!] = (f^*, x^*)$.

Most theories of programming languages manage to control the relationship between syntax and semantics, since the formal grammar parsers they employ to define recognition algorithms can easily be modified to construct the sentence semantics (as underlined in the discussion on recognition and evaluation of arithmetic expression sentences in Sect. 2.1.1). In other words, most programming languages are defined in such a way that recursion in syntax parallels recursion in semantics (this is particularly true of imperative languages, see Sect. 2.1.3.2).

On the other hand, the algorithms implemented by solvers have generally nothing to do with the recursive syntactical structure of the formal grammar used to recognize the sentences. Hence, unfortunately, the relationship between syntax and semantics is much harder to establish in a theoretical sense. There is a general consensus to the effect that efficient (e.g. polynomial time) algorithms provide a “desirable semantics”.

Not only can different solvers employ very different algorithms in order to compute $[\![P]\!]$; they may also have different *formats* for their semantics, which could be, e.g.: a single optimum, or many, or even all if there are finitely many optima; the optima might be defined only with respect to (w.r.t.) a neighbourhood, or they may be global; the results might be guaranteed or not (see Defn. 6.0.1 for a formal definition of optima).

One of the major efforts in the theory of MP is that of deriving new implied constraints (generally called *valid cuts*) to be added to existing hard MP formulations so that: (a) at least one (and hopefully all) optimal solutions remains feasible; (b) they help make other problematic constraints (such as integrality constraints) redundant; (c) they themselves are not problematic. This allows the use of an efficient solver to solve the instance. Valid cuts can be seen as a way to keep $[\![P]\!]$ invariant while making the solution searching process more efficient.

2.1.3.2 Imperative and declarative languages

Computer programming languages such as C/C++, Java, Pascal, Basic, Fortran, Python, Matlab (and more) are known as *imperative* languages: a program in any of these languages will be a set of statements in any of four broad categories: (a) storage, or assignments of values to program variables; (b) tests, or verification of given conditions on program variables; (c) loops, or repeated execution of some parts of the

code; (d) input/output (I/O), i.e. interaction with the hardware layer or external world. Most languages can also encapsulate some parts of code into *callable functions*: this also allows the implementation of loops by means of *recursion*.

By contrast, *declarative*[1] languages only make logical statements about variables, and then let a general algorithm search for the variable values that satisfy those statements. It should be clear that MP is a declarative language. Programming in declarative languages is both simpler and harder than programming in an imperative language. It is simpler because one need not conceive nor implement the algorithm — it is by definition the language interpreter. It is harder because humans are better suited to understand the very simple blocks *assignments, tests, loops* than to design multiple logical statements which, conjunctively, are supposed to describe the output of a given process (without actually detailing the process itself). Programming in a declarative language is also somtimes called *modelling*, although this term also has a different meaning (see Sect. 1.3.2.1). The MP language shifts the focus of optimization from algorithmics to modelling.

Suppose someone asks you to find the largest stable set in a given graph $G = (V, E)$, i.e. the largest subset $S \subseteq V$ such that no unordered pair $\{s, t\}$ of vertices in S is an edge in E. In an imperative language, you would need to decide how to encode a graph and a subgraph, how to enumerate subgraphs in the most efficient possible way, and how to verify whether a subgraph is a stable set (i.e. it has induces no edges in E) or not. In MP, you would simply write:

$$\max \left\{ \sum_{v \in V} x_v \;\middle|\; \forall \{u, v\} \in E \ (x_u + x_v \leq 1) \land \forall v \in V \ x_v \in \{0, 1\} \right\}, \tag{2.1}$$

and then deploy an appropriate solver on the formulation in Eq. (2.1).

Note that most imperative and declarative languages are Turing-complete, (see Sect. 4.1.1). This means one can program or design a universal Turing machine (UTM) with them (again, see Sect. 4.1.1). Hence their expressive power is equivalent.

2.1.8 Exercise
Consider the imperative pseudocode

$p = 1$
input $x \in \mathbb{Z}$
if $x < p$ ***then***
  $x \leftarrow 2x$
end if
return x

Write a declarative language equivalent of this code.

2.2 Definition of MP and basic notions

The formal definition of an MP formulation on n decision variables and m constraints is as follows:

$$\left.\begin{array}{rrcl} \min\limits_{x \in \mathbb{R}^n} & f(p, x) & & \\ \forall i \leq m & g_i(p, x) & \leq & 0 \\ \forall j \in Z & x_j & \in & \mathbb{Z} \\ & x & \in & X, \end{array}\right\} \quad [P] \tag{2.2}$$

where $Z \subseteq \{1, \ldots, n\}$, $X \subseteq \mathbb{R}^n$ is the set of implicit constraints (see Sect. 2.1.2.5) x is a vector of n decision variables taking values in $\mathbb{R}$, p is a vector of parameters which, once fixed to values, make the

[1] Some computer scientists might call such languages "descriptive", and reserve "declarative" for a different type of programming languages.

functions f and g_i (for $i \leq m$) functions $\mathbb{R}^n \to \mathbb{R}$. The symbol $P = P(n, m, p, Z, X)$ denotes the MP instance for given n, m, p, Z, X.

We let $\overline{\mathbb{MP}}$ be the class of all instances of Eq. (2.2) as n, m range over all sizes, Z over all subsets of $\{1, \ldots, n\}$ and p over all possible sizes and values, and f, g over all functions $\mathbb{R}^n \to \mathbb{R}$.

The set of vectors in $\mathbb{R}^n$ that satisfy all constraints of the instance P is called the *feasible set* of P and denoted by $\mathcal{F}(P)$ or simply $\mathcal{F}$. The set of feasible vectors that are also optima (i.e. achieve the minimum objective function value) in P is called the *optimal set* of P and denoted by $\mathcal{G}(P)$ or simply $\mathcal{G}$.

There are three possibilities for a given a MP instance P, which we assume without loss of generality (wlog) in minimization form:

1. there exists at least an optimum x^* of P with optimal objective function value f^*;
2. P is *unbounded*, i.e. for any feasible solution x' with objective function value f', there always exist another feasible solution x'' with objective function value f'' such that $f'' < f'$;
3. P is *infeasible*, i.e. $\mathcal{F}(P) = \varnothing$.

This ternary classification corresponds to two hierarchically dependent binary classifications: whether P is feasible or not, and, if P is feasible, whether it has an optimum or not.

2.2.1 Certifying feasibility and boundedness

In general, it is possible to certify feasibility in practice: given a solution x', it suffices to verify whether x' satisfies all the constraints. Certifying optimality is more difficult in general: whether it can be done or not depends on many factors, the most important of which the behaviour of the objective over the feasible region, the presence of linear/nonlinear terms in the description of the objective function, whether there are finitely or infinitely many feasible solutions.

Infeasibility is also hard to certify: in general, given a MP formulation as in Eq. (2.2), assuming we have an algorithm for optimizing over the implicit constraints $x \in X$, we can add non-negative *slack variables* $s_1, \ldots, s_m$ to the rhs of the inequality constraints and minimize their sum:

$$\left.\begin{array}{rrcl} \min\limits_{x \in \mathbb{R}^n, s \geq 0} & \sum\limits_{i \leq m} s_i & & \\ \forall i \leq m & g_i(p, x) & \leq & s_i \\ \forall j \in Z & x_j & \in & \mathbb{Z} \\ & x & \in & X. \end{array}\right\} \quad [F_P] \tag{2.3}$$

The original instance P is infeasible if and only if (iff) the globally optimal objective function value of Eq. (2.3) is strictly greater than zero. This poses two issues: (a) globally optimizing Eq. (2.3) is generally just as hard as optimizing Eq. (2.2); and (b) in practice, using floating point computations, we might well obtain optimal objective function values in the order $O(10^{-5})$ where the parameters are in the range $O(1)$-$O(100)$: how do we decide whether the problem is infeasible or it is feasible up to some floating point error?

2.2.2 Cardinality of the $\overline{\mathbb{MP}}$ class

Since p might encode continuously varying parameters, and f, g range over all possible real functions of n arguments, the class $\overline{\mathbb{MP}}$ must contain uncountably many instances.

In practice, however, any continuous parameter in p must in fact range over the rationals, of which there are countably many (in fact continuous parameters usually range over the floating point numbers, of

which there are finitely many). As for f, g, they must be recognized by the expression languages described in Sect. 2.1 above. Since there are countably many arithmetical expressions, and only finitely many of a given size, the subclass of instances in $\overline{\mathbb{MP}}$ which can be explicitly described (a necessary condition in order for an instance to be solved — if nothing else because the instance description is the input to the solver) is countably infinite in theory. Given our language $\mathscr{L}$, we call $\mathbb{MP}_{\mathscr{L}}$ the subclass of instances in $\overline{\mathbb{MP}}$ having a finite description in $\mathscr{L}$. If $\mathscr{L}$ is fixed *a priori* (which it usually is), we drop the subscript and simply write $\mathbb{MP}$.

This means we cannot express (and hence solve) uncountably many instances. But the good news is that, given any instance (and so any functions f, g described in some language $\mathscr{L}'$), we can extend our language $\mathscr{L}$ to integrate $\mathcal{L}'$ so that f, g can also be described in $\mathcal{L}$.

2.2.3 Reformulations

Several features of Eq. (2.2) might appear arbitrary to the untrained eye. We will show in this section that every assumption was made wlog.

2.2.3.1 Minimization and maximization

In Sect. 2.1.2.3 we stated that objective functions have a direction, either min or max. But in Eq. (2.2) we only wrote min. However, given any MP formulation

$$P \equiv \min\{f(x) \mid x \in \mathcal{F}\} \tag{2.4}$$

can be written as

$$Q \equiv \max\{-f(x) \mid x \in \mathcal{F}\} \tag{2.5}$$

while keeping the set $\mathcal{G}$ of optima invariant. The only thing that changes is the value of the optimal objective function: it is f^* in P iff it is $-f^*$ in Q.

Some solvers only accept one of the two optimization directions (typically the min direction is more common). So there is sometimes a practical need for carrying out this transformation.

2.2.3.2 Equation and inequality constraints

Eq. (2.2) only lists m inequality constraints $g_i(p, x) \leq 0$ (for $i \leq m$). However, we can express an equation constraint $h(p, x) = 0$ by requiring that there exist two indices $i, j \leq 0$ such that $g_i(p, x) \equiv h(p, x)$ and $g_j(p, x) \equiv h(p, x)$. This yields

$$\begin{array}{rcl} h(p,x) & \leq & 0 \\ -h(p,x) & \leq & 0, \end{array}$$

which hold for fixed p iff $h(p, x) = 0$. Note that for each equation constraint we need two inequality constraints, so the size m of the constraint list changes.

In practice, the large majority of solvers accept both inequality and equation constraints explicitly.

2.2.3.3 Right-hand side constants

Although all right-hand sides (rhs) in Eq. (2.2) have been set to zero, any other constant can simply be brought over (with opposite sign) to the left-hand side (lhs) and considered part of the function $g_i(p, x)$ (for $i \leq m$).

2.2.3.4 Symbolic transformations

All the simple transformations given in Sect. 2.2.3.1-2.2.3.3 are part of a much larger family of symbolic and numerical transformations on MP formulations collectively known as *reformulations* [84, 151], some of which will be discussed in more depth below.

2.2.4 Coarse systematics

As we shall see below, MP formulations are classified in many different ways [85, 151]. For example,

- according to the properties of their descriptions: e.g. an MP where all the functions are linear and $Z = \varnothing$ is called a Linear Program (LP), whereas if $Z \neq \varnothing$ it is called a Mixed-Integer Linear Program (MILP);
- according to their mathematical properties: e.g. if f is nonlinear but convex in x and $\mathcal{F}$ is a convex set, P is a convex Nonlinear Program (convex NLP or cNLP);
- according to whether a certain class of solvers can solve them: this classification is obviously *a posteriori* w.r.t. the solution process, and often changes in time, since solvers, operating systems and hardware all evolve.

Unions of properties are also possible: for example an MP involving both integer variables and nonlinear functions is called a Mixed-Integer Nonlinear Program (MINLP). If, when relaxing the integer variables to take continuous values, the resulting problem is a cNLP, then the MINLP is referred to as a convex MINLP (cMINLP). We remark that a cMINLP has a nonconvex feasible region (by virtue of the integrality constraints).

2.2.5 Solvers state-of-the-art

In this section we examine the state of the art of current MP solvers according to our systematics (Sect. 2.2.4) as regards robustness and solution size.

- Currently, LP solvers are the most advanced. Most of them are very robust. For sparse data, current LP solvers might well solve instances with $O(10^6)$ variables and constraints. For dense data, unfortunately, the situation varies wildly depending on the data themselves: but most input data in MP is sparse, and dense MPs mostly occur in specific fields, such as quantile regression or signal processing.
- The most advanced MILP solvers are based on the Branch-and-Bound (BB) algorithm, which essentially solves a sequence of LPs (this makes MILP solvers quite robust). However, this sequence is exponentially long in the worst case. It is very hard to make predictions on the maximal size of MILPs that current BB technology is able to solve in "acceptable times", as there are minuscule examples known to force the worst-case, as well as practical cases of MILPs with tens of thousands of variables and/or constraints being solved very fast.
- SDP solvers (and conic solvers in general) are quite robust, but compared to LP solvers their "size bottleneck" is much more restricted. You can hope to solve SDPs with $O(10^3)$ variables and constraints, and possibly even $O(10^4)$ (but remember that SDPs involves matrices of decision variables, so the number of decision variables is usually quite large).
- Local NLP solvers guarantee global optimality on the vast majority of practical cNLP instances; and most of them will also be rather efficient at finding such optima. One might hope to solve instances

with tens of thousands of variables and/or constraints as long as the "linear part" of the problem is large, sparse, and the solver is able to exploit it. Today, however, many cNLP applications are from Machine Learning (ML), and their sizes are so large that special purpose solvers have to be designed — and a guarantee of optimality often forsaken. While a local NLP solver deployed on a cNLP is reasonably robust, the same solver deployed on a nonconvex NLP typically has many more chances of failures, specially if an infeasible starting point was provided (which is often the case — finding a feasible solution in a nonconvex NLP is as hard as finding an optimal one, in terms of computational complexity in the worst case).

- The state of the art of global NLP solvers for nonconvex NLPs is less advanced than then the previous ones. Currently, all of the solvers that are able to certify global optimality (to within a given $\varepsilon > 0$ tolerance on the optimal objective function value) are based on a BB variant called "spatial BB" (or sBB). The sBB algorithm solves a sequence of LP or cNLP relaxations of the given (nonconvex) NLP, as well as locally solving the given NLP every so often. This procedure is as fragile as its local solvers warrant — and since local NLP solvers are not so robust, sBB is no different. Current sBBs perform reasonably well on problems with a quadratic structure, as those are the best studied. sBB implementations can often exhibit their exponential worst-case behaviour even on tiny instances, unfortunately. Expect some results in the size range $O(10^2)$-$O(10^3)$ variables/constraints.
- cMINLP solvers are somewhat more robust than nonconvex NLP solvers, but much less advanced than MILP solvers; they can probably be deployed on instance sizes of around $O(10^3)$.
- General MINLP solvers implement sBB algorithms that can also branch on integer variables. There is currently no sBB solver that can only deal with nonconvex NLPs but not with MINLP. Since MILP solution technology is reasonably advanced, endowing an sBB implementation with mixed-integer capabilities does not worsen its robustness or the limits of its maximal sizes.

You should take all of the information given above with a pinch of salt. It is the author's own opinion, formed after close to twenty years' experience in the field. It is not a scientific statement, and has been left suitably vague on purpose. Algorithmic research in MP is intense, and major improvements, even on much smaller subclasses than our systematics above lists, are often picked up by the major commercial codes rather rapidly.

If you have a large instance for which your solver takes too long you should: (b) ask yourself whether there exists a simple and efficient algorithm that can solve your problem independently of its MP formulation; (b) attempt to reformulate the problem in order to be able to solve it with a more robust/efficient solver; (c) give your solver a time limit, forsake its guarantees, and hope it finds a good solution within the allotted time. While advice (c) sounds close to "give up", remember that (i) in the large majority of practical cases, having any solution is better than having none at all; (ii) for many classes of problems, local optima tend to cluster together, and local optima close to the global optimum might be quite close to it.[2]

2.2.6 Flat versus structured formulations

A formulation is *flat* if it has no quantifier over variable indices, and *structured* otherwise.

We have seen two examples of MP formulations so far: Eq. (2.1) and Eq. (2.2). Eq. (2.1) involves the maximization of the sum of all the decision variables (one per vertex in the graph), subject to the condition that, for each edge in the graph, the decision variables corresponding to the adjacent vertices cannot both be set to one. Eq. (2.2) is completely general: it minimizes an objective subject to a list of functional constraints introduced by a universal ("for all") quantifier. In both formulations there appear

[2]This is mostly an empirical observation [28]. Intuitive explanations have sometimes been attempted, based on the distribution of optima in all points satisfying first-order conditions [17].

symbols quantified by indices (u, v in Eq. (2.1), i in Eq. (2.2)), and quantifiers ($\sum, \forall$ in Eq. (2.1), $\forall$ in Eq. (2.2)). Therefore, both are structured.

The following is a simple example of a flat formulation:

$$\left.\begin{array}{rrcl} \min & x_1 + x_2 + x_3 + x_4 & & \\ & x_1 + x_2 & \le & 1 \\ & x_1 + x_3 & \le & 1 \\ & x_2 + x_4 & \le & 1 \\ & x_3 + x_4 & \le & p \\ & x_1, x_2, x_3, x_4 & \in & \{0, 1\}, \end{array}\right\} \quad (2.6)$$

where p is a (scalar) parameter. If we assign a fix value to p, e.g. $p = 1$, we obtain a flat formulation representing an instance of the MP formulation in Eq. (2.1).

2.2.1 Exercise
Since Eq. (2.6) is an instance of Eq. (2.1) when $p = 1$, its optima are stable sets in a graph: recover the graph from the formulation.

2.2.2 Exercise
Is Eq. (2.6) an instance of Eq. (2.1) whenever $p \neq 1$? What about $p = 0$ or $p = 2$? Does it make sense to consider other values of p?

2.2.6.1 Modelling languages

The distinction between flat and structured formulations is that solvers only accept flat (instance) formulations, whereas humans naturally model optimization problems using structured formulations. This calls for two MP languages: one that understand parameters and variable symbols with indices, as well as quantifiers over those indices, and one that does not. It also calls for a translator between the two languages.

In MP, translators from structured to flat formulations are called *modelling languages*. In fact, they do more than just translate. Since each solver accepts its input in a flat formulation language with its own distinct syntax, most modelling languages act as interfaces to a set of solvers, each of which requires a specific translation module.

2.2.3 Remark (Quantifiers over indices)
Quantifiers are only allowed to range over indices belonging to a set given as part of the parameters (the input). In no case should a quantifier ever involve a decision variable symbol. The issue arises because translating from a structured formulation to a flat one would be impossible if a quantifier involved a decision variable (the value of which is not known before the solution process occurs). Though this remark might appear innocuous at this time, wait until you need a "conditional constraint" (see the discussion at the end of Sect. 2.2.7.5).

The best known purely MP-related translators are AMPL [57] and GAMS [29]. AMPL structured formulation language syntax is very similar to the mathematical form of MP languages, and hence very close to human-readable syntax, and can interface with many solvers. Its weak point is that it has very a limited imperative sub-language, which makes it hard to reformulate and post-process solutions. GAMS has a better imperative sub-language, but its structure formulation language syntax has a steep learning curve (at best).

On the other hand, with the increasing need for complicated algorithms involving MP as elementary steps, many imperative programming languages have been endowed with capabilities for modelling and solving MP formulations. Python has a growing number of translators (e.g. PyOMO [65] and PICOS [129]), and Matlab [102] has many extremely good translators, some commercial and some not. The

most complete Matlab translator appears to be TOMLAB [71], which interfaces with a large number of solvers. A free equivalent to TOMLAB is the OPTI toolbox [42], which, however, unfortunately only works on the Windows version of Matlab. Another excellent free translator for Matlab is YALMIP [96], which focuses mostly (but not only) on conic optimization.

2.2.7 Some examples

2.2.7.1 Diet problem

A diet involving m nutrients (vitamins, proteins, fats, fibers, iron, etc.) is healthy if it has at least quantities $b = (b_1, \ldots, b_m)$ of the nutrients. In order to compose such a diet, we need to buy quantities $x = (x_1, \ldots, x_n)$ of n types of food having unit costs $c = (c_1, \ldots, c_n)$. Food $j \le n$ contains a_{ij} units of nutrient $i \le m$. The solution of the following LP problem yields an x that satisfies the requirements of a healthy diet at minimum cost [43].

$$\left.\begin{array}{rrcl} \min_x & \sum\limits_{i=1}^{n} c^\top x & & \\ & Ax & \ge & b \\ & x & \ge & 0. \end{array}\right\} \qquad (2.7)$$

The parameters are A, b, c. The decision variables are the components of the vector x. The functional constraints are the rows of the linear inequality system $Ax \le b$. The *non-negativity* constraints $x \ge 0$ can be interpreted both as functional constraints (since $x = f(x)$ where f is the identity function) and as implicit constraints: in the latter case, the sentence $x \ge 0$ encodes membership in the non-negative orthant.

2.2.7.2 Transportation problem

Consider a transportation network modelled by a weighted bipartite directed graph $B = (U, V, A, d)$ with a set of departure vertices U, a set of destinations V, a set of arcs $A = \{(u, v) \mid u \in U, v \in V\}$ weighted by a nonnegative distance function $d : A \to \mathbb{R}_+$. A certain amount of material a_u is stored at each departure vertex $u \in U$. We associate to each destination $v \in V$ a given demand b_v of the same material. The cost of routing a unit of material from $u \in U$ to $v \in V$ is directly proportional to the distance d_{uv}. We have to determine the transportation plan of least cost satisfying the demands at the destinations. The variables x_{uv} in the LP formulation below, associated to each arc $(u, v) \in A$, denote the amount of material routed on the arc.

$$\left.\begin{array}{rrcl} \min_x & \sum\limits_{(u,v)\in A} d_{uv} x_{uv} & & \\ \forall u \in U & \sum\limits_{v \in V} x_{uv} & \le & a_u \\ \forall v \in V & \sum\limits_{u \in U} x_{uv} & \ge & b_v \\ \forall (u,v) \in A & x_{uv} & \ge & 0. \end{array}\right\} \qquad (2.8)$$

The parameters are all encoded in the weighted bipartite directed graph (digraph) B. The decision variables represented by the double-indexed symbols x_{uv} (for $(u, v) \in A$). This structure can also be seen as a partial[3] $|U| \times |V|$ matrix X with component (u, v) being present iff $(u, v) \in A$. There are two sets of functional constraints and a non-negativity constraint.

[3] A *partial matrix* is a matrix with some components replaced by a placeholder indicating their absence.

2.2.7.3 Network flow

Given a network on a directed graph $G = (V, A)$ with a source node s, a destination node t, and capacities u_{ij} on each arc (i, j). We have to determine the maximum amount of material flow that can circulate on the network from s to t. The variables x_{ij} in the LP formulation below, defined for each arc (i, j) in the graph, denote the quantity of flow units.

$$\left.\begin{array}{rlcl} \max_x & \sum\limits_{i\in\delta^+(s)} x_{si} & & \\ \forall\, i \le V, i \ne s, i \ne t & \sum\limits_{j\in N^+(i)} x_{ij} & = & \sum\limits_{j\in N^-(i)} x_{ji} \\ \forall (i,j)\in A & 0 \le x_{ij} \le u_{ij}. & & \end{array}\right\} \quad (2.9)$$

The parameters include the array $\{u_{ij} \mid (i, j) \in A$ of upper bounds and the digraph G, represented in Eq. (2.9) in the node adjacencies $N^+(i)$ (set of *outgoing* nodes j such that $(i, j) \in A$) and $N^-(i)$ (set of *incoming* nodes j such that $(j, i) \in A$). The decision variables are x_{ij} for $(i, j) \in A$. The functional constraints are in the form of equations (we remark that the form of the equation is not $f(x) = 0$ but $f^1(x) = f^2(x)$, trivially reducible to the former standard form). The *range* constraints $0 \le x_{ij} \le u_{ij}$ can be seen as functional constraints. This is obtained by re-writing them as $x_{ij} - u_{ij} \le 0$ and $x_{ij} \ge 0$ or as an implicit constraint $X \in [0, U]$ where X is the partial $|V| \times |V|$ matrix of decision variables, and U is the partial $|V| \times |V|$ matrix of upper bounds.

2.2.7.4 Set covering problem

A certain territory containing n cities is partitioned in m regions. We must decide whether to build a facility on region $i \le m$ or not. For each $i \le m$ and $j \le n$, the parameter a_{ij} is equal to 1 iff a facility on region i can serve city j (otherwise $a_{ij} = 0$). The cost of building a facility on region i is c_i. We require that each city is served by at least one facility, and we want to find the construction plan of minimum cost. We model the problem as the following MILP:

$$\left.\begin{array}{rrcl} \min_x & \sum\limits_{i=1}^{m} c_i x_i & & \\ \forall\, j \le n & \sum\limits_{i=1}^{m} a_{ij} x_i & \ge & 1 \\ & x & \in & \{0,1\}^n. \end{array}\right\} \quad (2.10)$$

The parameters are (c, A) where A is the $m \times n$ matrix having a_{ij} as its (i, j)-th component (A is an adjacency matrix). There is a decision variable vector x, a set of linear functional constraints and an implicit integrality constraints of binary type. Note that, although Eq. (2.10) is a MILP, it only has binary variables and no continuous ones. We usually call such problems Binary Linear Programs (BLP).

2.2.7.5 Multiprocessor scheduling with communication delays

A *scheduling problem* generally has two main types of decision variables: assignment (of tasks to processors) and sequencing (order of tasks for each processor). The *makespan* is the time taken to finish processing the last task: an optimal schedule usually minimizes the makespan. The Multiprocessor Scheduling Problem with Communication Delays (MSPCD) consists in finding a minimum makespan schedule in order to run a set V of tasks with given duration L_i (for $i \in V$) on an arbitrary network P of homogeneous processors. Tasks must be executed according to a certain partial precedence order

encoded as a digraph $G = (V, A)$, where $(i, j) \in A$ if task i must be completed before task j can start. If $i, j \in V$ are assigned to different processors $h, k \in P$, they incur a communication cost penalty γ_{ij}^{hk}, which depends on the (given) distance d_{hk}, which is in fact the length of a shortest path from h to k in P, as well as on the (given) amount of exchanged data c_{ij} that needs to be passed from task i to task j. In summary, $\gamma_{ij}^{hk} = \Gamma c_{ij} d_{hk}$, where Γ is a given constant.

2.2.4 Remark (Meanings of V)
We assume that V is actually a set of integers $\{1, \ldots, |V|\}$ indexing the tasks, so that we can talk about task i (for $i \in V$) but also the s-th task on some processor (for $s \in V$). While syntactically this notation is valid, it might engender some confusion to do with the fact that task i might not be the i-th task on the processor it is assigned to. You should consider that V stands in fact for two different collections: one of the task indices, and the other of the order indices. □

We define two sets of decision variables as follows:

- binary variables y denoting assignment and sequencing:

$$\forall i, s \in V, k \in P \; y_{ik}^s = \begin{cases} 1 & \text{task } i \text{ is the } s\text{-th task on processor } k \\ 0 & \text{otherwise,} \end{cases}$$

- continuous variables $t_i \geq 0$ determining the starting time for task i (for $i \in V$).

The MSPCD can now be formulated as follows:

$$\left.\begin{array}{rrcll}
\min\limits_{y,t} & \max\limits_{i \in V}(t_i + L_i) & & & (1) \\
\forall i \in V & \sum\limits_{k \in P} \sum\limits_{s \in V} y_{ik}^s & = & 1 & (2) \\
\forall k \in P & \sum\limits_{i \in V} y_{ik}^1 & \leq & 1 & (3) \\
\forall k \in P, s \in V \smallsetminus \{1\} & \sum\limits_{i \in V} y_{ik}^s & \leq & \sum\limits_{i \in V} y_{ik}^{s-1} & (4) \\
\forall j \in V, i \in N^-(j) & t_i + L_i + \sum\limits_{h \in P} \sum\limits_{s \in V} \sum\limits_{k \in P} \sum\limits_{r \in V} \gamma_{ij}^{hk} y_{ih}^s y_{jk}^r & \leq & t_j & (5) \\
\forall i, j \in V, k \in P, s \in V \smallsetminus \{n\} & t_i + L_i - M\left(2 - \left(y_{ik}^s + \sum_{r=s+1}^n y_{jk}^r\right)\right) & \leq & t_j & (6) \\
\forall i, s \in V, k \in P & y_{ik}^s & \in & \{0, 1\} & (7) \\
\forall i \in V & t_i & \geq & 0, & (8)
\end{array}\right\} \quad (2.11)$$

where $M \gg 0$ is a "sufficiently large" (given) penalty coefficient, and $N^-(j)$ is standard graph theoretical notation to mean the *incoming neighbourhood* of node $j \in V$, i.e. the set of nodes $i \in V$ such that $(i, j) \in A$.

Equation (2) ensures that each task is assigned to exactly one processor. Inequalities (3)-(4) state that each processor can not be simultaneously used by more than one task: (3) means that at most one task will be the first one at k, while (4) ensures that if some task is the sth one (for $s \geq 2$) scheduled to processor $k \in P$ then there must be another task assigned as $(s-1)$-st to the same processor. Inequality (5) expresses the precedence constraints together with communication time required for tasks assigned to different processors. Inequality (6) defines the sequence of the starting times for the set of tasks assigned to the same processor: it expresses the fact that task j must start at least L_i time units after the beginning of task i whenever j is executed after i on the same processor k; the M parameter must be large enough so that constraint (6) is active only if i and j are executed on the same processor k and $r > s$ (for $i, j, r, s \in V$, $k \in P$).

2.2.5 Remark (Presenting a MP formulation)
Each row of a MP formulation is split in four columns.

- *In the first column, quantifiers:* min *and* max *for objective functions,* $\forall$ *or none for constraints;*

- *In the second column, functional forms (objective and constraints);*
- *In the third column, equality sign or $\leq, \geq$ signs for functional constraints, $\in$ for implicit constraints (nothing for objectives);*
- *In the fourth column, constants or functional forms for functional constraints, set names or labels for implicit constraints (nothing for objectives).*

2.2.6 Remark (Objective function)
The objective function has a min max *form, and is therefore not linear. Formulations exhibiting a* min max *optimization direction are known as* saddle problems*. Though this might deceptively look like one, it is not: in saddle problems you minimize over a subset of variables and maximize over the rest. In Eq.* (2.11) *the inner maximization occurs w.r.t. an index ranging over a set given as an input parameter. In other words, the objective function expression $f(p, x)$ given in Eq.* (2.2) *is $\max_{i \in V}(t_i + L_i)$: it corresponds to the ending time of the last task, i.e. the makespan.*

2.2.7 Exercise
Reformulate the objective function (1) of Eq. (2.11) *exactly so that it becomes linear in the decision variables.*

2.2.8 Remark (Products of binary variables)
Note that Constraint (5) in Eq. (2.11) *involves a sum of products of two binary variables. Without any further analysis on the problem structure, we are forced to conclude that this formulation belongs to the (nonconvex) MINLP class. This is bad news according to Sect. 2.2.5. Fortunately, however, roducts of binary variables can be reformulated exactly to a linear form. Whenever any MP involves a product $x_i x_j$ where $x_i, x_j \in \{0, 1\}$, proceed as follows: replace the product with an additional variable $X_{ij} \in [0, 1]$ (a process called* linearization*), and adjoin the following constraints:*

$$X_{ij} \leq x_i \quad (2.12)$$
$$X_{ij} \leq x_j \quad (2.13)$$
$$X_{ij} \geq x_i + x_j - 1. \quad (2.14)$$

This reformulation was first proposed in [55]. It can be generalized to products where only one of the variables is binary, as long as the other is bounded above and below [85]. If both variables are continuous and bounded, Eq. (2.12)*-*(2.14) *can be generalized to obtain a convex envelope of the set $\mathcal{X}^{ij} = \{(X_{ij}, x_i, x_j) \in B^{ij} \mid X_{ij} = x_i x_j\}$ (where B^{ij} is a box defined by lower and upper bounds on x_i, x_j and the corresponding bounds on X_{ij} obtained by interval analysis) [106].*

2.2.9 Exercise
With reference to Rem. 2.2.8, prove that Eq. (2.12)*-*(2.14) *provide an exact reformulation of the set $\mathcal{X}^{ij} \cap [0, 1] \times \{0, 1\}^2$.*

The formulation in Eq. (2.11) uses a rather standard set of variables for most scheduling problems. It is not easy to solve, however, even for medium-sized instances, since it has $O(|V|^3)$ variables and $O(|V|^3|P|)$ constraints. See [45] for a more compact formulation.

2.2.7.5.1 The infamous "big M" Anyone who is familiar with the integer programming literature knows about the "big M", its widespread use, and its unanimous condemnation. The need for a "large" constant M arises when a constraint needs to be activated or deactivated according to the value of a given binary decision variable (such constrained are known as conditional constraints). Suppose we have a constraint $g(x) \leq g_0$ which should only be active when the variable $y \in \{0, 1\}$ has value 1.

A maximally inexperienced reader would probably come up with the expression "$\forall y \in \{1\}\ g(x) \leq g_0$", which unfortunately involves the decision variable y appearing in a constraint quantifier, against

Rem. 2.2.3. A naive reader might propose multiplying both sides of the constraint by y, so that the constraint (now reformulated as $yg(x) \leq yg_0$) will be inactive when $y = 0$ and active when $y = 1$, as desired. The issue here is that this introduces unnecessary products in the formulation, which, according to our analysis of the state of the art in solvers (Sect. 2.2.5) should be best avoided.

The common practice is to assume that $g(\cdot)$ is bounded above over its domain, say $g(x) \leq g^U$ for all possible values of the decision variable vector x. One would then reformulate the constraint by choosing some parameter $M \geq g^U - g_0$ and writing:

$$g(x) \leq g_0 + M(1 - y), \tag{2.15}$$

so that when $y = 1$ we retrieve $g(x) \leq g_0$, whereas with $y = 0$ we simply have $g(x) \leq g_0 + M$, which implies $g(x) \leq g^U$, which is always true (and therefore does not actively constrain the problem anymore).

MILP formulations involving "big M"s are often condemned because their continuous relaxations (obtained by relaxing the integrality constraints) yield a bound that is known to often have a large gap with the optimal objective function value of the original problem. MILP solvers therefore take much longer to achieve termination. It is also known that this adverse impact is lessened when M is as small as possible. So when people write "big M" what they really mean is "big enough": make an effort to correctly estimate M as an upper bound to the (possibly unknown) g^U.

2.2.7.6 Graph partitioning

The Graph Partitioning Problem (GPP), also known as MIN-k-CUT problem is part of a larger family of clustering problems, which form the methodological basis of unsupervised ML. Given an undirected graph $G = (V, E)$ and two integers $L, k \geq 2$, it asks for a partition of V into k (disjoint) subsets, called *clusters*, such that each cluster has cardinality bounded above by L, and such that the number of edges $\{i, j\} \in E$ such that i, j belong to different clusters is minimized [58, ND14].

In general, the GPP is **NP**-hard for all $k \geq 3$. The particular case $k = 2$ is known as the MIN CUT problem, and can be solved in polynomial time by computing the solution of its dual,[4] the MAX FLOW problem (see Sect. 2.2.7.3).

The parameters of the problem are given by an encoding of G and the two integers L, k. As decision variables we employ two-indexed binary variables in order to assign vertices to clusters:

$$\forall i \in V, h \leq k \quad x_{ih} = \begin{cases} 1 & \text{if vertex } i \text{ is in cluster } h \\ 0 & \text{otherwise.} \end{cases}$$

The formulation is as follows:

$$\left.\begin{array}{rrcll} \min\limits_x & \sum\limits_{\{i,j\}\in E} \sum\limits_{h\leq k} x_{ih}(1 - x_{ih}) & & & (1) \\ \forall h \leq k & \sum\limits_{i\in V} x_{ih} & \leq & L & (2) \\ \forall i \in V & \sum\limits_{h\leq k} x_{ih} & = & 1 & (3) \\ \forall i \in V, h \leq k & x_{ih} & \in & \{0, 1\}. & (4) \end{array}\right\} \tag{2.16}$$

We remark that, for each edge $\{i, j\} \in E$ and $h \leq k$, the product $x_{ih}(1 - x_{jh})$ has value 1 iff i, j are assigned to different clusters: thus the objective function (1).

2.2.10 Remark (Data structure representation for edges)
If you implement Eq. (2.16), be aware that if $\{i, j\}$ is represented as a couple (i, j) rather than an

[4] See e.g. [119] for an introduction to LP duality, as well as the special form of "combinatorial" duality given by the pair MAX FLOW − MIN CUT.

unordered pair, then you are likely to have to multiply the objective function by $\frac{1}{2}$, unless you remove the repeated couples by means of a condition $i < j$. In general, however, whether you are allowed to express $i < j$ also depends on the other features of the MP you are considering; sometimes the most expedited solution is to count edges twice and divide by two.

As for Constraint (2), it expresses the fact that each cluster must have cardinality bounded above by L. Constraint (3) states that each vertex must be assigned to exactly one cluster (i.e. the clustering is a partition).

The formulation in Eq. (2.16) belongs to the class of MINLP, since the objective function is quadratic, and possibly nonconvex. An exact reformulation to a MILP can be achieved by employing Fortet's reformulation technique (see Remark 2.2.8).

2.2.7.7 Haverly's Pooling Problem

Haverly's Pooling Problem (HPP), first introduced in [66], is described visually in Fig. 2.2. We have three input feeds with different levels of percentage of sulphur in the crude. Accordingly, the unit costs of the input feeds vary. Two of the feeds go into a mixing pool, which makes the level of sulphur percentage the same in the two streams coming out of the pool. The various streams are then blended to make two end products with different requirements on the sulphur percentage and different unit revenues. We have some market demands on the end products and we want to determine the quantities of input crude of each type to feed into the networks so that the operations costs are minimized. This problem can be

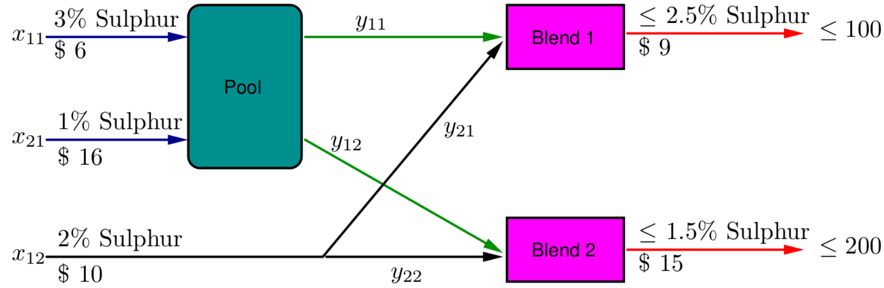


Figure 2.2: Haverly's Pooling Problem.

formulated in various ways. We present here what is known as the "p-formulation" of the HPP [10], with comments on the constraints explaining their meaning.

$$\left.\begin{array}{rll}
\min\limits_{x,y,p\geq 0} & 6x_{11} + 16x_{21} + 10x_{12} - 9(y_{11} + y_{21}) - 15(y_{12} + y_{22}) & \text{cost} \\
\text{s.t.} & x_{11} + x_{21} - y_{11} - y_{12} = 0 & \text{mass balance} \\
& x_{12} - y_{21} - y_{22} = 0 & \text{mass balance} \\
& y_{11} + y_{21} \leq 100 & \text{demands} \\
& y_{12} + y_{22} \leq 200 & \text{demands} \\
& 3x_{11} + x_{21} - p(y_{11} + y_{12}) = 0 & \text{sulphur balance} \\
& py_{11} + 2y_{21} \leq 2.5(y_{11} + y_{21}) & \text{quality req} \\
& py_{12} + 2y_{22} \leq 1.5(y_{12} + y_{22}) & \text{quality req,}
\end{array}\right\}$$

where x, y are decision variable vectors representing input and intermediate stream quantities (as shown in Fig. 2.2) and p is the decision variable scalar representing the percentage of sulphur in the streams out of the pool. Notice that this NLP has three constraints involving bilinear terms, so Global Optimization (GO) techniques are mandatory for its solution. Since bilinear terms can (and usually do) yield nonconvex

feasible regions when used in constraints, we can only say that this is a nonconvex NLP. Note that the implicit non-negativity constraints appear under the minimization direction operator min.

The formulation presented above is the flat formulation (it has no quantifiers ranging over indices) of a single instance (it has no parameters). This instance is part of the problem that can be obtained by replacing the numbers $6, 16, 10, 9, 15, 100, 200, 2.5, 1.5$ in the objective and constraints by parameter symbols ranging over non-negative real scalars. It is this problem that is actually called HPP. Many generalizations of the HPP have been studied in the literature, most notably with respect to the network topology, to the types of oil impurity (e.g. the sulphur) and to the activation/de-activation of conducts in the oil network [111], see Sect. 2.2.7.8 below.

2.2.7.8 Pooling and Blending Problems

The HPP (Sect. 2.2.7.7) is a subclass of more general problems termed Pooling/Blending problems. Various types of crude oils of different qualities, coming from different feeds, are mixed together in various pools to produce several end-products subject to quality requirements and quantity demands; the objective is to minimize the net costs. These problems are usually modelled as continuous NLPs involving bilinear terms. The literature on Pooling/Blending problems is vast (see e.g. [1, 56, 150, 142, 10, 91]). We present the general blending problem formulation found in [1, p. 1958]. The formulation refers to a setting with q pools each with n_j input streams ($j \le q$) and r end products. Each stream has l qualities.

$$\left.\begin{array}{rlr}
\min\limits_{x,y,p\ge 0} \sum\limits_{j=1}^{q}\sum\limits_{i=1}^{n_j} c_{ij}x_{ij} - \sum\limits_{k=1}^{r} d_k \sum\limits_{j=1}^{q} y_{jk} & & \\
\sum\limits_{i=1}^{n_j} x_{ij} = \sum\limits_{k=1}^{r} y_{jk} & & \forall j \le q \\
\sum\limits_{j=1}^{q} y_{jk} \le S_k & & \forall k \le r \\
\sum\limits_{i=1}^{n_j} \lambda_{ijw} x_{ij} = p_{jw} \sum\limits_{k=1}^{r} x_{jk} & & \forall j \le q\ \forall w \le l \\
\sum\limits_{j=1}^{q} p_{jw} x_{jk} \le z_{kw} \sum\limits_{j=1}^{q} y_{jk} & & \forall k \le r\ \forall w \le l \\
x^L \le x \le x^U, p^L \le p \le p^U, y^L \le y \le y^U, & &
\end{array}\right\} \quad (2.17)$$

where x_{ij} is the flow of input stream i into pool j, y_{jk} is the total flow from pool j to product k and p_{jw} is the w-th quality of pool j; $c_{ij}, d_k, S_k, Z_{kw}, \lambda_{ijw}$ are, respectively: the unit cost of the i-th stream into pool j, the unit price of product k, the demand for product k, the w-th quality requirement for product k and the w-th quality specification of the i-th stream into pool j.

The variable symbols are x, y, p, as emphasized under the optimization direction symbol min. The other symbols indicate parameters.

2.2.7.9 Euclidean Location Problems

There are n plants with geographical positions expressed in Euclidean coordinates (a_i, b_i) $(1 \le i \le n)$ w.r.t. to an arbitrary point $(0, 0)$. Daily, the i-th plant needs r_i tons of raw material, which can be delivered from m storage points each with storage capacity c_j $(1 \le j \le m)$. For security reasons, each storage point must be located at least at $D = 1$ Km distance from the plant. The cost of raw material transportation between each storage point and each plant is directly proportional to their distance as well as the quantity of raw material. Find geographical positions where to place each storage point so

that the transportation costs are minimized. The MP formulation is as follows:

$$\left.\begin{array}{llr}\min\limits_{x,y,d,w} & \sum\limits_{i=1}^{n}\sum\limits_{j=1}^{m} w_{ij}d_{ij} & \\ \text{s.t.} & \sum\limits_{i=1}^{n} w_{ij} \le c_j \quad \forall j \le m & \text{storage capacity} \\ & \sum\limits_{j=1}^{m} w_{ij} \ge r_i \quad \forall i \le n & \text{plant requirement} \\ & d_{ij} = \sqrt{(x_j-a_i)^2+(y_j-b_i)^2} \quad \forall i \le m, j \le n & \text{Euclidean distance} \\ & d_{ij} \ge D \quad \forall i \le n, j \le m & \text{minimum distance}\end{array}\right\}$$

where (x_j, y_j) is the geographical position of the j-th storage point, d_{ij} is the distance between the i-th plant and the j-th storage point, w_{ij} is the quantity of raw material transported from the j-th storage point to the i-th plant ($i \le n$, $j \le m$). The decision variable symbols are x, y, d, w. The rest are parameter symbols.

2.2.7.10 Kissing Number Problem

When billiard balls touch each other they are said to "kiss". Accordingly, the *kissing number* in D dimensions is the number of D-dimensional spheres of radius R that can be arranged around a central D-dimensional sphere of radius R so that each of the surrounding spheres touches the central one without their interiors overlapping. Determining the maximum kissing number in various dimensions has become a well-known problem in combinatorial geometry. Notationally, we indicate the Kissing Number Problem in D dimensions by KNP(D). In $\mathbb{R}^2$ the result is trivial: the maximum kissing number is 6.

2.2.11 Exercise
Prove that the kissing number in 2 dimensions is 6.

The situation is far from trivial in $\mathbb{R}^3$. The problem earned its fame because, according to Newton, the maximum kissing number in 3D is 12, whereas according to his contemporary fellow mathematician David Gregory, the maximum kissing number in 3D is 13 (this conjecture was stated without proof). This question was settled, at long last, more than 250 years after having been stated, when J. Leech finally proved that the solution in 3D is 12 [82]. As you can see in Fig. 2.3, there is some slack around the sphere, so it is not obvious that 13 non-overlapping spheres cannot fit. Given parameters D (number

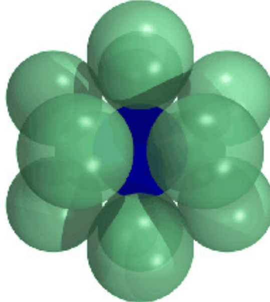


Figure 2.3: A solution of Kissing Number Problem in 3D with 12 spheres.

of dimensions) and N (number of spheres), the variables $x^i = (x_1^i, \ldots, x_D^i)$, $1 \le i \le N$ determine the position of the center of the i-th sphere around the central one. We maximize a decision variable $\alpha \ge 0$ which represents the minimum pairwise sphere separation distance in the N-sphere configuration being tested, subject to the necessary geometric constraints. Since the constraints are nonconvex, there may be multiple local minima. If the solution of the formulation determines that the global maximum is at

$\alpha \geq 1$, then there is enough space for N spheres; if the globally optimal α is strictly less than 1, it means that the N configuration has overlapping spheres, hence the kissing number is $N-1$. By solving this decision problem repeatedly for different values of N, we are able to quickly pinpoint the maximum N for which $\alpha > 1$. The following formulation correctly models the problem:

$$\max \quad \alpha \tag{2.18}$$

$$\forall i \leq N \quad ||x^i||_2 = 2R \tag{2.19}$$

$$\forall i < j \leq N \quad ||x^i - x^j||_2 \geq 2R\alpha \tag{2.20}$$

$$\alpha \geq 0 \tag{2.21}$$

$$\forall i \leq N \quad x^i \in \mathbb{R}^D \tag{2.22}$$

Constraints Eq. (2.19) ensure that the centers of the N spheres all have distance $2R$ from the center of the central sphere (i.e., the N spheres kiss the central sphere). Constraints Eq. 2.20 make the N spheres non-overlapping. This problem has been solved correctly up to $D = 4$ (and $N = 24$, which is KNP(4)) [87].

Chapter 3

The AMPL language

This chapter provides a brief tutorial to the AMPL language. A much better reference is the AMPL book [57], the chapters of which can be downloaded from `www.ampl.com` free of charge. AMPL stands for "A Mathematical Programming Language". It was initially conceived by Robert Fourer, David Gay and Brian Kernighan, although the current software and book are only authored by Fourer and Gay.

AMPL's strong point is that can interface to many different solvers, for LP, MILP, NLP and MINLP. Another endearing feature is that MP formulations written in AMPL are very close to the mathematical syntax (much closer to it than, say, what the GAMS [29] language achieves). Its weak point is that its algorithmic capabilities are quite limited.

AMPL is a commercial software: even with academic pricing, a yearly license runs into the hundreds of dollars (but GAMS costs much more, and MATLAB [103] more than either, specially if you order a decent set of add-ons). A subset of the AMPL language is implemented within the open-source GNU-licensed GLPK [100] solver; but GLPK only offers two solvers (a good LP solver, and a somewhat primitive MILP solver). Note that with both AMPL and GAMS the cost of the solvers is extra — and often you need to purchase solvers from other distributors. Luckily, AMPL makes it possible for teachers to obtain time-limited teaching licenses free of charge, which come with a lot of embedded solvers.

We will not cover installation here: we assume you obtained an AMPL distribution with a good set of solvers (particularly CPLEX, IPOPT, BonMin and Couenne), and that paths are correctly set, so that if you type `ampl` or `cplex` on the command line, you will invoke the correct executables.

3.1 The workflow

Although AMPL comes with a rather primitive GUI, we focus on a command-line driven workflow. You can see the `ampl` executable as an interpreter: a program which inputs a text file containing instructions and executes them one by one. Instruction files traditionally have the extension `.run`. So the basic calling sequence (from Linux, MacOSX or Windows) is:

```
ampl < file.run
```

If you are on a Unix system (e.g. Linux and MacOSX, but to some extent this might also work with Windows), you can exploit the operating system's "pipe"-style filters: you instruct AMPL to provide its output as formatted text, and pass the output to a second `command` which accepts that format:

```
ampl < file.run | command
```

In this setting, `command` might perform tasks such as writing a graphical file with a visualization of the output of your `file.run` program, or perform further algorithmics on the output of your program.

3.2 Input files

The simplest way to solve a MP formulation using AMPL involves three text files:

- a `.run` file, containing some imperative instructions (e.g. read/write data from/to the console or files, perform loops and/or tests);
- a `.mod` file, containing some declarative instructions (e.g. declare and define index sets, parameters, variables, objectives, constraints, formulations)
- a `.dat` file, containing the values to assign to the index sets and parameters.

Typically, all files share the same name (e.g. `mymodel.run`, `mymodel.mod`, `mymodel.dat`). The `.run` file usually instructs AMPL to read the `.mod` and the the `.dat` file.

Dividing a formulation into two files (`.mod` and `.dat`) is meant to help separating symbolic entities from numerical data. In a real world setting, one might need to solve large amounts of instances of the same problem: in that case one would only need to update the `.dat` file, never the `.mod` file.

On the other hand, this division in three text files serves the purpose of making the organization of information clearer to the user. AMPL does not care if you use one, two, three or more files (which might be the case if solving your problem involves more than one formulation).

3.3 Basic syntax

AMPL embeds three sublanguages: one is imperative (used mostly in `.run` files), one is declarative (used mostly in `.mod` files), and the third (the simplest) is only used within `.dat` files.

For all three sublanguages, comments are one line long and are introduced by the hash (`#`) character. Every instruction is completed using a semicolon (`;`), with one exception: within the AMPL imperative sublanguage, if the body of loops or tests is delimited by braces ({, }), there need not be a semicolon after the closing brace. E.g.,

```
# whole line comment
param i default 0; # rest of line is comment
let i := 4;
```

but

```
if (i == 4) then {
  let i := i + 1;
} else {
  let i := i - 1;
}
```

and

```
for {i in 1..5} {
  let i := i + 1;
}
```

Note that imperative program variables are declared to be formulation parameters (keyword `param`). Assignment of values to program variables requires the keyword `let` and the assignment operator `:=`, while the equality test uses `==` (the operator `=` is reserved for use in the definition of equality constraints). The notation `1..5` denotes the set $\{1, 2, 3, 4, 5\}$. For more about test/loop syntax, see the AMPL book [57].

3.4 LP example

Let us model the following LP using AMPL:

$$\min\{c^\top x \mid Ax \geq b \wedge x \geq 0\},$$

where c, A, b are parameters and x decision variables. AMPL will not accept matrix notation, so we really have to write the formulation as follows:

$$\left.\begin{array}{rrcl} \min & \sum\limits_{j\in N} c_j x_j & & \\ \forall i \in M & \sum\limits_{j\in N} A_{ij} x_j & \geq & b_i, \end{array}\right\}$$

which involves two index sets M (for the constraints) and N (for the variables), a cost vector $c \in \mathbb{R}^n$, a RHS vector $b \in \mathbb{R}^m$ and an $m \times n$ matrix A.

3.4.1 The `.mod` file

The syntax of a `.mod` file is declarative. It segments a MP formulation into five different entities: sets (`set`), parameters (`param`), variables (`var`), objective (introduced by either `minimize` or `maximize`) and constraints (introduced by `subject to`). Every entity is named. The name may be quantified over an index set. For example if `N` is an index set, you can declare variables x_i for $i \in$ `N` as follows:

```
var x{i in N};
```

We write the `.mod` file as follows.

```
## .mod file for an LP in form min cx : Ax >= b
# parameters and sets
param m integer, >0, default 50; # number of constraints
param n integer, >0, default 10; # number of variables
set M := 1..m; # index set for constraints
set N := 1..n; # index set for variables
param c{N} default Uniform01();  # objfun coeff vector
param A{M,N} default Uniform(-1,1); # constr matrix
param b{M} default Uniform(1,2); # RHS vector
# decision variables
var x{N} >= 0;
# objective function
minimize myObj: sum{j in N} c[j]*x[j];
```

```
# constraints
subject to myConstr{i in M}: sum{j in N} A[i,j]*x[j] >= b[i];
# solve the problem
option solver cplex;  # choose the solver
solve;  # solve it
# display the output
display x, objective, solve_result;
```

Some remarks follow.

- Every entity declaration supports a list of modifiers separated by commas: the parameter symbol `m` is required to be integer, positive, and, if uninitialized elsewhere, be assigned the value 50. The decision variable symbol `x`, quantified over `N`, declares a variable vector each component of which is constrained to be nonnegative.
- Modifiers such as `integer`, `>0` and `>=0` are applied to both parameters and variables: their meaning in these different context is correspondingly different. When a parameter is constrained, it will force AMPL to abort its execution whenever it is assigned (within the `.run` or `.dat` file) a value which does not satisfy the constraints. When a variable is constrained, the constraint will be passed to the solver. Constraining parameters is therefore a form of *input data validation*, whereas constraining variables is an essential part of an MP formulation.
- The parameters `c`, `A`, `b` are quantified over index sets, and describe vectors and matrices. Notwithstanding, their assigned default value is the output of the functions `Uniform01` and `Uniform`, which is a scalar. This means that every component of the vectors and matrix will be assigned the scalar returned by the function, which is called on every component. In other words, `c`, `A`, `b` are random vectors and a random matrix. Suppose we defined a parameter `C` quantified over `N`, to which we would like to assign default values taken from `c`. In this case, the declaration should be written as follows:

  ```
  param C{j in N} default c[j];
  ```

  Note that we explicitly mention the index `j` ranging over `N` in order to use it to index `c` (which is also quantified over the same set `N`).
- In order to initialize the index sets `M` and `N`, we use two scalar integer parameters `m` and `n`, which allow us to define `M` and `N` as sequence of consecutive integers from 1 to `m` (respectively, `n`). This is often done when defining consecutive integer ranges. You can also initialize a set within a `.mod` file by using normal set notation:

  ```
  set M := {1,3,6};
  ```

  or range notation:

  ```
  set M := 1..m;
  ```

  We remark that initialization of sets in `.dat` files follows a different syntax (see Sect. 3.4.2).
- Initializing a parameter or set with a value within a declaration instruction in a `.mod` can be done with two constructs: the assignment operator `:=` and the `default` keyword, e.g.:

  ```
  param m default 50;
  param n := 10;
  set M := 1..50;
  set N default {1,2,3,4};
  ```

Those sets/parameters initialized with an assignment operator `:=` are initialized once and for all during the AMPL execution. The initialization value assigned with the `default` keyword can be changed (e.g. using `let`) during the AMPL execution.

- The label `myObj` is the name we chose for the objective function. The label`myConstr` is the name we chose for the constraints. Since LPs only have one objective, we do not need to quantify `myObj` over an index set. On the other hand, we need to quantify `myConstr` over the constraint index set `M`.

- The choice of solver is made by specifying the `option solver`. The name which follows (in this case, `cplex`) must correspond to a solver executable file by the same name available to AMPL for calling (which requires adding the solver executable directory to the default path). The instruction `solve` will flatten the formulation, pass it to the solver, retrieve the (flat) solution from the solver, and re-organize the solution components in structured format.

- The `display` command is the simplest of AMPL's output commands. See the AMPL book [57] for more information.

- The variable `solve_result` is a system variable (i.e. it exists in AMPL's namespace by default — no need to declare it), in which solvers may store a string description of their return status.

3.4.2 The `.dat` file

An AMPL `.dat` file simply stores the input data in an AMPL-specific format. Users can define parameter values and set contents in a `.dat` file.

Sets are initialized in `.dat` files by providing a list of elements separated by spaces, without brace enclosure:

```
set N := 1 2 3;
set M := 1 2;
```

Parameters are initialized in various ways (see the AMPL book for more details). We shall only cover the basics here.

- Initializing a vector is done as follows.

  ```
  param c :=
    1  0.4
    2  0.1
    3  1.23 ;
  ```

- Supposing you did not initialize the index set `N` in the `.mod` file, and you cannot be bother to list its contents explicitly using the constructs above, you can do it implicitly in the definition of the first parameter indexed on `N`.

  ```
  param : N : c :=
    1  0.4
    2  0.1
    3  1.23 ;
  ```

- If two (or more) vectors (such as `c`, `C`) are defined over the same index set `N`, you can list the index set once only.

```
param : c C :=
  1  0.4   0.9
  2  0.1   0.8
  3  1.23 -0.7 ;
```

- You can also initialize `N` while defining both `c` and `C`.

```
param : N : c C :=
  1  0.4   0.9
  2  0.1   0.8
  3  1.23 -0.7 ;
```

- Initializing a matrix (or a tensor) simply requires more index columns.

```
param A :=
  1 1   1.1
  1 2   0.0
  1 3   0.3
  2 1   0.0
  2 2  -0.31
  2 3   0.0;
```

- If your matrix is sparse, make sure you initialize it to zero in the `.mod` file (using the `default 0` modifier in the declaration), and then simply initialize the nonzeros in the `.dat` file (otherwise your `.dat` files will be enormous).

```
param A :=
  1 1   1.1
  1 3   0.3
  2 2  -0.31;
```

- Note that the format (columns, line breaks) is arbitrary. By leveraging its knowledge of the index sets of the parameters, necessarily declared in the `.mod` file, AMPL will not mind whether you write the previous matrix definition as follows.

```
param A := 1 1 1.1 1 3 0.3 2 2 -0.31;
```

  Since the previous syntax is clearer (to a human), it is preferable.

3.4.3 The `.run` file

A minimal `.run` file, sufficient for reading the model, the data, selecting the solver and solving the instance is as follows.

```
## .run file
# read the model file
model file.mod;
# read the data file
model file.dat;
# choose the solver
option solver cplex;
# solve the problem
solve;
# display the solver status
display solve_result;
```

3.5 The imperative sublanguage

Although some heuristics can easily be coded in AMPL, more complicated algorithms might be unwieldy, as AMPL has (among other limitations) no construct for function calls. Mostly, the imperative sublanguage is very useful for formatting the output. You might for example instruct AMPL to write the solution of a circle packing problem (Sect. 1.3.10) in Python, and then use the latter to display the solution graphically, as in the following AMPL code snippet:

```
print "import matplotlib.pyplot as plt" > circlepacking_out.py;
for {i in N} {
  printf "circle%d = plt.Circle((%g,%g),%g)\n", i, x[i], y[i], r >> circlepacking_out.py;
}
print "fig = plt.gcf()" >> circlepacking_out.py;
for {i in N} {
  printf "fig.gca().add_artist(circle%d)\n", i >> circlepacking_out.py;
}
print "fig.savefig('circlepacking_out.png')" >> circlepacking_out.py;
```

Part II

Computability and complexity

Chapter 4

Computability

In this chapter we treat the very basic question "can we even solve an optimization problem using a computer?" In general, this question can be asked of any type of broad problem category, be it decision, search or optimization. The field of logic that studies this question is called *computability.* The questions are asked in a given *computing model*, which is usually the Turing machine (TM) model of computation (though it need not be). We want the answers to be valid for every problem in the class of interest. For example, every (finite) LP with rational input data can be solved using a TM that implements the simplex method. Conversely, there can be no TM that is able to solve every MINLP.

4.1 A short summary

We first give a very short summary of concepts in computability theory.

4.1.1 Models of computation

The computer was first conceived by Alan Turing in 1936 [143]. Turing's mathematical model of the computer is called *Turing machine.* A TM consists of an infinite tape, divided into a countably infinite number of cells, with a device (called *head*) that can read or write symbols out of a given alphabet A on each cell of the tape. According to the state $s \in S$ the TM is in, the head either reads, or writes, or moves its position along the tape. The description of any TM includes a set of instructions which tell it how to change its state. Turing showed that there exist TMs which can simulate the behaviour of any other TM: such TMs are called *Universal TMs*

Turing's work spawned further research, from the 1950s onwards, aimed at simplifying the description of UTMs, involving scientists of the caliber of Shannon [134] and Minsky [110]. More recently, Rogozhin [127] described UTMs with low values of $(|S|, |A|)$, e.g. $(24, 2)$, $(10, 3)$, $(7, 4)$, $(5, 5)$, $(4, 6)$, $(3, 10)$, $(2, 18)$. It appears clear that there is a trade-off between number of states and number of symbols in the alphabet.

UTMs are not the only existing models of computation — several others exist, sometimes very different from each other (see e.g. the *Game of Life*, a model for bacteria diffusion [19]). Such models are said to be *Turing-complete* if they can simulate a UTM. "Simulating", in this context, means using a different model C of computation in order to mimick the behaviour of a UTM. To prove this, it suffices to show that every instruction, state and symbol of the UTM can be simulated by C. If the UTM can also simulate C, then C is said to be *Turing-equivalent.*

Church's Thesis is the statement that every Turing-complete model of computation is also Turing-

equivalent. So far, no Turing-complete model of computation was found to be more "powerful" than the UTM.

4.1.2 Decidability

Functions $\mathbb{N} \to \mathbb{N}$ described by a TM are called *computable*. The term *decidable* applies to relations instead of functions: a k-ary relation R on D^k is decidable if, given $d_1, \ldots, d_k \in D$, there exists a TM that decides whether the k-tuple $d = (d_1, \ldots, d_k)$ is in R. Since "being in R" can be encoded as a YES/NO type of question, decidability applies to decision problems.

Sets $V \subseteq \mathbb{N}$ that are domains (or co-domains) of computable functions are called *recursively enumerable*. If V and $\mathbb{N} \smallsetminus V$ are both recursively enumerable, then they are both also called *recursive* or *decidable*.

Given a set $V \subseteq \mathbb{N}$ and an integer $v \in \mathbb{N}$, one may ask whether $v \in V$ or not. This is a fundamental decision problem (in number theory — but a computer represents every data structure with numbers in base 2, so this limitation is only formal). It turns out that V is recursively enumerable if and only if there is a program that answers YES when $v \in V$, but may answer wrongly or even fail to terminate when $v \notin V$; moreover, V is decidable if and only if there is a program that answers YES when $v \in V$ and NO when $v \notin V$.

It should appear clear that recursively enumerable sets are of limited value as far as proving that an answer to a problem is correct: if the algorithm answers YES, it may be a true positive or a false negative, and there is no way to tell. Moreover, how is a user supposed to know whether a program fails to terminate or is simply taking a long time? Accordingly, we hope to consider problems so that the solution set is decidable. On the other hand, many interesting sets arising in optimization problems are only recursively enumerable (or worse).

4.2 Solution representability

The solutions of LPs and MILP have rational components as long as the input data is rational. For MINLP, the situation is not so clear: solution components might involve irrational numbers (both algebraic and transcendental, depending on the involved functions). We list four approaches that attempt to deal with the issue of representing such solutions within a finite amount of storage.

4.2.1 The real RAM model

The computation model of Blum, Shub and Smale [22] (often referred to as *real RAM* model) essentially eschews the problem of representation, as it defines the real equivalent of computational complexity classes such as **P**, **NP** and their relationships. In the real RAM model, storing, reading or performing arithmetic on real numbers has unit cost [22, p. 24]. This model of computation is mostly used for theoretical results concerning algorithms in numerical analysis and scientific computing.

4.2.2 Approximation of the optimal objective function value

The approach taken by the GO community, specially those who develop sBB algorithms, consists in finding a (rational, or rather floating point encoded) solution x^* yielding an objective function value $f^* = f(x^*)$ that is within a given $\varepsilon > 0$ of the true globally optimal function value $\tilde{f}$ at a true global

optimum $\tilde{x}$:

$$|f^* - \tilde{f}| \le \varepsilon. \tag{4.1}$$

Since the true optimal value $\tilde{f}$ is not known, in practice Eq. (4.1) is enforced by requiring that $|f^* - \bar{f}| \le \varepsilon$, where $\bar{f}$ is a guaranteed lower bound to the optimal objective function value, computed e.g. by solving an LP relaxation of Eq. (2.2). One of the issues with this approach is that, depending on the instance being solved, Eq. (4.1) might be satisfied even if $\|x^* - \tilde{x}\|$ is arbitrarily large.

4.2.3 Approximation of the optimal solution

The approach taken by Dorit Hochbaum [70] is more accurate, as it insists that the solution x^* is within a given $\varepsilon > 0$ tolerance of the true optimum $\tilde{x}$:

$$\|x^* - \tilde{x}\|_\infty \le \varepsilon. \tag{4.2}$$

This means that x^* is the same as $\tilde{x}$ in $O(\log \frac{1}{\varepsilon})$ decimal digits. Other than that, all arithmetical operations on reals take $O(1)$ time. Since one only needs to consider $O(\log \frac{1}{\varepsilon})$ decimal digits, this assumption places this representation approach within the TM model of computation.

4.2.4 Representability of algebraic numbers

A more credible attempt at representing an algebraic number α has been made using of minimal polynomials. The most common is the *Thom encoding*, a pair (p_α, σ), where $p_\alpha(x)$ is the minimal polynomial of α (of degree d, say) and $\sigma : \{0, \ldots, d\} \to \{0, -1, 1\}$ encodes the sign of the k-th derivative of p_α at α [12, Prop. 2.28]. Simpler representations are possible for specific tasks, e.g. σ might be replaced by a rational number a which is closer to α than to any other real root of p_α [14].

4.2.4.1 Solving polynomial systems of equations

Solving polynomial systems of equations exactly is sometimes possible by "diagonalizing" them using *Gröbner bases* and then perform back-substitution, similar to Gaussian elimination.

Gröbner bases can be found by Buchberger's algorithm [30]. It takes as input a rational multivariate polynomial equation system:

$$\forall i \le m \quad p_i(x) = 0. \tag{4.3}$$

It then proceeds by diagonalizing Eq. (4.3) to a new polynomial system:

$$\forall i \le m' \quad q_i(x) = 0, \tag{4.4}$$

such that the leading terms of p_i's and q_i's, w.r.t. some given monomial order, generate the same ideal. Let $F = \{p_1, \ldots, p_m\}$. Buchberger's algorithm proceeds as follows:

1: Fix an ordering $<_F$ on the monomials of F
2: Let $G \leftarrow F$
3: **repeat**
4: Let $H \leftarrow G$
5: **for** $p, q \in G$ s.t. $p \neq q$ **do**
6: Let $\hat{p}, \hat{q}$ be the leading terms of p, q w.r.t. $<_F$
7: Let a be the least common multiple (lcm) of $\hat{p}, \hat{q}$
8: Let $s \leftarrow \frac{a}{\hat{p}}p - \frac{a}{\hat{q}}q$ # *This cancels the leading terms of* p, q *in* s
9: Reduce s w.r.t. G using multivariate polynomial division
10: **if** $s \not\equiv 0$ **then**

11: Update $G \leftarrow G \cup \{s\}$
12: **end if**
13: **end for**
14: **until** $G = H$

Buchberger's algorithm monotonically increases the size of the ideal generated by the leading terms of G. The algorithm terminates because, by Hilbert's basis theorem, ascending chains of ideals must eventually become stationary. The termination condition is verified even if the last considered polynomial is not univariate.

Like Gaussian elimination, this diagonalization can be used for performing back-substitution as long as the last considered equation $q(x)$ only depends on a single variable. Unlike Gaussian elimination, however, m' generally exceeds m, and it does not yield a guarantee that q_i will contain strictly fewer variables than q_{i+1}: the diagonal structure might contain blocks of polynomials depending on the same set of variables. Even if the back-substitution procedure fails to provide a solution, the diagonal form will still hold after a failure occurs, a condition which might be described as "back-substitute as far as possible".

Unfortunately, Buchberger's algorithm has doubly exponential worst-case complexity in general (see Ch. 5), though it behaves singly exponentially in some cases [11].

An interesting development of Gröbner's bases is given by *chordal networks* [34]. They supply polynomial systems that are cheaper to construct, provide the same back-substitution functionality for finding a solution of a polynomial system of equations. Unfortunately, their size is larger than for Gröbner bases.

4.2.4.2 Optimization using Gröbner bases

There are at least two articles [63, 32] where Gröbner bases are used to diagonalize the first-order optimality conditions, also known as Karush-Kuhn Tucker (KKT) system (see Thm. 6.2.7), of a Polynomial Programming (PP) problem. In both articles, the last phase of the procedure performs back-substitution on the diagonalized polynomial system using floating point numbers, thereby forsaking exactness; but those floating point numbers could in principle be used as "closest rationals" in the representation mentioned above.

4.3 Computability in MP

As mentioned above, we can solve LPs (by means of the simplex method, see Sect. 7.1). We can solve MILPs (by means of the BB algorithm). We cannot solve all cNLPs (and hence even the including classes NLPs, cMINLPs and MINLPs) at least because we have issues with representing the solution exactly, as detailed in Sect. 4.2.

We focus on MINLP. While we cannot solve them in full generality (see Sect. 4.3.2 below), the full answer is rather more interesting: MINLP is a class of problems containing two bordering theories[1], one of which is decidable, while the other is not.

4.3.1 Polynomial feasibility in continuous variables

MINLP contains (as a strict subset) all Polynomial Feasibility Problems (PFP) with variables ranging over the reals:

$$\forall i \leq m \qquad p_i(x) \quad \mathscr{R} \quad 0, \tag{4.5}$$

[1] By *theory* we mean a class of formal sentences provable from a given set of axioms; also see Footnote 3 on p. 66.

where the p_i's are rational polynomials and the relation symbol $\mathscr{R}$ is one of the relations in the set $\{\geq, =\}$. We question the existence of a general method for deciding whether there exists a solution to Eq. (4.5).

4.3.1 Remark (Polynomial equations and inequalities)
Note that Eq. (4.5) can in fact be expressed with a single relation $\mathscr{R}$, either $\geq$ or $=$, since every equation can be expressed by a pair of inequalities with opposite sign, and every inequality $p_i(x) \geq 0$ can be rewritten as $p_i(x) + s_i^2 = 0$, where s_i is an additional continuous variable.

4.3.1.1 Quantifier elimination

Tarski proved in [141] that systems like Eq. (4.5) are decidable. Most algorithms for deciding Eq. (4.5) are based on a technique known as *quantifier elimination*. This is an algorithm which turns a quantified logical sentence with variable terms into one without quantifiers or free variables. Forthwith, deciding truth or falsity can be achieved by elementary manipulations leading to either a tautology $1 = 1$ or a contradiction $0 = 1$. Note that Tarski's algorithm can be applied to a larger class of polynomial systems than Eq. (4.5): the relation symbol $\mathscr{R}$ can actually range over $\{\geq, >, =, \neq\}$.

Tarski's proof extends for 57 pages of a RAND Corporation technical report [141]. To showcase an easier quantifier elimination example, Lyndon discusses dense linear orders in his book [99, p. 38]. This theory includes logical formulæ involving $\forall, \exists, \neg, \wedge, \vee$, the variable symbols $x_1, x_2, \ldots$, the terms True, False, the real numbers as constants, and the relation symbols $<, =$. Sentences of this theory can be inductively reduced to a disjunctive normal form (DNF) such that each clause is $\exists x_i$ s.t. $q_i(x)$, where q_i is an unquantified conjunction of sentences $\bigwedge q_{ij}$, where, in turn, each q_{ij} has one of the forms $s = t$ or $s < t$ with s, t are either variables or real constants. Each q_{ij} is then reduced to either True or False: if s, t are both constants, the conditions $s < t$ or $s = t$ are immediately verified and can be replaced with True or False. If both s and t are x_i, then $s = t \Rightarrow x_i = x_i$ is True, and $s < t \Rightarrow x_i < x_i$ is False: so s, t can be assumed to be different. If s is the variable x_i, a formula $x_i = t$ (independently of whether t is a constant or another variable) can be interpreted to mean "replace x_i with t", so the variable x_i can be eliminated. The remaining case is that q_i is a conjunction of formulae of the form $s < x_i$ and $x_i < t$ (with s, t either other variables or constants), which amounts to writing $s < t$ — again, this eliminates x_i. Since every occurrence of x_i can be eliminated from q_i, $\exists x_i q_i$ can be more simply re-written as q_i: hence the name *quantifier elimination.*.

4.3.1.2 Cylindrical decomposition

Well after Tarski's 1948 quantifier elimination algorithm, Collins discovered [36] that the decision procedure of systems such as Eq. (4.5) is in some sense a nontrivial extension of the dense linear order case. The solution set of Eq. (4.5) consists of finitely many connected components, which can be recursively built out of cylinders with bases shaped as points or intervals the extremities of which are either points, or $\pm\infty$, or algebraic curves depending on variables involved in previous recursion levels. Although Collins' algorithm is doubly exponential in the number of variables, a singly exponential algorithm was described in [12].

The cylindrical decomposition result of [36] consists of a topological and a geometric part. The topological part states that the feasible regions of Eq. (4.5) (where $\mathscr{R}$ ranges in $\{>, \geq, =, \neq\}$), also called *semi-algebraic sets*, consist of a finite number of connected components. The geometrical part gives the recursive description mentioned above in terms of cylinders. The topological part was known previous to Collins' contribution, see e.g. [108].

4.3.2 Polynomial feasibility in integer variables

In this section, we shall consider Eq. (4.5) subject to integrality constraints on the vector x of decision variables. In fact, it suffices to consider equations only (see Rem. 4.3.1):

$$\left.\begin{array}{rrcl} \forall i \le m & p_i(x) & = & 0 \\ \forall j \le n & x_j & \in & \mathbb{Z}. \end{array}\right\} \tag{4.6}$$

Given a system Eq. (4.6) of polynomial equations in integers, can we decide whether it has a solution?

4.3.2.1 Undecidability versus incompleteness

The question of deciding whether a polynomial system has integer solutions is related but different from completeness[2]. A consistent formal system[3] S is *complete* when, for any sentence p of the system, either p is provable within S, or $\neg p$ is. A system S is incomplete when there are sentences p such that neither p nor $\neg p$ are provable within S. Gödel's (first) incompleteness theorem states that any S capable of representing $\mathbb{N}$ and its arithmetic is either inconsistent or incomplete. This leaves open the question of decidability, i.e. of whether there exists an algorithm that, given any p in S, decides whether p is provable within S or not.

4.3.2 Remark (Decidability does not imply completeness)
There is a common misconception that decidability should imply completeness. The (faulty) argument goes as follows. If a formal system S is decidable, then for any given p the system S can be used to decide whether p is provable in S (e.g. by exhibiting a proof of p within S). So, in case p is provable, then $\neg p$ cannot be, and vice versa*. Hence, either p or $\neg p$ must be provable within S, which implies that S is complete.*

*The error resides in thinking that the "*vice versa*" above exhausts all possibilities. For two sentences p and $\neg p$ in S, there are four assignments of "provability within S" to the two sentences: (i) both are provable, (ii) the first is provable and the second is not, (iii) the first is not and the second is, and (iv) neither is provable. The first assignment leads to the inconsistency of S: it should be discarded since we assumed that S is consistent. The second and third assignments are part of the above (faulty) argument. The error stems from forgetting the fourth assignment: i.e., that both p and $\neg p$ may fail to be provable within S. This condition is described by saying that p is* independent *of S. A decision algorithm for provability in S might answer NO when given either p or $\neg p$ as input. So a formal system can be decidable but incomplete (e.g., the Wikipedia page* `https://en.wikipedia.org/wiki/Decidability_(logic)#Relationship_with_completeness` *states that the theory of algebraically closed fields bears this property).*

As it turns out, if S encodes arithmetic in $\mathbb{N}$ and is consistent, it is not only incomplete (by Gödel's first incompleteness theorem) but also undecidable. This was settled by Turing [143] using a diagonalization argument involving another undecidable decision problem called the *halting problem* — is there an algorithm for deciding whether a given TM terminates or not?

[2] We mean "completeness" as in Gödel's *incompleteness* theorem, rather than Gödel's *completeness* theorem — these two notions, though bearing related names, are distinct.

[3] A formal system S is a finite language L, together with a grammar that defines a set of well-formed formulæ (called *sentences*) over L, a chosen set of sentences called *axioms*, and a set of *inference rules* (e.g. *modus ponens*) which define relations over sentences. Given a sentence p, a *proof* for p in S is a sequence of iterative applications of inference rules to sentences that are either axioms or for which a proof was already provided.

4.3.2.2 Hilbert's 10$^{\text{th}}$ problem

We now come back to our MINLP feasibility problem in Eq. (4.6). Each equation in the system is known as a *Diophantine equation* (DE). Let S be a formal system encoding arithmetic in $\mathbb{N}$. Systems of DEs are certainly well-formed formulæ within S. Although the set of *all* well-formed formulæ in S is undecidable, we still do not know whether the limited subset described by the form of Eq. (4.6) is "general enough" to be undecidable. The common property of all feasibility systems is that the integer variables $x_1, \ldots, x_n$ are implicitly quantified by *existential* quantifiers "$\exists$", but no *universal* quantifier "$\forall$". Moreover, Eq. (4.6) only consists of sentences involving polynomials, whereas exponentiation is also part of arithmetic in integers. We can now frame the question as follows: is the set of all existentially quantified polynomial sentences of S decidable or not? This can be seen as a modern restatement of Hilbert's 10$^{\text{th}}$ problem.

From the proof of Gödel's first incompleteness theorem [60], it is clear that Gödel only used a finite number of *bounded* universal quantifiers. Davis, in [46], shows that a single bounded universal quantifier is sufficient to encode undecidable problems:

$$\exists y \forall z \le y \exists x_1, \ldots, x_n \quad p(y, z, x) = 0, \tag{4.7}$$

where p is an integral polynomial, and $x_1, \ldots, x_n, y, z$ are all in $\mathbb{N}$. In [47], it is shown that there exist undecidable problems that are almost in the desired form:

$$\exists x_1, \ldots, x_n \in \mathbb{N} \quad \eta(x) = 0, \tag{4.8}$$

but where η is an *exponential* DE (EDE), i.e. a function that can be written using arithmetical operations and exponentiation. In a landmark result, Matiyasevich proved in 1970 [104] that the exponential relationship $a = b^c$ can be expressed by means of a DE (i.e. without exponentiation), thereby settling Hilbert's 10$^{\text{th}}$ problem in the negative. This result is now known as the Matiyasevich-Davis-Putnam-Robinson (MDPR) theorem. In the setting of this paper, the MDPR theorem means that

$$\exists x_1, \ldots, x_n \in \mathbb{N} \quad p(x) = 0, \tag{4.9}$$

where p is a polynomial, is generally undecidable. This makes Eq. (4.6) undecidable, which, by inclusion, makes MINLP undecidable, too.

4.3.3 Remark (DE systems)
A system of DEs such as Eq. (4.6) is equivalent to a single DE such as Eq. (4.9): it suffices to write

$$p(x) = \sum_{i \le m} (p_i(x))^2.$$

4.3.4 Remark (Undecidability in $\mathbb{Z}$)
The undecidability results relate to $\mathbb{N}$ rather than $\mathbb{Z}$, but this is without loss of generality: we can transform any DE with solutions in $\mathbb{Z}$ to one with solutions in $\mathbb{N}$ by writing $x_i = y_i^+ - y_i^-$ (where $y_i^+, y_i^- \in \mathbb{N}$), and, conversely, since every non-negative integer is the sum of four squares, the opposite transformation as $x_i = a_i^2 + b_i^2 + c_i^2 + d_i^2$ for the i-th component x_i occurring in the arguments of $p(x)$.

4.3.5 Remark (Polynomials over $\mathbb{Q}$)
The result also holds for polynomials over $\mathbb{Q}$: it suffices to write rational coefficients as fractions, find the lcm L of the denominators, and consider $Lp(x)$ instead of $p(x)$.

It might seem strange to stare at a single polynomial equation such as Eq. (4.9), and claim that it is undecidable: it sounds like saying that a single instance of a problem is undecidable. In fact, the variable vector of $p(x)$ is partitioned in two subsequences $\alpha = (\alpha_1, \ldots, \alpha_\ell)$ and $y = (y_1, \ldots, y_N)$, so that α encodes the parameter of an "instance", and y the solution. Since:

(a) every recursively enumerable set W can be encoded by a single polynomial equation $p^W(\alpha, y) = 0$ such that any string w is encoded in α, and $w \in W$ iff $p(\alpha, y) = 0$ has a solution in y;

(b) there exist recursively enumerable sets that are undecidable,

the MDRP result follows.

4.3.3 Universality

As remarked in [76], recursively enumerable sets can be enumerated in some order $W_1, W_2, \ldots$ such that the relation $w \in W_v$ for some v is also recursively enumerable. This implies the existence of a DE

$$U(w, v, y) = 0 \tag{4.10}$$

for some parameters w and v such that $U(\alpha, v, y) = 0$ has an integer solution y iff $w \in W_v$. Such polynomials U are known as *universal Diophantine equations* (UDE). This is equivalent to a UTM, which takes as input an encoding of any TM T_v and any instance w, and simulates $T_v(w)$. In this setting, T_v is a TM that is supposed to determine whether $w \in W_v$.

Finding a UDE presents potential applications, as it would allow the encoding of any computer program into a single polynomial. Studying its properties might help shed light on the program itself. Jones [76] conducted a thorough study of two complexity measures for UDEs: their degrees δ and the number ν of variables occuring in them.

The minimum known value for δ is 4. It suffices to take *any* UDE, and repeatedly replace any degree 2 term with a new variable until we obtain a system of DEs $\forall i \le m \ (t_i(x) = 0)$ where each $t_i(x)$ consists of monomials of degrees 1 and 2. The equation

$$\sum_{i \le m} (t_i(x))^2 = 0 \tag{4.11}$$

(see Rem. (4.3.3)) is therefore a UDE with degree $\delta = 4$. In passing, we also conclude that, in general, systems of (many) quadratic DEs (QDE) are also undecidable. Jones reports the existence of a UDE with $(\delta = 4, \nu = 58)$. Decreasing ν unfortunately yields large increases on δ: Jones [76] reports a new (δ, ν) pair due to Matiyasevich valued at $(1.638 \times 10^{45}, 9)$.

4.3.6 Remark (Proofs in $\mathbb{N}$ involve at most 100 operations)
By way of an application, Jones exploits the $(4, 58)$ *UDE, suitably modified to minimize the number* B *basic operations (additions and multiplications) required to evaluate the polynomial, and obtains* $B = 100$. *This implies that for any statement* p *that can be proved within the formal system* S *of arithmetic in* $\mathbb{N}$, p *has at least a proof that only involves 100 integer additions and multiplications.*

Coming back to MINLP, since UDEs are subsets of MINLP, MINLP inherits their properties, which means that there exist universal MINLP formulations, though they may be hard to exploit in practice. The dynamics of a universal register machine (another computation model which is more similar to modern computers than TMs are) have been modelled in [88] using an infinite MINLP. This MINLP becomes finite, and hence practically solvable, on *bounded* executions, as boundedness ensures termination of the underlying TM.

4.3.4 What is the cause of MINLP undecidability?

Considering Sect. 4.3.1 and Sect. 4.3.2, we can ascribe the undecidability of MINLP to the presence of integer variables. This is apparently in contrast with the fact that any integer can be expressed within a

theory encoding polynomials and continuous variables: given any $a \in \mathbb{Z}$, the equation

$$x - a = 0$$

is polynomial and encodes the fact that the continuous variable x should take the integer value a. Taking this further, we can write $x \in \{a_1, \ldots, a_k\}$ for any integer values $a_1, \ldots, a_k$ using the polynomial equation

$$(x - a_1) \cdots (x - a_k) = 0.$$

A different approach uses the length ℓ of the finite sum $y + y + \cdots + y$ (say it has ℓ occurrences of y) to express the integer ℓ using the polyomial equation $xy = \sum_\ell y$. Aside from the zero solution, any other solution with $y > 0$ yields $x = \ell$.

However, every finite set F is decidable, at least if its elements are all given explicitly: any total order on F provides an enumeration algorithm. Obviously, the complement $\bar{F}$ of F w.r.t. $\mathbb{N}$ is recursively enumerable: just list $\mathbb{N}$ and verify if the current element is in F or not.

To achieve undecidability, we have to look at infinite subsets of $\mathbb{N}$. Is it possible to encode any such set as solutions over $\mathbb{R}$ of some (multivariate) polynomial equation? The answer is no: supposing there exists a real polynomial system with a countably infinite set of (integer) solutions would yield an infinite number of connected components in the corresponding variety, contrary to Milnor's topological result [108]. Another way of proving this is that, if it were possible to encode $\mathbb{N}$ as solutions of a real polynomial system in any (even nonstandard) way, then the theory of polynomials over $\mathbb{R}$ would be undecidable, contrary to Tarski's decision algorithm. It is common knowledge that, in order to encode all integers in a system of nonlinear equations with variables ranging over $\mathbb{R}^n$, one needs at least one periodic function, e.g. the set of solutions of $\sin(\pi x) = 0$ is $\mathbb{Z}$. If the polynomials range over $\mathbb{C}^n$, the exponential function (which is periodic over the complex numbers) is also a candidate.

These arguments suggest that a cause of undecidability is the issue of boundedness versus unboundedness of the decision variables. This is well known in polynomial optimization theory. With unbounded variables, even the continuous relaxation of a MILP may need to be reformulated using nonlinear functions for practical usefulness [68].

4.3.5 Undecidability in MP

Although the theories of polynomial equations over the reals and the natural numbers belongs *de re* to MINLP, since PFP is clearly a subclass of MINLP, the results above are traditionally a part of logic and axiomatic set theory. Here follow two results from the MP community.

The earliest paper investigating MP and (un)decidability is possibly Jeroslow's 1971 paper [75] about the undecidability of Integer Quadratic Programming. Consider the formulation

$$\left.\begin{array}{lrcl} \min & c^\top x & & \\ \forall i \le m & x^\top Q^i x + a_i^\top x & \le & b_i \\ \forall j \le n & x_j & \in & \mathbb{Z}, \end{array}\right\} \quad (4.12)$$

where $c \in \mathbb{Q}^n$, Q^i are rational $n \times n$ matrices for each $i \le m$, $A = (a_i \mid i \le m)$ is a rational $m \times n$ matrix, and $b \in \mathbb{Q}^m$. Witzgall's algorithm [152] solves Eq. (4.12) when each quadratic form $x^\top Q^i x + a_i^\top x$ is *parabolic*, i.e. each Q^i is diagonal with non-negative diagonal entries (for $i \le m$).

In contrast, Jeroslow observed that this is a limiting case, since if the quadratic forms are diagonal but are allowed to have some negative entries, then they can encode an undecidable set, via the undecidability theory of DEs. The proof is as follows: given an undecidable DE $p(x) = 0$, we consider the following

subclass of Eq. (4.12):

$$\left.\begin{array}{rrcl} \min & x_{n+1} & & \\ & (1-x_{n+1})p(x) & = & 0 \\ & x_{n+1} & \ge & 0 \\ \forall j \le n & x_j & \in & \mathbb{Z}. \end{array}\right\} \quad (4.13)$$

Obviously, the minimum of Eq. (4.13) is 0 iff $p(x) = 0$ has a solution, and 1 otherwise. Now we follow the argument given above Eq. (4.11), and iteratively linearize products occurring in the k monomials of $p(x)$ until p can be reformulated to a linear form $y_1 + \cdots + y_k$, subject to a set of *defining constraints* in the form $y_h = \tau_h(x, y)$, where each τ_h only involves linear occurrences of variables, or their squares, or bilinear products of two variables. This is already undecidable, since finding the optimum of Eq. (4.13) would solve the undecidable DE $p(x) = 0$, but Jeroslow notes that one can write each bilinear product of decision variables uv (where u, v are decision variable symbols occurring in either x or y), by means of an additional variable w, as $w = u + v$ while replacing uv by $\frac{1}{2}(w^2 - u^2 - v^2)$. This yields the required form.

Jeroslow also notes that whenever the integer variables are bounded, the problem becomes decidable (since there is only a finite number of possible solutions of $p(x) = 0$).

Another paper about optimization and undecidability is [154], which focuses on undecidable problems in MINLP and GO as detailed here below.

1. **PP in integers is undecidable**. Consider:

$$\left.\begin{array}{rrcl} \min & q(x) & & \\ \forall j \le n & x_j & \in & \mathbb{Z}, \end{array}\right\} \quad (4.14)$$

where q is a polynomial. We define $q(x) = (p(x))^2$ so that $\min_x q(x) = 0$ iff $p(x) = 0$, since q is a square and its minimum value must be ≥ 0. If we could compute the minimum of $q(x)$, we could decide on the solvability of $p(x) = 0$ according to whether $\min_x q(x) = 0$ or > 0. But this is impossible since $p(x) = 0$ is undecidable.

2. **Solving system of nonlinear equations is undecidable**. Consider:

$$\forall i \le m \quad g_i(x) = 0, \quad (4.15)$$

where $g_i : \mathbb{R}^n \to \mathbb{R}$ are nonlinear functions: is this problem decidable? The paper [154] remarks that if $p(x) = 0$ is an undecidable DE, then

$$(p(x))^2 + \sum_{j \le n} (\sin(\pi x_j))^2 = 0, \quad (4.16)$$

where x ranges in $\mathbb{R}^n$, is precisely a restatement of the DE, and so it is undecidable. Note that Eq. (4.16) is obviously a subclass of Eq. (4.15).

3. **Unconstrained NLP is undecidable**. Consider:

$$\min_x q(x), \quad (4.17)$$

for some nonlinear function $q(x)$. Let $p(x) = 0$ be an undecidable DE. Let $q(x) = (p(x))^2 + \sum_{j \le n} (\sin(\pi x_j))^2$, and suppose $q^* = \min_x q(x)$ is computable. Then if $q^* = 0$ we have $p(x) = 0$ and $x_j \in \mathbb{Z}$ for all $j \le n$, otherwise we do not, which is equivalent to the decidability of $p(x) = 0$, against assumption.

4. **Box-constrained NLP is undecidable**. Consider

$$\min_{x^L \le x \le x^U} q(x), \quad (4.18)$$

for some nonlinear function $q(x)$ and some variable bound vectors x^L, x^U. Let $p(y) = 0$ be an undecidable DE. Let

$$q(x) = (p(\tan x_1, \ldots, \tan x_n))^2 + \sum_{j \le n} (\sin(\pi \tan x_j))^2,$$

then we can enforce $-\frac{\pi}{2} \le x_j \le \frac{\pi}{2}$ for all $j \le n$, i.e. $x^L = -\frac{\pi}{2}$ and $x^U = \frac{\pi}{2}$ without changing the values of $q(x)$. The argument runs as above: if we could compute the minimum q^* of $q(x)$ over $x^L \le x \le x^U$, we could establish whether $p(y) = 0$ has a solution or not, which is impossible.

Chapter 5

Complexity

In this chapter, we look at the computational complexity of some MINLP problems. We shall mostly focus on nonconvex NLPs, since the presence of integer variables, even bounded to $\{0, 1\}$, makes it very easy to prove MINLP hardness, as shown in Sect. 5.2.

5.1 Some introductory remarks

Many variants of TMs have been proposed in the first years of research on theoretical computer science: larger alphabets, half-infinite or multiple tapes to name a few. For most of these variants, simulation proofs were quickly devised to show that none of them was *essentially* more powerful than the "basic" TM. Driven by the need for faster computation, the issue of computational complexity became more pressing: given an algorithm and some input data, how many steps[1] would a TM need to perform before termination? Given that the same algorithm is routinely run on different inputs, the paradigm of *worst case complexity* was brought to attention. Infinite sets of input data of the same type and increasing size, together with a specification of the goal the algorithm is supposed to achieve, were grouped in classes named *problems*; conversely, each member of a given problem is an *instance* (also see Sect. 2.1.3). We recall that a decision problem consists in answering a YES/NO question.

Given any problem P, if there exists an algorithm taking a number of steps bounded by a polynomial function of the instance size n in the worst case, we denote its complexity by $O(n^d)$, where d is the degree of the polynomial, and call the algorithm *polynomial-time* (or simply *polytime*). If we are only able to establish an exponential bound, we denote it by $O(2^n)$, and call the algorithm *exponential-time.*

5.1.1 Problem classes

5.1.1.1 The class P

The focus of computational complexity rapidly shifted from algorithms to problems. Given a decision problem P, the main issue of computational complexity is: what is the *worst-case* complexity of the *best* algorithm for solving P? Edmonds [49] and Cobham [35] remarked around 1965 that problems having a polytime complexity are invariant w.r.t. changes in the TM definitions concerning alphabet size (as long as it contains at least 3 characters), number of tapes, and more. This is the reason why today we partition decision problems into two broad categories called "tractable" and "intractable". The tractable problems are those having polytime complexity. The class of such problems is called **P**.

[1] The issue of whether the TM would actually stop or not was discussed in Ch. 4.

5.1.1.2 The class NP

For those decision problems for which no-one was able to find a polytime algorithm, it was remarked that a somewhat "magic" TM, one that is able to pursue every test branch concurrently (this is called *nondeterministic* TM), gives another useful partition on the class of all decision problems. Those for which there exists a nondeterministic TM that runs in polytime are all grouped in a class called **NP**.

5.1.1 Remark (NP and certificates)
An equivalent definition of **NP***, which is often used, is the following:* **NP** *is the class of all problems for which YES instances come with a polytime verifiable* certificate*, i.e. a proof that the instance is indeed YES, which can be checked in polytime.*

To see this, we first define **NP** *as the class of all problems which can be solved by a nondeterministic TM in polytime. We run the solution algorithm nondeterministically (i.e. by following all test branches concurrently) on a given instance. At termination we look at the* trace *of the algorithm, i.e. the sequence of instructions followed by the algorithm: we "unfold" loops, and list every occurrence of repeated steps. This will yield a set of step sequences each pair of which shares an initial subsequence, i.e. a tree where branches correspond to tests. Each tree leaf identifies the end of the sequence it corresponds to. If the algorithm terminates with a YES, it is because one of the sequences ends with a solution of the instance. We identify this sequence with the certificate: it has polynomial length since the nondeterministic algorithm runs in polytime; and by following its steps we can convince ourselves that the answer is indeed YES, as we verify each computation along the terminating YES sequence. We note that NO answers generally occur because every branch was explored, and not necessarily because a particular sequence has some specific property (but see Ex. 5.1.2), which makes this argument non-symmetric w.r.t. YES and NO.*

Conversely, we now define **NP** *as the class of problems for which YES instances have a polytime verifiable certificate. We assume that the given certificate is a binary string with length bounded by a (given) polynomial in function of the instance size. We devise a brute-force algorithm which explores the set of all such strings by branching (on zeros and ones) at each component. Since the TM is nondeterministic, all branches will be followed concurrently, and since we only need to explore polynomially bounded strings, it will terminate in polytime. The certificate will be found if it exists (i.e. if the instance is YES).*

Consider the CLIQUE problem: given a graph G and an integer k, does G possess a clique of size at least k? If the instance is YES, then it has a clique of size at least k, and this clique can be supplied as certificate to a verification algorithm which is able to establish in polytime whether the certificate is valid. Therefore CLIQUE is in **NP**.

While it is easy to show that $\mathbf{P} \subseteq \mathbf{NP}$, no-one was ever able to establish whether **P** is different or equal to **NP**. This is the famous **P** vs. **NP** question.

5.1.2 Exercise
Prove that $\mathbf{P} \subseteq \mathbf{NP}$.

5.1.2 Reductions

The class **NP** is very useful because, in absence of a complement of **P** allowing us to tell problems apart into "easy" and "hard", it provides a good proxy.

Given two problems P and Q in **NP**, suppose we know a polytime algorithm A to solve P but we know of no such algorithm for Q. If we can identify a polytime algorithm R that transforms a YES instance of Q into a YES instance of P and, conversely, a NO instance of Q into a NO instance of P, then we can compose R and A to obtain a polytime algorithm for Q. An algorithm R mapping instances $Q \to P$

while keeping their membership in YES and NO classes invariant is called a *polynomial reduction*[2] from Q to P.

5.1.2.1 The hardest problem in the class

This gives an interesting way to define the "hardest problem in **NP**". Let P be a problem in **NP** such that any problem in **NP** polynomially reduces to P. Pick any $Q \in \mathbf{NP}$: can Q be harder to solve than P? Since there is a polynomial reduction $R : Q \to P$, if we know how to solve P then we know how to solve Q, so there is no real additional difficulty in solving Q other than knowing how to solve P. In this sense, P is hardest in the class **NP**. The set of such problems are said to be **NP**-*complete*. Since this notion of hardness only depends on polynomial reductions rather than membership in **NP**, we also define as **NP**-*hard* those problems which are as hard as any problem in **NP** without necessarily being members of **NP**. Thus, **NP**-complete problems are the subset of **NP**-hard problems which also belong to **NP**.

In a landmark result, S. Cook proved in [37] that the class of **NP**-complete problems is non-empty, since it contains the satisfiability problem (SAT). The SAT problem involves a decision about the truth or falsity of the sentences defined over variable symbols, the $\neg$ unary operator, the $\wedge$ and $\vee$ binary operators, and the constants True and False (represented by 1 and 0). Traditionally, in SAT notation, one writes $\bar{x}$ instead of $\neg x$. An instance (i.e. a sentence) is YES if there is an assignment of 1 and 0 to the variables for which the sentence is True, and NO otherwise. The evaluation uses the common meaning of the boolean operators $\neg, \wedge, \vee$. Cook's result is based on the idea that SAT can be used as a declarative language to model the dynamics of *any* polytime TM. The modelling exploits the fact that TMs (tapes, instructions, states) can be described by 0-1 vectors each component of which is modelled as a SAT variable. Since the definition of **NP** involves a polytime-checkable certificate, SAT can be used to model the polytime TM used to verify the certificate. The SAT instance has finite length because we know that the number of steps of the TM is bounded by a polynomial in the input size.

5.1.3 Remark (Cook's Theorem)
In order to prove that SAT *is* **NP**-*complete, we must prove that it is in* ***NP*** *and that is* **NP**-*hard.*

The hard part is the reduction of any problem in ***NP*** *to* SAT. *We use the definition of* ***NP****: given a problem in this class, there exists a polytime nondeterministic TM which decides each instance of the problem. Cook showed that the dynamics of a nondeterministic polytime TM can be modelled by a polynomially sized* SAT *instance. Since this is a book about MP, we reduce to a MILP instead: so, instead of proving that* SAT *is* ***NP****-complete, we shall prove that MILP is* ***NP****-hard.*

A nondeterministic TM M is described by a tuple $(Q, \Sigma, s, F, \delta)$ where Q is the set of states of the machine, Σ is the alphabet (characters to be written on the tape), $s \in Q$ is the initial state, $F \subseteq Q$ is the set of termination states, and δ is the transition relation, a subset of $(Q \smallsetminus F \times \Sigma) \times (Q \times \Sigma \times \{-1, 1\})$ (the component $\{-1, 1\}$ signals the left or right movement of the head on the tape). Let n be the size of the input. We know that M terminates in polytime $O(p(n))$, where p is a polynomial. So we only need tape cells indexed by i where $-p(n) \le i \le p(n)$, and steps indexed by k where $0 \le k \le p(n)$. We index alphabet characters by $j \in \Sigma$. The dynamics of the TM can be described by the following statements [58].

1. *Initialization:*
   (a) *the tape has an initial string at step $k = 0$;*
   (b) *M has an initial state s at step $k = 0$;*
   (c) *the initial position of the read/write head at $k = 0$ is on cell $i = 0$;*

[2] Technically, this is known as a *Karp reduction*. A *Cook reduction* occurs from Q to P if Q can be solved by a polynomial number of standard operations and calls to an oracle that solves P. A Karp reduction is like a Cook reduction allowing for a single oracle call. Karp reductions allow for a distinction between hard problems where polynomial certificates are available for YES instances and for NO ones — in other words, it allows for the definition of the class co-**NP**.

2. *Execution:*

   (a) *at each step k each cell i contains exactly one symbol j;*

   (b) *if cell i changes symbol between step k and $k+1$, the head must have been on cell i at step k;*

   (c) *at each step k, M is in exactly one state;*

   (d) *each step k, cell i and symbol σ lead to possible head positions, machine states and symbols as prescribed by the transition relation δ;*

3. *Termination:*

   (a) *M must reach a termination state in F at some step $k \leq p(n)$.*

Next, we translate the above description into a set of MILP constraints. As parameters we have the initial tape string τ (a vector indexed by $-p(n) \leq i \leq p(n)$). We introduce the following binary (polynomially many) decision variables:

- *$\forall$ cell i, symbol j, step k $t_{ijk} = 1$ iff tape cell i contains symbol j at step k;*
- *$\forall$ cell i, step k $h_{ik} = 1$ iff head is at tape cell i at step k;*
- *$\forall$ state ℓ, step k $q_{\ell k} = 1$ iff M is in state ℓ at step k.*

Finally, we express the above statements by means of constraints in function of the variables t, h, q:

1. *Initialization:*

   (a) $\forall i \ (t_{i,\tau_i,0} = 1)$;

   (b) $q_{s,0} = 1$;

   (c) $h_{0,0} = 1$;

2. *Execution:*

   (a) $\forall i, k \ (\sum_j t_{ijk} = 1)$;

   (b) $\forall i, j \neq j', k < p(n) \ (t_{ijk}\, t_{i,j',k+1} = h_{ik})$;

   (c) $\forall k \ \sum_i h_{ik} = 1$;

   (d) $\forall i, \ell, j, k \ (|\delta(\ell, j)|\, h_{ik}\, q_{\ell k}\, t_{ijk} = \sum\limits_{((\ell,j),(\ell',j',d))\in\delta} h_{i+d,k+1}\, q_{\ell',k+1}\, t_{i,j',k+1})$;

3. *Termination:*

   (a) $\sum\limits_{k, f\in F} q_{fk} = 1$.

Again, the number and size of these constraints are bounded by polynomials in the input size. We observe that some constraints involve products of binary variables, but these can all be reformulated exactly to linear, by means of a polynomial quantity of additional variables and constraints (see Rem. 2.2.8).

5.1.4 Exercise
Prove that feasibility-only MILPs are in **NP**.

5.1.2.2 The reduction digraph

After Cook's result, SAT became known as the "primitive problem" in the theory of **NP**-hardness. While the *first* proof of **NP**-hardness was difficult to devise (since it necessarily has to encode *every* TM, following the definition), subsequent proofs are of an altogether different nature, as they can rely on the mechanism of reduction.

Let P be an **NP**-hard problem. We want to establish the **NP**-hardness of Q. Can Q be any easier than P? Suppose we find a polynomial reduction $R : P \to Q$: if Q could be solved by an algorithm A that is asymptotically faster than that of P, then we could compose R with A to derive a better algorithm for P, which is impossible since P was defined to be hardest for **NP**. In [77], R. Karp used this idea to prove that many common problems are **NP**-complete. Since then, when discussing a new problem, an effort is made to establish either membership in **P** or **NP**-hardness.

Note that polytime reductions define an asymmetric relation on the class **NP**, i.e. two problems P, Q in **NP** are related if there is a reduction $R : P \to Q$. This turns **NP** in an (infinite) digraph, called the *reduction digraph*, where the problems are represented by nodes, and reductions by arcs. This digraph is strongly connected by Cook's result, which proves exactly that there is a reduction from any problem in **NP** to SAT. This makes the reduction digraph strongly connected.

5.1.2.3 Decision vs. optimization

As mentioned above, a problem P is **NP**-complete if it is **NP**-hard and belongs to **NP**. Many theoretical results in computational complexity concern decision problems, but in practice we also need to solve function evaluation and optimization problems. In the Wikipedia page about "Decision problem" (`en.wikipedia.org/wiki/Decision_problem`), we read:

> There are standard techniques for transforming function and optimization problems into decision problems, and vice versa, that do not significantly change the computational difficulty of these problems.

The "decision version" of the MINLP in Eq. (2.2) adds a *threshold value* ϕ to the input and asks whether the system

$$\left.\begin{array}{rrcl} & f(x) & \leq & \phi \\ & g(x) & \in & [g^L, g^U] \\ & x & \in & [x^L, x^U] \\ \forall j \in Z & x_j & \in & \mathbb{Z} \end{array}\right\} \tag{5.1}$$

is feasible. The class of optimization problems that can be reducible to their decision version Eq. (5.1) is called **NPO** (the "O" stands for "optimization"). It has the following properties: (i) the feasibility of any solution can be established in polytime; (ii) every feasible solution has polynomially bounded size; (iii) the objective function and constraints can be evaluated in polytime at any fasible solution.

5.1.2.4 When the input is numeric

For problems involving arrays of rational numbers in the input data, such as vectors or matrices, more notions are used to distinguish complexity in function of the numerical value of the input versus the number of bits of memory required to store it.

An algorithm is *pseudopolynomial* if it is polynomial in the value of the numbers in the input, but not in their storage size. E.g., testing whether a number n is prime by trying to divide it by $2, \ldots, \lfloor\sqrt{n}\rfloor$ takes $\sqrt{n}$ divisions. In the classic TM computational model, the number of divisions is polynomial in the value of the input n, but exponential in the size of the input $\lceil\log_2(n)\rceil$, since $\sqrt{n} = 2^{\frac{1}{2}\log_2(n)}$.

5.1.5 Remark (Pseudopolynomial and unary encoding)
An equivalent definition of a pseudopolynomial algorithm is that it is polytime in the unary encoding of the data (but not in the binary encoding). The equivalence of these two definitions is readily seen because an integer in encoded in base 1 needs as many bits of storage as its value, whereas in base 2 it can be encoded in $\lceil \log_2(n) \rceil$ bits.

In the arithmetic computational model, where elementary operations on numbers take unit time, an algorithm is *strongly polytime* if its worst case running time is bounded above by a polynomial in function of the *length* of the input arrays, and the worst-case amount of memory required to run it (a.k.a. the *worst-case space*) is bounded by a polynomial in the number of bits required to store their values, a.k.a. the size of the input (e.g. Dijkstra's shortest path algorithm on weighted graphs is strongly polytme). By contrast, if the running time also depends nontrivially (i.e. aside from read/write and elementary arithmetic operations) on the actual input storage size, including the bits required to represent the numbers in the arrays, the algorithm is *weakly polytime* (e.g. the ellipsoid method for LP is weakly polytime: whether there exists a strongly polytime algorithm for LP is a major open question).

A problem P is *strongly* **NP**-hard if there is a strongly polytime reduction algorithm R from every problem in **NP** to P, or, equivalently, from a single **NP**-hard problem to P. P is *strongly* **NP**-complete if it is strongly **NP**-hard and also belongs to the class P. An equivalent definition of strong **NP**-hardness is the class of those **NP**-hard problems that remain **NP**-hard even if the input is encoded in unary (see Rem. 5.1.5), i.e. when the value of all of their numerical data is bounded by a polynomial in the input size. A problem P is *weakly* **NP**-hard when it is **NP**-hard but there exists a pseudopolynomial algorithm that solves it. E.g. often dynamic programming based solutions search the set of values that a given variable can take, so that the number of iterations might remain polynomial in the value rather than the number of bits required to store it. When proving **NP**-hardness for a new problem P, using reductions from a strongly **NP**-hard problem gives more flexibility, as one can use a pseudopolynomial reduction and still claim **NP**-hardness of P. This technique was used in [27].

5.1.6 Remark (Strong and weak)
Algorithms may be strongly or weakly polytime, and problems may be strongly or weakly **NP***-hard. But the opposition of the terms "strong" and "weak" are expressed in different terms for algorithms and problems. I.e. the weak notion of problem* **NP***-hardness rests on pseudopolynomial (rather than "weak") reductions.*

5.2 Complexity of solving general MINLP

MINLP is not in **NP** because it is not a decision problem. It is **NP**-hard because it includes MILP as a subclass. MILP, in turn, is **NP**-hard by means of a trivial reduction from SAT. Transform the SAT instance to conjunctive normal form[3] (CNF), write $\bar{x}$ as $1 - x$, $\vee$ as $+$ and let $\wedge$ mark the separation between constraints. This yields a set of MILP constraints that are feasible if and only if the SAT instance is YES.

This argument, however, only brushes the surface of the issue, as it is essentially an argument about MILP. We know by Sect. 4 that nonlinearity makes unbounded MINLPs undecidable, whereas finite bounds make it decidable. But what about the continuous variables? We know that PP without integer variables is decidable, but is it **NP**-hard? Again, the answer is yes, and it follows from the fact that polynomials can express a bounded number of integer variables (see the beginning of Sect. 4.3.4). All that the SAT $\to$ MILP reduction above needs is a sufficient number of binary (boolean) variables, which can be defined by requiring a continuous variable x to satisfy the polynomial $x(1 - x) = 0$.

In the rest of this section, we shall survey the field of computational complexity of several different MINLP problems, with a particular attention to NLPs (which only involve continuous variables).

[3] I.e. a sequence of clauses involving exclusively $\vee$, each separated from the next by $\wedge$.

5.3 Quadratic programming

The general Quadratic Programming (QP) problem is as follows:

$$\left.\begin{array}{rrcl} \min & \frac{1}{2}x^\top Qx & + & c^\top x \\ & Ax & \geq & b. \end{array}\right\} \tag{5.2}$$

5.3.1 NP-hardness

QP was shown in [130] to contain an **NP**-hard subclass of instances (and hence QP itself is **NP**-hard by inclusion). The reduction is from an **NP**-complete problem called SUBSET-SUM: given a list s of non-negative integers $s_1, \ldots, s_n$ and an integer σ, is there an index set $J \subseteq \{1, \ldots, n\}$ such that $\sum_{j\in J} s_j = \sigma$? Consider the QP formulation:

$$\left.\begin{array}{lrcl} \max & f(x) = \sum\limits_{j\le n} x_j(x_j-1) & + & \sum\limits_{j\le n} s_j x_j \\ & \sum\limits_{j\le n} s_j x_j & \le & \sigma \\ \forall j \le n & 0 \le x_j & \le & 1. \end{array}\right\} \tag{5.3}$$

This defines a transformation from an instance of SUBSET-SUM to one of QP. Obviously, it can be carried out in polytime. We now prove that it maps YES instances of SUBSET-SUM to QP instances where $f(x) < \sigma$ and NO instances to instances of QP where $f(x) = \sigma$.

Assume (s, σ) is a YES instance of SUBSET-SUM with solution J. Then setting $x_j = 1$ for all $j \in J$ satisfies all constraints of Eq. (5.3): in particular, the constraint is satisfied at equality. Solution integrality mkes the first sum in the objective function yield value zero, which yields $f(x) = \sigma$. Conversely, assume (s, σ) is a NO instance, and suppose first that Eq. (5.3) has an integer solution: then the constraint must yield $\sum_j s_j x_j < \sigma$; solution integrality again zeroes the first sum in the objective function, so $f(x) < \sigma$. Next, if Eq. (5.3) has no integer solution, there is at least one $j \le n$ such that $0 < x_j < 1$, which makes the objective function term $x_j(x_j - 1)$ negative, yielding again $f(x) < \sigma$, as claimed.

The paper [130] also contains another proof that shows that a Nonlinear Programming (NLP) problem with just one nonlinear constraint of the form $\sum_j x_j(x_j - 1) \ge 0$ is also **NP**-hard.

5.3.1.1 Strong NP-hardness

A different proof, reducing from SAT, was given in [149, Thm. 2.5]. It shows that the following QP subclass is **NP**-hard:

$$\left.\begin{array}{ll} \min & f(x) = \sum\limits_{j\le n} x_j(1-x_j) \\ & \text{SAT} \to \text{MILP} \\ \forall j \le n & 0 \le x_j \le 1, \end{array}\right\} \tag{5.4}$$

where SAT $\to$ MILP indicates the MILP constraints encoding a SAT instances which were discussed in the first paragraph of this section. The proof shows that the given SAT instance is YES iff $f(x) = 0$. Assume first that the SAT instance is YES: then there is an assignment of boolean values to the SAT variables that satisfies the SAT $\to$ MILP constraints. Moreover, since the solution is integral, we get $f(x) = 0$. Conversely, assume the SAT instance is NO, and suppose, to aim at a contradiction, that a solution x^* to Eq. (5.4) exists, and is such that $f(x^*) = 0$. Since the quadratic form $\sum_j x_j(1 - x_j)$ is zero iff each $x_j \in \{0, 1\}$, we must conclude that x^* is integral. Since the SAT $\to$ MILP constraints are feasible iff the SAT instance is YES, and x^* satisfies those constraints, it follows that the SAT instance is YES, against assumption. Hence, if the SAT instance is NO, either Eq. (5.4) is infeasible or $f(x^*) > 0$.

These two arguments prove the same fact, i.e. that QP is **NP**-hard. However, the first reduction

is from SUBSET-SUM, while the second is from SAT. This has some consequences, since while SAT is strongly **NP**-hard, SUBSET-SUM is not: namely, the first reduction only proves the weak **NP**-hardness of QP, leaving the possibility of a pseudopolynomial algorithm open. The second reduction rules out this possibility.

5.3.2 NP-completeness

While QP cannot be in **NP** since it is not a decision problem, the decision problem corresponding to QP is a candidate. The question is whether the following decision problem is in **NP**:

$$\left.\begin{array}{rcl} \frac{1}{2}x^\top Qx + c^\top x & \leq & \phi \\ Ax & \geq & b, \end{array}\right\} \quad (5.5)$$

where ϕ is a threshold value that is part of the input.

As shown in [149], the proof is long and technical, and consists of many intermediate results that are very important by themselves.

1. If the QP of Eq. (5.2) is convex, i.e. Q is positive semidefinite (PSD), and has a global optimum, then it has a globally optimal solution vector where all the components are rational numbers — this was shown in [126]. The main idea of the proof is as follows: only consider the active constraints in $Ax \geq b$, then consider the KKT conditions, which consist of linear equations in x, and derive a global optimum of the convex QP as a solution of a set of linear equations.
2. Again by [126], there is a polytime algorithm for solving convex QPs (cQP): in other words, cQP is in **P**. This is a landmark result by itself — we note that the algorithm is an interior point method (IPM) and that it is weakly polytime. Specifically, though, this result proves that the size of the rational solution is bounded by a polynomial in the input size. By [149, p. 77], this is enough to prove the existence of a polynomially sized certificate in case Eq. (5.5) is bounded.
3. The unbounded case is settled in [146].

This allows us to conclude that the decision version of QP is **NP**-complete.

5.3.3 Box constraints

A QP is *box-constrained* if the constraints $Ax \geq b$ in Eq. (5.2) consist of variable bounds $x^L \leq x \leq x^U$. The hyper-rectangle defined by $[x^L, x^U]$ is also known as a "box". As for the **NP**-hardness proof of QP, there are two reductions from **NP**-complete problems to box-constrained QP: one from SUBSET-SUM [116, Eq. (3)] and one from SAT [149, §4.2]. Since reductions from SAT imply strong **NP**-hardness, we only focus on the latter.

We actually reduce from 3SAT in CNF, i.e. instances consisting of a conjunction of m clauses each of which is a disjunction of exactly 3 literals. As before, we write the i-th literal as x_i or $1 - x_i$ if negated. A disjunction $x_i \vee \bar{x}_j \vee x_k$, for example, is written as a linear constraint $x_h + (1 - x_j) + x_k \geq 1$, yielding

$$\forall i \leq m \quad a_i^\top x \geq b_i \quad (5.6)$$

for appropriate vectors $a_i \in \mathbb{Z}^m$ and $b \in \mathbb{Z}$. By adding a slack variable $v_\ell \in [0, 2]$ to each of the m clauses, Eq. (5.6) becomes $\forall i \leq m \ (a_i^\top x = b_i + v_i)$. Next, we formulate the following box-constrained QP:

$$\left.\begin{array}{rl} \min & f(x, v) = \sum\limits_{j \leq n} x_j(1 - x_j) + \sum\limits_{i \leq m} (a_i^\top x - b_i - v_i)^2 \\ & x \in [0, 1]^n, \quad v \in [0, 2]^m. \end{array}\right\} \quad (5.7)$$

We are going to show that the 3SAT instance is YES iff the globally optimal objective function value of Eq. (5.7) is zero.

Obviously, if the 3SAT formula is satisfiable, there exists a feasible solution (x^*, v^*) where $x^* \in \{0,1\}^n$ and $v^* \in \{0,1,2\}^m$ that yields a zero objective function value. Conversely, suppose there exists (x^*, v^*) such that $f(x^*, v^*) = 0$, which yields

$$a_i^\top x^* = b_i + v_i^* \tag{5.8}$$

for all $i \leq m$. Supposing some of the x variables take a fractional value, the corresponding term $x_j^*(1-x_j^*)$ would be nonzero, against the assumption $f(x^*, v^*) = 0$. From integrality of the x variables, Eq. (5.8) ensures that v_i^* is integer, for all $i \leq m$. Since integrality and feasibility w.r.t. Eq. (5.8) are equivalent to Eq. (5.6) and therefore encode the clauses of the 3SAT instance, x^* is a YES certificate for the 3SAT instance. Thus, finding the global optimum of the box-constrained QP in Eq. (5.7) is **NP**-hard.

5.3.4 Trust region subproblems

Trust Region Subproblems (TRS) take their name from the well-known trust region method for black-box optimization. TRSs are essentially instances of QP modified by adding a single (convex) norm constraint $\|x\| \leq r$, where r (which is part of the input) is the *radius* of the trust region. If the norm is ℓ_2 and $Ax \geq b$ has a special structure, then the problem can be solved in polytime [21]. In this case the solution is generally irrational (due to the nonlinear norm constraint — note that because of that constraint, the TRS is not formally a subclass of QP in general), though for the simple case of $\|x\|_2 \leq 1$ and no linear constraints, the technical report [148] states that the decision problem is actually in **P**.

Most TRSs arising in practical black-box optimization problems, however, are formulated with an ℓ_∞ norm constraint. This makes the resulting QP easier to solve numerically, to a given $\varepsilon > 0$ approximation tolerance, using local NLP solvers. This is because the ℓ_∞ norm yields simple box constraints on the decision variables, and therefore the ℓ_∞ TRS *does* belong to the class QP, specifically it is a box-constrained QP. From a worst-case computational complexity point of view, however, we recall that box-constrained QPs form an **NP**-hard subclass of QP, as mentioned above.

5.3.5 Continuous Quadratic Knapsack

The reduction is from SUBSET-SUM. Consider the following formulation, called *continuous Quadratick Knapsack Problem* (cQKP):

$$\left.\begin{array}{rcl} \min \quad x^\top Q x & + & c^\top x \\ \sum\limits_{j\leq n} a_j x_j & = & \gamma \\ x & \in & [0,1]^n, \end{array}\right\} \tag{5.9}$$

where Q is a square diagonal matrix, $a, c \in \mathbb{Q}^n$, and $\gamma \in \mathbb{Q}$.

We encode a SUBSET-SUM instance $(\{s_1, \ldots, s_n\}), \sigma)$ in Eq. (5.9) as follows [149, §4.2]:

$$\left.\begin{array}{l} \min \quad f(x) = \sum\limits_{j\leq n} x_j(1-x_j) \\ \sum\limits_{j\leq n} s_j x_j = \sigma \\ x \in [0,1]^n, \end{array}\right\} \tag{5.10}$$

We are going to show that the instance is YES iff the global optimum of Eq. (5.10) is zero. If the instance is YES, then there is a subset $J \subset \{1, \ldots, n\}$ such that $\sum\limits_{j\in J} s_j = \sigma$. Let $x_j^* = 1$ for all $j \in J$ and $x_j^* = 0$ for all $j \notin J$: then x^* is feasible in the constraints of Eq. (5.9), and yields $f(x^*) = 0$. Conversely, if x^* is a feasible solution of Eq. (5.9) yielding $f(x^*) = 0$, then each term $x_j^*(1-x_j^*)$ in $f(x)$ has value zero,

which implies $x^* \in \{0,1\}^n$. Now let $J = \{j \le n \mid x^*_j = 1\}$ be the support of x^*. By construction, J is a YES certificate for the SUBSET-SUM instance. Thus finding a global optimum of a cQKP is **NP**-hard.

5.3.5.1 Convex QKP

Since a convex QKP is a subclass of convex QP, it can be solved in polytime — but no strongly polytime algorithm is known. On the other hand, if Q is a diagonal matrix, then the objective function of Eq. (5.9) is separable.[4] As remarked in [149, §3.1] there is an $O(n \log n)$ algorithm for solving this specific variant of convex QKP [67].

5.3.6 The Motzkin-Straus formulation

In 1965, Motzkin and Straus established an interesting relationship between the maximum clique C in a graph $G = (V, E)$ and the following QP [115]:

$$\left.\begin{array}{rrcl} \max & f(x) & = & \sum\limits_{\{i,j\}\in E} x_i x_j \\ & \sum\limits_{j\in V} x_j & = & 1 \\ \forall j \in V & x_j & \ge & 0\,; \end{array}\right\} \qquad (5.11)$$

namely, that there exists a global optimum x^* of Eq. (5.11) such that

$$f^* = f(x^*) = \frac{1}{2}\left(1 - \frac{1}{\omega(G)}\right),$$

where $\omega(G)$ is the size of a maximum cardinality clique in G. In other words, this gives the following formula for computing the *clique number* of a graph:

$$\omega(G) = \frac{1}{1 - 2f^*}.$$

Moreover, a maximum clique is encoded in a global optimum x^* of Eq. (5.11), which has the form

$$\forall j \in V \quad x^*_j = \begin{cases} \frac{1}{\omega(G)} & \text{if } j \in C \\ 0 & \text{otherwise.} \end{cases}$$

Eq. (5.11) is called the *Motzkin-Straus formulation* for the MAX CLIQUE optimization problem. Its decision version CLIQUE is well known to be **NP**-complete, which makes the Motzkin-Straus formulation an appropriate candidate for reductions from CLIQUE to various problems related to QP and NLP.

We follow the proof of Motzkin and Straus as related in [6]. Let x^* be a global optimum of Eq. (5.11) with as many zero components as possible. Consider $C = \{j \in V \mid x^*_j > 0\}$. We claim that C is a maximum clique in G.

- First, we claim C is a clique. Suppose this is false to aim at a contradiction, and assume without loss of generality that $1, 2 \in C$ and $\{1, 2\} \notin E$. For some ϵ in the interval $[-x^*_1, x^*_2]$, let $x^\epsilon = (x^*_1 + \epsilon, x^*_2 - \epsilon, x^*_3, \ldots, x^*_n)$. Note that x^ϵ satisfies the simplex constraint $\sum_j x_j = 1$, as well as the non-negativity constraints. Since the edge $\{1, 2\}$ is not in E, the product $x_1 x_2$ does not appear in the objective function $f(x)$. This means that ϵ^2 never occurs in $f(x^\epsilon)$. In particular, $f(x)$ is linear in ϵ. We temporarily look at f as a function f_ϵ of ϵ, parametrized by x^*. By the choice of x^* (a global optimum), f_ϵ achieves its maximum at $\epsilon = 0$. Since $\epsilon = 0$ is in the interior of its range $[-x^*_1, x^*_2]$ and f_ϵ is linear in ϵ, f_ϵ must necessarily be constant over this range. Hence setting

[4] A multivariate function is separable if it can be written as a sum of univariate functions.

$\epsilon = -x_1^*$ and $\epsilon = x_2^*$ yields global optima with a smaller number of nonzero components x^*, which is a contradiction as x^* was chosen with the maximum possible number of zero components. Thus C is a clique.

- Now, we claim C has maximum cardinality $|C| = \omega(G)$. Consider the simplex constraint $\sum_j x_j = 1$ and square both sides:

$$1 = \left(\sum_{j\in V} x_j\right)^2 = 2\sum_{i<j\in V} x_i x_j + \sum_{j\in V} x_j^2. \tag{5.12}$$

Since by construction of C we have $x_j^* = 0$ iff $j \notin C$, the above reduces to

$$\psi(x^*) = 2\sum_{i<j\in C} x_i^* x_j^* + \sum_{j\in C}(x_j^*)^2.$$

Moreover, $\psi(x) = 1$ for all feasible x by Eq. (5.12). So the objective function $f(x) = \sum_{i,j} x_i x_j$ achieves its is maximum when the second term of $\psi(x)$ is minimum (given that the sum of the two terms is constant by Eq. (5.12)), i.e. when $\sum_{j\in C}(x_j^*)$ attains its minimum, which occurs at $x_j^* = \frac{1}{|C|}$. Again by the simplex constraint, we have

$$f(x^*) = 1 - \sum_{j\in C}(x_j^*)^2 = 1 - |C|\frac{1}{|C|^2} = 1 - \frac{1}{|C|} \le 1 - \frac{1}{\omega(G)},$$

with equality when $|C| = \omega(G)$, as claimed.

By reduction from CLIQUE, it follows therefore that Eq. (5.11) describes an **NP**-hard subclass of QP. Using the same basic ideas, Vavasis gives a proof by induction on $|V|$ in [149, Lemma 4.1]. A bijection between the local optima of Eq. (5.11) and the maximal cliques of G is discussed in [23].

5.3.6.1 QP on a simplex

Consider the following formulation:

$$\left.\begin{array}{rrcl} \min & x^\top Q x & + & c^\top x \\ & \sum\limits_{j\le n} x_j & = & 1 \\ \forall j \le n & x_j & \ge & 0, \end{array}\right\} \tag{5.13}$$

where Q is a square $n \times n$ rational matrix and $c \in \mathbb{Q}^n$. Since Eq. (5.11) describes a subclass of Eq. (5.13), the latter is **NP**-hard by inclusion.

5.3.7 QP with one negative eigenvalue

So far, we established that cQPs are in **P**, and that a variety of nonconvex QPs are **NP**-hard (with their decision version being **NP**-complete). Where does efficiency end and hardness begin? In an attempt to provide an answer to this question, Pardalos and Vavasis proved in [120] that an objective function $\min x^\top Q x$ where Q has rank one and has a single negative eigenvalue suffices to make the problem **NP**-hard. The problem of solving a QP with one negative eigenvalue is denoted by QP1NE.

The construction is very ingenious. It reduces CLIQUE to QP1NE in two stages. First, it provides a QP formulation attaining globally optimal objective function value zero iff the main decision variable vector x takes optimal values in $\{0, 1\}$. Second, it encodes a clique of given cardinality k in a given graph

$G = (V, E)$ by means of the following constraints:

$$\forall \{i,j\} \notin E \quad x_i + x_j \leq 1 \tag{5.14}$$

$$\sum_{j \in V} x_j = k \tag{5.15}$$

$$0 \leq x \leq 1. \tag{5.16}$$

The rest of the formulation, which essentially ensures integrality of the decision variables, is as follows:

$$\min \quad z - w^2 \tag{5.17}$$

$$w = \sum_{j \in V} 4^j x_j \tag{5.18}$$

$$z = \sum_{j \in V} 4^{2j} x_j + 2 \sum_{i<j} 4^{i+j} y_{ij} \tag{5.19}$$

$$\forall i < j \in V \quad y_{ij} \geq \max(0, x_i + x_j - 1). \tag{5.20}$$

Eq. (5.17) clearly is of rank one and has a single nonzero eigenvalue which is negative. Note that the definitions of w^2 (by means of Eq. (5.18)) and z in Eq. (5.19) almost match: we should have $y_{ij} = x_i x_j$ for them to be equal. Eqs. (5.16), (5.20) and (5.19) ensure that z cannot be negative, which also holds for w^2 since it is a square. A couple of technical lemmata ensure that the QP in Eqs. (5.17)-(5.20) has optimal value zero iff the optimal solution is binary. Integrating the constraints Eqs. (5.14)-(5.16) encodes CLIQUE in this QP so that G has a clique of cardinality k iff the optimal objective function value is zero, as claimed.

5.3.8 Bilinear programming

The BILINEAR PROGRAMMING PROBLEM (BPP) reads as follows:

$$\left. \begin{array}{ll} \min & \sum_{j \leq n} x_j y_j \\ & Ax + By \geq b. \end{array} \right\} \tag{5.21}$$

The **NP**-hardness of BPP has been established in [18], by a reduction from a problem in computational geometry called 2-LINEAR SEPARABILITY (2LS), consisting in determining whether two sets of points in a Euclidean space can be separated by a piecewise linear curve consisting of two pieces. In turn, 2LS was proven **NP**-complete in [107].

Bennett and Mangasarian show in [18] that the 2LS reduces to one of three possible BPP formulations, all of which with general inequality constraints and non-negativity constraints on the decision variables.

5.3.8.1 Products of two linear forms

In [147, p. 37], Vavasis proposed as an open question whether the following QP:

$$\left. \begin{array}{ll} \min & f(x) = (c^\top x + \gamma)(d^\top x + \delta) \\ & Ax \geq b \end{array} \right\} \tag{5.22}$$

is **NP**-hard. Note that that although Eq. (5.22) is a subclass of QP, which is itself an **NP**-hard problem, there is the possibility that this might be a tractable case. This question was eventually settled in the negative in [105], which gives an **NP**-hardness proof for Eq. (5.22).

The proof is constructed very ingeniously by borrowing the functional form $\min x_1 - x_2^2$ from QP1NE.

First, it presents a reduction of the (**NP**-complete) SET PARTITION problem to the formulation

$$\left.\begin{array}{rl} \min & \sum\limits_{i=1}^{n}\sum\limits_{j=1}^{n} p^{i+j} y_{ij} - \left(\sum\limits_{i=1}^{n} p^i x_i\right)^2 \\ & Sx = 1 \\ \forall i \neq j \leq n & y_{ij} \leq x_i \\ \forall i \neq j \leq n & y_{ij} \leq x_j \\ \forall i \neq j \leq n & y_{ij} \geq x_i + x_j - 1 \\ \forall i \leq n & y_{ii} = x_i \\ & x \in [0,1]^n \\ & y \in [0,1]^{n^2}, \end{array}\right\} \tag{5.23}$$

where p is any positive integer and $Sx = 1$ is a set of constraints modelling SET PARTITION. This is achieved by showing that the objective function is positive if and only if there are fractional feasible solutions x' with $0 < x'_i < 1$ for some $i \leq n$. The crucial point of the proof is that the linearization constraints $x_i + x_j + 1 \leq y_{ij} \leq \min(x_i, x_j)$ and $y_{ii} = x_i$ are exact only for $x \in \{0,1\}$. A technical (but easy to follow) argument shows that the objective function is positive at the optimum if and only if some fractional solution exists.

This proof is then extended to the generalization of Eq. (5.23) where the objective function is replaced by a general function $g(x_0, y_0)$ where $x_0 = \sum_i p^i x_i$, $y_0 = \sum_{i,j} p^{i+j} y_{ij}$ and two more conditions on x_0, y_0 designed to endow g with positivity/negativity properties similar to that of the objective function of Eq. (5.23). This new problem also has non-positive objective function value at the optimum if and only if the optimum is binary. This provides the reduction mechanism from SET PARTITION (encoded in the constraints $Sx = 1$).

Finally, the function $g(x_0, y_0) = (y_0 - p + 2p^{4n})^2 - 4p^{4n}x_0^2 - 4p^{8n}$ is shown to satisfy the requirements on g and also to factor as a product of two linear forms plus a constant, which provides the necessary form shown in Eq. (5.22).

The same proof mechanism can also prove **NP**-hardness of the related problems

$$\min \quad \{x_1 x_2 \mid Ax \geq b\} \tag{5.24}$$

$$\min \quad \left\{x_1 - \frac{1}{x_2} \mid Ax \geq b\right\} \tag{5.25}$$

$$\min \quad \left\{\frac{1}{x_1} - \frac{1}{x_2} \mid Ax \geq b\right\}. \tag{5.26}$$

5.3.9 Establishing local minimality

The problem of deciding whether a given x is a local minimum of a QP or not has attracted quite a lot of attention in the late 1980s and early 1990s. There appear to be three distinct proofs of this fact: in [116, Problem 1], in [123, §3], and in [149, §5.1]. The first [116] reduces SUBSET-SUM to the problem of deciding whether a quadratic form over a translated simplex is negative, shown to be equivalent to unboundedness of a constrained quadratic form, and to the problem of deciding whether a given point is not a local optimum of a given QP. Moreover, [116] also shows that deciding copositivity of a given matrix is co-**NP**-hard; it further proves co-**NP**-hardness of verifying that a point is *not* a local optimum in unconstrained minimization (of a polynomial of degree 4). The second [123] presents a QP where a certain point is not a local minimum iff a given 3SAT instance is YES. The third [149] is based on an unconstrained variant of the Motzkin-Straus formulation, where the zero vector is a local minimum iff a given CLIQUE instance is NO.

These proofs all show that it is as hard to prove that a given point is *not* a local minimum of a QP as to show that a given **NP**-hard problem instance is YES. Implicitly, using the reduction transformation,

this provides certificates for the NO instances of the QP local minimality problem (QPLOC) rather than for the YES instances. In computational complexity, this shows that QPLOC is co-**NP**-hard[5] rather than **NP**-hard.

Currently, no-one knows whether **NP** = co-**NP**. Assume we could prove that **NP** $\neq$ co-**NP** (†); we know that **P** = co-**P** (the whole polynomially long trace of the algorithm provides a polynomially long certificate of both YES and NO instances). Suppose now **P** = **NP**: then it would follow from **P** = co-**P** that **NP** = co-**NP**, a contradiction with (†), which would prove **P** $\neq$ **NP**, the most famous open question in computer science and one of the most famous in mathematics. This tells us that proving **NP** $\neq$ co-**NP** looks exceedingly difficult.

It is remarkable that many **NP**-hard problems have QP formulations (proving that solving QPs is **NP**-hard), but verifying whether a given point is a local optimum is actually co-**NP**-hard. Looking in more depth, most of the **NP**-hardness reductions about QP actually reduce to deciding whether a given QP has zero optimal objective function value or not. On the other hand, the co-**NP**-hardness reductions in [116, 123, 149] all establish *local optimality of a given solution vector*. The former setting sometimes allows for clear dichotomies: for example, for the box-constrained QP in [116, Eq. (8)], it is shown that there is a finite gap between the optimal value being zero or less than a finite negative value (this implies that the corresponding decision problem is actually in **NP**). In practice, a sufficiently close approximation to zero can be rounded to zero exactly, which means that a certificate for "equal to zero" can be exhibited. Moreover, a YES instance of a problem might have multiple certificates, each of which is mapped (through the reduction) to a different solution of the corresponding QP having the same objective function value. The latter setting (about local optimality), on the other hand, is about a specific point. Since QP involves continuous functions of continuously varying variables, it seems hard to find cases where gap separations are possible. Furthermore, encoding a YES instance, possibly with multiple certificates, in the verification of optimality of a single point appears to be a hard task. These two considerations might be seen as an intuitive explanation about why QPLOC is co-**NP**-hard.

A completely different (again, intuitive) argument could be brought against the fact that QPLOC should be a hard problem at all. Given a candidate local minimum $\bar{x}$ in a QP, why not simply verify first and second order conditions? First-order conditions are equivalent to KKT conditions, and second-order conditions are well-known to involve the Hessian, i.e. the square symmetric matrix having second derivatives w.r.t. two decision variables as components. The main issue with this approach is that all QPs that have been proved hard in this section are constrained, so the Hessian alone is not sufficient: indeed, local solution algorithms for constrained QPs all look at the Hessian of the Lagrangian function, which involves the constraints; moreover, the Hessian of a QP objective is constant, so it cannot depend on $\bar{x}$. The second issue is that, in general, local and global optima of QPs may involve algebraic numbers, for which we do not know a compact representation in terms of the length of the input (see Sect. 4.2).

5.4 General Nonlinear Programming

The general NLP formulation is like Eq. (2.2) where $Z = \varnothing$. It obviously contains QP, so NLP is **NP**-hard in general. Murty and Kabadi's proof of co-**NP**-hardness of verifying whether a given point is a local minimum (see previous section) uses the following formulation

$$\min_u \, (u^2)^\top Q u^2,$$

where u^2 denotes the vector $(u_1^2, \ldots, u_n^2)$. This is a minimization of a quartic polynomial, and so it is not, strictly speaking, quadratic (although it is readily seen to be equivalent to the quadratic problem $\min\limits_{x \geq 0} x^\top Q x$).

[5] See Footnote 2.

In Sect. 4.3.5 we discussed *undecidable* NLP problems, so the hardness issue is somewhat moot. Two hardness results in NLP are nonetheless worth mentioning: deciding whether a given function is convex, and optimization over the copositive cone. These two problems are related by the notion of convexity — which, according to Rockafellar, is the real barrier between easy and difficult optimization problems. Given any function, can we efficiently decide whether it is convex? If so, then we may hope to optimize it efficiently using a special-purpose algorithm for convex functions. This paradigm was doubly shattered by relatively recent results. On the one hand, Ahmadi et al. proved **NP**-hardness of deciding convexity of polynomials of 4th degree. On the other, the realization that many **NP**-hard problems have natural copositive formulations [48] made Rockafellar's remark obsolete.

5.4.1 Verifying convexity

In [121], Pardalos and Vavasis presented a list of open questions in the field of computational complexity in numerical optimization problems. Problem 6, due to Shor, reads as follows.

> Given a degree-4 polynomial of n variables, what is the complexity of determining whether this polynomial describes a convex function [over the whole variable range]?

Polynomials of degree smaller than 4 are easy to settle: degree-1 are linear and hence convex, degree-2 have constant Hessian which can be computed in polytime in order to decide their convexity, and odd-degree polynomials are never convex over their whole domain (although they may be pseudo- or quasi-convex, see [81, Thm. 13.11]). Degree-4, the smallest open question concerning the efficient decidability of polynomial convexity, was settled in [5] in the negative.

The proof provided in [5] reduces from the problem of determining whether a given *biquadratic form* $\sum_{\substack{i\le j\\ k\le \ell}} \alpha_{i,j,l\ell} x_i x_j y_k y_\ell$ is non-negative over all its range is strongly **NP**-hard by reduction from CLIQUE [92] by way of the Motzkin-Straus formulation Eq. (5.11). It shows how to construct a (variable) Hessian form from any biquadratic form such that the former is non-negative iff the latter is. This Hessian form allows the construction of a quartic polynomial that is convex over its range iff the original biquadratic form is non-negative.

This result is extended to deciding other forms of convexity as well: strict and strong convexity, as well as pseudo- and quasi-convexity.

5.4.1.1 The copositive cone

First, a square symmetric matrix A is *copositive* if $x^\top Ax \ge 0$ for all $x \ge 0$. If we removed the non-negativity condition $x \ge 0$, we would retrieve a definition of A being PSD: while every PSD matrix is copositive, the converse is not true. Establishing copositivity of non-PSD matrices is **NP**-hard, as it involves verifying whether the optimal objective function value of the QP $P \equiv \min\{x^\top Ax \mid x \ge 0\}$ is ≥ 0 or either < 0 or unbounded [116].

We consider a variant of Eq. (5.13) where c is the zero vector (so the objective function is purely quadratic). This variant is called STANDARD QUADRATIC PROGRAMMING (StQP). Surprisingly, the (**NP**-hard) StQP can be exactly reformulated to a *convex* continuous cNLP, as reported here below.

(a) We linearize each product $x_i x_j$ occurring in the quadratic form $x^\top Qx$ to a new variable X_{ij}. This

yields:

$$\left.\begin{array}{rrcl} \min & Q \bullet X & & \\ & \sum\limits_{j\le n} x_j & = & 1 \\ \forall j \le n & x_j & \ge & 0 \\ & X & = & xx^\top, \end{array}\right\}$$

where $\bullet$ denotes $\mathsf{trace}(Q^\top X)$. Note that $X = xx^\top$ encodes the whole constraint set

$$\forall i < j \le n \quad X_{ij} = x_i x_j.$$

(b) We square both sides of the simplex constraint $\sum_j x_j = 1$ to obtain $\sum_{i,j} x_i x_j = 1$, which can be written as $\mathbf{1} \bullet X = 1$, where $\mathbf{1}$ is the all-one $n \times n$ matrix.

(c) We replace the (nonconvex) set $C = \{X \mid X = xx^\top \wedge x \ge 0\}$ by its convex hull $\mathcal{C} = \mathsf{conv}(C)$. This yields:

$$\left.\begin{array}{rrcl} \min & Q \bullet X & & \\ & \mathbf{1} \bullet X & = & 1 \\ & X & \in & \mathcal{C}. \end{array}\right\} \tag{5.27}$$

The set $\mathcal{C}$ is a convex combination of rank-one matrices, and as such forms a convex cone.

(d) We write the dual of Eq. (5.27):

$$\left.\begin{array}{rrcl} \max & y & & \\ & Q - y\mathbf{1} & \in & \mathcal{C}^*, \end{array}\right\} \tag{5.28}$$

where $\mathcal{C}^*$ is the dual cone of $\mathcal{C}$. Unlike the PSD cone, which is self-dual, $\mathcal{C}^* \ne \mathcal{C}$. In fact, $\mathcal{C}^*$ turns out to be the cone of all copositive matrices:

$$\mathcal{C}^* = \{A \mid \forall x \ge 0 \ (x^\top A x \ge 0)\},$$

see [64, Thm. 16.2.1] for a detailed proof. Both cones are convex and achieve strong duality. Hence Eq. (5.28) is a cNLP, as claimed.

This is extremely surprising, as cNLPs are known to be "easy to solve", since every local optimum is also global: thus a local solution algorithm should immediately find the global optimum (this proabably motivated Rockafellar to put the barrier of complexity in MP at the frontier of convexity and nonconvexity, see Sect. 5.4).

The issue is that no-one knows of any efficient algorithm for solving the cNLP in Eq. (5.28), and this is exactly because of the copositive cone $\mathcal{C}^*$ [24, 48]. Those cNLPs which we know how to solve efficiently are usually defined over the non-negative orthant or the PSD cone. We can obviously test whether a vector is in the non-negative orthant in linear time, and we can also test whether a given matrix is PSD in polytime [133, p. 1152]. The polynomially long traces of the checking algorithms provide compact certificates for both YES and NO instances. On the other hand, since testing copositivity is **NP**-hard, there is no hope of achieving such compact descriptions for the copositive cone $\mathcal{C}^*$.

A different way to see this issue is to consider that cNLPs over matrix cones are routinely solved by IPMs, the polytime analysis of which rest on the existence of some functions called "self-concordant barriers", that deviate the search path for the optimum away from the border of the cone. Barrier functions are used as penalty functions to be added to the objective function, which is made to increase towards the boundary of the cone. Self-concordant barriers can be optimized efficiently using Newton's method. Self-concordant barriers are known for many convex cones (orthants, PSD and more), but not for $\mathcal{C}^*$. In [25], an IPM-based heuristic is proposed to solve copositive programs such as [25].

Another interpretation of the complexity inherent in the copositive cone is the classification of extremal matrices of copositive cones of small dimension, pursued by Roland Hildebrand [69]. He emphasizes that

the description complexity of these extreme rays increases dramatically as the dimension increases.

Part III

Basic notions

Chapter 6

Fundamentals of convex analysis

This chapter contains a condensed treatment of the basics of convex analysis and duality.

6.0.1 Definition
Given a set $X \subseteq \mathbb{R}^n$, a function $f : X \to \mathbb{R}$ and a point $x' \in X$:

- *we say that x' is a local minimum of f if there is a ball $S(x', \epsilon)$ (for some $\epsilon > 0$) such that $\forall x \in S(x', \epsilon) \cap X$ we have $f(x') \leq f(x)$ — the local minimum is strict if $f(x') < f(x)$;*
- *we say that x' is a global minimum of f if $\forall x \in X$ we have $f(x') \leq f(x)$ — again, the global minimum is strict if $f(x') < f(x)$.*

Similar definitions hold for (strict) local/global maxima. If the objective function direction is not specified, the corresponding points are called *optima*.

6.1 Convex analysis

6.1.1 Definition
A set $S \subseteq \mathbb{R}^n$ is convex if for any two points $x, y \in S$ the segment between them is wholly contained in S, that is, $\forall \lambda \in [0, 1]$ $(\lambda x + (1 - \lambda)y \in S)$.

A linear equation $a^\top x = b$ where $a \in \mathbb{R}^n$ defines a hyperplane in $\mathbb{R}^n$. The corresponding linear inequality $a^\top x \leq b_0$ defines a closed half-space. Both hyperplanes and closed half-spaces are convex sets. Since any intersection of convex sets is a convex set, the subset of $\mathbb{R}^n$ defined by the system of closed half-spaces $Ax \geq b, x \geq 0$ is convex (where $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$).

6.1.2 Definition
A subset $S \subseteq \mathbb{R}^n$ defined by a finite number of closed half-spaces is called a polyhedron. A bounded, non-empty polyhedron is a polytope.

Polyhedra and polytopes are very important in optimization as they are the geometrical representation of a feasible region expressed by linear constraints.

6.1.3 Definition
Let $S = \{x_i \mid i \leq n\}$ be a finite set of points in $\mathbb{R}^n$.

1. *The set span(S) of all linear combinations $\sum_{i=1}^n \lambda_i x_i$ of vectors in S is called the linear hull (or linear closure, or span) of S.*

2. *The set* aff(S) *of all affine combinations* $\sum_{i=1}^n \lambda_i x_i$ *of vectors in* S *such that* $\sum_{i=1}^n \lambda_i = 1$ *is called the affine hull (or affine closure) of* S.

3. *The set* cone(S) *of all conic combinations* $\sum_{i=1}^n \lambda_i x_i$ *of vectors in* S *such that* $\forall i \le n$ $(\lambda_i \ge 0)$ *is called the conic hull (or conic closure, or cone) of* S. *A conic combination is strict if for all* $i \le n$ *we have* $\lambda_i > 0$.

4. *The set* conv(S) *of all convex combinations* $\sum_{i=1}^n \lambda_i x_i$ *of vectors in* S *such that* $\sum_{i=1}^n \lambda_i = 1$ *and* $\forall i \le n$ $(\lambda_i \ge 0)$ *is called the convex hull (or convex closure) of* S. *A convex combination is strict if for all* $i \le n$ *we have* $\lambda_i > 0$.

6.1.4 Definition
Consider a polyhedron P *and a closed half-space* H *in* $\mathbb{R}^n$. *Let* $\overline{H \cap P}$ *be the affine closure of* $H \cap P$ *and* $d = \dim(\overline{H \cap P})$. *If* $d < n$ *then* $H \cap P$ *is a face of* P. *If* $d = 0$, $H \cap P$ *is called a vertex of* P, *and if* $d = 1$, *it is called an edge. If* $d = n - 1$ *then* $H \cap P$ *is a facet of* P.

The following technical result is often invoked in the proofs of LP theory.

6.1.5 Lemma
Let $x^* \in P = \{x \ge 0 \mid Ax \ge b\}$. *Then* x^* *is a vertex of* P *if and only if for any pair of distinct points* $x', x'' \in P$, x^* *cannot be a strict convex combination of* x', x''.

Proof. $(\Rightarrow)$ Suppose x^* is a vertex of P and there are distinct points $x', x'' \in P$ such that there is a $\lambda \in (0,1)$ with $x^* = \lambda x' + (1-\lambda)x''$. Since x^* is a vertex, there is a half-space $H = \{x \in \mathbb{R}^n \mid h^\top x \le d\}$ such that $H \cap P = \{x^*\}$. Thus $x', x'' \notin H$ and $h^\top x' > d$, $h^\top x'' > d$. Hence $h^\top x^* = h^\top(\lambda x' + (1-\lambda)x'') > d$, whence $x^* \notin H$, a contradiction. $(\Leftarrow)$ Assume that x^* cannot be a strict convex combination of any pair of distinct points x', x'' of P, and suppose that x^* is not a vertex of P. Since x^* is not a vertex, it belongs to a face $H \cap P$ of P (with H a closed half-space) with $d = \dim \text{aff}(H \cap P) > 0$. Then there must be a ball S (of dimension d) within $H \cap P$, having radius $\varepsilon > 0$ and center x^*. Let $x' \in S$ such that $||x' - x^*|| = \frac{\varepsilon}{2}$. Let $x'' = (x^* - x') + x^*$. By construction, x'' is the point symmetric to x' on the line through x' and x^*. Thus, $||x'' - x^*|| = \frac{\varepsilon}{2}$, $x'' \ne x'$, $x'' \in P$, and $x^* = \frac{1}{2}x' + \frac{1}{2}x''$, which is a strict convex combination of x', x'', a contradiction. □

Having defined convex sets, we now turn our attention to convex functions.

6.1.6 Definition
A function $f : X \subseteq \mathbb{R}^n \to \mathbb{R}$ *is convex if for all* $x, y \in X$ *and for all* $\lambda \in [0,1]$ *we have:*

$$f(\lambda x + (1-\lambda)y) \le \lambda f(x) + (1-\lambda)f(y).$$

Note that for this definition to be consistent, $\lambda x + (1-\lambda)y$ *must be in the domain of* f, *i.e.* X *must be convex. This requirement can be formally relaxed if we extend* f *to be defined outside* X.

The main theorem in convex analysis, and the fundamental reason why convex functions are useful in optimization, is that a local optimum of a convex function over a convex set is also a global optimum, which we prove in Thm. 6.1.7. The proof is described graphically in Fig. 6.1.

6.1.7 Theorem
Let $X \subseteq \mathbb{R}^n$ *be a convex set and* $f : X \to \mathbb{R}$ *be a convex function. Given a point* $x^* \in X$, *suppose that there is a ball* $S(x^*, \varepsilon) \subset X$ *such that for all* $x \in S(x^*, \varepsilon)$ *we have* $f(x^*) \le f(x)$. *Then* $f(x^*) \le f(x)$ *for all* $x \in X$.

Proof. Let $x \in X$. Since f is convex over X, for all $\lambda \in [0,1]$ we have $f(\lambda x^* + (1-\lambda)x) \le \lambda f(x^*) + (1-\lambda)f(x)$. Notice that there exists $\bar\lambda \in (0,1)$ such that $\bar\lambda x^* + (1-\bar\lambda)x = \bar x \in S(x^*, \varepsilon)$. Consider $\bar x$: by

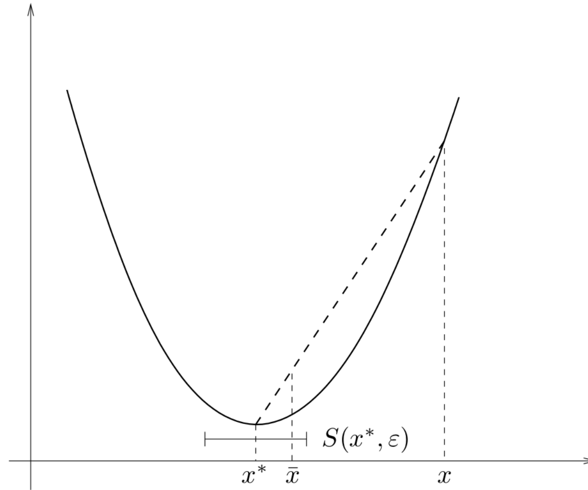


Figure 6.1: Graphical sketch of the proof of Thm. 6.1.7. The fact that $f(x^*)$ is the minimum in $S(x^*, \varepsilon)$ is enough to show that for any point $x \in X$, $f(x^*) \leq f(x)$.

convexity of f we have $f(\bar{x}) \leq \bar{\lambda} f(x^*) + (1 - \bar{\lambda}) f(x)$. After rearrangement, we have

$$f(x) \geq \frac{f(\bar{x}) - \bar{\lambda} f(x^*)}{1 - \bar{\lambda}}.$$

Since $\bar{x} \in S(x^*, \varepsilon)$, we have $f(\bar{x}) \geq f(x^*)$, thus

$$f(x) \geq \frac{f(x^*) - \bar{\lambda} f(x^*)}{1 - \bar{\lambda}} = f(x^*),$$

as required. □

6.2 Conditions for local optimality

In this section we shall give necessary and sufficient conditions for a feasible point x^* to be locally optimal. Most of the work deals with deriving necessary conditions. The sufficient conditions are in fact very close to requiring convexity of the objective function and feasible region, as we shall see later.

For a scalar function $f : \mathbb{R}^n \to \mathbb{R}$ we define the function vector ∇f as $(\nabla f)(x) = \left(\frac{\partial f(x)}{\partial x_1}, \ldots, \frac{\partial f(x)}{\partial x_n} \right)^\top$, where $x = (x_1, \ldots, x_n)^\top$. We denote by $\nabla f(x')$ the evaluation of ∇f at x'. If g is a vector-valued function $g(x) = (g_1(x), \ldots, g_m(x))$, then ∇g is the set of function vectors $\{\nabla g_1, \ldots, \nabla g_m\}$, and $\nabla g(x')$ is the evaluation of ∇g at x'.

6.2.1 Equality constraints

We first deal with the case of an optimization problem as in Eq. (2.2) with all equality constraints, unbounded variables and $Z = \varnothing$. Consider the following NLP:

$$\left.\begin{array}{lrcl} \min\limits_{x \in \mathbb{R}^n} & f(x) & & \\ \text{s.t.} & g(x) & = & 0, \end{array}\right\} \tag{6.1}$$

where $f : \mathbb{R}^n \to \mathbb{R}$ and $g : \mathbb{R}^n \to \mathbb{R}^m$ are C^1 (i.e., continuously differentiable) functions.

A *constrained critical point* of Eq. (6.1) is a point $x^* \in \mathbb{R}^n$ such that $g(x^*) = 0$ and the directional derivative[1] of f along g is 0 at x^*. It is easy to show that such an x^* is a (local) maximum, or a minimum, or a saddle point of $f(x)$ subject to $g(x) = 0$.

6.2.1 Theorem (Lagrange Multiplier Method)
If x^* is a constrained critical point of Eq. (6.1), $m \le n$, and $\nabla g(x^*)$ is a linearly independent set of vectors, then $\nabla f(x^*)$ is a linear combination of the set of vectors $\nabla g(x^*)$.

Proof. Suppose, to get a contradiction, that $\nabla g(x^*)$ and $\nabla f(x^*)$ are linearly independent. In the case $\nabla f(x^*) = 0$, the theorem is trivially true, so assume $\nabla f(x^*) \ne 0$. Choose vectors $w_{m+2}, \ldots, w_n$ such that the set $J = \{\nabla g_1(x^*), \ldots, \nabla g_m(x^*), \nabla f(x^*), w_{m+2}, \ldots, w_n\}$ is a basis of $\mathbb{R}^n$. For $m + 2 \le i \le n$ define $h_i(x) = \langle w_i, x\rangle$. Consider the map

$$F(x) = (F_1(x), \ldots, F_n(x)) = (g_1(x), \ldots, g_m(x), f(x), h_{m+2}(x), \ldots, h_n(x)).$$

Since the Jacobian (i.e., the matrix of the first partial derivatives of each constraint function) of F evaluated at x^* is J, and J is nonsingular, by the inverse function theorem F is a local diffeomorphism of $\mathbb{R}^n$ to itself. Thus, the equations $y_i = F_i(x)$ $(i \le n)$ are a local change of coordinates in a neighbourhood of x^*. With respect to coordinates y_i, the surface S defined by $g(x) = 0$ is the coordinate hyperplane $0 \times \mathbb{R}^{n-m}$. Notice that the $(k + 1)$-st coordinate, $y_{k+1} = f(x)$, cannot have a critical point on the coordinate plane $0 \times \mathbb{R}^{n-m}$, so x^* is not a constrained critical point, which is a contradiction. □

In the proof of the above theorem, we have implicitly used the fact that the criticality of points is invariant with respect to diffeomorphism (this can be easily established by showing that the derivatives of the transformed functions are zero at the point expressed in the new coordinates). The classical proof of the Lagrange Multiplier Theorem 6.2.1 is much longer but does not make explicit use of differential topology concepts (see [9], p. 153). The proof given above was taken almost verbatim from [124].

By Theorem 6.2.1 there exist scalars $\lambda_1, \ldots, \lambda_m$, such that

$$\nabla f(x^*) + \sum_{i=1}^{m} \lambda_i \nabla g_i(x^*) = 0.$$

The above condition is equivalent to saying that if x^* is a constrained critical point of f s.t. $g(x^*) = 0$, then x^* is a critical point of the following (unconstrained) function:

$$L(x, \lambda) = f(x) + \sum_{i=1}^{m} \lambda_i g_i(x). \tag{6.2}$$

Eq. (6.2) is called the *Lagrangian* of f w.r.t. g, and $\lambda_1, \ldots, \lambda_m$ are called the *Lagrange multipliers*. Intuitively, when we are optimizing over a subspace defined by $Ax = b$, the optimization direction must be a linear combination of the vectors which are normal to the hyperplane system $Ax = b$. The situation is shown in Fig. 6.2.

[1] A formal definition is given in [109], p. 7-8.

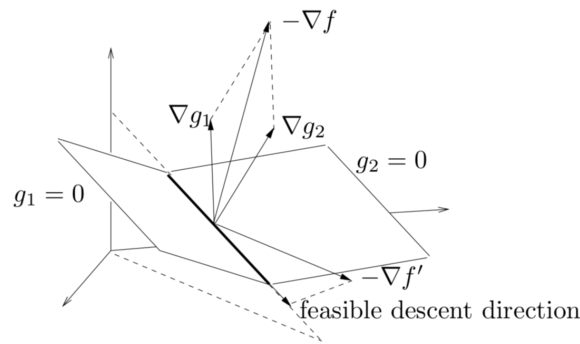


Figure 6.2: If ∇f is linearly dependent on the constraint gradients, there is no feasible descent direction. $\nabla f'$, which does not have this property, identifies a feasible descent direction when projected on the feasible space (the thick line).

Hence, in order to find the solution of Eq. (6.1), by Theorem 6.2.1, one should find all critical points of $L(x, \lambda)$ and then select the one with minimum objective function value. This approach is of limited use on all but the simplest formulations. It does, however, provide at least necessary conditions for the characterization of a constrained minimum.

6.2.2 Inequality constraints

Notice, however, that Eq. (6.1) only deals with equality constraints; moreover, the proof of Theorem 6.2.1 is heavily based on the assumption that the only constraints of the problem are equality constraints. In order to take into account inequality constraints, we introduce the following simple example.

6.2.2 Example
Consider the problem $\min\{-x_1 - x_2 \mid x_1 - 1 \leq 0, x_2 - 1 \leq 0\}$. *The minimum is obviously at* $x^* = (1, 1)$ *as shown in Fig. 6.3 (the figure only shows the non-negative quadrant; the feasible region actually extends to the other quadrants). By inspection, it is easy to see that at the point* $x^* = (1, 1)$ *any further movement*

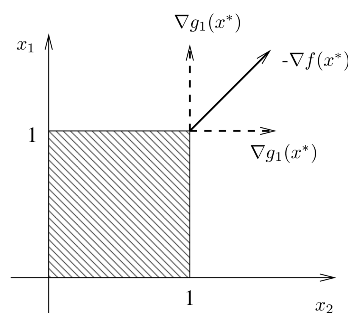


Figure 6.3: The problem of Example 6.2.2.

towards the direction of objective function decrease would take x^* *outside the feasible region, i.e. no feasible direction decreases the objective function value. Notice that the descent direction at* x^* *is in the cone defined by the normal vectors to the constraints in* x^*. *In this particular case, the descent direction of the objective function is the vector* $-\nabla f(x^*) = (1, 1)$. *The normal vector to* $g_1(x) = x_1 - 1$ *at* x^* *is* $\nabla g_1(x^*) = (1, 0)$ *and the normal vector to* $g_2(x) = x_2 - 1$ *at* x^* *is* $\nabla g_2(x^*) = (0, 1)$. *Notice that we can*

express $-\nabla f(x^*) = (1,1)$ *as* $\lambda_1(1,0) + \lambda_2(0,1)$ *with* $\lambda_1 = 1 > 0$ *and* $\lambda_2 = 1 > 0$. *In other words,* $(1,1)$ *is a conic combination of* $(1,0)$ *and* $(0,1)$.

If we now consider the problem of minimizing $\bar{f}(x) = x_1 + x_2$ *subject to the same constraints as above, it appears clear that* $x^* = (1,1)$ *cannot be a local minimum, as there are many feasible descent directions. Take for example the direction vector* $y = (-1,-1)$. *This direction is feasible w.r.t. the constraints:* $\nabla g_1(x^*)y = (1,0)(-1,-1) = (-1,0) \leq 0$ *and* $\nabla g_2(x^*)y = (0,1)(-1,-1) = (0,-1) \leq 0$. *Moreover, it is a nonzero descent direction:* $-\nabla \bar{f}(x^*)y = -(1,1)(-1,-1) = (1,1) > 0$.

In summary, either the descent direction at x^* *is a conic combination of the gradients of the constraints (and in this case* x^* *may be a local minimum), or there is a nonzero feasible descent direction (and in this case* x^* *cannot be a local minimum).*

The example above is an application of a well known theorem of alternatives called Farkas' Lemma. The following three results are necessary to introduce Farkas' Lemma, which will then be used in the proof of Theorem 6.2.7.

6.2.3 Theorem (Weierstraß)
Let $S \subseteq \mathbb{R}^n$ *be a non-empty, closed and bounded set and let* $f : S \to \mathbb{R}$ *be continuous on* S. *Then there is a point* $x^* \in S$ *such that* f *attains its minimum value at* x^*.

Proof. Since f is continuous on S and S is closed and bounded, then f is bounded below on S. Since S is non-empty, there exists a greatest lower bound α for the values of f over S. Let ε be such that $0 < \varepsilon < 1$ and consider the sequence of sets $S_k = \{x \in S \mid \alpha \leq f(x) \leq \alpha + \varepsilon^k\}$ for $k \in \mathbb{N}$. By the definition of infimum, S_k is non-empty for each k, so we can select a point $x^{(k)} \in S_k$ for each k. Since S is bounded, there exists a convergent subsequence of $x^{(k)}$ which converges to a point x^*. Since S is closed, $x^* \in S$. By continuity of f, and because $\alpha \leq f(x^{(k)}) \leq \alpha + \varepsilon^k$, we have that the values $f(x^{(k)})$ (taken on the convergent subsequence) converge to α. Thus x^* is a point where f attains its minimum value $f(x^*) = \alpha$ (see Fig. 6.4). □

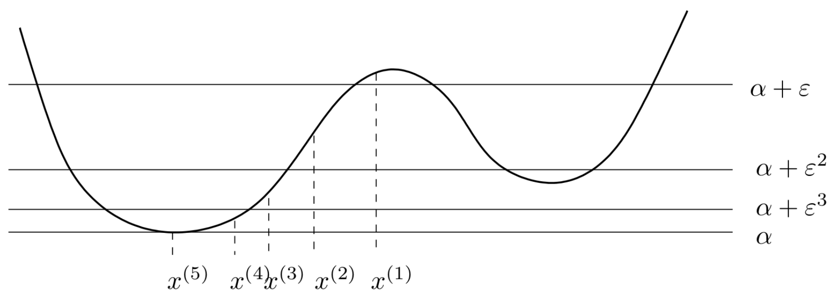


Figure 6.4: Weierstraß' Theorem 6.2.3.

6.2.4 Proposition
Given a non-empty, closed convex set $S \subseteq \mathbb{R}^n$ *and a point* $x^* \notin S$, *there exists a unique point* $x' \in S$ *with minimum distance from* x^*. *Furthermore,* x' *is the minimizing point if and only if for all* $x \in S$ *we have* $(x^* - x')^\top (x - x') \leq 0$.

Proof. Let $x' \in S$ be the point minimizing $f(x) = ||x^* - x||$ subject to $x \in S$ (which exists by Weierstraß Theorem 6.2.3). To show that it is unique, notice first that f is convex: for $\lambda \in [0,1]$ and $x_1, x_2 \in S$ we have $f(\lambda x_1 + (1-\lambda)x_2) \leq f(\lambda x_1) + f((1-\lambda)x_2) = \lambda f(x_1) + (1-\lambda)f(x_2)$ by triangular inequality and homogeneity of the norm. Suppose now $y \in \mathbb{R}^n$ such that $f(y) = f(x')$. Since $x', y \in S$ and S is convex, the point $z = \frac{x'+y}{2}$ is in S. We have $f(z) \leq \frac{f(x')}{2} + \frac{f(y)}{2} = f(x')$. Since $f(x')$ is minimal,

$f(z) = f(x')$. Furthermore, $f(z) = ||x^* - z|| = ||x^* - \frac{x'+y}{2}|| = ||\frac{x^*-x'}{2} + \frac{x^*-y}{2}||$. By the triangle inequality, $f(z) \leq \frac{1}{2}||x^* - x'|| + \frac{1}{2}||x^* - y||$. Since equality must hold as $f(z) = f(x') = f(y)$, vectors $x^* - x'$ and $x^* - y$ must be collinear, i.e. there is $\theta \in \mathbb{R}$ such that $x^* - x' = \theta(x^* - y)$. Since $f(x') = f(y)$, $|\theta| = 1$. Supposing $\theta = -1$ we would have $x^* = \frac{x'+y}{2}$, which by convexity of S would imply $x^* \in S$, contradicting the hypothesis. Hence $\theta = 1$ and $x' = y$ as claimed. For the second part of the Proposition, assume x' is the minimizing point in S and suppose there is $x \in S$ such that $(x^* - x')^\top (x - x') > 0$. Take a point $y \neq x'$ on the segment $\overline{x, x'}$. Since S is convex, $y \in S$. Furthermore, since $y - x'$ is collinear to $x - x'$, $(x^* - x')^\top (y - x') > 0$. Thus, the angle between $y - x'$ and $x^* - x'$ is acute. Choose y close enough to x' so that the largest angle of the triangle T having x^*, x', y as vertices is the angle in y (such a choice is always possible) as in Fig. 6.5. By elementary geometry, the longest side of such a triangle is the segment $\overline{x^*, x'}$ opposite to the angle in y. This implies $||x^* - y|| < ||x^* - x'||$, which is a contradiction, as x' was chosen to minimize the distance from x^*. Conversely, suppose for all $x \in S$ we have $(x^* - x')^\top (x - x') \leq 0$. This means that the angle in x' is obtuse (and hence it is the largest angle of T), and consequently the opposite side $\overline{x, x^*}$ is longer than the side $\overline{x', x^*}$. □

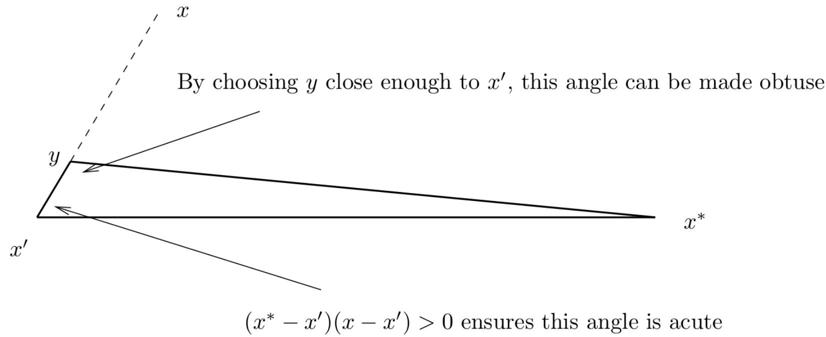


Figure 6.5: Second part of the proof of Prop. 6.2.4: the point y can always be chosen close enough to x' so that the angle in the vertex y is obtuse. The figure also shows that it is impossible for x' to be the minimum distance point from x^* if the angle in x' is acute and the set S containing points x', x, y is convex.

6.2.5 Proposition (Separating hyperplane)
Given a non-empty, closed convex set $S \subseteq \mathbb{R}^n$ and a point $x^* \notin S$, there exists a separating hyperplane $h^\top x = d$ (with $h \geq 0$) such that $h^\top x \leq d$ for all $x \in S$ and $h^\top x^* > d$.

Proof. Let x' be the point of S having minimum (strictly positive, since $x^* \notin S$) distance from x^*. Let $y = \frac{x'+x^*}{2}$ be the midpoint between x', x^*. The plane normal to the vector $x^* - y$ and passing through y separates x^* and S (see Fig. 6.6). □

6.2.6 Theorem (Farkas' Lemma)
Let A be an $m \times n$ matrix and c be a vector in $\mathbb{R}^n$. Then exactly one of the following systems has a solution: (a) $Ax \leq 0$ and $c^\top x > 0$ for some $x \in \mathbb{R}^n$; (b) $\mu^\top A = c^\top$ and $\mu \geq 0$ for some $\mu \in \mathbb{R}^m$.

Proof. Suppose system (b) has a solution. Then $\mu^\top Ax = c^\top x$; supposing $Ax \leq 0$, since $\mu \geq 0$, we have $c^\top x \leq 0$. Conversely, suppose system (b) has no solution. Let $\mathsf{Im}_+(A) = \{z \in \mathbb{R}^n \mid z^\top = \mu^\top A, \mu \geq 0\}$; $\mathsf{Im}_+(A)$ is convex, and $c \notin \mathsf{Im}_+(A)$. By Prop. 6.2.5, there is a separating hyperplane $h^\top x = d$ such that $h^\top z \leq d$ for all $z \in \mathsf{Im}_+(A)$ and $h^\top c > d$. Since $0 \in \mathsf{Im}_+(A)$, $d \geq 0$, hence $h^\top c > 0$. Furthermore, $d \geq z^\top h = \mu^\top Ah$ for all $\mu \geq 0$. Since μ can be arbitrarily large, $\mu^\top Ah \leq d$ implies $Ah \leq 0$. Take $x = h$;

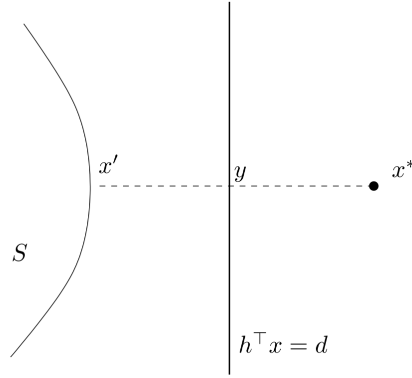


Figure 6.6: Prop. 6.2.5: separating hyperplane between a point x^* and a convex set S.

then x solves system (a). □

We can finally consider the necessary conditions for local minimality subject to inequality constraints: Consider the following NLP:

$$\left.\begin{array}{rrcl} \min\limits_{x\in\mathbb{R}^n} & f(x) & & \\ \text{s.t.} & g(x) & \le & 0, \end{array}\right\} \tag{6.3}$$

where $f : \mathbb{R}^n \to \mathbb{R}$ and $g : \mathbb{R}^n \to \mathbb{R}^m$ are C^1 functions. A *constrained optimum* of Eq. (6.3) is an optimum x^* of $f(x)$ such that $g(x^*) = 0$ — a condition described as the constraint g being *active* at x^*. It can be shown that if x^* is a constrained minimum then there is no nonzero feasible descent direction at x^* (see [13], p. 141). We shall define a *feasible direction at* x^* as a direction vector y such that $(\nabla g(x^*))^\top y \le 0$, and a *nonzero descent direction at* x^* as a direction vector y such that $(-\nabla f(x^*))^\top y > 0$.

6.2.7 Theorem (KKT)
If x^* is a constrained minimum of Eq. (6.3), I is the maximal subset of $\{1, \ldots, m\}$ such that $g_i(x^*) = 0$ for all $i \in I$, and $\nabla \bar{g}$ is a linearly independent set of vectors (where $\bar{g} = \{g_i(x^*) \mid i \in I\}$), then $-\nabla f(x^*)$ is a conic combination of the vectors in $\nabla \bar{g}$, i.e. there exist scalars λ_i for all $i \in I$ such that the following conditions hold:

$$\nabla f(x^*) + \sum_{i\in I} \lambda_i \nabla g_i(x^*) = 0 \tag{6.4}$$

$$\forall i \in I \quad (\lambda_i \ge 0). \tag{6.5}$$

Proof. Since x^* is a constrained minimum and $\nabla \bar{g}$ is linearly independent, there is no nonzero feasible descent direction at x^* such that $(\nabla \bar{g}(x^*))^\top y \le 0$ and $-\nabla f(x^*) y > 0$. By a direct application of Farkas' Lemma 6.2.6, there is a vector $\lambda \in \mathbb{R}^{|I|}$ such that $\nabla(\bar{g}(x^*))\lambda = -\nabla f(x^*)$ and $\lambda \ge 0$. □

The KKT necessary conditions (6.4)-(6.5) can be reformulated to the following:

$$\nabla f(x^*) + \sum_{i=1}^{m} \lambda_i \nabla g_i(x^*) = 0 \tag{6.6}$$

$$\forall i \le m \quad (\lambda_i g_i(x^*) = 0) \tag{6.7}$$

$$\forall i \le m \quad (\lambda_i \ge 0). \tag{6.8}$$

This is easily verified by defining $\lambda_i = 0$ for all $i \notin I$. Conditions (6.7) are called *complementary slackness*

conditions, and they express the fact that if a constraint is not active at x^* then its corresponding Lagrange multiplier is 0. A point x^* satisfying the KKT conditions is called a *KKT point*.

6.2.3 General NLPs

Consider now a general NLP with both inequality and equality constraints:

$$\left.\begin{array}{rrcl} \min\limits_{x\in\mathbb{R}^n} & f(x) & & \\ \text{s.t.} & g(x) & \leq & 0 \\ & h(x) & = & 0, \end{array}\right\} \tag{6.9}$$

where $f:\mathbb{R}^n\to\mathbb{R}$, $g:\mathbb{R}^n\to\mathbb{R}^m$ and $h:\mathbb{R}^n\to\mathbb{R}^p$ are C^1 functions.

By applying theorems 6.2.1 and 6.2.7, we can define the Lagrangian of Eq. (6.9) by the following:

$$L(x,\lambda,\mu) = f(x) + \sum_{i=1}^{m}\lambda_i g_i(x) + \sum_{i=1}^{p}\mu_i h_i(x), \tag{6.10}$$

and the corresponding KKT conditions as:

$$\left.\begin{array}{rcll} \nabla f(x^*) + \sum\limits_{i=1}^{m}\lambda_i\nabla g_i(x^*) + \sum\limits_{i=1}^{p}\mu_i\nabla h_i(x^*) & = & 0 & \\ \lambda_i g_i(x^*) & = & 0 & \forall i\leq m \\ \lambda_i & \geq & 0 & \forall i\leq m. \end{array}\right\} \tag{6.11}$$

In order to derive the general KKT conditions (6.11), it is sufficient to sum Eq. (6.4) and (6.6) and then divide by 2.

This completes the discussion as regards the necessary conditions for local optimality. If a point x^* is a KKT point, the objective function is convex in a neighbourhood of x^*, and the objective direction is minimization, then x^* is a local minimum These are the sufficient conditions which are used in practice in most cases. It turns out, however, that they are not the most stringent conditions possible: many variants of convexity have been described in order to capture wider classes of functions for which all local optima are also global.

6.2.8 Definition
Consider a function $f: X\subseteq\mathbb{R}^n\to\mathbb{R}^n$.

1. *f is quasiconvex if for all $x,x'\in X$ and for all $\lambda\in[0,1]$ we have:*

$$f(\lambda x + (1-\lambda)x') \leq \max\{f(x), f(x')\}.$$

2. *f is pseudoconvex if for all $x,x'\in X$ such that $f(x')<f(x)$ we have:*

$$(\nabla f(x))^\top(x'-x) < 0.$$

We state the sufficiency conditions in the following theorem; the proof can be found in [13, p. 155].

6.2.9 Theorem
Let x^* be a KKT point of Eq. (6.3), I be as in Theorem 6.2.7, and X be the feasible region of a relaxation of Eq. (6.9) where all constraints g_i such that $i\notin I$ have been discarded from the formulation. If there is a ball $S(x^*,\varepsilon)$ with $\varepsilon>0$ such that f is pseudoconvex over $S(x^*,\varepsilon)\cap X$ and g_i are differentiable at x^* and quasiconvex over $S(x^*,\varepsilon)\cap X$ for all $i\in I$, then x^* is a local minimum of Eq. (6.9).

6.3 Duality

Given an MP formulation P, the term "dual" often refers to an auxiliary formulation Q such that the decision variables of P are used to index the constraints of Q, and the constraints of P are used to index the variables of Q. For minimization problems, this is shown by setting up a special saddle problem can sometimes be re-cast in terms of an ordinary MP where variables and constraint indices are swapped (this is not the only relationship between primal and dual formulations, of course). Duality is important because of weak and strong duality theorems. The former guarantees that dual formulations provide lower bounds to primal minimization formulations. The latter guarantees that the "gap" between this lower bound and the optimal objective function value of the original primal formulation is zero.

In the following, we shall employ the terms *primal variables*, *dual variables*, *primal constraints*, *dual constraints*, *primal objective*, *dual objective* to denote variables, constraints and objectives in the primal and dual problems in primal/dual problem pairs.

6.3.1 The Lagrangian function

The primordial concept in duality theory is the Lagrangian function (see Eq. (6.2)) of a given formulation, which, for a problem

$$\min\{f(x) \mid g(x) \leq 0\} \tag{6.12}$$

is given by $L(x, y) = f(x) + yg(x)$. The row vector $y \in \mathbb{R}^m$ is called the vector of the Lagrange multipliers.

The Lagrangian aggregates the constraints on the objective, penalizing them by means of the multipliers. The solution $x^*(y)$ (itself a function of the multiplier vector y) to $\min_x L(x, y)$ must surely have $g(x^*(y)) \leq 0$ as long as $y \geq 0$, since we are minimizing w.r.t. x (the term $yg(x)$ must become negative for L to attain its minimum). In other words, the solution $x^*(y)$ is feasible in the original problem Eq. (6.12). We write $L(y) = \min_x L(x, y) = \min_x (f(x) + yg(x))$.

It is easy to show that for all $y \geq 0$, $L(y)$ is a lower bound to the optimal objective function value f^* of the original formulation. Thus, it makes sense to find the *best* (i.e. maximum) achievable lower bound. This leads us to maximize $L(y)$ with respect to y and subject to $y \geq 0$. The Lagrangian dual problem of Eq. (6.12) is a saddle problem defined as:

$$p^* = \max_{y \geq 0} \min_x L(x, y). \tag{6.13}$$

The considerations above show that

$$p^* \leq f^* \tag{6.14}$$

which is known as the weak duality theorem.

6.3.2 The dual of an LP

Consider the LP in *standard form*

$$\min\{c^\top x \mid Ax = b \wedge x \geq 0\}. \tag{6.15}$$

Its Lagrangian function is $L(x,y) = c^\top x + y(b - Ax)$. We have

$$\begin{aligned} & \max_{y\ge 0}\min_x L(x,y) = \\ = \;& \max_{y\ge 0}\min_x (c^\top x + y(b-Ax)) = \\ = \;& \max_{y\ge 0}\min_x (c^\top x + yb - yAx) = \\ = \;& \max_{y\ge 0}(yb + \min_x (c^\top - yA)x). \end{aligned}$$

In general, if y increases, the expression above may become unbounded. Assume therefore that the equation $yA = c^\top$ holds; this implies $\min_x (c^\top - yA)x = \min_x 0 = 0$, and so the above reduces to finding

$$\max_{y\ge 0, yA = c^\top} yb.$$

We define the above maximization problem to be the dual of the LP Eq. (6.15), which is usually written as follows:

$$\left.\begin{array}{rrcl} \max_y & yb & & \\ & yA & = & c^\top \\ & y & \ge & 0. \end{array}\right\} \tag{6.16}$$

6.3.2.1 Alternative derivation of LP duality

Eq. (6.16) can also be achieved as follows: we seek the best possible lower bound for Eq. (6.15) by considering a weighted sum of the constraints $Ax \ge b$, using weights $y_1, \ldots, y_m$. We obtain $yAx \ge yb$, which are only valid if $y \ge 0$. To get a lower bound, we need $yb \le c^\top x$: since $yAx \ge yb$, we must require $yA = c^\top$. To make the lower bound tightest, we maximize yb subject to $y \ge 0$ and $yA = c^\top$, obtaining Eq. (6.16) again.

6.3.2.2 Economic interpretation of LP duality

Consider the diet problem of Sect. 2.2.7.1. Its dual, $\max\{yb \mid yA \le c^\top \wedge y \ge 0\}$, can be interpreted as follows. A megalomaniac pharmaceutical firm wishes to replace human food with nutrient pills: it wishes to set the prices of the pills as high as possible, whilst being competitive with the cost of the foods. In this setting, y are the prices of the m nutrient pills, b is the quantity of nutrients required, and c are the costs of the food.

6.3.3 Strong duality

In this section we shall prove the strong duality theorem for cNLP: namely that for any cNLP Eq. (6.12) having feasible region with a non-empty interior, strong duality holds:

$$p^* = f^* \tag{6.17}$$

holds. The condition on the non-emptiness of the interior of the feasible region is called *Slater's constraint qualification*, and it asserts that:

$$\exists x' \; (g(x') < 0). \tag{6.18}$$

6.3.1 Theorem (Strong Duality)
Consider a cNLP Eq. (6.12) s.t. Eq. (6.18) holds. Then we have $p^* = f^*$.

Proof. Consider the sets $\mathcal{A} = \{(\lambda, t) \mid \exists x\ (\lambda \geq g(x) \wedge t \geq f(x))\}$ and $\mathcal{B} = \{(0, t) \mid t < f^*\}$. It is easy to show that $\mathcal{A} \cap \mathcal{B} = \emptyset$, for otherwise f^* would not be optimal. Furthermore, both $\mathcal{A}$ and $\mathcal{B}$ are convex sets. Thus, there must be a separating hyperplane defined by $(u, \mu) \neq 0$ and $\alpha \in \mathbb{R}$ such that

$$\forall (\lambda, t) \in \mathcal{A}\ (u\lambda + \mu t \quad \geq \quad \alpha) \tag{6.19}$$

$$\forall (\lambda, t) \in \mathcal{B}\ (u\lambda + \mu t \quad \leq \quad \alpha). \tag{6.20}$$

Since both λ and t can increase indefinitely, in order for the expression $u\lambda + \mu t$ to be bounded below in Eq. (6.19), we must have

$$u \geq 0, \mu \geq 0. \tag{6.21}$$

Condition (6.20) is equivalent to $\mu t \leq \alpha$ for all $t < f^*$, that is $\mu f^* \leq \alpha$, since $\lambda = 0$ in $\mathcal{B}$. Combining the latter with (6.19) we conclude that for all x (in particular, for all feasible x),

$$ug(x) + \mu f(x) \geq \mu f^*. \tag{6.22}$$

Suppose now that $\mu = 0$: this implies, by Eq. (6.22), that $ug(x) \geq 0$ for all feasible x. In particular, by Eq. (6.18) there exists x' feasible such that $g(x') < 0$, which implies $u \leq 0$, and by Eq. (6.21), this means $u = 0$, yielding $(u, \mu) = 0$ which contradicts the separating hyperplane theorem (Prop. 6.2.5). Thus $\mu > 0$ and we can set $y = \frac{1}{\mu} u$ in Eq. (6.22):

$$f(x) + yg(x) \geq f^*. \tag{6.23}$$

This implies that for all feasible x we have $L(x, y) \geq f^*$. The result follows from the weak duality theorem Eq. (6.14). □

The above proof applies to LPs Eq. (6.15) as a special case.

Chapter 7

Fundamentals of Linear Programming

This chapter is devoted to LP. We summarize the main LP solution methods: simplex, ellipsoid, and interior point.

7.1 The Simplex method

The simplex method[1] is the fundamental algorithm used in LP. We remark straight away that it is one of the practically most efficient algorithms for LP, although all known implementations have exponential worst-case behaviour.

The simplex algorithms rests on four main observations.

- The LP in *canonical form*
$$\min\{c^\top x \mid Ax \le b\} \tag{7.1}$$
is equivalent to minimizing a linear form over a polyhedron.
- The minimum of a linear form over a polyhedron is attained at a vertex of the polyhedron (cf. Thm. 7.1.9): since there are finitely many vertices in a polyhedron in $\mathbb{R}^n$, there exists a finite search procedure to solve the (continuous) LP.
- Verifying whether a vertex of a polyhedron is a local minimum w.r.t. a linear form is easy: it suffices to check that all adjacent vertices have higher associated objective function value.
- Polyhedra are convex sets and linear forms are convex functions, so any local minimum is also a global minimum.

Obviously, corresponding statements can be made for maximization.

The simplex algorithm starts from a feasible polyhedron vertex and moves to an adjacent vertex with lower associated objective function value. When no such vertex exists, the vertex is the minimum and the algorithm terminates. The simplex algorithm can also be used to detect unboundedness and infeasibility.

[1] The simplex method was invented by G. Dantzig in the late forties [44]; rumour has it that the young Dantzig approached J. Von Neumann to present his results, and met with the response that his algorithm was correct but not very innovative. Dantzig himself, for the very same reason, chose not to immediately publish his algorithm in a scientific journal paper, although, to date, the simplex algorithm is the most famous algorithm in Operations Research and one of the most famous in the whole field of applied mathematics.

7.1.1 Geometry of Linear Programming

The material in this section is taken from [119, 53]. Consider the LP (in standard form)

$$\min_{x \in P} c^\top x \tag{7.2}$$

where P is the polyhedron $\{x \in \mathbb{R}^n_+ \mid Ax = b\}$ and $c \in \mathbb{R}^n$.

7.1.1 Definition
A set $\{A_i \mid i \in \beta\}$ of m linearly independent columns of A is a basis *of A. The variables $\{x_i \mid i \in \beta\}$ corresponding to the indices β of the basis are called* basic variables*. All other variables are called* nonbasic variables*.*

Defn. 7.1.1 suggests that we can partition the columns of A in $(B|N)$ where B is the nonsingular, square matrix of the basic columns and N are the nonbasic columns. Correspondingly, we partition the variables x into (x_B, x_N).

7.1.2 Definition
Given a polyhedron $P = \{x \in \mathbb{R}^n_+ \mid Ax = b\}$, the feasible vectors x having $x_B = B^{-1}b \geq 0$ and $x_N = 0$ are called basic feasible solutions *(bfs) of P.*

7.1.3 Lemma
Given a polyhedron $P = \{x \in \mathbb{R}^n_+ \mid Ax = b\}$ and a bfs x^* for P, there exists a cost vector $c \in \mathbb{R}^n$ such that x^* is the unique optimal solution of the problem $\min\{c^\top x \mid x \in P\}$.

Proof. Let $c_j = 0$ for all j such that x_j is a basic variable, and $c_j = 1$ otherwise. □

The most important result in this section states that bfs's correspond to vertices of P.

7.1.4 Theorem
Given a polyhedron $P = \{x \in \mathbb{R}^n_+ \mid Ax = b\}$, any bfs for P is a vertex of P, and vice versa.

Proof. $(\Rightarrow)$ Let $x^* = (x^*_B, 0)$, with $x^*_B \geq 0$, be a bfs for P. By Lemma 7.1.3 there is a cost vector c such that for all $x \in P$, x^* is the unique vector such that $c^\top x^* \leq c^\top x$ for all $x \in P$. Thus, the hyperplane $c^\top(x - x^*) = 0$ intersects P in exactly one point, namely x^*. Hence x^* is a vertex of P. $(\Leftarrow)$ Assume now that x^* is a vertex of P and suppose, to get a contradiction, that it is not a bfs. Consider the columns A_j of A such that $j \in \beta = \{j \leq n \mid x^*_j > 0\}$. If A_j are linearly independent, we have immediately that x^* a bfs for P, which contradicts the hypothesis. Thus, suppose A_j are linearly dependent. This means that there are scalars d_j, not all zero, such that $\sum_{j\in\beta} d_j A_j = 0$. On the other hand, since x^* satisfies $Ax = b$, we have $\sum_{j\in\beta} x_j A_j = b$. Thus, for all $\varepsilon > 0$, we obtain $\sum_{j\in\beta}(x_j - \varepsilon d_j)A_j = b$ and $\sum_{j\in\beta}(x_j + \varepsilon d_j)A_j = b$. Let x' have components $x_j - \varepsilon d_j$ for all $j \in \beta$ and 0 otherwise, and x'' have components $x_j + \varepsilon d_j$ for all $j \in \beta$ and 0 otherwise. By choosing a small enough ε we can ensure that $x', x'' \geq 0$. Since $Ax' = Ax'' = b$ by construction, both x' and x'' are in P. Thus, $x^* = \frac{1}{2}x' + \frac{1}{2}x''$ is a strict convex combination of two points of P, hence by Lemma 6.1.5 it cannot be a vertex of P, contradicting the hypothesis. □

We remark that Thm. 7.1.4 does *not* imply that there is a bijection between vertices and bfs. In fact, multiple bfs may correspond to the same vertex, as Example 7.1.5 shows.

7.1.5 Example
Consider the trivial LP $\min\{x_1 \mid x_1 + x_2 \leq 0 \wedge x_1, x_2 \geq 0\}$. The feasible polyhedron $P \equiv \{(x_1, x_2) \geq 0 \mid x_1 + x_2 \leq 0\} = \{0\}$ consists of a single vertex at the origin. On the other hand, we can partition the constraint matrix $(1\ 1)$ so that the basic column is indexed by x_1 (and the nonbasic by x_2) or, conversely,

so that the basic column is indexed by x_2 (and the nonbasic by x_1): both are bfs of the problem, both correspond to a feasible vertex, but since there is only one vertex, obviously both must correspond to the origin.

7.1.6 Remark
Geometrically, multiple bfs corresponding to a single vertex is a phenomenon known as degeneracy, *which corresponds to more than n constraint hyperplanes passing through a single point (where n is the number of variables).* Degenerate *vertices correspond to bfs having strictly less than m nonzero components (where m is the number of constraints).*

In the case of our example, $n = 2$ but there are three lines passing through the (only) feasible vertex $(0, 0)$: $x_2 = 0$, $x_1 = 0$ and $x_1 + x_2 = 0$.

The event of more than n hyperplanes intersecting in a single point has probability zero if their coefficients are sampled from a uniform distribution: this might lead the reader to believe that degeneracy is a rare occurrence. This, however, is not the case: many formulations put together by humans are degenerate. This is sometimes explained by noticing that LPs are used to model technological processes conceived by humans, which — according to a human predisposition to simplicity — involve a fair amount of symmetry, which, in turn, is likely to generate degeneracy.

7.1.7 Exercise
"A bfs is degenerate iff it has fewer than m nonzero components": is this statement true or false?

7.1.8 Exercise
Prove the statement "degenerate vertices correspond to bfs having strictly less than m nonzero components" in Rem. 7.1.6.

By the following theorem, in order to solve an LP all we have to do is compute the objective function at each vertex of the feasible polyhedron.

7.1.9 Theorem
Consider Eq. (7.2)*. If P is non-empty, closed and bounded, there is at least one bfs which solves the problem. Furthermore, if x', x'' are two distinct solutions, any convex combination of x', x'' is also a solution.*

Proof. Since the polyhedron P is closed and bounded, the function $f(x) = c^\top x$ attains a minimum on P, say at x' (and by convexity of P, x' is the global minimum). Since $x' \in P$, x' is a convex combination of the vertices $v_1, \ldots, v_p$ of P, say $x' = \sum_{i=1}^{p} \lambda_i v_i$ with $\lambda_i \geq 0$ for all $i \leq p$ and $\sum_{i=1}^{p} \lambda_i = 1$. Thus,

$$c^\top x' = \sum_{i=1}^{p} \lambda_i c^\top v_i.$$

Let $j \leq p$ be such that $c^\top v_j \leq c^\top v_i$ for all $i \leq p$. Then

$$\sum_{i=1}^{p} \lambda_i c^\top v_i \geq c^\top v_j \sum_{i=1}^{p} \lambda_i = c^\top v_j,$$

whence $c^\top x' \geq c^\top v_j$. But since $c^\top x'$ is minimal, we have $c^\top x' = c^\top v_j$, which implies that there exists a vertex of P, which by Thm. 7.1.4 corresponds to a bfs, having mimum objective function value; in other words, there is a bfs which solves the problem. For the second part of the theorem, consider a convex combination $x = \lambda x' + (1 - \lambda)x''$ with $\lambda \geq 0$. We have $c^\top x = \lambda c^\top x' + (1 - \lambda)c^\top x''$. Since x', x'' are solutions, we have $c^\top x' = c^\top x''$, and hence

$$c^\top x = c^\top x'(\lambda + (1 - \lambda)) = c^\top x',$$

which shows that x is also a solution. □

Theorem 7.1.9 states that P should be closed and bounded, so it requires that P should in fact be a polytope (polyhedra may be unbounded). In fact, this theorem can be modified [20, Prop. 2.4.2] to apply to unbounded polyhedra by keeping track of the unboundedness directions (also called extreme rays).

7.1.2 Moving from vertex to vertex

Since vertices of a polyhedron correspond to bfs by Theorem 7.1.4, and a bfs has at most m nonzero components out of n, there are at worst (nm) vertices in a given polyhedron. Thus, unfortunately, polyhedra may possess a number of vertices which is exponential in the size of the instance, so the above approach is not practical.

However, it is possible to look for the optimal vertex by moving from vertex to vertex along the edges of the polyhedron, following the direction of decreasing cost, and checking at each vertex if an optimality condition is satisfied: this is a summary description of the *simplex method*. In order to fully describe it, we need an efficient way of moving along a path of edges and vertices.

Consider a bfs x^* for $P = \{x \geq 0 \mid Ax = b\}$ and let β be the set of indices of the basic variables. Let A_i be the i-th column of A. We have:

$$\sum_{i\in\beta} x_i^* A_i = b. \tag{7.3}$$

Now, fix a $j \notin \beta$; A_j is a linear combination of the A_i in the basis. Thus, there exist multipliers x_{ij} such that for all $j \notin \beta$,

$$\sum_{i\in\beta} x_{ij} A_i = A_j. \tag{7.4}$$

Multiply Eq. (7.4) by a scalar θ and subtract it from Eq. 7.3 to get:

$$\sum_{i\in\beta} (x_i^* - \theta x_{ij}) A_i + \theta A_j = b. \tag{7.5}$$

Now suppose we want to move (by increasing θ from its initial value 0) from the current bfs to another point inside the feasible region. In order to move to a feasible point, we need $x_i^* - \theta x_{ij} \geq 0$ for all $i \in \beta$. If $x_{ij} \leq 0$ for all i, then θ can grow indefinitely (this means the polyhedron P is unbounded). Assuming a bounded polyhedron, we have a bounded $\theta > 0$. This means

$$\theta = \min_{\substack{i\in\beta \\ x_{ij}>0}} \frac{x_i^*}{x_{ij}}. \tag{7.6}$$

If $\theta = 0$ then there is $i \in \beta$ such that $x_i^* = 0$. This means that the bfs x^* is degenerate (see Example 7.1.5 and Remark 7.1.6). We assume a nondegenerate x^* in this summary treatment. Let $k \in \beta$ be the index minimizing θ in the expression above. The coefficient of A_k in Eq. 7.5 becomes 0, whereas the coefficient of A_j is nonzero.

7.1.10 Proposition
Let x^* be a bfs, $j \notin \beta$, x_{ij} be as in Eq. (7.5) for all $i \in \beta$ and θ be as in Eq. (7.6). The point $x' = (x'_1, \ldots, x'_n)$ defined by

$$x'_i = \begin{cases} x_i^* - \theta x_{ij} & \forall i \in \beta \smallsetminus \{k\} \\ \theta & i = k \\ 0 & \textit{otherwise} \end{cases}$$

is a bfs.

Proof. First notice that x' is a feasible solution by construction. Secondly, for all $i \notin \beta, i \neq$ we have $x'_i = x^*_i = 0$ and for all $i \in \beta, i \neq k$ we have $x'_i \geq 0$. By the definition of x', we have $x'_j \geq 0$ and $x'_k = 0$. Thus, if we define $\beta' = \beta \backslash \{k\} \cup \{j\}$, it only remains to be shown that $\{x_i \mid i \in \beta'\}$ is a set of basic variables for A. In other words, if we partition the columns of A according to the index set β', obtaining $A = (B'|N')$, we have to show that B' is nonsingular. Notice $(B|N) = A = (B'|N')$ implies $B^{-1}A = (I|B^{-1}N) = (B^{-1}B'|B^{-1}N')$ (here the equality sign is considered "modulo the column order": i.e. the two matrices are equal when considered as sets of columns). Eq. (7.4) can be stated in matrix form as $BX^\top = N$ where X is the $(n-m) \times m$ matrix whose (p,q)-th entry is x_{pq}, thus $B^{-1}N = X^\top$. By construction of B' we have $B' = B \backslash \{A_k\} \cup \{A_j\}$. Thus, $B^{-1}B' = (e_1, \ldots, e_{k-1}, B^{-1}A_j, e_{k+1}, \ldots, e_n)$, where e_i is the vector with i-th component set to 1 and the rest set to zero, and $B^{-1}A_j$ is the j-th column of X, i.e. $(x_{1j}, \ldots, x_{nj})^\top$. Hence, $|\det(B^{-1}B')| = |x_{kj}| > 0$, since $\theta > 0$ implies $x_{kj} \neq 0$. Thus, $\det B' \neq 0$ and B' is nonsingular. □

Intuitively, Theorem 7.1.10 says that any column A_j outside the basis can replace a column A_k in the basis if we choose k as the index that minimizes θ in Eq. 7.6. Notice that this implies that the column A_k exiting the basis is always among those columns i in Eq. 7.4 which have multiplier $x_{ij} > 0$. In other words, a column A_j can replace column A_k in the basis only if the linear dependence of A_j on A_k is nonzero (A_k is a "nonzero component" of A_j). Informally, we say that x_j enters the basis and x_k leaves the basis.

In order to formalize this process algorithmically, we need to find the value of the multipliers x_{ij}. By the proof of Prop. 7.1.10, x_{ij} is the (i,j)-th component of a matrix X satisfying $X^\top = B^{-1}N$. Knowing x_{ij} makes it possible to calculate β' and the corresponding partition B', N' of the columns of A. The new bfs x' can be obtained as $(B')^{-1}b$, since $Ax' = b$ implies $(B'|N')x' = b$ and hence $Ix' = (B')^{-1}b$ (recall $N'x' = 0$ since x' is a bfs).

7.1.3 Decrease direction

All we need now is a way to identify "convenient" variables to enter the basis. In other words, from a starting bfs we want to move to other bfs (with the method described above) so that the objective function value decreases. To this end, we iteratively select the variable x_j having the most negative *reduced cost* to enter the basis (the reduced costs are the coefficients of the objective function expressed in terms of the current nonbasic variables). Writing c as (c_B, c_N) according to the current basic/nonbasic partition, the reduced costs $\bar{c}^\top$ are obtained as $c^\top - c_B B^{-1}A$. The algorithm terminates when there is no negative reduced cost (i.e. no vertex adjacent to the current solution has a smaller objective function value). This criterion defines a local optimum. Since LP problems are convex, any local minimum is also a global one by Theorem 6.1.7.

7.1.4 Bland's rule

When a vertex is degenerate, an application of the simplex algorithm as stated above may cause the algorithm to cycle. This happens because a reduced cost in the objective function identifies a variable x_j to enter the basis, replacing x_k, with (degenerate) value $x'_j = \theta = 0$. This results in a new basis yielding exactly the same objective function value as before; at the next iteration, it may happen that the selected variable to enter the basis is again x_k. Thus, the current basis alternatively includes x_k and x_j without any change to the objective function value. It can be shown that the following simple rule entirely avoids these situations: whenever possible, always choose the variable having the lowest index for entering/leaving the basis [33, Thm. 3.3].

7.1.5 Simplex method in matrix form

Here we give a summary of the algebraic operations involved in a simplex algorithm step applied to a LP in standard form

$$\min\{c^\top x \mid Ax = b \wedge x \geq 0\}. \tag{7.7}$$

Suppose we are given a current bfs x ordered so that variables $x_B = (x_1, \ldots, x_m, 0, \ldots, 0)$ are basic and $x_N = (0, \ldots, 0, x_{m+1}, \ldots, x_n)$ are nonbasic. We write $A = B + N$ where B consists of the basic columns $1, \ldots m$ of A and 0 in the columns $m+1, \ldots n$, and N consists of 0 in the first m columns and then the nonbasic columns $m+1, \ldots n$ of A.

1. *Express the basic variables in terms of the nonbasic variables.* From $Ax = b$ we get $Bx_B + Nx_N = b$. Let B^{-1} be the inverse of the square submatrix of B consisting of the first m columns (i.e. the basic columns). We pre-multiply by B^{-1} to get:

$$x_B = B^{-1}b - B^{-1}Nx_N. \tag{7.8}$$

2. *Select an improving direction.* Express the objective function in terms of the nonbasic variables: $c^\top x = c_B^\top x_B + c_N^\top x_N = c_B^\top(B^{-1}b - B^{-1}Nx_N) + c_N^\top x_N$, whence:

$$c^\top x = c_B^\top B^{-1}b + \bar{c}_N^\top x_N, \tag{7.9}$$

where $\bar{c}_N^\top = c_N^\top - c_B^\top B^{-1}N$ are the reduced costs. If all the reduced costs are nonnegative there is no nonbasic variable which yields an objective function decrease if inserted in the basis, since the variables must also be nonegative. Geometrically speaking it means that there is no adjacent vertex with a lower objective function value, which in turn, by Thm. 6.1.7, means that we are at an optimum, and the algorithm terminates. Otherwise, select an index $h \in \{m+1, \ldots n\}$ of a nonbasic variable x_h with negative reduced cost (or, as in Section 7.1.4, select the least such h). We now wish to insert x_h in the basis by increasing its value from its current value 0. Geometrically, this corresponds to moving along an edge towards an adjacent vertex.

3. *Determine the steplength.* Inserting x_h in the basis implies that we should determine an index $l \leq m$ of a basic variable which exits the basis (thereby taking value 0). Let $\bar{b} = B^{-1}b$, and let $\bar{a}_{ij}$ be the (i, j)-th component of $B^{-1}N$ (notice $\bar{a}_{ij} = 0$ for $j \leq m$). By Eq. (7.8) we can write $x_i = \bar{b}_i - \sum\limits_{j=m+1}^{n} \bar{a}_{ij}x_j$ for all $i \leq m$. Since we only wish to increase the value of x_h and all the other nonbasic variables will keep value 0, we can write $x_i = \bar{b}_i - \bar{a}_{ih}x_h$. At this point, increasing the value of x_h may impact on the feasibility of x_i only if it becomes negative, which can only happen if $\bar{a}_{ih}$ is positive. Thus, we get $x_h \leq \frac{\bar{b}_i}{\bar{a}_{ih}}$ for each $i \leq m$ and $\bar{a}_{ih} > 0$, and hence:

$$l = \operatorname{argmin}\{\frac{\bar{b}_i}{\bar{a}_{ih}} \mid i \leq m \wedge \bar{a}_{ih} > 0\} \tag{7.10}$$

$$x_h = \frac{\bar{b}_l}{\bar{a}_{lh}}. \tag{7.11}$$

The above procedure fails if $\bar{a}_{ih} \leq 0$ for all $i \leq m$. Geometrically, it means that x_h can be increased in value without limit: this implies that the value of the objective function becomes unbounded. In other words, the problem is unbounded.

7.1.6 Sensitivity analysis

Material from this section has been taken from [53]. We write the optimality conditions as follows:

$$\bar{b} = B^{-1}b \geq 0 \quad (7.12)$$
$$\bar{c}^\top = c^\top - c_B^\top B^{-1}A \geq 0. \quad (7.13)$$

Eq. (7.12) expresses primal feasibility and Eq. (7.13) expresses dual feasibility.

Suppose now we have a variation in b, say $b \to b + \Delta b$: Eq. (7.12) becomes $B^{-1}b \geq -B^{-1}\Delta b$. This system defines a polyhedron in Δb where the optimal basis does not change. The variable values and objective function obviously change. The variation of the objective function is $(c_B^\top B^{-1})\Delta b = y^*\Delta b$, where y^* are the optimal dual variable values: these, therefore, can be seen to measure the sensitivity of the objective function value to a small change in the constraint coefficients.

7.1.7 Simplex variants

We briefly describe some of the most popular variants of the simplex algorithm. Material in this section has been taken from [119, 53].

7.1.7.1 Revised Simplex method

The revised simplex mehod is basically a smart storage and update scheme for the data of the current iteration of the simplex algorithm. In practice, we only need to store B^{-1}, as the rest of the data can be obtained via premultiplication by B^{-1}. The disadvantages of this method reside in the high numerical instability of updating B^{-1} directly. This issue is usually addressed by storing B^{-1} in various factorized forms.

7.1.7.2 Two-phase Simplex method

If no starting bfs is available for Eq. (7.7), we can artificially look for one by solving the auxiliary LP:

$$\left.\begin{array}{ll} \min\limits_{x,y} & \mathbf{1}y \\ \text{s.t.} & Ax + yI = b \\ & x \in \mathbb{R}^n_+ \\ & y \in \mathbb{R}^m_+ \end{array}\right\}$$

where $\mathbf{1}$ is the row vector consisting of all 1's. Here, the bfs where $B = I$ is immediately evident (all x are nonbasic, all y are basic), and if Eq. (7.7) is feasible, the optimal objective function value of the auxiliary LP will be 0 with $y = 0$, yielding a bfs in the x variables only. This solution can then be used as a starting bfs for the original LP.

7.1.7.3 Dual Simplex method

Another way to deal with the absence of a starting bfs is to apply the dual simplex method. What happens in the (primal) simplex algorithm is that we maintain primal feasibility by moving from vertex to vertex, while trying to decrease the objective function until this is no longer possible. In the dual simplex algorithm, we maintain the optimality of the objective function (in the sense that the current dual simplex objective function value is always a lower bound with respect to the primal minimum value) whilst trying to achieve feasibility. We use the same notation as in Section 7.1.5.

We start with a (possibly infeasible) basic primal solution where all the reduced costs are nonnegative. If $\bar{b} = B^{-1}b = x_B \geq 0$ the algorithm terminates: if x_B is primal feasible, then we have an optimal basis. Otherwise, the primal problem is infeasible. If $b \not\geq 0$, we select $l \leq m$ such that $\bar{b}_l < 0$. We then find $h \in \{m+1, \ldots, n\}$ such that $\bar{a}_{lh} < 0$ and a_{lh} is minimum among $\{\frac{\bar{c}_j}{|\bar{a}_{lj}|} \mid j \leq n \wedge \bar{a}_{lj} < 0\}$ (this ensures that the reduced costs will stay nonnegative), and we swap x_l with x_h in the current basis. If $\bar{a}_{lj} \geq 0$ for all $j \leq n$, then the primal problem is infeasible.

The advantage of the dual simplex method is that we can add cutting planes (valid inequalities) to the main data structure of the simplex algorithm (called *simplex tableau*) during the execution of the algorithm. A valid cut should make the current optimal solution infeasible, but since dual simplex bases are not primal feasible, this is not an issue.

7.1.8 Column generation

It may sometimes happen that the number of variables in a LP is much larger than the number of constraints. Consequently, while the basis has a manageable cardinality, the computational costs of running the simplex algorithm on the LP are huge. If there exists an efficient procedure for finding the reduced cost of minimum value, we can insert columns in the simplex tableau as the need arises, thus eliminating the need of dealing with all variables at once. The problem of determining the reduced cost of minimum value (of a variable that is not yet in the simplex tableau) is called *pricing problem*. Column generation techniques are only useful if the pricing problem can be solved efficiently. The procedure stops when the pricing problem determines a minimum reduced cost of non-negative value.

One example of application of column generation is the multicommodity network flow problem formulated so that each variable corresponds to a path on the network. There are exponentially many paths, but the pricing problem is a shortest path problem, which can be solved very efficiently.

7.2 Polytime algorithms for LP

Material for this section (except for Sect. 7.3) has been taken from [13, 54, 140, 74, 26].

L. Khachiyan showed in 1979 that finding an optimal solution to a LP problem has polynomial worst-case complexity. Even though Kachiyan's *ellipsoid algorithm* has polynomial worst-case complexity, it does not work well in practice. In 1984, Karmarkar presented another polynomial algorithm for solving LP which was claimed to have useful practical applicability. Gill et al. showed in 1985 that Karmarkar's algorithm was in fact an IPM with a log-barrier function applied to an LP. IPMs had been applied to nonlinear problems with considerable success in the late 60's [52]. This spawned considerable interest in IPMs applied to LP; so-called *barrier solvers* for LP were incorporated in most commercial software codes [73]. Barrier solvers compete well with simplex-based implementations especially on large-scale LPs. We look at these methods below.

7.3 The ellipsoid algorithm

Material for this section has been taken from [117, 79, 119]. The ellipsoid algorithm actually solves a different problem, which is called

> LINEAR STRICT INEQUALITIES (LSI). Given $b \in \mathbb{Q}^m$ and a rational $m \times n$ matrix A, decide whether there is a rational vector $x \in \mathbb{Q}^n$ such that $Ax < b$.

First, we show a computational complexity equivalence between LP and LSI, by reducing the former to the latter in polytime.

7.3.1 Equivalence of LP and LSI

By the term LP we mean both a MP formulation and a problem. Formally, but rather unusually, LP "as a problem" is stated as a conditional sequence of (formal) subproblems:

> LINEAR OPTIMIZATION PROBLEM (LOP). Given a vector $c \in \mathbb{Q}^n$, an $m \times n$ rational matrix A, and a vector $b \in \mathbb{Q}^m$, consider the LP formulation in Eq. (7.7), and:
>
> 1. decide whether the feasible set is empty;
> 2. if not, decide whether Eq. (7.7) is unbounded in the objective direction
> 3. if not, find the optimum and the optimal objective function value.

Namely, we check feasibility, unboundedness (two decision problems) and then optimality (an optimization problems). We must show that all of these tasks can be carried out in a polynomial number of calls to the "oracle" algorithm $\mathscr{A}$.

7.3.1.1 Reducing LOP to LI

Instead of reducing LOP to LSI directly, we show a reduction to

> LINEAR INEQUALITIES (LI). Given $b \in \mathbb{Q}^m$ and a rational $m \times n$ matrix A, decide whether there is a rational vector $x \in \mathbb{Q}^n$ such that $Ax \leq b$.

7.3.1.1.1 Addressing feasibility First, we note that if $\mathscr{A}$ is an algorithm for LI, $\mathscr{A}$ also trivially solves (with just one call) the feasibility subproblem 1 of LOP: it suffices to reformulate $\{x \geq 0 \mid Ax = b\}$ to $\{x \geq 0 \mid Ax \leq b \wedge Ax \geq b\}$.

7.3.1.1.2 Instance size For boundedness and optimality, we need to introduce some notions about the maximum possible size of LOP solutions (if they exist) in function of the input data A, b, c. We define the size $\mathscr{L} = mn + \lceil \log_2 P \rceil$ of the LOP instance (A, b, c), where P is the product of all numerators and denominators occurring in the components of A, b, c ($\mathscr{L}$ is an upper bound to the storage required to write A, b, c in binary representation).

7.3.1.1.3 Bounds on bfs components By [119, Lemma 8.5], bfs consist of rational components such that the absolute values of numerators and denominators are bounded above by 2^L (while this is not the strictest possible bound, it is a valid bound). This bound arises a consequence of three facts: (i) bfs can be computed as $x_B = B^{-1}b$ (see Eq. (7.8) and set nonbasic variables x_N to zero), where B is a basis of A; (ii) components of B^{-1} can be expressed in terms of the determinants of the adjoints of B; (iii) the absolute value of the determinant of B is bounded above by the product of the absolute values of the numerators of the components of B. Thus, we know that

$$x \text{ is a bfs of Eq. (7.7)} \quad \Longleftrightarrow \quad \forall j \leq n \ (0 \leq x_j \leq 2^L), \tag{7.14}$$

which implies in particular that if the instance is feasible and bounded and x^* is a bfs which solves Eq. (7.7), then $x^* \in [0, 2^L]$.

7.3.1.1.4 Addressing unboundedness This observation allows us to bound the optimal objective function $\min c^\top x$ below: since $c_j \ge -2^L$ for each $j \le n$, $c^\top x^* \ge -n2^{2L}$. On the other hand, if the LOP instance is unbounded, there are feasible points yielding any value of the objective function, namely strictly smaller than $n2^{2L}$. This allows us to use LSI in order to decide the boundedness subproblem 2 of LOP: we apply $\mathscr{A}$ (the LI oracle) to the system $Ax \le b \wedge Ax \ge b \wedge x \ge 0 \wedge c^\top x \le -n2^{2L} - 1$. If the system is feasible, then the LOP is unbounded.

7.3.1.1.5 Approximating the optimal bfs If the LOP instance was not found infeasible or unbounded, we know it has an optimal bfs x^*. We first find an approximation $\hat{x}$ of x^* using *bisection search*, one of the most efficient generic algorithms in combinatorial optimization More precisely, we determine $\hat{x}$ and an integer $K \in [-2^{4L}, 2^{4L}]$ such that $K2^{2L} < c^\top \hat{x} \le (K+1)2^{2L}$ as follows:

1. Let $a^L = -2^{2L}$, $a^U = 2^{2L}$;
2. Let $a = \frac{a^L + a^U}{2}$;
3. Solve the LI instance:
$$Ax \le b \ \wedge \ Ax \ge b \ \wedge \ x \ge 0 \ \wedge \ c^\top x \le a\,; \tag{7.15}$$
   using the oracle $\mathscr{A}$;
4. If Eq. (7.15) is infeasible:
   - update $a^L \leftarrow a$ and repeat from Step 2;
5. If Eq. (7.15) is feasible:
   - let $\hat{x}$ be the solution of Eq. (7.15)
   - if $a^U - a^L < 2^{-2L}$ return $\hat{x}$ and stop, else $a^U \leftarrow a$ and repeat from Step 2.

We note this bisection search makes $O(\log_2(2^{2L+1}) = 2L + 1$ calls to the oracle $\mathscr{A}$.

7.3.1.1.6 Approximation precision Terminating the bisection search when the objective function approximation of $\hat{x}$ is within an $\epsilon = 2^{-2L}$ has the following significance: by [119, Lemma 8.6], if there are two bfs x, y of Eq. (7.7) and $K \in \mathbb{Z}$ such that

$$K2^{-2L} < c^\top x \le (K+1)2^{-2L} \quad \wedge \quad K2^{-2L} < c^\top y \le (K+1)2^{-2L}, \tag{7.16}$$

then $c^\top x = c^\top y$. Note that Eq. (7.16) states that the two rational numbers $q_1 = c^\top x$ and $q_2 = c^\top y$ are as close to each other as 2^{-2L}. We suppose $q_1 \ne q_2$ to aim at a contradiction: since these are different rational numbers with denominators bounded above by 2^L [119, Lemma 8.5], we must have $|c^\top x - c^\top y| \ge 2^{-2L}$, which contradicts Eq. (7.16).

7.3.1.1.7 Approximation rounding Since we found a point $\hat{x}$ with $a^L < c^\top \hat{x} \le a^U$, and we know that requiring the objective function value to be equal to a^L yields an infeasible LI, by the existence of optimal bfs, there must be an optimal bfs x^* such that $a^L < c^\top x^* \le a^U$. We shall now give an algorithm for finding x^* using $\mathscr{A}$, which works as long as there is no degeneracy (see Rem. 7.1.6).

- Let $S = \varnothing$.
- For $j \in \{1, \ldots, n\}$ repeat:
  1. Append j to S;

2. Solve the LI instance:

$$Ax \leq b \ \wedge \ Ax \geq b \ \wedge \ x \geq 0 \ \wedge \ c^\top x \leq a^U \ \wedge \ c^\top x \geq a^L \ \wedge \ \forall j \in S \ (x_j \leq 0)\,; \tag{7.17}$$

   using the oracle $\mathscr{A}$;

3. If Eq. (7.17) is infeasible then remove j from S.

- Let B be square $m \times m$ submatrix of A indexed by any subset of m columns indexed by $\bar{S} = \{1, \ldots, n\} \smallsetminus S$
- Let $x^* = B^{-1}b$.

This algorithm is correct since it chooses basic columns from A indexed by variables which could not be set to zero in Eq. (7.17) (and hence they could not be nonbasic).

This completes the polynomial reduction from LOP to LI.

7.3.1.2 Reducing LI to LSI

By [119, Lemma 8.7], a LI instance $Ax \leq b$ is feasible if and only if the LSI instance $Ax < b + \epsilon$, where $\epsilon = 2^{-2L}$, is feasible. Let x' satisfy $Ax \leq b$; then by definition it satisfies $Ax \leq (b-\epsilon)+\epsilon$, i.e. $Ax < b+\epsilon$. Now let x^* satisfy $Ax < b+\epsilon$. If x^* also satisfies $Ax < b$ then it satisfies $Ax \leq b$ by definition, so let I be the largest set I of constraint indices of $Ax < b+\epsilon$ such that $A_I = \{a_i \mid i \in I\}$ is linearly independent. A technical argument (see [119, p. 174]) shows that the solution $\hat{x}$ to $A_I x = b_I$ also satisfies $Ax \leq b$.

The ellipsoid algorithm presentation in [132] works with closed polyhedra and hence does not need this last reduction from LI to LSI (although there is a simpler equivalence between $Ax \leq b$ and $Ax \leq b+\epsilon$ based on Farkas' lemma [132, p. 169]).

7.3.2 Solving LSIs in polytime

Let P_ε be the (open) polyhedron corresponding to the feasible set of the given system of strict linear inequalities, and let E_0 be an ellipsoid such that $P_\varepsilon \subseteq E_0$. The ellipsoid algorithm either finds a feasible solution $x^* \in P_\varepsilon$ or determines that P_ε is empty. We assume that the volume of P_ε is strictly positive if P_ε is nonempty, i.e. $P_\varepsilon \neq \emptyset \to \mathrm{Vol}(P_\varepsilon) > 0$. Let v be a number such that $\mathrm{Vol}(P_\varepsilon) > v$ if $P_\varepsilon \neq \emptyset$ and $V = \mathrm{Vol}(E_0)$, and let

$$K = \lceil 2(n+1)(\ln V - \ln v) \rceil.$$

Initially, $k = 0$.

1. Let $x^{(k)}$ be the centre of the ellipsoid E_k. If $x^{(k)} \in P_\varepsilon$, the algorithm terminates with solution $x^{(k)}$. Otherwise, there exists a violated strict constraint $A_i x < b_i$ such that $A_i x^{(k)} \geq b_i$. The hyperplane $A_i x = b_i$ slices E_k through the centre; the part which does not contain P_ε can be discarded.

2. Find the minimum volume ellipsoid E_{k+1} containing the of part of E_k containing P_ε, and let $x^{(k+1)}$ be the centre of E_{k+1}.

3. If $k \geq K$, stop: $P_\varepsilon = \varnothing$.

4. Repeat from 1.

An ellipsoid E_k with centre $x^{(k)}$ is described by $\{x \in \mathbb{R}^n \mid (x - x^{(k)})^\top D_k^{-1}(x - x^{(k)}) \le 1\}$ where D_k is an $n \times n$ PSD matrix. We compute $x^{(k+1)}$ and D_{k+1} as follows:

$$\begin{aligned}
\Gamma_k &= \frac{D_k A_i}{\sqrt{A_i{}^\top D_k A_i}} \\
x^{(k+1)} &= x^{(k)} + \frac{\Gamma_k}{n+1} \\
D_{k+1} &= \frac{n^2}{n^2-1}\left(D_k - \frac{2\Gamma_k \Gamma_k{}^\top}{n+1}\right).
\end{aligned}$$

It turns out that E_{k+1} defined by the matrix D_{k+1} contains the part of E_k containing P_ε, and furthermore

$$\mathrm{Vol}(E_{k+1}) \le e^{-\frac{1}{2(n+1)}}\mathrm{Vol}(E_k). \tag{7.18}$$

The volume of E_K is necessarily smaller than v: by Eq. (7.18) we have

$$\mathrm{Vol}(E_K) \le e^{-\frac{K}{2(n+1)}}\mathrm{Vol}(E_0) \le V e^{-\frac{K}{2(n+1)}} \le V e^{-\ln(V/v)} = v,$$

hence by the assumption on v we must have $P_\varepsilon = \emptyset$ if $k \ge K$. Since it can be shown that K is polynomial in the size of the instance (which depends on the number of variables, the number of constraints as well as the bits needed to store A and b), the ellipsoid algorithm is a polytime algorithm which can be used to solve LPs.

One last point to be raised is that in Eq. (7.18) we rely on an irrational computation, which is never precise on a computer. It can be shown that computations carried out to a certain amount of accuracy can still decide whether P_ε is empty or not (see [119, §8.7.4]).

7.4 Karmarkar's algorithm

Karmarkar's algorithm addresses all LPs with constraints $Ax = 0, x \ge 0$ and $\mathbf{1}^\top x = 1$, and known *a priori* to have optimal objective function value zero. The constraints evidently imply that $\bar{x} = \mathbf{1}/n$ is an initial feasible solution (where $\mathbf{1} = (1, \ldots, 1)^\top$.

It can be shown that any LP can be reduced to this special form.

- If no constraint $\sum_j x_j = 1$ is present in the given LP instance, one can be added as follows:
  - adjoin a constraint $\sum_j x_j \le M = O(2^L)$ (where L is the size of the instance) to the formulation: this will not change optimality properties, though it might turn unboundedness into infeasibility;
  - add a new (slack) variable x_{n+1} and rewrite the new constraint as $\sum\limits_{j \le n+1} x_j = M$;
  - scale all variables so that $x \leftarrow \frac{1}{M}x$, and accordingly scale the constraint RHSs $b \leftarrow \frac{1}{M}b$, yielding $\sum_j x_j = 1$.
- The system $Ax = b$ appearing in Eq. (7.7) can be written as

$$\forall i \le m \quad \sum_{j \le n} a_{ij}x_j - b\sum_{j \le n} x_j = 0$$

since we have the constraint $\mathbf{1}^\top x = 1$; this yields

$$\forall i \le m \quad \sum_{j \le n} (a_{ij} - b_i) x_j = 0,$$

which is homogeneous in x, as desired.

- If the optimal objective function value is known to be $\bar{c} \neq 0$, it can be "homogenized" in the same way as $Ax = b$, namely optimize the objective $c^\top x - \bar{c}$ (adding constants does not change the optima) and rewrite it as $c^\top x - \bar{c} \sum_j x_j$ based on the constraint $\mathbf{1}^\top x = 1$.
- If the optimal objective function value is unknown, proceed with a bisection search (see Sect. 7.3.1).

Let $X = \mathrm{diag}(\bar{x})$ and $B = \begin{pmatrix} AX \\ \mathbf{1} \end{pmatrix}$. The algorithm is as follows:

1. Project Xc into the null space of B: $c^* = (I - B^\top (BB^\top)^{-1} B) Xc$.
2. Normalize the descent direction: $d = \gamma \frac{c^*}{||c^*||}$. If $c^* = 0$ terminate with optimal solution x^*.
3. Move in projected space: $y = e/n - sd$ where s is a fixed step size.
4. Project back into x-space: $\bar{x} \leftarrow \frac{Xy}{e^\top Xy}$.
5. Repeat from 1.

Taking $\gamma = \frac{1}{\sqrt{n(n-1)}}$ and $s = \frac{1}{4}$ guarantees that the algorithm has polynomial complexity.

Let us look at the first iteration of Karmarkar's algorithm in more detail. The initial point $\bar{x}$ is taken to be the feasible solution $\bar{x} = \mathbf{1}/n$; notice $\mathbf{1}/n$ is also the centre of the simplex $\mathbf{1}^\top x = 1 \wedge x \ge 0$. Let $S_r = \{x \in \mathbb{R}^n \mid ||x - x^*|| \le r \wedge \mathbf{1}^\top x = 1 \wedge x \ge 0\}$ be the largest sphere that can be inscribed in the simplex, and let S_R be the smallest concentric sphere that circumscribes the simplex. It can be shown that $R/r = n - 1$. Let x_r be the minimum of $c^\top x$ on $F_r = S_r \cap \{x \mid Ax = 0\}$ and x_R the minimum on $F_R = S_R \cap \{x \mid Ax = 0\}$; let $f_r = c^\top x_r$, $f_R = c^\top x_R$ and $\bar{f} = c^\top \bar{x}$. By the linearity of the objective function, we have $\frac{\bar{f} - f_R}{\bar{f} - f_r} = n - 1$. Since F_R contains the feasible region of the problem, $f_R \le f^* = 0$, and so $(n-1)\bar{f} - (n-1) f_r = \bar{f} - f_R \ge \bar{f} - f^* = \bar{f}$, whence

$$f_r \le \frac{n-2}{n-1} \bar{f} < e^{-\frac{1}{n-1}} \bar{f}. \tag{7.19}$$

Finally, we update $\bar{x}$ with x_r and repeat the process. If this reduction in objective function value could be attained at each iteration, $O(nL)$ iterations would be required to get within 2^{-L} tolerance from $f^* = 0$, and the algorithm would be polynomial. The only issue lies in the fact that after the first iteration the updated current point x_r is not the centre of the simplex anymore. Thus, we use a projective transformation (step 4 of the algorithm) to "re-shape" the problem so that the updated current point is again at the centre of the simplex. The linearity of the objective function is not preserved by the transformation, so a linear approximation is used (step 1 of the algorithm). Karmarkar showed that Eq. (7.19) holds for the modified objective function too, thus proving correctness and polytime complexity.

7.5 Interior point methods

Karmarkar's algorithm turns out to be equivalent to an IPM applied to an LP in standard form with orthant constraints $x \ge 0$ reformulated by means of log-barrier penalties on the objective function [59].

We consider the LP in Eq. (7.7), and reformulate it as follows:

$$\left.\begin{array}{rl} \min_x & c^\top x - \beta \sum\limits_{j=1}^n \ln x_j \\ \text{s.t.} & Ax = b, \end{array}\right\} \quad (7.20)$$

where $\beta > 0$ is a parameter. Notice that since $-\ln x_j$ tends to ∞ as $x_j \to 0^+$, minimizing the objective function of Eq. (7.20) automatically implies that $x > 0$. Furthermore, as β decreases towards 0, Eq. (7.20) describes a continuous family of NLP formulations converging to Eq. (7.7). This suggests a solution method based on solving a discrete sequence of convex problems

$$\left.\begin{array}{rl} \min_{x(\beta)} & c^\top x(\beta) - \beta \sum\limits_{j=1}^n \ln x_j(\beta) \\ \text{s.t.} & Ax(\beta) = b \end{array}\right\} \quad (7.21)$$

for $\beta = \beta_1, \ldots, \beta_k, \ldots$. We expect the solutions $x^*(\beta_k)$ of Eq. (7.21) to tend to x^* as $k \to \infty$, where x^* is the solution of Eq. (7.7). The set $\{x^*(\beta) \mid \beta > 0\}$ is a path in $\mathbb{R}^n$ called the *central path*.

7.5.1 Primal-Dual feasible points

We show that each point $x(\beta)$ on the central path yields a dual feasible point. The Lagrangian $L_1(x, \lambda, \nu)$ for Eq. (7.7) (where λ are the dual variables for the constraints $-x \leq 0$ and ν for $Ax = b$) is:

$$L_1(x, \lambda, \nu) = c^\top x - \sum_{j=1}^n \lambda_j x_j + \nu(Ax - b), \quad (7.22)$$

while the Lagrangian $L_2(x, \nu)$ for Problem (7.21) is:

$$L_2(x, \nu) = c^\top x(\beta) - \beta \sum_{j=1}^n \ln x_j(\beta) + \nu(Ax - b).$$

Deriving the KKT condition (6.6) from L_1 we get:

$$\forall j \leq n \ (c_j - \lambda_j + \nu A^j = 0),$$

where A^j is the j-th column of A. From L_2 we get:

$$\forall j \leq n \ (c_j - \frac{\beta}{x_j} + \nu A^j = 0).$$

Therefore, by letting

$$\lambda_j = \frac{\beta}{x_j} \quad (7.23)$$

for all $j \leq n$, we show that each point $x(\beta)$ on the central path gives rise to a dual feasible point (λ, ν) for the dual of Eq. (7.7):

$$\left.\begin{array}{rrcl} \max\limits_{\nu} & & b^\top \nu & \\ \text{s.t.} & A^\top \nu + \lambda & = & c \\ & \lambda & \geq & 0. \end{array}\right\} \quad (7.24)$$

Notice that the dual Problem (7.24) has been derived from Eq. (6.16) by setting $\nu = -\mu$ and using λ as slack variables for the inequalities in Eq. (6.16). Since λ, ν also depend on β, we indicate them by $\lambda(\beta), \nu(\beta)$. That $(\lambda(\beta), \nu(\beta))$ is dual feasible in Eq. (7.24) follows because $(x(\beta), \lambda(\beta), \nu(\beta))$ satisfies

Eq. (6.6) as shown above. Now, notice that by definition $\lambda_j(\beta) = \frac{\beta}{x_j(\beta)}$ implies

$$\forall j \le n \; (\lambda_j(\beta) x_j(\beta) = \beta) \tag{7.25}$$

which means that, as β converges to 0, the conditions (7.25) above imply the KKT complementarity conditions (6.8). Since $\lambda(\beta) \ge 0$ by definition Eq. (7.23), we have that $(x^*, \lambda^*, \nu^*) = (x(0), \lambda(0), \mu(0))$ is an optimal primal-dual pair solving Eq. (7.7) and Eq. (7.24).

7.5.2 Optimal partitions

LPs may have more than one optimal solution. In such cases, all optimal solutions are on a single (non full-dimensional) face of the polyhedron. The simplex method would then find more than one optmial bfs. The analysis of the IPM sketched above provides a unique characterization of the optimal solutions even when there is no unique optimal solution. We show that the central path converges to a strictly complementary optimal solution, i.e. an optimal solution for which

$$\begin{aligned} (x^*)^\top \lambda^* &= 0 \\ x^* + \lambda^* &> 0. \end{aligned}$$

These solutions are used to construct the *optimal partition*,, i.e. a partition of the n solution components in two index sets B, N such that:

$$\begin{aligned} B &= \{j \le n \mid x_i^* > 0\} \\ N &= \{j \le n \mid \lambda_i^* > 0\}. \end{aligned}$$

The partition obtained in this way is unique, and does not depend on the strictly complementary optimal solution used to define it. Optimal partitions provide a unique and well-defined characterization of optimal faces.

In the rest of this section we write $x = x(\beta)$ and $\lambda = \lambda(\beta)$ to simplify notation. The proof of the following theorem was taken from [74].

7.5.1 Theorem (Goldman-Tucker, 1956)
With the same notation of this section, the limit point (x^*, λ^*) of the primal-dual central path $(x(\beta), \lambda(\beta))$ is a strictly complementary primal-dual optimal solution for Eq. (7.7).

Proof. By Eq. (7.25) we have that $x^\top \lambda = n\beta$, thus $(x^*)^\top \lambda^*$ converges to zero as $\beta \to 0$. Now, both x^* and x are primal feasible, so $Ax^* = Ax = b$, hence $A(x^* - x) = 0$. Furthermore, since both λ^* and λ are dual feasible, we have $\nu^* A + \lambda^* = \nu A + \lambda = c$, i.e. $(\nu - \nu^*)A = \lambda^* - \lambda$. In other words, $x^* - x$ is in the null space of A and $\lambda^* - \lambda$ is in the range of $A^\top$: thus, the two vectors are orthogonal. Hence we have:

$$0 = (x^* - x)^\top (\lambda^* - \lambda) = (x^*)^\top \lambda^* + x^\top \lambda - (x^*)^\top \lambda - x^\top \lambda^*,$$

and thus

$$(x^*)^\top \lambda + x^\top \lambda^* = n\beta.$$

Dividing throughout by $\beta = x_j \lambda_j$ we obtain:

$$\sum_{j=1}^n \left(\frac{x_j^*}{x_j} + \frac{\lambda_j^*}{\lambda_j} \right) = n.$$

Since

$$\lim_{\beta \to 0} \frac{x_j^*}{x_j} = \begin{cases} 1 & \text{if } x_i^* > 0 \\ 0 & \text{otherwise} \end{cases}$$

and similarly for the λ component, for each $j \leq n$ exactly one of the two components of the pair (x^*_j, λ^*_j) is zero and the other is positive. □

7.5.3 A simple IPM for LP

The prototypical IPM for LP is as follows:

1. Consider an initial point $x(\beta_0)$ feasible in Eq. 7.21, a parameter $\alpha < 1$ and a tolerance $\varepsilon > 0$. Let $k = 0$.
2. Solve Eq. (7.21) with initial point $x(\beta_k)$, to get a solution x^*.
3. If $n\beta_k < \varepsilon$, stop with solution x^*.
4. Update $\beta_{k+1} = \alpha\beta_k$, $x(\beta_{k+1}) = x^*$ and $k \leftarrow k + 1$.
5. Go to Step 2.

By Eq. (7.22), $L_1(x, \lambda, \nu) = c^\top x - n\beta_k$, which means that the duality gap is $n\beta_k$. This implies that $x(\beta_k)$ is never more than $n\beta_k$-suboptimal. This is the basis of the termination condition in Step 3. Each subproblem in Step 2 can be solved by using Newton's method.

7.5.4 The Newton step

In general, the Newton descent direction d for an unconstrained problem $\min f(x)$ at a point $\bar{x}$ is given by:

$$d = -(\nabla^2 f(\bar{x}))^{-1} \nabla f(\bar{x}). \tag{7.26}$$

If $\nabla^2 f(\bar{x})$ is PSD, we obtain

$$(\nabla f(\bar{x}))^\top d = -(\nabla f(\bar{x}))^\top (\nabla^2 f(\bar{x}))^{-1} \nabla f(\bar{x}) < 0,$$

so d is a descent direction. In this case, we need to find a feasible descent direction such that $Ad = 0$. Thus, we need to solve the system

$$\begin{pmatrix} \nabla^2 f(\bar{x}) & A^\top \\ A & 0 \end{pmatrix} \begin{pmatrix} d \\ \nu^\top \end{pmatrix} = \begin{pmatrix} -\nabla f(\bar{x}) \\ 0 \end{pmatrix},$$

for (d, ν), where ν are the dual variables associated with the equality constraints $Ax = b$. Step 4 in the IPM of Section 7.5.3 becomes $x(\beta_{k+1}) = x(\beta_k) + \gamma d$, where γ is the result of a line search (see Rem. 9.1.1), for example

$$\gamma = \mathrm{argmin}_{s \geq 0} f(\bar{x} + sd). \tag{7.27}$$

Notice that feasibility with respect to $Ax = b$ is automatically enforced because $\bar{x}$ is feasible and d is a feasible direction.

Chapter 8

Fundamentals of Mixed-Integer Linear Programming

This chapter is devoted to some basic notions arising in MILP. We discuss total unimodularity, valid cuts, the Branch-and-Bound (BB) algorithm, and Lagrangean relaxation.

8.1 Total unimodularity

The continuous relaxation of a MILP is a MILP formulation where the integrality constraints have been dropped: in other words, an LP. In Sect. 7.1.1 and 7.1.5 we characterized LP solutions as bfs, which encode the combinatorics and geometry of an intersection of at least m hyperplanes in $\mathbb{R}^m$.

The question we try and answer in this section is: when does a solution of the continuous relaxation of a MILP automatically satisfy the integrality constraints too? In other words, when can we solve a MILP by simply solving an LP? The question is important because, as we noted above (see Sect. 5.2) MILP is **NP**-hard, whereas we can solve LPs in polytime (see Sect. 7.2): and this is a worst-case analysis which applies to practical computation (see Sect. 2.2.5).

As mentioned in Sect. 7.1.5, if we consider the continuous relaxation of a MILP as an LP in standard form (7.7), a bfs x^* corresponds to a basis B of the constraint matrix A appearing in the linear system $Ax = b$. The values of the basic variables in x^* are computed as $x^*_B = B^{-1}b$, whereas the nonbasic variables have value zero. So the question becomes: what are the conditions on a square nonsingular matrix B and on a vector b such that $B^{-1}b$ is an integer vector?

We first note that any MILP with rational input (A, b, c) can be reformulated to a MILP with integer input by simply rescaling by the minimum common multiple (mcm) of all the denominators (a better rescaling can be carried out by considering each constraint in turn). So we shall assume in the rest of this chapter that A, b, c all have integer components.

8.1.1 Definition
An $m \times n$ integral matrix A such that each $m \times m$ invertible square submatrix has determinant ± 1 is called unimodular.

8.1.2 Proposition
If A is unimodular, the vertices of the polyhedron $P_s = \{x \geq 0 \mid Ax = b\}$ all have integer components.

8.1.3 Exercise
Prove Prop. 8.1.2.

Proving unimodularity is hard (computationally) for any instance, and even harder (theoretically) for problems. We now consider a stronger condition.

8.1.4 Definition
An $m \times n$ integral matrix A where all square submatrices of any size have determinant in $\{0, 1, -1\}$ is called totally unimodular (TUM).

8.1.5 Example
The identity matrix is TUM: square submatrices on the diagonal have determinant 1, while off-diagonal square submatrices have determinant zero.

The following propositions give some characterizations of TUM matrices which can be used to prove the TUM property for some interesting problems.

8.1.6 Proposition
A matrix A is TUM iff $A^\top$ is TUM.

8.1.7 Exercise
Prove Prop. 8.1.6.

8.1.8 Proposition
If a matrix is TUM, then its entries can only be $\{0, 1, -1\}$.

8.1.9 Exercise
Prove Prop. 8.1.8.

8.1.10 Proposition
The $m \times n$ matrix A is TUM iff the matrix (A, I), obtained by appending an $m \times m$ identity to A, is TUM.

Proof. Let B be a square submatrix of (A, I): if it is wholly contained in A or in I, then its determinant is $\{0, 1, -1\}$ because A is TUM. Otherwise, by permuting its rows, we can write B as follows:

$$B = \left(\begin{array}{c|c} A' & 0 \\ \hline A'' & I_\ell \end{array} \right),$$

where A' is a $k \times k$ submatrix of A and A'' is an $\ell \times k$ submatrix of A. By elementary linear algebra, $|B| = |A'| \in \{0, 1, -1\}$ since A' is a square submatrix of a TUM matrix. □

We now give a sufficient condition for checking the TUM property.

8.1.11 Proposition
An $m \times n$ matrix A is TUM if: (a) for all $i \le m$, $j \le n$ we have $a_{ij} \in \{0, 1, -1\}$; (b) each column of A contains at most two nonzero coefficients; (c) there is a partition R_1, R_2 of the set of rows such that for all columns j having exactly two nonzero coefficients, we have $\sum_{i \in R_1} a_{ij} - \sum_{i \in R_2} a_{ij} = 0$.

Proof. Suppose that conditions (a), (b), (c) hold but A is not TUM. Let B be the smallest square submatrix of A such that $\det(B) \notin \{0, 1, -1\}$. B cannot contain a column with just one nonzero entry, otherwise B would not be minimal (just eliminate the row and column of B containing that single nonzero entry). Hence B must contain two nonzero entries in every column. By condition (c), adding the rows in R_1 to those in R_2 gives the zero vector, and hence $\det(B) = 0$, contradicting the hypothesis. □

8.1.12 Theorem
If A is TUM, the vertices of the polyhedron $P_c = \{x \ge 0 \mid Ax \ge b\}$ all have integer components.

Proof. Let x^* be a vertex of P_c, and $s^* = Ax^* - b$. Then (x^*, s^*) is a vertex of the standardized polyhedron $\bar{P}_c = \{(x,s) \ge 0 \mid Ax - s = b\}$: suppose it were not, then by Lemma 6.1.5 there would be two distinct points (x_1, s_1), (x_2, s_2) in $\bar{P}_c$ such that (x^*, s^*) is a strict convex combination of (x_1, s_1), (x_2, s_2), i.e. there would be a $\lambda \in (0,1)$ such that $(x^*, s^*) = \lambda(x_1, s_1) + (1-\lambda)(x_2, s_2)$. Since $s_1 = Ax_1 - b \ge 0$ and $s_2 = Ax_2 - b \ge 0$, both x_1 and x_2 are in P_c, and thus $x^* = \lambda x_1 + (1-\lambda)x_2$ is not a vertex of P_c since $0 < \lambda < 1$, which is a contradiction. Now, since A is TUM, $(A, -I)$ is unimodular by Prop. 8.1.10, and (x^*, s^*) is an integer vector. □

8.1.13 Example
The transportation formulation Eq. (2.8) and network flow formulation Eq. (2.9) both have TUM constraint matrices. Solving them using the simplex method yields an integer solution vector.

8.1.14 Exercise
Prove that network flow constraints (see Eq. (2.9)) yield a TUM constraint matrix.

8.1.15 Exercise
Prove that transportation constraints (see Eq. (2.8)) yield a TUM constraint matrix.

8.2 Cutting planes

The convex hull of the feasible region of any MILP is a polyhedral set. Moreover, optimizing over the convex hull yields the same optima as optimizing over the mixed-integer feasible region of the MILP. Therefore, potentially, any MILP could be reformulated to an LP. Let me refrain the reader from jumping to the conclusion that the complexity of MILP (**NP**-hard) is the same as that of LP (**P**): there are obstacles of description and size. First, in order to even cast this equivalent LP formulation, we need to explicitly know all integer vectors in the feasible region of the MILP, including the optimal one: so already writing this LP formulation is as hard as solving the MILP. Moreover, there might be exponentially (or even infinitely) many feasible vectors to a given MILP instance, yielding an exponentially large description of the convex hull. On the other hand, finding some inequalities belonging (or just close) to the convex hull improves the performance of MILP solution methods, which is the subject of this section.

Consider a MILP $\min\{c^\top x \mid x \in \mathbb{Z}^n \cap P\}$ where $P = \{x \ge 0 \mid Ax \ge b\}$. Let $\bar{P}$ be the convex hull of its integer feasible solutions (thus $\min\{c^\top x \mid x \in \bar{P}\}$ has the same solution as the original MILP). We are interested in finding linear constraints defining the facets of $\bar{P}$. The polyhedral analysis approach is usually expressed as follows: given an integral vector set $X \subseteq \mathbb{Z}^n$ and a valid inequality $h^\top x \le d$ for X, show that the inequality is a facet of $\mathrm{conv}(X)$. We present two approaches below.

1. Find n points $x_1, \ldots, x_n \in X$ such that $h^\top x_i = d \forall i \le n$ and show that these points are affinely independent (i.e. that the $n-1$ directions $x_2 - x_1, \ldots, x_n - x_1$ are linearly independent).

2. Select $t \ge n$ points $x_1, \ldots, x_t$ satisfying the inequality. Suppose that all these points are on a generic hyperplane $\mu^\top x = \mu_0$. Solve the equation system

$$\forall k \le t \ \sum_{j=1}^{n} x_{kj}\mu_j = \mu_0$$

   in the $t+1$ unknowns (μ_j, μ_0). If the solution is $(\lambda h_j, \lambda d)$ with $\lambda \ne 0$ then the inequality $h^\top x \le d$ is facet defining.

One of the limits of polyhedral analysis is that the theoretical devices used to find facets for a given MILP are often unique to the problem it models.

8.2.1 Separation Theory

Finding all of the facets of $\bar{P}$ is overkill, however. Since the optimization direction points us towards a specific region of the feasible polyhedron, what we really need is an oracle that, given a point $x' \in P$, tells us that $x' \in \bar{P}$ or else produces a separating hyperplane $h^\top x = d$ such that for all $h^\top \bar{x} \leq d$, $\bar{x} \in \bar{P}$ and $h^\top x' > d$, adjoining the constraint $h^\top x \geq d$ to the MILP formulation tightens the feasible region P of the continuous relaxation. The problem of finding a valid separating hyperplane is the *separation problem*. It is desirable that the separation problem for a given **NP**-hard problem should have polynomial complexity.

8.2.1 Example (Valid cuts for the TSP)
A classic example of a polynomial separation problem for a **NP***-hard problem is the* Travelling Salesman Problem *(TSP): given a nonnegatively edge-weighted clique K_n, with weight $c_{ij} \geq 0$ on each edge $\{i,j\} \in E(K_n)$, find the shortest Hamiltonian cycle in K_n.*

Now consider the following MILP:

$$\left.\begin{array}{rrcll} \min & \sum\limits_{i \neq j \in V} c_{ij} x_{ij} & & & \\ s.t. & \sum\limits_{i \neq j \in V} x_{ij} & = & 2 & \forall\, i \in V \\ & x_{ij} \in \{0,1\} & & \forall\, i \neq j \in V. & \end{array}\right\} \tag{8.1}$$

Some of its feasible solutions are given by disjoint cycles. However, we can exclude them from the feasible region by requesting that each cut should have cardinality at least 2, as follows:

$$\forall\, S \subsetneq V\ (\sum_{i \in S, j \notin S} x_{ij} \geq 2).$$

There is an exponential number of such constraints (one for each subset S of V), however we do not need them all: we can add them iteratively by identifying cuts $\delta(S)$ where $\sum_{\{i,j\} \in \delta(S)} x_{ij}$ is minimum. We can see this as the problem of finding a cut of minimum capacity in a flow network (so the current values x_{ij} are used as arc capacities — each edge is replaced by antiparallel arcs). The formulation we look for is the LP dual of Eq. (2.9); we can solve it in weakly polytime with the ellipsoid method or in strongly polytime with a combinatorial algorithm ($O(n^3)$ if we use the Goldberg-Tarjan push-relabel algorithm [61]). So if each nontrivial cut has capacity at least 2, the solution is an optimal Hamiltonian cycle.

Otherwise, supposing that $\delta(S)$ has capacity $K < 2$, the following is a valid cut:

$$\sum_{\{i,j\} \in \delta(S)} x_{ij} \geq 2,$$

which can be added to the formulation. The problem is then re-solved iteratively to get a new current solution until the optimality conditions are satisfied. This approach is also known as row generation.

In the following sections 8.2.2-8.2.6 we shall give examples of four different cut families which can be used to separate the incumbent (fractional) solution from the convex hull of the integer feasible set.

8.2.2 Chvátal Cut Hierarchy

A *cut hierarchy* is a finite sequence of cut families that generate tighter and tighter relaxed feasible sets $P = P_0 \supseteq P_1 \supseteq \ldots \supseteq P_k = \bar{P}$, where $\bar{P} = \mathrm{conv}(X)$.

Given the relaxed feasible region $P = \{x \geq 0 \mid Ax = b\}$ in standard form, define the *Chvátal first-level closure* of P as $P_1 = \{x \geq 0 \mid Ax = b, \forall u \in \mathbb{R}^n_+ \lfloor uA \rfloor \leq \lfloor ub \rfloor\}$. Although formally the number of

inequalities defining P_1 is infinite, it can be shown that these can be reduced to a finite number [153]. We can proceed in this fashion by transforming the Chvátal first-level inequalities to equations via the introduction of slack variables. Reiterating the process on P_1 to obtain the Chvátal second-level closure P_2 of P, and so on. It can be shown that any fractional vertex of P can be "cut" by a Chvátal inequality.

8.2.3 Gomory Cuts

Gomory cuts are a special kind of Chvátal cuts. Their fundamental property is that they can be inserted in the simplex tableau very easily. This makes them a favorite choice in cutting plane algorithms, which generate cuts iteratively in function of the current incumbent.

Suppose x^* is the optimal solution found by the simplex algorithm deployed on a continuous relaxation of a given MILP. Assume the component x^*_h is fractional. Since $x^*_h \neq 0$, column h is a basic column; thus there corresponds a row t in the simplex tableau:

$$x_h + \sum_{j \in \nu} \bar{a}_{tj} x_j = \bar{b}_t, \tag{8.2}$$

where ν are the nonbasic variable indices, $\bar{a}_{tj}$ is a component of $B^{-1}A$ (B is the nonsingular square matrix of the current basic columns of A) and $\bar{b}_t$ is a component of $B^{-1}b$. Since $\lfloor \bar{a}_{tj} \rfloor \leq \bar{a}_{tj}$ for each row index t and column index j,

$$x_h + \sum_{j \in \nu} \lfloor \bar{a}_{tj} \rfloor x_j \leq \bar{b}_t.$$

Furthermore, since the LHS must be integer, we can restrict the RHS to be integer too:

$$x_h + \sum_{j \in \nu} \lfloor \bar{a}_{tj} \rfloor x_j \leq \lfloor \bar{b}_t \rfloor. \tag{8.3}$$

We now subtract Eq. (8.3) from Eq. (8.2) to obtain the *Gomory cut*:

$$\sum_{j \in \nu} (\lfloor \bar{a}_{tj} \rfloor - \bar{a}_{tj}) x_j \leq (\lfloor \bar{b}_t \rfloor - b_t). \tag{8.4}$$

We can subsequently add a slack variable to the Gomory cut, transform it to an equation, and easily add it back to the current dual simplex tableau as the last row with the slack variable in the current basis.

8.2.3.1 Cutting plane algorithm

In this section we illustrate the application of Gomory cut in an iterative fashion in a cutting plane algorithm. This by solving a continuous relaxation at each step. If the continuous relaxation solution fails to be integral, a separating cutting plane (a valid Gomory cut) is generated and added to the formulation, and the process is repeated. The algorithm terminates when the continuous relaxation solution is integral.

Let us solve the following MILP in standard form:

$$\left.\begin{array}{rrcl} \min & x_1 - 2x_2 & & \\ t.c. & -4x_1 + 6x_2 + x_3 & = & 9 \\ & x_1 + x_2 + x_4 & = & 4 \\ & x \geq 0 & , & x_1, x_2 \in \mathbb{Z} \end{array}\right\}$$

In this example, x_3, x_4 can be seen as slack variables added to an original formulation in canonical form with inequality constraints expressed in x_1, x_2 only.

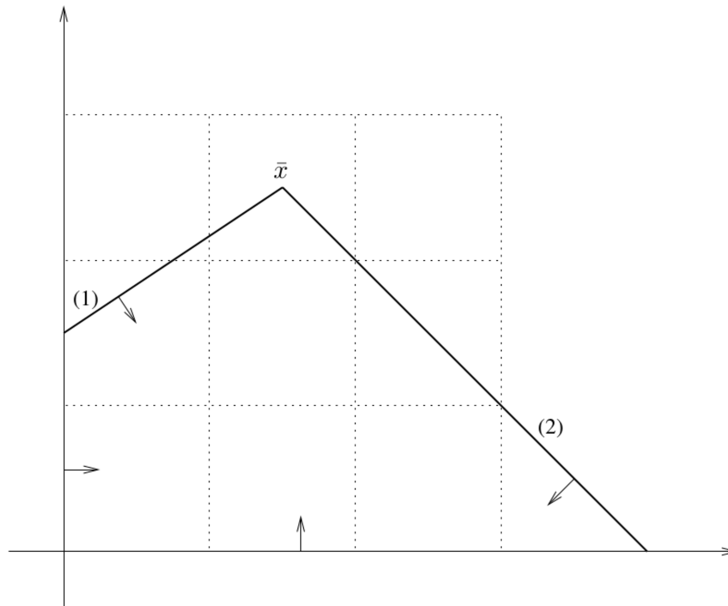
We identify $x_B = (x_3, x_4)$ as an initial feasible basis; we apply the simplex algorithm obtaining the following tableau sequence, where the pivot element is $\boxed{\text{framed}}$.

	x_1	x_2	x_3	x_4
0	1	-2	0	0
9	-4	$\boxed{6}$	1	0
4	1	1	0	1

	x_1	x_2	x_3	x_4
3	$-\frac{1}{3}$	0	$\frac{1}{3}$	0
$\frac{3}{2}$	$-\frac{2}{3}$	1	$\frac{1}{6}$	0
$\frac{5}{2}$	$\boxed{\frac{5}{3}}$	0	$-\frac{1}{6}$	1

	x_1	x_2	x_3	x_4
$\frac{7}{2}$	0	0	$\frac{3}{10}$	$\frac{1}{5}$
$\frac{5}{2}$	0	1	$\frac{1}{10}$	$\frac{2}{5}$
$\frac{3}{2}$	1	0	$-\frac{1}{10}$	$\frac{3}{5}$

The solution of the continuous relaxation is $\bar{x} = (\frac{3}{2}, \frac{5}{2})$, where $x_3 = x_4 = 0$.



We derive a Gomory cut from the first row of the optimal tableau: $x_2 + \frac{1}{10}x_3 + \frac{2}{5}x_4 = \frac{5}{2}$. The cut is formulated as follows:

$$x_i + \sum_{j \in N} \lfloor \bar{a}_{ij} \rfloor x_j \leq \lfloor \bar{b}_i \rfloor, \tag{8.5}$$

where N is the set of nonbasic variable indices and i is the index of the chosen row. In this case we obtain the constraint $x_2 \leq 2$.

We introduce this Gomory cut in the current tableau. Note that if we insert a valid cut in a simplex tableau, the current basis becomes primal infeasible, thus a dual simplex iteration is needed. First of all, we express $x_2 \leq 2$ in terms of the current nonbasic variables x_3, x_4. We subtract the i-th optimal tableau row from Eq. (8.5), obtaining:

$$\begin{aligned} x_i + \sum_{j \in N} \bar{a}_{ij} x_j &\leq \bar{b}_i \\ \Rightarrow \sum_{j \in N} (\lfloor \bar{a}_{ij} \rfloor - \bar{a}_{ij}) x_j &\leq (\lfloor \bar{b}_i \rfloor - \bar{b}_i) \\ \Rightarrow -\frac{1}{10}x_3 - \frac{2}{5}x_4 &\leq -\frac{1}{2}. \end{aligned}$$

Recall that the simplex algorithm requires the constraints in equation (rather than inequality) form, so

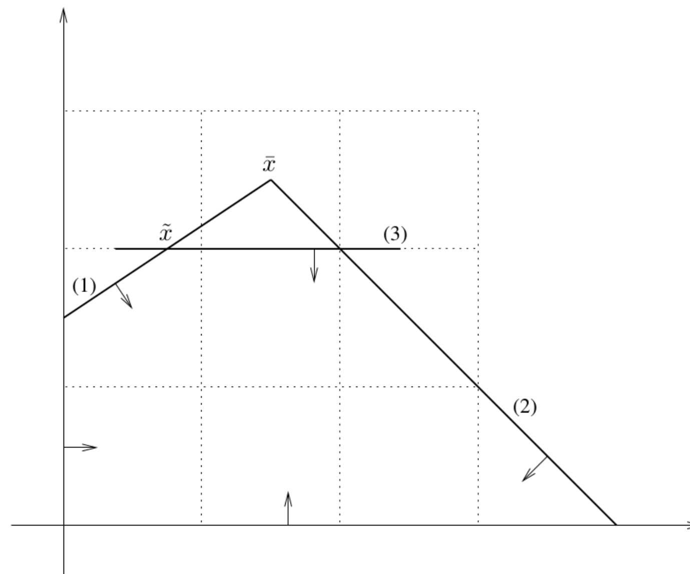
we add a slack variable $x_5 \geq 0$ to the formulation:

$$-\frac{1}{10}x_3 - \frac{2}{5}x_4 + x_5 = -\frac{1}{2}.$$

We ajoin this constraint as the bottom row of the optimal tableau. We now have a current tableau with an additional row and column, corresponding to the new cut and the new slack variable (which is in the basis):

	x_1	x_2	x_3	x_4	x_5
$\frac{7}{2}$	0	0	$\frac{3}{10}$	$\frac{1}{5}$	0
$\frac{5}{2}$	0	1	$\frac{1}{10}$	$\frac{2}{5}$	0
$\frac{3}{2}$	1	0	$-\frac{1}{10}$	$\frac{3}{5}$	0
$-\frac{1}{2}$	0	0	$-\frac{1}{10}$	$-\frac{2}{5}$	1

The new row corresponds to the Gomory cut $x_2 \leq 2$ (labelled "constraint (3)" in the figure below).



We carry out an iteration of the dual simplex algorithm using this modified tableau. The reduced costs are all non-negative, but $\bar{b}_3 = -\frac{1}{2} < 0$ implies that $x_5 = \bar{b}_3$ has negative value, so it is not primal feasible (as $x_5 \geq 0$ is now a valid constraint). We pick x_5 to exit the basis. The variable j entering the basis is given by:

$$j = \text{argmin}\{\frac{\bar{c}_j}{|\bar{a}_{ij}|} \mid j \leq n \wedge \bar{a}_{ij} < 0\}.$$

In this case, $j = \text{argmin}\{3, \frac{1}{2}\}$, corresponding to $j = 4$. Thus x_4 enters the basis replacing x_5 (the pivot element is indicated in the above tableau). The new tableau is:

	x_1	x_2	x_3	x_4	x_5
$\frac{13}{4}$	0	0	$\frac{1}{4}$	0	$\frac{1}{2}$
2	0	1	0	0	1
$\frac{3}{4}$	1	0	$-\frac{1}{4}$	0	$\frac{3}{2}$
$\frac{5}{4}$	0	0	$\frac{1}{4}$	1	$-\frac{5}{2}$

The optimal solution is $\tilde{x} = (\frac{3}{4}, 2)$. Since this solution is not integral, we continue. We pick the second

tableau row:

$$x_1 - \frac{1}{4}x_3 + \frac{3}{2}x_5 = \frac{3}{4},$$

to generate a Gomory cut

$$x_1 - x_3 + x_5 \leq 0,$$

which, written in terms of the variables x_1, x_2 is

$$-3x_1 + 5x_2 \leq 7.$$

This cut can be written as:

$$-\frac{3}{4}x_3 - \frac{1}{2}x_5 \leq -\frac{3}{4}.$$

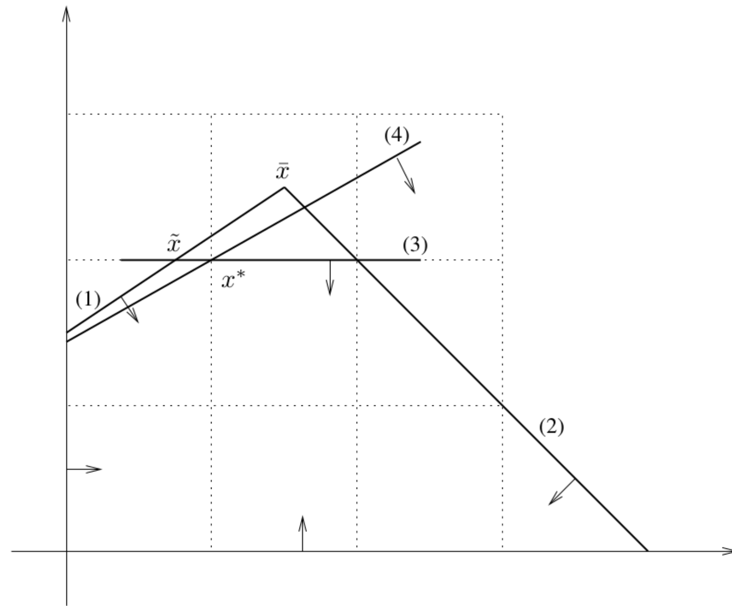
The new tableau is:

	x_1	x_2	x_3	x_4	x_5	x_6
$\frac{13}{4}$	0	0	$\frac{1}{4}$	0	$\frac{1}{2}$	0
2	0	1	0	0	1	0
$\frac{3}{4}$	1	0	$-\frac{1}{4}$	0	$\frac{3}{2}$	0
$\frac{5}{4}$	0	0	$\frac{1}{4}$	1	$-\frac{5}{2}$	0
$-\frac{3}{4}$	0	0	$\boxed{-\frac{3}{4}}$	0	$-\frac{1}{2}$	1

The pivot is framed; the exiting row 4 was chosen because $\bar{b}_4 < 0$, the entering column 5 because $\frac{\bar{c}_3}{|\bar{a}_{43}|} = \frac{1}{3} < 1 = \frac{\bar{c}_5}{|\bar{a}_{45}|}$). Pivoting, we obtain:

	x_1	x_2	x_3	x_4	x_5	x_6
3	0	0	0	0	$\frac{1}{3}$	$\frac{1}{3}$
2	0	1	0	0	1	0
1	1	0	0	0	$\frac{5}{3}$	$-\frac{1}{3}$
1	0	0	0	1	$-\frac{8}{3}$	$\frac{1}{3}$
1	0	0	1	0	$\frac{2}{3}$	$-\frac{4}{3}$

This tableau has optimal solution $x^* = (1, 2)$, which is integral (and hence optimal). The figure below shows the optimal solution and the last Gomory cut to be generated.



8.2.4 Disjunctive cuts

A condition such as "either…or…" can be modelled using disjunctive constraints (stating e.g. membership of a variable vector in a disjunction of two or more sets), wchich are themselves written using binary variables.

8.2.2 Example
Consider two polyhedra $P = \{x \in \mathbb{R}^m \mid Ax \le b\}$ and $Q = \{x \in \mathbb{R}^n \mid Cx \le d\}$. Then the constraint $x \in P \cup Q$ can be written as $(x \in P) \vee (x \in Q)$ by means of an additional binary variable $y \in \{0,1\}$:

$$\begin{aligned} yAx &\le yb \\ (1-y)Cx &\le (1-y)d. \end{aligned}$$

We remark that the above constraints are bilinear, as they involve products of variables yx_j for all $j \le n$. This can be dealt with using the techniques in Rem. 2.2.8. On the other hand, if P, Q are polytopes (i.e. they are bounded), it suffices to find a large constant M such that $Ax \le b + M$ and $Cx \le d + M$ hold for all $x \in P \cup Q$, and then adjoin the linear constraints:

$$\begin{aligned} Ax &\le b + My \\ Cx &\le d + M(1-y) \end{aligned}$$

We caution the reader against the indiscriminate use of "big M" constants (see Sect. 2.2.7.5.1). How would one find a "good" big M? First of all, if one really needed to find a single constant M valid for $x \in P \cup Q$, one possible way to go about it would be to find the smallest possible hyper-rectangle containnig P and Q, describe it by $x^L \le x \le x^U$, and then compute M as the maximum upper bound w.r.t. each row in $Ax - b$: this involves using interval arithmetic on $A[x^L, x^U] - b$ [114]. Secondly, we need not use the same constant M to bound both $Ax \le b$ and $Cx \le d$: we might be able to find smaller M_1, M_2 such that $Ax \le b + M_1$ and $Cx \le d + M_2$ are always valid for all $x \in P \cup Q$. This would allow us to write

$$\begin{aligned} Ax &\le b + M_1 y \\ Cx &\le d + M_2(1-y). \end{aligned}$$

8.2.3 Exercise
Propose an algorithm for finding the smallest hyper-rectangle $[x^L, x^U]$ *containing a given polytope* $P = \{x \in \mathbb{R}^n \mid Ax \leq b\}$.

We now describe a method for computing a cut valid for the union of two polyhedra $P \cup Q$, where $P = \{x \geq 0 \mid Ax \leq b\}$ and $Q = \{x \geq 0 \mid ; Cx \leq d\}$ (note that we are explicitly requiring $x \geq 0$ for both P, Q). We construct our cut from row i in the description of P and row ℓ in the description of Q. For each $j \leq n$ choose some $h_j \leq \min(A_{ij}, C_{\ell j})$ and some $h_0 \geq \max(b_i, d_\ell)$. Then the inequality

$$h^\top x \leq h_0 \tag{8.6}$$

is valid for $P \cup Q$.

8.2.4 Exercise
Prove that Eq. (8.6) *is valid for* $P \cup Q$.

8.2.5 Lifting

It is possible to derive valid inequalities for a given MILP

$$\min\{cx \mid Ax \leq b \land x \in \{0,1\}^n\} \tag{8.7}$$

by *lifting* lower-dimensional inequalities to a higher-dimensional space. If the inequality $\sum_{j=2}^n \pi_j x_j \leq \pi_0$ (with $\pi_j \geq 0$ for all $j \in \{2, \ldots, n\}$) is valid for the restricted

$$\min\{\sum_{j=2}^n c_j x_j \mid \sum_{j=2}^n a_{ij} x_j \leq b_i \forall i \leq m \land x_j \in \{0,1\} \ \forall\ j \in \{2, \ldots, n\}\},$$

then by letting

$$\left.\begin{array}{rrcll} \pi_1 = \max & (\pi_0 - \sum\limits_{j=2}^n \pi_j x_j) & & & \\ & \sum\limits_{j=2}^n a_{ij} x_j & \leq & b_i - a_{i1} & \forall i \leq m \\ & x_j & \in & \{0,1\} & \forall j \in \{2, \ldots, n\}. \end{array}\right\}$$

we can find the inequality $\sum_{j=1}^n \pi_j x_j \leq \pi_0$ which is valid for (8.7), as long as the above formulation is not infeasible; if it is, then $x_1 = 0$ is a valid inequality. Of course the lifting process can be carried out with respect to any variable index (not just 1).

8.2.6 RLT cuts

Reformulation-Linearization Techniques (RLT) cuts, described in [137], are a form of *nonlinear lifting*. From each constraint $a_i^\top x \geq b_i$ of a feasible set

$$F = \{x \in \{0,1\}^n \mid Ax \leq b\}$$

we derive the i-th *constraint factor*

$$\gamma(i) = a_i^\top x - b_i$$

(for $i \leq m$). We then form the *bound products*

$$p(I, J) = \prod_{j \in I} x_j \prod_{\ell \in J} (1 - x_\ell)$$

for all partitions I, J of the index set $\{1, \ldots, d\}$. The set of all of the cuts

$$p(I, J)\, \gamma(i) \geq 0 \tag{8.8}$$

obtained by multiplying each constraint factor $\gamma(i)$ (for $i \leq m$) by all the bound products $p(I, J)$ over all I, J s.t. $I \cup J = \{1, \ldots, d\}$, is called the *RLT d-th level closure*. We remark that d refers to the maximum degree of the bound products.

Notice that Eq. (8.8) are nonlinear inequalities. As long as they only involve binary variables, we can apply a linearization which generalizes the one in Rem. 2.2.8: after replacing each occurrence of x_j^2 by x_j (because $x_j \in \{0, 1\}$) for each j, we linearize the inequalities Eq. (8.8) by lifting them in a higher-dimensional space: replace all products $\prod_{j \in H} x_j$ by a new added variable $w_H = \prod_{j \in H} x_j$, to obtain linearized cuts of the form

$$\mathscr{L}^i_{IJ}(x, w) \geq 0, \tag{8.9}$$

where $\mathscr{L}^i_{IJ}$ is a linear function of x, w. We define the RLT d-th level closure as:

$$P_d = \{x \mid \forall i \leq m \text{ and } I, J \text{ partitioning } \{1, \ldots, d\},\ \mathscr{L}^i_{IJ}(x, w) \geq 0\}.$$

The *RLT cut hierarchy* is defined as the union of all the RLT d-th level closures P_d up to and including level n. It was shown in [136] that

$$\mathsf{conv}(F) = \mathsf{proj}_x(P_n) \subseteq \mathsf{proj}_x(P_{n-1}) \subseteq \ldots \subseteq \mathsf{proj}_x(P_0) = \mathsf{relax}(F), \tag{8.10}$$

where $\mathsf{conv}(X)$ denotes the convex hull of a set X, $\mathsf{proj}_x(X)$ denotes the projection on the x variables of a set description X involving the x variables and possibly other variables (e.g. the w linearization variables), and $\mathsf{relax}(X)$ denotes the continuous relaxation of a mixed-integer set X. In other words, the whole RLT hierarchy yields the convex hull of any linear set involving binary variables.

This cut hierarchy has two main shortcomings: (a) the high number of additional variables and (b) the huge number of generated constraints. It is sometimes used heuristically to generate tighter continuous relaxations various mixed-integer formulations.

8.3 Branch-and-Bound

BB is an iterative method that endows the search space with a tree structure. Each node of this tree defines a subproblem. BB processes each subproblem in turn. Lower and upper bounds to the objective function value are computed at the current subproblem, and globally valid upper and lower bounds (w.r.t. all remaining subproblems) are maintained during the search. Usually, and assuming a minimization direction, upper bounds are derived from feasible solutions, computed using various heuristics. Lower bounds are computed by solving a relaxation of the subproblem (unlike upper bounds, lower bounds do not always correspond to a feasible solution). If the lower bound at the current subproblem is larger than the globally valid upper bound, the current subproblem cannot yield a global optimum, so it is *pruned by bound* (i.e., discarded because its lower bound is worse than a global upper bound). If the lower and upper bounds are equal (or sufficiently close), then the current upper bound solution is assumed to be globally optimal for the subproblem — and if it improves the globally valid optimum (called *incumbent*), it is used to update it. Otherwise, a partition of the feasible region of the current subproblem is defined, and the search is *branched*, yielding as many new subproblems as there are sets of the partition. The BB algorithm terminates when there are no more subproblems to process.

Most BB implementations define the search tree implicitly by storing subproblems into a priority queue, with highest priority given to subproblems with lowest lower bound. This is because, intuitively, relaxations are expected to yield lowest lower bounds in part of the feasible region containing global optima. The queue is initialized with the original formulation. In a typical iteration, a subproblem is

extracted from the priority queue, processed as described above, and then discarded.

For MILP, lower bounds are usually computed by solving the continuous relaxations. If the lower bound does not prune the current subproblem by bound, the most common branching strategy in MILP selects an integer variable $x_j \in [x_j^L, x_j^U] \cap \mathbb{Z}$ where the lower bounding solution $\bar{x}$ obtained from the continuous relaxation is such that $\bar{x}_j \notin \mathbb{Z}$. The feasible set is partitioned in two: a part where $x_j \le \lfloor \bar{x}_j \rfloor$, and the other where $x_j \ge \lceil \bar{x}_j \rceil$. This is equivalent to splitting the parent subproblem range $[x_j^L, x_j^U]$ in two ranges $[x_j^L, \lfloor \bar{x}_j \rfloor]$ and $[\lceil \bar{x}_j \rceil, x_j^U]$. If $\bar{x} \in \mathbb{Z}^n$, lower and upper bounds for the current subproblem clearly have the same value, which is used to update the incumbent if needed. Then the problem is discarded.

8.3.1 Example

Initially, we let $x^* = (0,0)$ e $f^* = -\infty$. Let L be the list (priority queue) containing the unsolved subproblems, initialized to the original formulation N_1:

$$\left.\begin{array}{rrcl} \max & 2x_1 + 3x_2 & & \\ & x_1 + 2x_2 & \le & 3 \\ & 6x_1 + 8x_2 & \le & 15 \\ & x_1, x_2 & \in & \mathbb{Z}_+. \end{array}\right\} \tag{8.11}$$

We remark that in this situation we are maximizing rather than minimizing the objective, which implies that the roles of lower and upper bounds are exchanged.

The solution of the continuous relaxation is P (corresponding to the intersection of line (1) $x_1+2x_2 = 3$ with (2) $6x_1 + 8x_2 = 15$), as shown in the Fig. 8.1 We obtain an upper bound $f = \frac{21}{4}$ corresponding to a

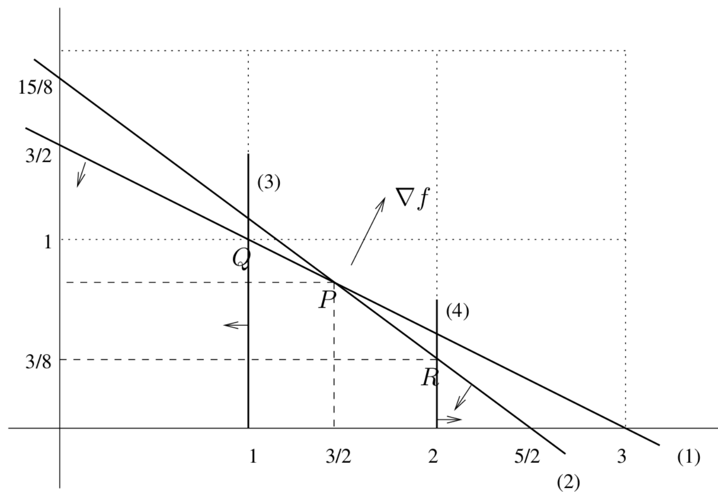


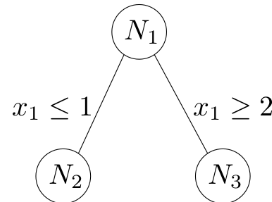
Figure 8.1: Graphical representation of the problem in Eq. (8.11).

fractionary solution $x = P = (\frac{3}{2}, \frac{3}{4})$. We choose the fractionary component x_1 as the branching variable, and form two subproblems N_2, N_3. We adjoin the constraint $x_1 \le 1$ (labelled (3)) to N_2 and $x_1 \ge 2$ (labelled (4)) to N_3. Finally, we insert N_2 and N_3 in L with priority $f = \frac{21}{4}$.

Next, we choose N_2 and remove it from L. The solution of the continuous relaxation of N_2 is at the intersection Q of (1) and (3): we therefore obtain $x = Q = (1,1)$ and $f = 5$. Since the solution is integral, we do not branch. Furthermore, since $f > f^*$ we update $x^* = x$ and $f^* = f$.

Finally, we choose N_3 and remove it from L. The solution of the continuous relaxation of N_3 is at the intersection R of (2) and (4): we obtain $x = R = (2, \frac{3}{8})$ and $f = \frac{41}{8}$. Since the upper bound is 41/8, and $\lfloor \frac{41}{8} \rfloor = 5$, each integral solution found in the feasible region of N_3 will never attain a better objective function value than f^*; hence, again, we do not branch.

Since the L is now empty, the algorithm terminates with solution $x^* = (1, 1)$. The algorithmic process can be summarized by the following tree:



8.3.2 Branch-and-Cut

Branch-and-Cut (B&C) algorithms are a mixture of BB and cutting plane algorithms (Sect. 8.2.3.1). In practice, they follow a BB framework where valid cuts are generated at each subproblem [118].

8.3.3 Branch-and-Price

Branch-and-Price might be described as a mixture of BB and column generation algorithms (Sect. 7.1.8). Extremely large LP formulations are solved using column generation at each BB subproblem [145].

8.4 Lagrangean relaxation

Although the most common way to obtain a lower bound for a MILP is to solve its continuous relaxation, as mentioned in Sect. 8.3, there are other techniques. The technique we sketch in this section leverages duality theory (see Sect. 6.3) in order to exploit the formulation structure, which may be a great help for large-scale instances.

Consider the following MILP formulation:

$$\left.\begin{array}{rrcl} \min_{x,y} & c_1^\top x + c_2^\top y & & \\ & A_1 x & \geq & b_1 \\ & A_2 y & \geq & b_2 \\ & Bx + Dy & \geq & d \\ & x \in \mathbb{Z}_+^{n_1} & , & y \in \mathbb{Z}_+^{n_2} \end{array}\right\} \quad (8.12)$$

where x, y are two sets of integer variables, $c_1^\top, c_2^\top, b_1, b_2, d$ are vectors and A_1, A_2, B, D are matrices of appropriate sizes. Observe that, were it not for the "complicating constraints" $Bx + Dy \geq d$, we would be able to decompose Eq. (8.12) into two smaller independet subproblems, and then solve each separately (usually a much easier task). Such formulations are sometimes referred to as "nearly decomposable".

A tight lower bound for nearly decomposable formulations can be obtained by solving a *Lagrangean relaxation.* The complicating constraints are penalized as part of the objective function, with each

constraint weighted by a Lagrange multiplier:

$$L(\lambda) = \left.\begin{array}{lrcl} \min_{x,y} & c_1^\top x + c_2^\top y & + & \lambda(Bx + Dy - d) \\ & A_1 x & \geq & b_1 \\ & A_2 y & \geq & b_2 \\ & x \in \mathbb{Z}_+^{n_1} & , & y \in \mathbb{Z}_+^{n_2} \end{array}\right\} \quad (8.13)$$

For each vector $\lambda \geq 0$, $L(\lambda)$ is a lower bound to the solution of the original formulation. Since we want to find the tightest possible lower bound, we maximize $L(\lambda)$ w.r.t. λ:

$$\max_{\lambda \geq 0} L(\lambda). \quad (8.14)$$

The lower bound obtained by solving (8.14) is guaranteed to be at least as tight as that obtained by solving the continuous relaxation of the original problem: let us see why. Consider the following formulation:

$$\left.\begin{array}{lrcl} \min_x & c^\top x & & \\ & Ax & \leq & b \\ & x & \in & X, \end{array}\right\} \quad (8.15)$$

where X is a discrete but finite set $X = \{x^1, \ldots, x^\ell\}$, and its Lagrangean relaxation obtained as if each constraint were complicating:

$$\max_{\lambda \geq 0} \min_{x \in X} c^\top x + \lambda(Ax - b). \quad (8.16)$$

Let p^* be the solution of Eq. (8.16). By definition of X, Eq. (8.16) can be written as follows:

$$\left.\begin{array}{lrcll} \max_{\lambda,u} & u & & & \\ & u & \leq & c^\top x^t + \lambda(Ax^t - b) & \forall t \leq \ell \\ & \lambda & \geq & 0. & \end{array}\right\}$$

The above formulation is linear. Hence, its dual:

$$\left.\begin{array}{lrcll} \min_v & \sum_{t=1}^\ell v_t(c^\top x^t) & & & \\ & \sum_{t=1}^\ell v_t(A_i x^t - b_i) & \leq & 0 & \forall i \leq m \\ & \sum_{t=1}^\ell v_t & = & 1 & \\ & v_t & \geq & 0 & \forall t \leq \ell \end{array}\right\}$$

(where A_i is the i-the row of A), has the same optimal objective function value p^*. Notice now that $\sum_{t=1}^\ell v_t x^t$ subject to $\sum_{t=1}^\ell v_t = 1$ and $v_t \geq 0$ for all $t \leq \ell$ is the convex hull of $\{x^t \mid t \leq \ell\}$, and so the above dual formulation can be written as follows:

$$\left.\begin{array}{lrcl} \min_x & c^\top x & & \\ & Ax & \leq & b \\ & x & \in & \mathsf{conv}(X). \end{array}\right\}$$

Thus, the bound given by the Lagrangean relaxation is at least as strong as that given by the continuous relaxation restricted to the convex hull of the original discrete domain. Specifically, for problems with the integrality property, the Lagrangean relaxation bound is no tighter than the continuous relaxation bound. On the other hand, the above result leaves the possibility open that Lagrangian relaxations may be tighter.

Solving (8.14) is not straightforward, as $L(\lambda)$ is a piecewise linear (but non-differentiable) function. The most popular method for solving such problems is the *subgradient method*. Its description is very simple, although the implementation is not.

1. Start with an initial multiplier vector λ^*.

2. If a pre-set termination condition is verified, exit.
3. Evaluate $L(\lambda^*)$ by solving Eq. (8.13) with fixed λ, yielding a solution x^*, y^*.
4. Choose a vector d in the subgradient of L w.r.t. λ and a step length t, and set $\lambda' = \max\{0, \lambda^* + td\}$.
5. Update $\lambda^* = \lambda'$ and go back to step 2.

What's t ent?

Choosing appropriate subgradient vectors and step lengths at each iteration to accelerate convergence is, unfortunately, a non-trivial task that takes a lot of testing.

Chapter 9

Fundamentals of Nonlinear Programming

This chapter is devoted to NLP. As we have seen in Chapter 6, much of the existing theory in NLP concerns local optimality. We start our treatment by summarizing a well-known local optimization algorithm called *sequential quadratic programming* (SQP), which can be seen as a solution method for cNLP as well as a heuristic algorithm for nonconvex NLP. We then overview the field of GO, focusing on general NLP.

9.1 Sequential quadratic programming

There are many different algorithmic approaches to local optimization of NLPs in the form (6.9), most of which are based on the theoretical results of Section 6.2. The vast majority of local optimization methods will take in input a NLP formulation as well as an "starting point" assumed to be feasible: as an output, it will return a local optimum close to the starting point. The assumption that a feasible starting point is known *a priori* is often false in practice: which implies that some of the theoretical guarantees might not hold. On the other hand, many local NLP algorithms deliver good computational performance and good quality solutions even from infeasible starting points.

One of the best known local optimization algorithms for NLP is SQP: it aims at solving the KKT conditions (6.6)-(6.8) iteratively by solving a sequence of quadratic approximations of the objective function subject to linearized constraints.

We start with a given starting point $x \in X$ and generate a sequence $x^{(k)}$ of points using the update relation:

$$x^{(k+1)} = x^{(k)} + \alpha d,$$

where α is the step length and d the search direction vector. In other words, at each iteration we move from $x^{(k)}$ in the direction of d by an amount αd. Both α and d are updated at each iteration. The step length $\alpha \in (0, 1]$ is updated at each iteration using a line search optimization method.

9.1.1 Remark (Line search)
A line search is a lifting of an optimization problem in a single scalar variable into a higher-dimensional space. Given a multivariate function $f(x)$ where $t \in [x^L, x^U] \subseteq \mathbb{R}^n$ is a decision variable vector, it sometimes happens that one would wish to optimize $f(x)$ for x belonging to a line, half-line or segment. Thus, if $x = x^0 + \alpha d$, where $x^0, d \in \mathbb{R}^n$ and $\alpha \in \mathbb{R}_+$, x belongs to a half-line, and $f(x) = f(x^0 + \alpha d) = u_f(\alpha)$ becomes the problem of optimizing the univariate function u_f in the single variable α.

If f is monotonic, line searches can be carried out to a given $\epsilon > 0$ precision using a bisection search (see Sect. 7.3.1.1.5). Otherwise, bisection searches might help finding local optima. If f is a polynomial, global optima can be found by listing all the roots $A = \{\alpha_1, \dots, \alpha_\ell\}$ of the polynomial equation $\frac{df}{d\alpha} = 0$ and choosing the α_i such that $u_f(\alpha_i)$ is minimum in $U = \{u_f(\alpha_j) \mid j \leq \ell\}$.

The search direction vector d is obtained at each step by solving the following QP, where m, p, f, g and h are as in Eq. (6.9):

$$\left.\begin{array}{lrcll} \min\limits_{d} & (\nabla f(x^{(k)}))^\top d + \frac{1}{2} d^\top H(x^{(k)}) d & & & \\ \text{s.t.} & (\nabla g_i(x^{(k)}))^\top d & \leq & 0 & \forall i \leq m \\ & (\nabla h_i(x^{(k)}))^\top d & = & 0 & \forall i \leq p. \end{array}\right\} \tag{9.1}$$

In Eq. (9.1), $H(x^{(k)})$ is a PSD approximation to the Hessian of the objective function evaluated at $x^{(k)}$. As remarked in Sect. 5.4.1, a quadratic function can be shown to be convex by verifying that its Hessian is PSD, so Eq. (9.1) is the best convex quadratic approximation of Eq. (6.9). Thus, a KKT point for (9.1) is a globally optimal solution of (9.1) by Theorem 6.2.9.

The KKT conditions for each subproblem (9.1) are solved directly (e.g. by Newton's method) to obtain the solution of (9.1). If $\|d\|$ is smaller than a pre-defined $\varepsilon > 0$ tolerance, the current point $x^{(k)}$ solves the KKT conditions for (6.9) and the process terminates. Notice that solving the KKT conditions for Eq. (9.1) also provides current solution values for the Lagrange multipliers μ, λ, which upon termination are also valid for the original formulation Eq. (6.9).

9.2 The structure of GO algorithms

Most of the algorithms for globally solving NLPs (and MINLPs) have two phases: a global one and a local one [131]. During the global phase, calls are made to other possibly complex algorithms which belong to the local phase. The function of the global phase is to survey the whole of the search space, while local phase algorithms identify local optima. The global phase is also tasked with selecting the best local optima to return to the user as "global".

9.2.1 Deterministic vs. stochastic

GO algorithms are usually partitioned into two main categories: deterministic and stochastic. While this partition mostly concerns the global phase, it may occasionally also refer to the local phase. An algorithm is stochastic when it involves an element of random choice, whereas a deterministic algorithm does not. We do not enter into philosophical discussions of what exactly is a "random choice": for our purposes, a pseudo-random number generator initialized with the current exact time as a seed is "random enough" to warrant the qualification of "stochastic" to the calling algorithm.

Stochastic algorithms typically offer a theoretical guarantee of global optimality only in infinite time with probability 1 (or none at all). Deterministic algorithm typically offer theoretical guarantees of either local or global optimality in finite time under certain conditions on their input (such as, e.g., Slater's constraint qualification in Sect. 6.3.3). Moreover, "global optimality" for NLP incurs the issue of solution representability (Sect. 4.2). The approach encountered most often in GO is sketched in Sect. 4.2.2, and is "the easiest approach" in the sense that one uses floating point numbers instead of reals, and hopes everything will turn out well in the end. In any case, all general-purpose deterministic GO algorithms require an $\epsilon > 0$ tolerance in input, which is used to approximate with floating point numbers some computational tasks that should in theory be performed with real numbers (such as, e.g., whether two real numbers are equal or not).

9.2.2 Algorithmic reliability

As we shall see below, GO algorithms are usually quite complicated: either because the global phase is complicated (this is the case for BB), or because the local phase is complicated, or both. In practice, complicated algorithms require complicated implementations, and these in turn make it more difficult for programmers to avoid or even remove bugs. Therefore, the overall (practical) reliability of many implementations of GO algorithms might not be perfect.

While this is a point that could be made for any sufficiently complicated algorithm, there is however an inherent unreliability in all local optimization algorithms for NLPs which affects the reliability of the calling algorithm. In other words, GO algorithms are only as reliable as their most unreliable component.

Let us consider the SQP algorithm of Sect. 9.1 as an example. The theory of SQP guarantees convergence subject to conditions: in general, these conditions are that the starting point should be feasible, and that some constraint qualification conditions should hold. In practice, SQP implementations are often called from global phases of GO algorithms with either of these conditions not holding. There are good reasons for this: (a) verifying feasibility in NLP is just as hard, for computational complexity purposes, as verifying optimality (see Sections 4.3.1, 4.3.2, 4.3.2.2, 5.1.2.3); (b) verifying constraint qualification conditions might in general require precise real number computation, which may be impossible. This implies that the local phase might fail: either in a controlled fashion (reporting some proof of failure), or, more spectacularly, by not converging or simply crashing.

The following issues provide the most popular reasons why SQP implementations might fail on even the most innocent-looking NLPs:

- the linearized constraints of (9.1) may be infeasible, even though the original constraints of (6.9) are feasible;
- the Jacobian of the constraints may not have full rank (see Thm. 6.2.1).

Tracing a definite cause for such occurrences is generally very difficult. Subproblems may be defective locally (because the approximation is poor) or because the original formulation is ill-posed. Some of these issues may be overcome by simply changing the starting point.

9.2.3 Stochastic global phase

Stochastic global phases may be based on sampling and/or escaping.

9.2.3.1 Sampling approaches

In sampling approaches, a local phase is deployed from each of many different starting points, sampled according to various rules (Fig. 9.1). Typical examples are provided by *multistart* algorithms, such as Multi-Level Single Linkage (MLSL) [95]. The best local optimum is returned as putative global optimum One of the most common artificial termination conditions is the Bayesian stopping rule, which is based on the expected number of local minima in the sampling set. CPU time limit may also be employed.

Sampling stochastic algorithms (without artificial termination) are guaranteed to converge in infinite time with probability 1, but in practice there is no guarantee that the returned point will actually be the global optimum. These algorithms work reasonably well for small- and medium-sized instances. The chance of finding global optima worsens considerably as the number of dimensions of the search space increases.

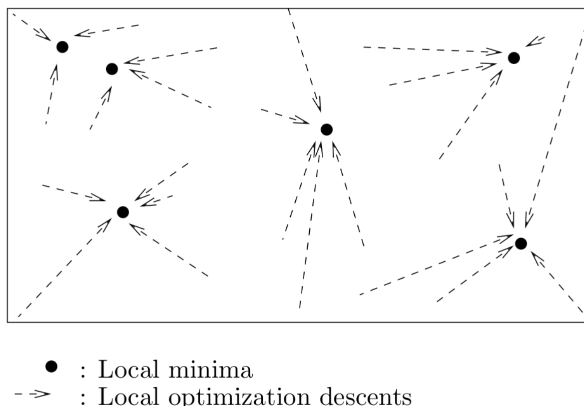


Figure 9.1: Sampling approach of the stochastic global phase. The arrows indicate a local optimization descent path from a starting point to the target local minimum.

9.2.3.2 Escaping approaches

In the escaping approach (see e.g. Tabu Search [80], Simulated Annealing [93] and tunneling methods [98]), various strategies are devised in order to "escape from local optima", so that after the local phase terminates, the global phase is able to reach another feasible point, from which a new local phase can be deployed (Fig. 9.2). Termination conditions for these methods are usually based on the number of calls to the local phase, or on a CPU time limit. As in the sampling approach, there are no definite guarantees on global optimality apart from convergence in infinite time with probability 1.

9.2.1 Remark
In Tabu Search, successive candidate points are located by performing some "moves" in the search space (e.g. $x \leftarrow x + \alpha d$ for some scalar α and vector d). The inverse of the move is then put into a tabu list and forbidden from being applied for as long as it stays in the list. This makes it unlikely to fall back on the same local minimum we are escaping from. In Simulated Annealing, the search procedure is allowed to escape from local optima with a decreasing probability. Tunneling methods are inspired by the quantum-mechanical idea of a particle in a potential well which escapes from the well with a certain probability.

9.2.3.3 Mixing sampling and escaping

There are also some stochastic methods, such as e.g. Variable Neighbourhood Search (VNS), which use both approaches at the same time. VNS is structured in a major and a minor iteration loop. Each major iteration is as follows: from the current local optimum x' loop over increasingly larger neighbourhoods centered at x'; run a multistart in each neighbourhood (minor iteration) until an improved local optimum $\bar{x}$ is found (this concludes a major iteration); if $\bar{x}$ improves the incumbent, update it with $\bar{x}$, then update x' with $\bar{x}$ and repeat. If no improving optimum is found during the minor iterations, terminate.

9.2.3.4 Clustering starting points

In both approaches, a nontrivial issue is that of reducing the number of local phase deployments converging to the same local optimum, which is a waste of computational resources. The idea of *clustering* for the stochastic global phase suggests that the sampling of starting points should be grouped into clusters of nearby points: only one local phase from each cluster should be performed [131]. The MLSL algorithm

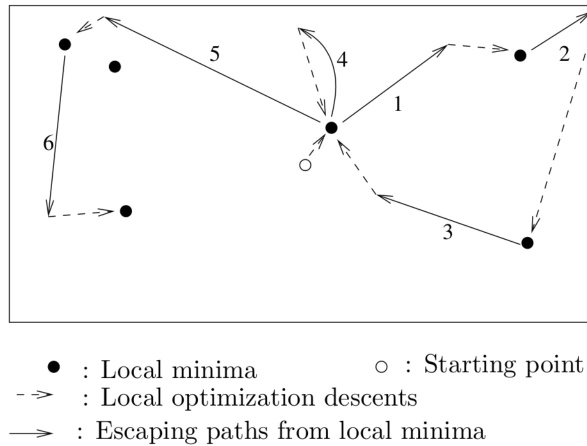


Figure 9.2: Escaping approach of the stochastic global phase. The trail consists of local optimization descents alternating with random escaping paths. Observe that certain escaping paths (e.g. arc 4) might position the new starting point in the same basin of attraction as the previous local optimum.

proposes a clustering based on linkage: a point x is clustered with a point y if x is "not too far" from y and the objective function value at y is better than that at x. The clusters are represented by a directed tree, and the local phase is deployed with the root of this tree (Fig. 9.3).

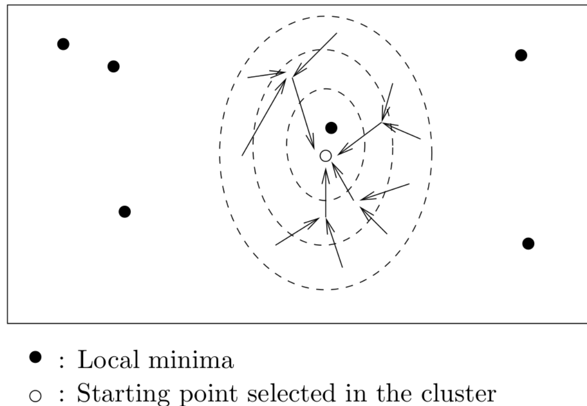


Figure 9.3: Linkage clustering in the stochastic global phase. The points in the cluster are those incident to the arcs; each arc (x, y) expresses the relation "x is clustered to y". The arcs point in the direction of objective function descent. The root of the tree isthe "best starting point" in the cluster.

9.2.4 Deterministic global phase

This section contains a very general treatment (mostly taken from [144, §5.5]) of a class of algorithms, called Branch-and-Select (B&S), which is an abstract model for BB, B&C and sBB algorithms. Although B&S is not the only deterministic global phase approach to GO, it is nonetheless the most widely used.

B&S algorithms can be used to solve Eq. (2.2) in full generality to global optimality. Without any "acceleration devices" (such as e.g. pre-processing) they often show their exponential worst-case complexity even on very small-sized instances, and tend to be very inefficient in practice. Furthermore, their performance may depend strongly on the formulation: a different algebraic form of the same equations

and inequalities might lead to a different algorithmic performance.

Let $\Omega \subseteq \mathbb{R}^n$. A finite family of sets $\mathcal{S}$ is a *net* for Ω if it is pairwise disjoint and it covers Ω, that is, $\forall s, t \in \mathcal{S}$ $(s \cap t = \emptyset)$ and $\Omega \subseteq \bigcup_{s \in \mathcal{S}} s$. A net $\mathcal{S}'$ is a *refinement* of the net $\mathcal{S}$ if $\mathcal{S}'$ has been obtained from $\mathcal{S}$ by finitely partitioning some set s in $\mathcal{S}$ and then replacing s by its partition; that is, given $s \in \mathcal{S}$ with $s = \bigcup_{i \in I} s_i$ where I is an index subset of $\{1, \ldots, |\mathcal{S}'|\}$ and each $s_i \in \mathcal{S}'$, we have

$$\mathcal{S}' = (\mathcal{S} \backslash s) \cup \{s_i \mid i \in I\}.$$

Let $\langle \mathcal{S}_n \rangle$ be an infinite sequence of nets for Ω such that, for all $i \in \mathbb{N}$, $\mathcal{S}_i$ is a refinement of $\mathcal{S}_{i-1}$; let $\langle M_n \rangle$ be an infinite sequence of subsets of Ω such that $M_i \in \mathcal{S}_i$. Then $\langle M_n \rangle$ is a *filter* for $\langle \mathcal{S}_n \rangle$ if $\forall i \in \mathbb{N}$ we have $(M_i \subseteq M_{i-1})$. We call $M_\infty = \bigcap_{i \in \mathbb{N}} M_i$ the *limit* of the filter.

We will now present a general algorithmic framework (Fig. 9.4) to solve the generic problem $\min\{f(x) \mid x \in \Omega\}$.

Given any net $\mathcal{S}$ for Ω and any objective function value $\gamma \in \mathbb{R}$, we consider a selection rule which determines:

(a) a distinguished point x^*_M for every $M \in \mathcal{S}$;

(b) a subfamily of qualified sets $\mathcal{R} \subset \mathcal{S}$ such that, for all $x \in \bigcup_{s \in \mathcal{S} \backslash \mathcal{R}} s$, we have $f(x) \geq \gamma$;

(c) a distinguished set $B_\mathcal{R}$ of $\mathcal{R}$.

For each set of $\mathcal{R}$, B&S iteratively calculates a distinguished point (for example, by deploying a local phase within the specified region); $B_\mathcal{R}$ is then picked for further net refinement.

<u>Branch-and-Select</u>:

1. (Initialization) Start with a net $\mathcal{S}_1$ for Ω, set $x_0 = \emptyset$ and let γ_0 be any strict upper bound for $f(\Omega)$. Set $\mathcal{P}_1 = \mathcal{S}_1$, $k = 1$, $\sigma_0 = \emptyset$.
2. (Evaluation) Let $\sigma_k = \{x^*_M \mid M \in \mathcal{P}_k\}$ be the set of all distinguished points.
3. (Incumbent) Let x_k be the point in $\{x_{k-1}\} \cup \sigma_k$ such that $\gamma_k = f(x_k)$ is lowest; set $x^* = x_k$.
4. (Screening) Determine the family $\mathcal{R}_k$ of qualified sets of $\mathcal{S}_k$ (in other words, from now on ignore those sets that can be shown not to contain a solution with objective value lower than γ_k).
5. (Termination) If $\mathcal{R}_k = \emptyset$, terminate. The problem is infeasible if $\gamma_k \geq \gamma_0$; otherwise x^* is the global optimum.
6. (Selection) Select the distinguished set $M_k = B_{\mathcal{R}_k} \in \mathcal{R}_k$ and partition it according to a pre-specified branching rule. Let $\mathcal{P}_{k+1}$ be a partition of $B_{\mathcal{R}_k}$. In $\mathcal{R}_k$, replace M_k by $\mathcal{P}_{k+1}$, thus obtaining a new refinement net $\mathcal{S}_{k+1}$. Set $k \leftarrow k + 1$ and go back to Step 2.

Figure 9.4: The B&S algorithm.

A B&S algorithm is *convergent* if γ^*, defined as $\lim_{k \to \infty} \gamma_k$, is such that $\gamma^* = \inf f(\Omega)$. A selection rule is *exact* if:

(i) $\inf(\Omega \cap M) \geq \gamma^*$ for all M such that $M \in \mathcal{R}_k$ for all k (i.e. each region that remains qualified forever in the solution process is such that $\inf(\Omega \cap M) \geq \gamma^*$);

(ii) the limit M_∞ of any filter $\langle M_k \rangle$ is such that $\inf f(\Omega \cap M_\infty) \geq \gamma^*$.

9.2.2 Theorem
A B&S algorithm using an exact selection rule converges.

Proof. Suppose, to get a contradiction, that there is $x \in \Omega$ with $f(x) < \gamma^*$. Let $x \in M$ with $M \in \mathcal{R}_n$ for some $n \in \mathbb{N}$. Because of condition (i) above, M cannot remain qualified forever; furthermore, unqualified regions may not, by hypothesis, include points with better objective function values than the current incumbent γ_k. Hence M must necessarily be split at some iteration $n' > n$. So x belongs to every M_n in some filter $\{M_n\}$, thus $x \in \Omega \cap M_\infty$. By condition (2) above, $f(x) \geq \inf f(\Omega \cap M_\infty) \geq \gamma^*$. The result follows. □

We remark that this algorithmic framework does not provide a guarantee of convergence in a finite number of steps. Consequently, most B&S implementations make use of the concept of ε-optimality, (Sect. 4.2.2). By employing this notion and finding lower and upper bound sequences converging to the incumbent at each step of the algorithm, finite termination can be ensured. For finite termination with $\varepsilon = 0$, some additional regularity assumptions are needed (see e.g. [135, 7]). While ε-optimality (with $\varepsilon > 0$) is sufficient for most practical purposes, it is worth pointing out that a ε-optimum x' is such that $f(x')$ is at most ε away from the true globally optimal objective function value f^*: this says nothing at all about the distance between x' and a true global optimum x^*; in fact, $\|x' - x^*\|_2$ might be arbitrarily large.

9.2.4.1 Fathoming

Let $\mathcal{S}_k$ be the net at iteration k. For each region $M \in \mathcal{S}_k$, find a lower bounding solution x^*_M for $f(x)$ defined on $\Omega \cap M$ and the corresponding lower bounding objective function value $\ell(M)$. A set $M \in \mathcal{S}_k$ is qualified if $\ell(M) \leq \gamma_k$. The distinguished region is usually selected as the one with the lowest $\ell(M)$.

The algorithm is accelerated if one also computes an upper bound $u(M)$ for $\inf f(x)$ on $\Omega \cap M$ and uses it to bound the problem from above by rejecting any M for which $\ell(M)$ exceeds the best upper bound $u(M)$ encountered so far. In this case, we say that the rejected regions have been *fathomed* (Fig. 9.5). This acceleration device has become part of all BB implementations. Usually, the upper bound $u(M)$ is computed by solving the problem to local optimality in the current region: this also represents a practical alternative to the implementation of the evaluation step (Step (2) of the B&S algorithm), since we can take the distinguished points $\omega(M)$ to be the local solutions $u(M)$ of the problem in the current regions. With a numerically precise local phase, the accuracy of ε-global optima is likely to be better than if we simply use $\ell(M)$ to define the distinguished points.

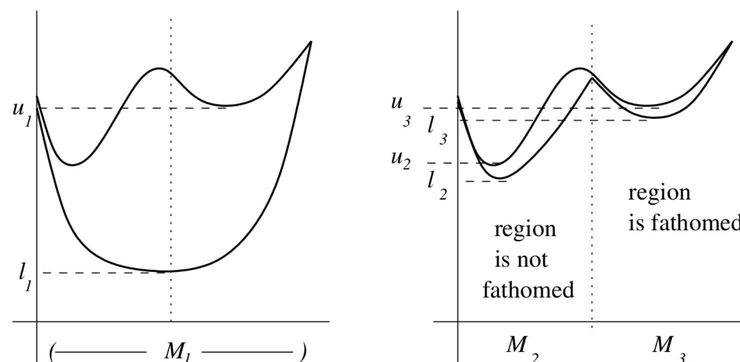


Figure 9.5: Fathoming via upper bound computation.

The convergence of B&S with fathoming is ensured if every filter $\{M_k | k \in K\}$ contains an infinite

nested sequence $\{M_k | k \in K_1 \subseteq K\}$ such that:

$$\lim_{\substack{k\to\infty \\ k\in K_1}} \ell(M_k) = \gamma^*. \quad (9.2)$$

To establish this, we will show that under such conditions the selection procedure is exact, and then invoke Thm. 9.2.2. Let $\{M_k | k \in K\}$ be any filter and M_∞ its limit. Because of equation (9.2), $\inf f(\Omega \cap M_k) \geq \ell(M_k) \to \gamma^*$, hence $\inf f(\Omega \cap M_\infty) \geq \gamma^*$. Furthermore, if $M \in \mathcal{R}_k$ for all k then $\inf f(\Omega \cap M) \geq \ell(M) \geq \ell(M_k) \to \gamma^*$ as $k \to \infty$, i.e. $\inf f(\Omega \cap M) \geq \gamma^*$. Thus the selection procedure is exact and, by theorem 9.2.2, the B&S algorithm with fathoming converges.

9.2.5 Example of solution by B&S

The formulation

$$\min\{f(x) = \frac{1}{4}x + \sin(x) \mid x \geq -3, x \leq 6\}$$

describes a simple NLP with two minima, only one of which is global (Fig. 9.6). We solve it (graphically) with a sBB approach: at each iteration we find lower and upper bounds to the optimum within a subregion of the search space; if these bounds are not sufficiently close, say to within a $\varepsilon > 0$ tolerance, we split the subregion in two, repeating the process on each subregion until all the regions have been examined). In this example we set ε to 0.15, but note that this is not realistic: in practice ε is set to values between 1×10^{-6} and 1×10^{-3}. At the first iteration we consider the region consisting of the whole x variable

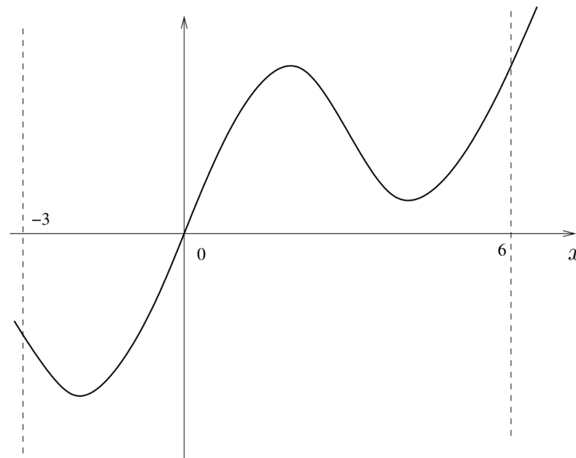


Figure 9.6: The problem $\min\{\frac{1}{4}x + \sin(x) \mid x \geq -3, x \leq 6\}$.

range $-3 \leq x \leq 6$. We calculate a lower bound by underestimating the objective function with a convex function: since for all x we have $-1 \leq \sin(x) \leq 1$, the function $\frac{1}{4}x - 1$ is a convex underestimator of the objective function. Limited to this example only, We can draw the tangents to $f(x)$ at the range endpoints $x = -3$ and $x = 6$ to make the underestimator tighter, as in Fig. 9.7. The whole underestimator is the pointwise maximum of the three linear functions emphasized in Fig. 9.7. The tangent to the objective function in the point $x = -3$ is the line $y = -0.74x - 3.11$, whereas in the point $x = 6$ it is $y = 1.21x - 6.04$. Thus the convex underestimator is $\bar{f}(x) = \max\{-0.74x - 3.11, \frac{1}{4}x - 1, 1.21x - 6.04\}$. Finding the minimum of $\bar{f}(x)$ in the region $-3 \leq x \leq 6$ yields a solution $\bar{x} = -2.13$ with objective function value $l = -1.53$ which is a valid lower bound for the original problem (indeed, the value of the original objective function at $\bar{x}$ is -1.42). Now we find an upper bound to the original objective function by locally solving the original problem. Suppose we pick the range endpoint $x = 6$ as a starting point and we employ Newton's method in one dimension: we find a solution $\tilde{x} = 4.46$ with objective function value $u = 0.147$. Since

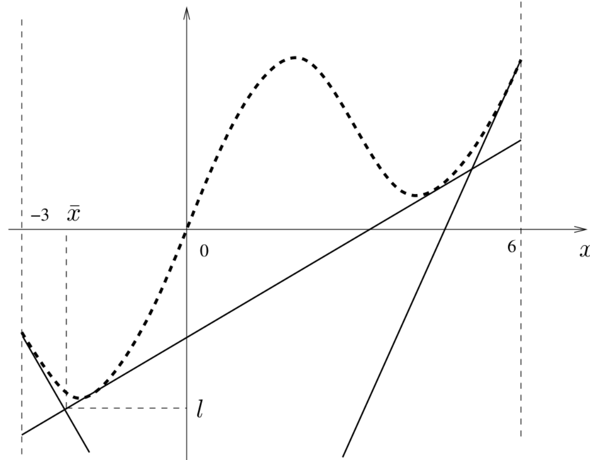


Figure 9.7: Convex underestimation of the objective function in Sect. 9.2.5 and optimal solution of the convex underestimating problem.

$|u - l| = |0.147 - (-1.53)| = 1.67 > \varepsilon$ shows that u and l are not sufficiently close to be reasonably sure that $\tilde{x}$ is the global optimum of the region under examination, we split this region in two. We choose the current $\tilde{x} = 4.46$ as the branching point, we add two regions $-3 \leq x \leq 4.46$, $4.46 \leq x \leq 6$ to a list of "unexamined regions" and we discard the original region $-3 \leq x \leq 6$. At the second iteration we pick the region $-3 \leq x \leq 4.46$ for examination and compute lower and upper bounds as in Fig. 9.8. We find

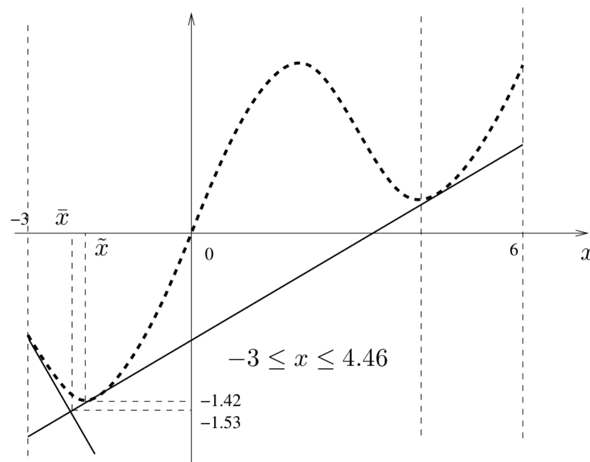


Figure 9.8: Second iteration of the sBB algorithm.

the same underestimating solution $\bar{x}$ as before (with $l = -1.53$) and by deploying Newton's method from the endpoint $x = -3$ we locate the local optimum $\tilde{x} = -1.823$ with $u = -1.42$. Since $|u - l| = 0.11 < \varepsilon$, we accept $\tilde{x}$ as the global optimum for the region under examination, and we update the "best solution found" $x^* = -1.823$ with associated function value $U = -1.42$. Since we have located the global optimum for this region, no branching occurs. This leaves us with just one region to examine, namely $4.46 \leq x \leq 6$. In the third iteration, we select this region and we compute lower and upper bounds (Fig. 9.9) to find $\bar{x} = \tilde{x} = 4.46$ with $l = 1.11$ and $u = 1.147$. Since $|u - l| = 0.04 < \varepsilon$, we have located the global optimum for this region, so there is no need for branching. Since $U = -1.42 < 1.147 = u$, we do not update the "best solution found", so on discarding this region from the list, the list is empty. The algorithm

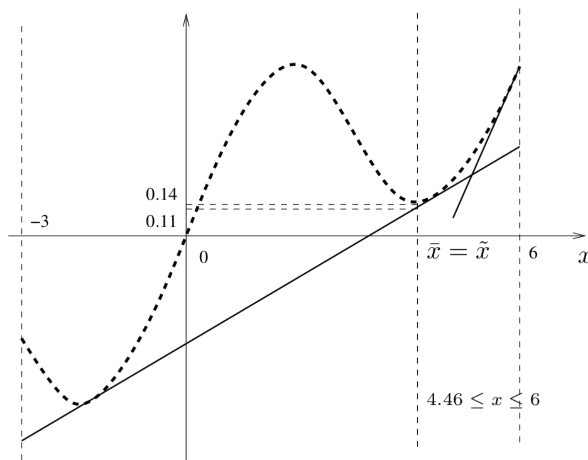


Figure 9.9: Third iteration of the sBB algorithm.

terminates with global optimum $x^* = -1.823$.

This example shows most of the important features of a typical sBB algorithm run, save three:

(a) the convex underestimation can (and usually is) modified in each region, so that it is tighter;

(b) in formulations with many variables, the choice of the branching variable is a crucial task. This will be discussed in detail in Sect. 9.4;

(c) in practice, pruning of region occurs when the lower bound in a region is higher than the current best solution.

In this example there was no pruning, as the region $4.46 \leq x \leq 6$ did not need to be branched upon. Had there been need for branching in that region, at the subsequent iterations two new regions would have been created with an associated lower bound $l = 1.11$. Since the current best solution has an objective function value of -1.42, which is strictly smaller than 1.11, both regions would have been pruned before being processed.

9.3 Variable Neighbourhood Search

The VNS approach was briefly sketched in Sect. 9.2.3.3. Here we describe a version of VNS which addresses nonconvex NLP formulations. An extension to MINLP was proposed in [89].

As mentioned in Sect. 9.2.3.3, VNS rests on sampling starting points, a local phase, and a neighbourhood structure designed both to delimit sampling, and to make it easier to escape from current local minima towards improved ones. The pseudocode for the VNS algorithm is given in Alg. 1

We adapt Alg. 1 to Eq. (6.9) in the following fashion.

- We employ a local NLP solver, such as SQP (Sect. 9.1), as the local phase delivering the current local minma x^*, x'.
- We consider a neighbourhood structure formed by a set of embedded hyper-rectangles, each side of which has length proportional to the corresponding variable range length and scaled by $r_k = \frac{k}{k_{\max}}$ all "centered" at the incumbent x^*.

Algorithm 1 The VNS algorithm.

0: *Input:* maximum number of neighbourhoods $k_{\max}$, number of local searches in each neighbourhood L
0: *Output:* a putative global optimum x^*.

loop
  Set $k \leftarrow 1$, pick a random point $\tilde{x}$, perform a local search to find a local minimum x^*.
  while $k \le k_{\max}$ **do**
    Consider a neighbourhood $N_k(x^*)$ of x^* s.t. $\forall\, k > 1$ $(N_k(x^*) \supset N_{k-1}(x^*))$.
    for $i = 1$ to L **do**
      Sample a random point $\tilde{x}$ from $N_k(x^*)$.
      Perform a local search from $\tilde{x}$ to find a local minimum x'.
      If x' is better than x^*, set $x^* \leftarrow x'$, $k \leftarrow 0$ and exit the FOR loop.
    end for
    Set $k \leftarrow k + 1$.
    Verify termination condition; if true, exit.
  end while
end loop

- Termination conditions based on maximum allowable CPU time.

More formally, let $H_k(x^*)$ be the hyper-rectangle $y^L \le x \le y^U$ where, for all $i \le n$,

$$\begin{aligned} y_i^L &= x_i^* - \frac{k}{k_{\max}}(x_i^* - x_i^L) \\ y_i^U &= x_i^* + \frac{k}{k_{\max}}(x_i^U - x_i^*). \end{aligned}$$

This construction forms a set of hyper-rectangles "centered" at x^* and proportional to $x^L \le x \le x^U$. Two strategies are possible to define each neighbourhood $N_k(x^*)$:

- $N_k(x^*) = H_k(x^*)$;
- $N_k(x^*) = H_k(x^*) \smallsetminus H_{k-1}(x^*)$,

for all $k \le k_{\max}$.

This extremely simple algorithm has a very small number of configurable parameters: the maximum neighbourhood size $k_{\max}$, the number of sampling points and local searches started in each neighbourhood (L in Alg. 1), a ε tolerance to allow accepting a new optimum, and the maximum CPU time allowed for the search. Notwithstanding its simplicity, this was found to be a very successful algorithm for nonconvex NLP [86].

9.4 Spatial Branch-and-Bound

In this section we shall give a detailed description of the sBB algorithm, which belongs to the B&S class (Sect. 9.2.4). This provides an example of a deterministic global phase. Although it is designed to address nonconvex NLP as in Eq. (6.9), an extension to address Eq. (2.2) in full generality can be provided quite simply by adding the possibility of branching on integer variables, as is done by the BB algorithm of Sect. 8.3. The convergence proof theorem 9.2.2 also covers the sBB algorithm described in this section.

The history of sBB algorithms for nonconvex NLP starts in the 1990s [128, 8, 3, 4, 2, 51, 78]. Here, we follow a particular type of sBB algorithm called *spatial Branch-and-Bound with symbolic reformulation* [138, 139, 83].

sBB algorithms all rely on the concept of a *convex relaxation* of the original nonconvex NLP. This is a convex NLP formulation, the solution of which provides a guaranteed lower bound to the optimal objective function value of the original NLP. At each iteration, the sBB algorithm solves restrictions to particular subregions of space of the original formulation and of its convex relaxation, in order to obtain upper and lower bounds to the optimal value of the objective function value in the subregion. If the bounds are very close, a global optimum relative to the subregion has been identified. The selection rule choosing next subregions makes it possible to exhaustively explore the search space. When subregions are defined by hyper-rectangles (i.e. simple variable ranges), starting with the smallest possible ranges speeds up the sBB considerably. This issue is addressed in Sect. 9.4.1.

Most sBB algorithms have the following form:

1. (*Initialization*) Initialize a list of regions to a single region comprising the entire set of variable ranges. Set the convergence tolerance $\varepsilon > 0$; set the best objective function value found up so far $U := \infty$ and the corresponding solution $x^* := (\infty, \ldots, \infty)$. Optionally, perform *Optimization-Based Bounds Tigthening* (OBBT), see 9.4.1.1.
2. (*Choice of Region*) If the region list is empty, terminate the algorithm with solution x^* and objective function value U. Otherwise, choose a region R (the "current region") from the list (see Sect. 9.4.2). Remove R from the list. Optionally, perform *Feasibility-Based Bounds Tightening* on R (see Sect. 9.4.1.2).
3. (*Lower Bound*) Generate a convex relaxation from the original formulation in the selected region R (see Sect. 9.4.3), and solve it to obtain an underestimation ℓ of the objective function, with corresponding solution $\bar{x}$. If $\ell > U$ or the relaxation is infeasible, go back to Step 2.
4. (*Upper Bound*) Attempt to solve the original formulation restricted to the selected region to obtain a (locally optimal) solution $\tilde{x}$ with objective function value u (see Sect. 9.4.4). If this fails, set $u := +\infty$ and $\tilde{x} = (\infty, \ldots, \infty)$.
5. (*Pruning*) If $U > u$, set $x^* = \tilde{x}$ and $U := u$. Remove all regions from the list having lower bounds greater than U, since they cannot possibly contain the global minimum.
6. (*Check Region*) If $u - \ell \leq \varepsilon$, accept u as the global minimum for this region and return to Step 2. Otherwise, we may not have located the global minimum for the current region yet, so we proceed to the next step.
7. (*Branching*) Apply a branching rule to the current region, in order to split it into subregions (see Sect. 9.4.5). Append these to the list of regions, assigning to them ℓ as an (initial) lower bound. Go back to Step 2.

The convex relaxation is generated automatically by means of a symbolic analysis of the mathematical expressions occurring in the original formulation. Below, we consider some of the key steps of the algorithm in more detail.

9.4.1 Bounds tightening

Bounds tightening procedures appear in steps 1 and 2. They are optional in the sense that the algorithm will converge even without them. In practice, however, bounds tightening is essential. Two major bounds tightening schemes have been proposed in the literature: OBBT and FBBT.

9.4.1.1 Optimization-based bounds tightening

OBBT identifies the smallest range of each variable, subject to feasibility of the convex relaxation. This prevents the sBB algorithm from exploring subregions that can be proved infeasible *a priori*.

OBBT requires the solution of at least $2n$ convex relaxations, where n is the number of variables. Let $\alpha \le \bar{g}(x) \le \beta$ be the set of constraints in the convex relaxation: the OBBT procedure, given below, constructs sequences $x^{L,k}, x^{U,k}$ of possibly tighter lower and upper variable bounds.

1. Set $x^{L,0} \leftarrow x^L$, $x^{U,0} \leftarrow x^U$, $k \leftarrow 0$.
2. Repeat

$$\begin{aligned} x_i^{L,k} &\leftarrow \min\{x_i \mid \alpha \le \bar{g}(x) \le \beta \wedge x^{L,k-1} \le x \le x^{U,k-1}\}, \quad \forall i \le n; \\ x_i^{U,k} &\leftarrow \max\{x_i \mid \alpha \le \bar{g}(x) \le \beta \wedge x^{L,k-1} \le x \le x^{U,k-1}\}, \quad \forall i \le n; \\ k &\leftarrow k+1. \end{aligned}$$

until $x^{L,k} = x^{L,k-1}$ and $x^{U,k} = x^{U,k-1}$.

Because of its computational cost, OBBT is usually only performed at the root node of the sBB.

9.4.1.2 Feasibility-based bounds tightening

FBBT is computationally cheaper than OBBT, and as such it can be applied at each region. Variable ranges are tightened using the constraints, which are exploited in order to calculate extremal values attainable by the variables. This is done by isolating a variable on the LHS of a constraint and evaluating the extremal values of the RHS by means of interval arithmetic.

FBBT is easiest for the case of linear constraints. Given constraints $l \le Ax \le u$ where A is an $m \times n$ matrix, interval analysis immediately yields:

$$\begin{aligned} x_j \in &\left[\max\left(x_j^L, \min_i\left(\frac{1}{a_{ij}}\left(l_i - \sum_{k\neq j}\max(a_{ik}x_k^L, a_{ik}x_k^U)\right)\right)\right),\right. \\ &\left.\min\left(x_j^U, \max_i\left(\frac{1}{a_{ij}}\left(u_i - \sum_{k\neq j}\min(a_{ik}x_k^L, a_{ik}x_k^U)\right)\right)\right)\right] \quad \text{if } a_{ij} > 0 \\ x_j \in &\left[\max\left(x_j^L, \min_i\left(\frac{1}{a_{ij}}\left(l_i - \sum_{k\neq j}\min(a_{ik}x_k^L, a_{ik}x_k^U)\right)\right)\right),\right. \\ &\left.\min\left(x_j^U, \max_i\left(\frac{1}{a_{ij}}\left(u_i - \sum_{k\neq j}\max(a_{ik}x_k^L, a_{ik}x_k^U)\right)\right)\right)\right] \quad \text{if } a_{ij} < 0 \end{aligned}$$

for all $1 \le j \le n$. As pointed out in [138, p. 202], FBBT can also be carried out for *factorable* nonlinear constraints.

9.4.1 Remark (Factorable expressions)
A constraint is factorable if it involves factorable expressions. Although a precise definition of factorability is provided in [106], a more useful characterization is "an expression which can be parsed using an arithmetic expression language" (see Sect. 2.1.1). In this sense, all expressions occurring in this book are factorable.

9.4.2 Choice of region

The region selection at Step 2 follows the simple policy of choosing the region in the list with the smallest lower objective function bound ℓ. Intuitively, this is the most promising region for further analysis.

9.4.3 Convex relaxation

The convex relaxation solved at Step 3 of the sBB algorithm aims at finding a guaranteed lower bound to the objective function value in the current region. It is generated automatically for Eq. (2.2) in two stages.

The formulation is first reduced to a standard form where each nonlinear term is linearized, i.e. replaced by an additional variable. Each linearization is then encoded in a new constraint of the form:

$$\text{additional variable} = \text{linearized nonlinear term}.$$

These constraints, called *defining constraints*, are all adjoined to the formulation: this yields a formulation where nonlinear terms only occur in defining constraints.

In the second stage, each defining constraint is replaced by pair of constraints, each defining a convex portion of space. One provides a convex underestimator, and the other a concave overestimator. This pair of convex estimating constraints is known as *convexification* (the union of all such pairs is also known as "convexification").

9.4.3.1 Reformulation to standard form

The symbolic reformulation algorithm scans the expression trees (see Sect. 2.1.1 recursively from the leaves. If the current node is a nonlinear operator $\otimes$ with arity k, it will have k subnodes $s_1^{\otimes}, \ldots, s_k^{\otimes}$, each of which is either a variable x_j in the original formulation or an additional variable w_h (by recursion) for some index h. We then create a new additional variable w_p, where p is the next available unused additional variable index, and adjoin the defining constraint

$$w_p = \otimes(x, w)$$

to the standard form reformulation, where (x, w) is an appropriate sequence of k variables (some of which may be original and some additional). The new additional variable w_p replaces the subexpression represented by the subtree rooted at the current node $\otimes$. See [138, 139] for more details.

9.4.2 Remark
Note that the linearization process is not well-defined, as there may be different linearizations corresponding to a single mathematical expression, depending on associativity. For example, the expression $x_1x_2x_3$ *might be linearized as* $w_1 = x_1x_2 \wedge w_2 = w_1x_3$, $w_1 = x_1x_3 \wedge w_2 = w_1x_2$ *or as* $w_1 = x_2x_3 \wedge w_2 = w_2x_3$, *but also simply as* $w_1 = x_1x_2x_3$, *as long as the symbolic algorithm is able to recognize the product operator as an arbitrary* k*-ary operator (rather than just binary).*

In general, if a tight convexification is available for a complicated subexpression, it is advisable to generate a single additional variable linearizing the whole subexpression [15, 31].

A standard form reformulation based on a symbolic parser which recognizes nonlinear operators of

arity $k \in \{1, 2\}$ is as follows:

$$\begin{aligned}
&\min v_\omega && (9.3)\\
a \leq\ & Av \leq b && (9.4)\\
v_k &= v_i v_j \quad \forall (i,j,k) \in \mathcal{M} && (9.5)\\
v_k &= \frac{v_i}{v_j} \quad \forall (i,j,k) \in \mathcal{D} && (9.6)\\
v_k &= v_i^\nu \quad \forall (i,k,\nu) \in \mathcal{P} && (9.7)\\
v_k &= \phi_\mu(v_i) \quad \forall (i,k,\mu) \in \mathcal{U} && (9.8)\\
v^L \leq\ & v \leq v^U && (9.9)
\end{aligned}$$

where $v = (v_1, \ldots, v_q)$ are the decision variables (including both original and additional variables), $\omega \leq q$, A is the constraint matrix, a, b are the linear constraint bound vectors, v^L, v^U are the variable bounds vectors, and ϕ_μ is a given sequence of labels denoting unary functions such as log, exp, sin, cos, which the parser is aware of.

The defining constraints (9.5)-(9.8) encode all of the nonlinearities occurring in the original formulation: $\mathcal{M}, \mathcal{D}$ are sets of variable index triplets defining bilinear and linear fractional terms respectively. $\mathcal{P}$ is a set of variable index triplets defining power terms (each triplet consists of two variable indices i, k and the corresponding power exponent $\nu \in \mathbb{R}$). $\mathcal{U}$ is a set of triplets which define terms involving the univariate function labels ϕ_μ (each triplet consists of two variable indices i, k and a label index μ).

Note that we also replace the objective function with the additional variable x_ω, corresponding to a defining constraint of the form $x_\omega =$ objective function.

9.4.3 Example

In this example we show the reformulation obtained for Sect. 9.2.5, together with its graphical representation. Since there is only one nonconvex term in the problem (namely, $\sin(x)$*), the reformulation is immediate:*

$$\left.\begin{array}{rl}
\min\limits_{x,y} & \frac{1}{4}x + y \\
s.t. & y = \sin(x) \\
 & -3 \leq x \leq 6 \\
 & -1 \leq y \leq 1.
\end{array}\right\}$$

The standard form reformulation is a lifting, since introducing new variables lifts the formulation into a higher-dimensional space. This is immediately apparent in this simple example. Compare Fig. 9.6 (the original formulation) and its reformulation shown in Fig. 9.10.

9.4.4 Example (Reformulation of the HPP)

The reformulation obtained for the HPP (see Sect. 2.2.7.7) is as follows:

$$\left.\begin{array}{rll}
\min\limits_{x,y,p,w} & 6x_{11} + 16x_{21} + 10x_{12} - 9(y_{11} + y_{21}) - 15(y_{12} + y_{22}) & \textit{cost} \\
s.t. & x_{11} + x_{21} - y_{11} - y_{12} = 0 & \textit{mass balance} \\
 & x_{12} - y_{21} - y_{22} = 0 & \textit{mass balance} \\
 & y_{11} + y_{21} \leq 100 & \textit{demands} \\
 & y_{12} + y_{22} \leq 200 & \textit{demands} \\
 & 3x_{11} + x_{21} - w_1 = 0 & \textit{sulphur balance} \\
 & w_1 = pw_2 & \textit{defining constraint} \\
 & w_2 = y_{11} + y_{12} & \textit{(linear) defining constraint} \\
 & w_3 + 2y_{21} \leq 2.5(y_{11} + y_{21}) & \textit{quality requirement} \\
 & w_3 = py_{11} & \textit{defining constraint} \\
 & w_4 + 2y_{22} \leq 1.5(y_{12} + y_{22}) & \textit{quality requirement} \\
 & w_4 = py_{12}. & \textit{defining constraint}
\end{array}\right\}$$

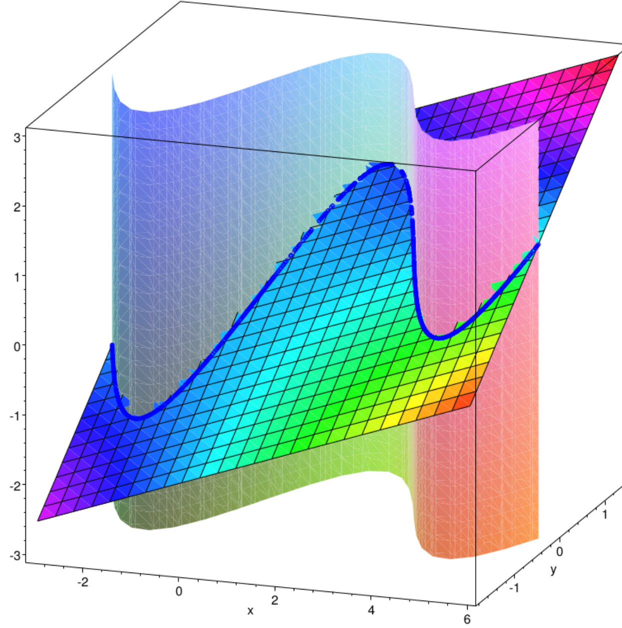


Figure 9.10: The problem $\min\{\frac{1}{4}x+\sin(x) \mid x \geq -3, x \leq 6\}$ reformulated to standard form.

Note that linear terms do not undergo any linearization. Among the defining constraints, some are nonlinear (hence nonconvex, since they are equality constraints) and some are linear. This conveniently splits the problem into a linear and a nonlinear part.

9.4.3.2 Convexification

The convex relaxation of the original formulation consists of the convexification of the defining constraints in the standard form. The convexification depends on the current region $[v^L, v^U]$, and is generated as follows:

1. The defining constraint $v_i = v_j v_k$ is replaced by four linear inequalities:

$$
\begin{aligned}
v_i &\geq v_j^L v_k + v_k^L v_j - v_j^L v_k^L & (9.10)\\
v_i &\geq v_j^U v_k + v_k^U v_j - v_j^U v_k^U & (9.11)\\
v_i &\leq v_j^L v_k + v_k^U v_j - v_j^L v_k^U & (9.12)\\
v_i &\leq v_j^U v_k + v_k^L v_j - v_j^U v_k^L. & (9.13)
\end{aligned}
$$

   Note that Eq. (9.10)-(9.13) provide the *convex envelope* of the set $B(i,j,k) = \{(v_i, v_j, v_k) \mid v_i = v_j v_k \wedge v \in [v^L, v^U]\}$ (i.e. the smallest convex set containing $B(i,j,k)$).

2. The defining constraint $v_i = v_j / v_k$ is reformulated to $v_i v_k = v_j$, and the convexification rules for bilinear terms (9.10)-(9.13) are applied. Note that this introduces the possibility that $v_k = 0$ is feasible in the convex relaxation, whereas the original constraint where v_k appears in the denominator forbids it.

3. The defining constraints $v_i = \phi_\mu(v_j)$ where ϕ_μ is concave univariate is replaced by two inequalities:

the function itself and the secant:

$$v_i \leq f_\mu(v_j) \quad (9.14)$$

$$v_i \geq f_\mu(v_j^L) + \frac{f_\mu(v_j^U) - f_\mu(v_j^L)}{v_j^U - v_j^L}(v_j - v_j^L). \quad (9.15)$$

4. The defining constraint $v_i = \phi_\mu(v_j)$ where ϕ_μ is convex univariate is replaced by:

$$v_i \leq f_\mu(v_j^L) + \frac{f_\mu(v_j^U) - f_\mu(v_j^L)}{v_j^U - v_j^L}(v_j - v_j^L) \quad (9.16)$$

$$v_i \geq f_\mu(v_j). \quad (9.17)$$

5. The defining constraint $v_i = v_j^\nu$, where $0 < \nu < 1$, is treated as a concave univariate function in the manner described in Step 3 above.

6. The defining constraint $v_i = v_j^{2m}$ for any $m \in \mathbb{N}$ is treated as a convex univariate function in the manner described in Step 4 above.

7. The defining constraint $v_i = v_j^{2m+1}$ for any $m \in \mathbb{N}$ may be convex, concave, or piecewise convex and concave with a turning point at 0. If the range of v_j does not include 0, the function is convex or concave and falls into a category described above. A complete discussion of convex underestimators and concave overestimators for this term when the range includes 0 can be found in [90].

8. Other defining constraints involving trigonometric functions need to be analysed on a case-by-case basis, similarly to Step 7.

9.4.4 Local solution of the original problem

This is usually obtained by deploying a local phase on the original formulation restricted to the current region (see Sect. 9.1). This is also typically the most computationally expensive step in each iteration of the sBB algorithm.

9.4.4.1 Branching on additional variables

An issue arises when branching on additional variables (say w_h): when this happens, the current region is partitioned into two subregions along the w_h axis, the convex relaxation is modified to take the new variable ranges into account, and lower bounds are found in each subregion.

The upper bounds, however, are found by solving the original formulation, which is not dependent on the additional variables. Thus the same original formulation is solved at least three times in the course of the algorithm (i.e. once for the original region and once for each of its two sub-regions).

We address this issue by storing the upper bounds to each region. Whenever the branching variable is an additional variable, we use the stored bounds rather than deploying the local phase.

9.4.4.2 Branching on original variables

Even when branching occurs on an original variable, there are some considerations that help avoid solving local optimization problems unnecessarily. Suppose that the original variable x is selected for branching in a certain region. Then its range $[x^L, x^U]$ is partitioned into $[x^L, x']$ and $[x', x^U]$. If the solution of the original formulation restricted to $[x^L, x^U]$ is x^*, and $x^* \in [x^L, x']$, then deploying the local phase in

the subregion $[x^L, x']$ is unnecessary. Of course, the lolca phase still needs to be deployed on the other subregion $[x', x^U]$ (see Fig. 9.11).

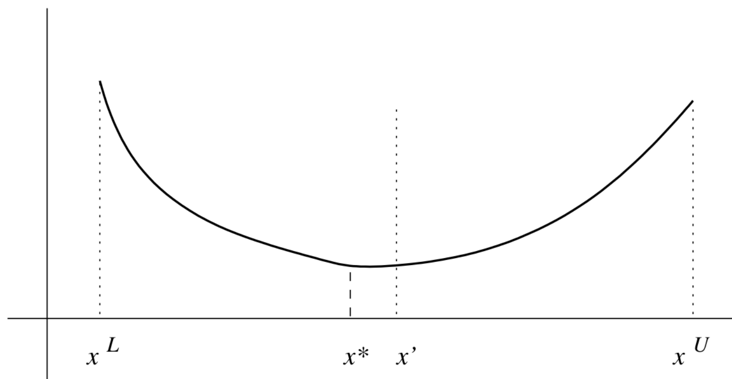


Figure 9.11: If the locally optimal solution in $[x^L, x^U]$ has already been determined to be at x^*, solving in $[x^L, x']$ is unnecessary.

9.4.5 Branching

There are many branching strategies [50, 16] available for use in sBB algorithms, most of which are based on branching along coordinate directions, i.e. by partitioning the variable ranges. It is known that best results on some particularly difficult MILP instances (e.g. [38]) are achieved by branching along constraints [39], but such branching schemes have apparently not been used in sBB algorithms yet. Other approaches include [94, 40, 41, 125]. Henceforth, we shall assume that "branching" implies "along coordinate directions".

Generally, branching involves two steps: determining the index of the variable on which to branch (called *branching variable*), and determining the point (called *branching point*) on which to partition the branching variable range. Several heuristics exist (see [138, p. 205-207] and [16]). Here, we use the upper bounding solution $\tilde{x}$ (obtained in Step 4 of the sBB algorithm) as the branching point, if such a solution is found; otherwise the lower bounding solutoin $\bar{v}$ (Step 3) is used. Recall that $v = (x, w)$, where x are the original variables and w the additional ones.

We then employ the standard form to identify the nonlinear term with the largest error with respect to its convex relaxation. By definition of the standard form Eq. (9.3) (see Sect. 9.4.3.1), this is equivalent to evaluating the defining constraints (9.5)-(9.8) at $\bar{v}$ and choosing the one giving rise to the largest error. In case the chosen defining constraint represents a unary operator, the only variable operand is chosen as the branching variable; if it represents a binary operator, the branching variable is chosen as the one having branching point value closest to the range midpoint.

Part IV

Advanced Mathematical Programming

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Index

NP-complete, 82–84
  strongly, 78
NP-hard, 78, 81, 83
  strongly, 78, 80, 87
  weakly, 78
NP-hardness
  reduction, 86
  weak, 80
P, 81, 83
2-Linear Separability, 84
clique, 87
set partition, 85
2LS, 84
3sat, 85
3sat, 80

abscissa, 28
absolute
  value, 113
acceleration
  device, 141, 143
accuracy, 143
active, 80
acute, 98
adjoint, 113
affine
  hull, 94
  independence, 123
algebraic, 62, 63, 86
  form, 141
algebraically closed field, 66
algorithm, 35, 41, 73, 130, 137
  accelerated, 143
  B&S, 143
  BB, 147
  calling, 138
  checking, 88
  complex, 138
  correct, 115
  cutting
    plane, 125
  cycle, 109
  deterministic
    GO, 138
  Dijkstra, 78
  efficient, 88
  ellipsoid, 112, 115
  enumeration, 69
  execution, 112
  generic, 114
  GO, 139
  heuristic, 137
  Karmarkar, 116, 117
  local, 88
  optimization, 137
  polytime, 74, 80
  pseudopolynomial, 78, 80
  recognition, 32, 35
  sBB, 147, 153
  stochastic, 138
  symbolic, 150
  Tarski, 65, 69
  terminate, 148
  terminates, 110, 112, 115, 146
  termination, 73, 109
  Witzgall, 69
algorithmic
  framework, 16
  performance, 142
algorithmics, 36
alphabet, 31, 61, 73, 75
  size, 73
ambiguity, 21
amount
  total, 21
AMPL, 41, 51–53
  dat
    syntax, 55
  executable, 51
  format, 55
  GUI, 51
  imperative, 52
  namespace, 55
  snippet, 57
analysis
  convex, 93
  polyhedral, 123
  polytime, 88
  symbolic, 148
  worst-case, 121
angle
  largest, 98
  obtuse, 99
application
  field, 13
approach
  algorithmic, 137
  escaping, 140
approximation, 114
  bfs, 114
  linear, 117
  poor, 139
  precision, 114
  quadratic, 137, 138
  rounding, 114
arc, 42
  antiparallel, 124
  capacity, 124

area, 28
arithmetic
  index, 24
arithmetical expression, 32
arity, 32, 150
  ero, 33
  positive, 32
  zero, 34
array, 33
ascending chain, 64
assigment, 15
assignment, 21, 25, 26, 35, 36, 43
  constraint, 23, 25
  optimal, 22
  problem, 22
associativity, 150
atom, 29
axis, 29

B&C, 133, 141
B&S, 141, 147
  convergence, 143
  fathoming, 144
back-substitution, 63, 64
ball, 49, 94, 101
barrier
  self-concordant, 88
  solver, 112
barycenter, 29
base
  circular, 28
basic, 111
  column, 106, 110, 125
  feasible
    solution, 106
  solution
    primal, 112
  variabkle, 121
  variable, 106, 110
    index, 110
basis, 106, 108–110, 112, 113, 121, 127
  current, 112, 125, 126
  enter, 127
  enters, 109
  exists, 110
  exit, 127
  leaves, 109
  new, 109
  optimal, 111, 112
Bayesian, 139
BB, 39, 64, 121, 131, 139, 141
  implementation, 131, 143
  spatial, 147
  subproblem, 133
  terminates, 131
best solution, 145
bfs, 106–109, 111, 113, 114, 121
  approximation, 114
  current, 108, 110
  multiple, 106, 107
  optimal, 114, 119
  starting, 109, 111
big M, 45
bijection, 106
bilinear, 151
bilinear programming, 84
binary
  operator, 150
binary optimum, 85
binary string, 74
biquadratic
  form, 87
biquadratic form, 87
bisection
  search, 114, 117, 138
    termination, 114
bit, 77, 78
  storage, 116
black-box optimization, 81
blending, 15, 18
  problem, 48
BLP, 43
BonMin, 51
boolean, 78
bound, 19, 131, 134, 148
  achievable, 102
  below, 114
  continuous, 134
  Lagrangean, 134
  lower, 101, 102, 111, 131, 132, 134, 143, 144, 146, 148, 149, 153
    best, 103
    guaranteed, 63, 150
    initial, 148
    lowest, 131
    maximum, 102
    smallest, 149
    valid, 144
  product, 130, 131
  sequence, 143
  tightening, 148, 149
  tighter, 149
  upper, 113, 129, 131–133, 143, 144, 148, 149, 153
    best, 143
  variable, 29
bounded, 46, 93, 98, 107, 108, 129
  above, 113, 114
  below, 103
  instance, 113
boundedness, 68, 113
  certification, 37
box constraints, 80
BPP, 84
brackets, 32
branch, 74, 132, 133, 154
  rule, 142
  tree, 74
Branch-and-Bound, 39, 121
Branch-and-Cut, 133
Branch-and-Price, 133
Branch-and-Select, 141
branched, 131
branching, 145, 146, 153, 154
  point, 154
  rule, 148
  strategy, 154
  variable, 132, 154
    additional, 153
    original, 153
Buchberger's algorithm, 63

budget, 17
bug, 17, 20

canonical
 form, 125
capacity, 15, 24, 27
cardinality, 47, 112, 124
 maximum, 82, 83
cell, 76
center, 28, 29
centre, 115
certificate, 74, 86
 compact, 88
 polynomial, 80, 86
character, 31
characterization
 unique, 119
 well-defined, 119
chordal network, 64
Church's thesis, 61
Church, A., 61
Chvátal
 cut, 125
 first-order, 124
 second-level, 125
circle
 equal, 29
 packing, 15, 57
classification, 37
clause, 65, 78, 80
clique, 124
 maximal, 83
 maximum, 82
CLIQUE, 74, 83
clique number, 82
closed, 98, 107, 108
closure, 124, 125, 131
 affine, 94
 conic, 94
 linear, 93
 RLT, 131
clusre
 convex, 94
cluster, 46, 140
 point
 nearby, 140
clustering, 46, 140, 141
cMINLP, 39, 64
CNF, 78, 80
cNLP, 39, 64, 87, 88, 103, 137
 linear part, 40
co-domain, 62
co-**NP**-hard, 85
code, 36
coding
 practice, 17
coefficient, 107, 108
 nonzero, 122
COIN-OR, 35
collinear, 98
column, 106, 108–110, 122, 127
 basic, 106, 115, 125
 current, 125
 entering, 128
 generation, 112, 133
 nonbasic, 106, 110
 partition, 106, 109
 set, 109
combination
 affine, 94
 conic, 94, 97
 convex, 94, 107
 strict, 94, 106
 linear, 93, 96, 108
combinatorics, 121
command-line
 workflow, 51
complement, 69
complementarity
 condition, 119
complementary
 slackness, 100
 strictly, 119
complete, 66
completeness, 66
completeness theorem
 Gödel, 66
completion
 time, 22
complex, 69
complexity
 computational, 73, 139
 description, 89
 exponential, 64, 141
 polynomial, 112, 117, 124
 polytime, 117
 worst-case, 73
complexity class, 62
component, 18, 29, 54, 86, 110, 113, 125
 fractionary, 132
 integer, 121, 122
 nonzero, 83, 107
 rational, 113
 solution, 55
 unreliable, 139
 zero, 82
computability, 61
computable, 62
computation
 irrational, 116
 practical, 121
computation model, 61, 62, 78
 TM, 63
computational
 complexity, 73
computational complexity, 40, 81, 86
computational geometry, 84
computationally
 expensive, 153
computationl model, 68
computing model, 61
concave, 23, 153
concurrent, 74
condition, 26
 boolean, 22
 boundary, 26
 complementarity, 119
 first-order, 86
 KKT, 86, 118, 137
 necessary, 95, 97

non-negativity, 87
optimality, 108, 124
second-order, 86
sufficiency, 101
sufficient, 95, 122
termination, 120, 135
cone, 94
border, 88
boundary, 88
convex, 88
copositive, 88
dual, 88
matrix, 88
membership, 33
PSD, 88
congruence
invariant, 29
conic
combination, 94
conic solver, 39
conjunction, 33, 65, 80
literal, 65
conjunctive normal form, 78
connected
strongly, 77
connected component, 65
connected components, 69
console, 52
constant, 38, 45, 82
large, 129
numerical, 17
real, 65
constraint, 23, 27, 33, 37, 44, 52, 53, 55, 79, 84, 101, 112, 116–118, 121, 124, 126, 129, 130
active, 80, 100
adjoin, 116, 124, 127, 129
aggregation, 102
allocation, 26
assignment, 23
bilinear, 129
boolean, 23
bound, 151
box, 80
capacity, 25
coefficient, 111
complicating, 133, 134
conditional, 45
convex, 81, 150
defining, 150–152
demand, 27
disjunctive, 129
dual, 102
equality, 38, 53, 97, 100, 120, 152
equation, 126
factor, 130, 131
factorable, 149
functional, 33, 45
generated, 131
gradient, 97
implicit, 33, 34, 45
implied, 35
index, 115
inequality, 38, 84, 97, 100, 125
integrality, 23, 24, 33–35, 39, 46, 121
LHS, 149
linear, 93, 123, 149
linearization, 85
linearized, 137, 139
list, 18
matrix, 106, 121, 123
MILP, 76
non-negativity, 42, 48, 82, 84
nonlinear, 149
nonnegativity, 24
norm, 81
number, 107, 116
original, 152
orthant, 117
precedence, 44
primal, 102
problematic, 35
qualification, 103, 139
range, 20, 33, 43
redundant, 35
RHS, 116
SDP, 34
set, 88
simplex, 82, 88
single-row, 18
string, 34
technical, 17, 18
trivial, 17
forgotten, 20
unmentioned, 23
valid, 127
violated, 115
weighted sum, 103
constriant
adjoin, 132
continuous
relaxation
solution, 126
continuous knapsack, 81
contradiction, 65, 114
convergence, 139, 140, 143
finite, 143
convergent, 142
convex, 39, 87, 93, 94, 109, 150, 153
analysis, 93
combination, 88, 123
function, 94, 144
hull, 88, 94, 123, 124, 131, 134
quadratic
approximation, 138
relaxation, 148
set, 94
smallest, 152
set intersection, 93
convex analysis, 94
convex cone, 88
convexification, 150, 152
convexity, 95, 107
strict, 87
strong, 87
variant, 101
coordinate, 28
change, 96
Euclidean, 48
copositive
programming, 88

copositive matrix, 87
copositivity, 85, 88
correctness, 117
cost, 20, 27, 48
  communication, 44
  competitive, 103
  computational, 112, 149
  decreasing
    direction, 108
  least, 42
  minimization, 48
  net, 48
  reduced, 109, 112, 127
    negative, 109
    nonnegative, 112
  set-up, 15, 27
  transportation, 49
  unit, 24
  vector, 53, 106
Couenne, 51
countably infinite, 38
countably many, 37
couple, 46
cover, 142
covering, 15, 27
CPLEX, 35, 51
CPU
  time, 147
    limit, 139, 140
cQKP, 81
cQP, 80, 83
crash, 139
critical point
  constrained, 96
curve
  piecewise linear, 84
cut, 124, 126, 128
  Chvátal, 125
  disjunctive, 129
  family, 124
  generation, 125
  Gomory, 125–128
  hierarchy, 124, 131
  new, 127
  nontrivial, 124
  RLT, 130
  valid, 112, 121, 124, 126, 130
cutting
  plane, 112, 123, 133
    algorithm, 125
cycle
  disjoint, 124
cylinder, 28, 65
cylindrical decomposition, 65

DAG, 32
  expression, 32
Dantzig, 105
data, 52
  dense, 39
  irrelevant, 21
  numerical, 52
  sparse, 39
  structure, 112
data structure, 33
DE, 67, 68
  exponential, 67
  quadratic, 68
  system, 67
  universal, 68
decidability, 66
  efficient, 87
decidable, 62, 78
  incomplete, 66
decision, 62
  algorithm, 66
  procedure, 65
  variable, 20, 22
    vector, 137
decision problem, 61, 73, 81
decision variable, 33, 34
  assignment, 43
declaration
  instruction, 54
declarative, 36
decomposable
  nearly, 133
definition
  formal, 36
degeneracy, 107
degenerate, 107, 108
  vertex, 107
degree, 87
  maximum, 131
  odd, 87
demand, 15, 25–27, 42, 48
  satisfaction, 24, 25, 27
denominator, 113, 114, 121
dense, 39
derivative
  directional, 96
  partial, 96
  second, 86
descent
  direction, 97, 120
description, 123
  compact, 88
determinant, 113, 121, 122
deterministic, 147
  algorithm, 138
diagonal, 69, 81, 122
diagonalization, 64
diet problem, 42
diffeomorphism, 96
differentiable, 101
  continuously, 96
digit, 63
digraph, 42–44
  infinite, 77
  reduction, 77
  strongly connected, 77
Dijkstra's algorithm, 78
dimension, 29
  search
    space, 139
  small, 88
diophantine equation, 67
directed acyclic graph, 32
direction
  cooordinate, 154

descent, 100, 117
feasible, 100
improving, 110
vector, 137
disjoint
pairwise, 142
disjunction, 33, 80, 129
disjunctive
normal
form, 65
distance, 143
Euclidean, 29
geometry
molecular, 15
minimum, 98
pairwise, 29
unit, 29
distinguished
point, 143
distribution
uniform, 107
division, 77
DNF, 65
domain, 46, 62, 94
discrete, 134
dual, 88, 103, 118, 134
basis, 112
constraint, 102
feasible, 118, 119
objective, 102
problem, 102
simplex, 125
iteration, 126
method, 111, 112
variable, 102
dual cone, 88
duality, 93
gap, 120
strong, 88, 101, 103
theorem, 103
theory, 102
weak, 101, 102
dynamic programming, 78
dynamics, 68, 75

EDE, 67
edge, 36, 40, 82, 108, 110, 124
induced, 36
edge-weighted, 124
efficient, 36
practically, 105
eigenvalue
negative, 83
elementary step, 41
ellipsoid, 115, 116
algorithm, 112, 115
centre, 115
method, 124
minimum
volume, 115
ellipsoid method, 78
empty, 113, 115
list, 148
encoding
binary, 78
Thom, 63
unary, 78
endpoint, 145
entity
declaration, 54
symbolic, 52
enumeration, 69
ϵ-optimality, 143
ϵ-optimum, 143
equality, 45
sign, 109
equation, 33, 43, 96, 102, 125, 141
linear, 80, 93
polynomial, 138
system, 123
error
largest, 154
escaping, 139, 146
approach, 140
Euclidean Location, 48
Euclidean space, 84
evaluation, 32, 95
exact, 142
exponential
bound, 73
doubly, 65
number, 124
worst-case, 105
exponential complexity, 64
exponential-time, 73
exponentially, 123
exponentiation, 67
expression
arithmetical, 32, 34, 38
DAG, 32
factorable, 149
mathematical, 150
nonlinear, 19
tree, 32
expressions
mathematical, 148
extension, 147

face, 94
full-dimensional, 119
optimal, 119
facet, 94, 123, 124
defining, 123
factorable, 149
failure
proof, 139
family
continuous, 118
Farkas' lemma, 98, 99
faster
asymptotically, 77
fathomed, 143
FBBT, 148, 149
feasibility, 81, 111, 113, 120, 148
certification, 37
dual, 111
primal, 111
verification, 139
feasibility system, 67
feasibility-only, 34

feasible, 34, 35, 104, 111, 114, 115, 120, 137, 139, 152
basic, 106
basis
initial, 126
descent, 97
direction, 97, 120
instance, 113
point, 95
polyhedron, 124
primal, 112
region, 93, 101, 103, 117, 123, 124, 133
mixed-integer, 123
set, 37, 113, 130
solution, 37, 117
value, 34
vector, 106
feasible region
nonconvex, 48
file, 52
run, 51, 52
filter, 142–144
limit, 142
finite set
decidable, 69
finitely many, 38
flat
formulation, 18
flattened, 18
floating point, 31, 37, 62, 64
error, 37
number, 138
flow, 25, 43
network, 112, 124
food, 103
form
factorized, 111
functional, 45
normal
disjunctive, 65
standard, 124, 150
formal system, 66, 67
complete, 66
incomplete, 66
formula
satisfiable, 81
formulation, 17, 18, 21, 22, 27, 34, 36, 52, 54, 97, 101, 102, 107, 116, 123–125, 127, 130, 134, 141, 144, 146, 150, 151
correct, 22
difficult, 22
dual, 101, 134
flat, 18, 19, 40, 41, 48
flatten, 55
generality, 17
ill-posed, 139
LP, 42, 123
MILP, 121, 124
minimization, 101
mixed-integer, 131
Motzkin-Strau, 82
Motzkin-Straus, 85, 87
MP, 33–36, 39, 52, 53, 113
NLP, 118, 137, 146
convex, 148
original, 131, 132, 138, 148, 150–153
parameter, 19, 22
primal, 101
QP, 83
restricted, 148
structure, 133
structured, 18, 19, 21, 40, 41
unconstrained, 29
wrong, 21
fraction, 18–21, 67, 81
fractional, 125, 151
full-dimensional, 119
function, 23, 62
barrier, 88
call, 57
callable, 36
class, 101
closed form, 32
computable, 62
concave, 23
convex, 94, 105
evaluation, 77
exponential, 69
linear, 33, 35, 144
nonlinear, 33, 69
penalty, 88
periodic, 69
piecewise
linear, 23
real, 37
separable, 82
unconstrained, 96
univariate, 151
vector, 95

Gödel, 67
Game of Life, 61
GAMS, 41, 51
gap, 46
duality, 120
Gaussian elimination, 63, 64
general-purpose
algorithm, 138
geometry, 121
combinatorial, 29
global, 101, 109, 144
minimum, 93
optimality, 40, 141
guarantee, 140
phase, 138
global optimality, 39
global optimization, 37, 47
global optimum, 63, 80–82
GLPK, 35, 51
GO, 47, 62, 70, 137, 138, 141
algorithm, 138
Gomory
cut, 125
valid, 125
GO
algorithm, 138
GPP, 46
Gröbner basis, 63
gradient
constraint, 97
grammar

formal, 35
graph, 31, 36, 40, 41, 74, 82, 83
  bipartite, 42
  directed, 42
  neighbourhood, 44
  notation, 44
  undirected, 46
  weighted, 42, 78
graph partitioning, 46
guarantee
  theoretical, 138

half-line, 137
half-space, 94
  closed, 93, 94
halting problem, 66
Hamiltonian
  cycle
    optimal, 124
hardware, 36
Haverly, 47
head
  read/write, 75
  tape, 75
Hessian, 86, 138
  constant, 86, 87
  form, 87
  of the Lagrangian, 86
heuristic, 57, 131
  IPM-based, 88
hierarchy
  cut, 131
Hilbert's 10th problem, 67
homogeneous, 117
HPP, 47, 48
hull
  affine, 94
  conic, 94
  convex, 94, 123
  linear, 93
hyper-rectangle, 80, 129, 147
  embedded, 146
  smallest, 130
hyper-rectangles, 148
hyperplane, 93, 96, 106, 115, 121
  constraint, 107
  generic, 123
  intersection, 107
  normal, 96
  separating, 99, 100, 103, 124
hypothesis, 122

I/O, 36
ideal, 63
identity, 122
  matrix, 122
iff, 37, 38
imperative, 35
implementation, 105, 112, 134, 143
  B&S, 143
incomplete, 66
incompleteness, 66
inconsistent, 66
incumbent, 131, 132, 140, 142, 143
  current, 125, 143
  fractional
    solution, 124
independence
  affine, 123
  linear, 123
independent, 66
index, 25, 106, 108
  column, 56, 125
  lowest, 109
  row, 125, 126
  set, 19, 22, 53, 55
  tuple, 34
index set, 24
inequalities
  linear, 113
inequality, 118, 123, 125, 130, 131, 142, 152
  linear, 93, 152
    strict, 112, 115
  lower-dimensional, 130
  non-strict, 33
  nonlinear, 131
  valid, 112, 123, 130
infeasibility, 105, 116
infeasible, 37, 112, 114, 130, 139, 142, 148
  primal, 112
infimum, 98
infinite, 125
  countably, 69
  time, 138
infinitely, 123
initial
  vector, 134
initialization, 148
input, 33
  array, 78
  integer, 121
  rational, 121
  storage, 78
input/output, 36
instability
  numerical, 111
instance, 18, 35, 41, 48, 52, 63, 67, 73, 116, 122
  bounded, 113
  description, 38
  feasible, 113
  large-scale, 133
  MILP, 154
  NO, 74, 79, 85
  size, 73, 108, 113, 116
  sizer, 113
  small-sized, 141
  YES, 74, 79, 85
instruction, 51, 52, 75
  declarative, 52
  imperative, 52
  sequence, 74
integer, 74, 114, 125
  component, 121
  consecutive, 54
  feasible
    set, 124
  programming, 121
integer programming, 45
integral, 125, 128
integrality, 26–28, 33, 81, 84

constraint, 121
property, 134
solution, 79
integrality constraint, 66
interface, 41
interior
non-empty, 103
point
method, 117
interior point method, 80
interpretation, 33
interpreter, 35, 36, 51
intersection, 121, 132, 133
interval, 19
arithmetic, 129, 149
intractable, 73
invariant, 21, 29, 38, 96
inverse function
theorem, 96
investment, 14, 17
IPM, 80, 88, 112, 117, 120
analysis, 119
IPOPT, 51
IQP, 69
irrational, 62, 81
irrelevance, 21
iteration, 117, 127, 135, 137, 143, 144, 148
current, 111
dual
simplex, 126
first, 117, 144
major, 140
minor, 140
next, 109
second, 145
subsequent, 146
typical, 131

Jacobian, 96, 139
job, 21
last, 22
order, 22

Karush-Kuhn Tucker system, 64
Khachiyan, 112
kissing number, 49
maximum, 49
KKT, 64, 80, 86
complementarity, 119
condition, 101, 118, 138
conditions, 100
point, 100, 101, 138
theorem, 100
knapsack
continuous quadratic, 81
KNP, 49

label, 151
Lagrange
multiplier, 102, 134
Lagrangean
relaxation, 121
Lagrangian, 96, 101, 118
dual, 102
function, 86, 102

language, 13
arithmetical expression, 34
basic, 31
composite, 31
decision variable, 33
declarative, 36, 52, 75
expression, 33
formal, 17, 19, 31
imperative, 35, 36, 52, 57
interpreter, 35
modelling, 41
MP, 33
natural, 17, 19, 21, 31
objective function, 34
parameter, 33
programming, 35
large
arbitrarily, 143
large instance, 40
lcm, 63, 67
leading term, 63
leaf, 74
least common multple, 63
leaves, 150
lemma
Farkas, 99, 100
LHS, 125
lhs, 38
LI, 113
infeasible, 114
instance, 114, 115
oracle, 114
lifting, 130, 131, 137
nonlinear, 130
process, 130
limit
filter, 142
point, 119
line, 94, 137
search, 120, 137
linear, 45, 82, 87
algebra, 122
combination, 93, 96
constraint, 93, 129
dependence, 109
forma, 105
fractional, 151
function, 131
hull, 93
independence, 96, 100, 106, 115, 123
inequalities, 113
part, 152
piecewise, 23, 134
system, 121
term, 37
linear order
dense, 65
linear programming, 105
linear time, 88
linearity, 117
linearization, 45, 131, 150, 152
process, 150
variable, 131
linearized
nonlinear

term, 150
link, 25
capacity, 25
linkage, 141
Linux, 51
list, 55, 132, 145, 148, 149
empty, 145
region, 148
remove, 148
tabu, 140
literal, 33, 65, 80
local
minimum, 93, 139
optimum, 95
escape, 140
phase, 138, 140, 143
search, 147
local minimum, 85
local optimum, 86
local solution, 143
log-barrier
function, 112
loop, 35, 36, 52, 140
unfolding, 74
LOP, 113, 114
instance, 113, 114
solution, 113
lower
bound, 145, 146
LP, 39, 42, 53, 55, 61, 62, 64, 78, 105, 107, 109, 112, 113, 116, 118–121, 123
algorithm, 105
auxiliary, 111
canonical form, 105
dual, 103, 124
formulation, 113, 133
instance, 116
large-scale, 112
polytime
algorithm, 112
relaxation, 63
solution, 112, 121
standard form, 102, 106, 110, 117, 121
theory, 94
trivial, 106
LSI, 112, 113
instance, 115
polytime, 115

machine, 21
identical, 21
slowest, 22
Machine Learning, 40
MacOSX, 51
major
iteration, 140
makespan, 43, 45
mathematical
programming, 13, 16
Mathematical Programming, 31
MATLAB, 51
Matlab, 41
matrix, 33, 53, 54, 77, 88, 99, 116, 122, 133
cone, 88
constraint, 106, 151
TUM, 123
copositive, 87, 88
copositivity, 85
decision variable, 34
extremal, 88
form, 109
identity
TUM, 122
initialization, 56
integral, 121, 122
inverse, 110
nonsingular, 106, 125
notation, 53
PSD, 34, 87
rank one, 88
rational, 112, 113
sparse, 56
square, 106, 110
nonsingular, 121
symmetric, 86
square diagonal, 81
square symmetric, 34, 87
TUM, 122
upper bound, 43
MAX CLIQUE, 82
maxima, 93
maximization, 22, 40, 105
inner, 45
maximum, 82, 96
global, 49
pointwise, 144
maximum flow, 43, 46
mcm, 121
MDPR
theorem, 67
medium-sized
instance, 139
membership, 33, 129
method
iterative, 131
subgradient, 134
midpoint, 99
MILP, 39, 62, 64, 69, 75, 78, 121, 123–125, 130, 132
constraint, 78, 79
feasibility-only, 76
formulation, 133
instance, 123
reformulation, 123
restricted, 130
size, 39
solution
method, 123
minimization, 22, 101, 105
direction, 131
minimum, 83, 95, 96, 98, 105, 107, 112, 117, 124, 144
constrained, 97, 100
cut, 124
distance, 99
global, 93, 105, 107, 148
local, 93, 97, 101, 105, 109, 146, 147
current, 146
objective
value, 97
vertex, 105
minimum k-cut, 46

minimum cut, 46
MINLP, 39, 45, 61, 62, 64, 68, 69, 78, 138, 146
  complexity, 73
  decision version, 77
  feasibility, 67
  hardness, 73
  unbounded, 78
  undecidability, 68
  undecidable, 67
  undecidable problem, 70
minor
  iteration, 140
Minsky, 61
ML, 40
  unsupervised, 46
MLSL, 139, 140
modelling, 19, 36
modelling language, 41
monomial order, 63
monotonic, 138
Motzkin-Straus formulation, 82, 87
MP, 31, 33, 75, 101
  complexity, 88
  formulation, 49, 51
  instance, 37
  reformulation, 39
  semantics, 35
  systematics, 39
  theory, 35
$\mathbb{MP}$, 38
MSPCD, 43
multi-level
  single
    linkage, 139
multi-objective, 34
multi-period
  production, 15
multicommodity
  flow, 112
multiple
  minimum
    common, 121
multiplier, 102, 108
  Lagrange, 96, 100, 102, 134, 138
  vector, 134
multistart, 140
  algorithm, 139
multivariate, 29
  function, 137

natural, 69
natural language
  description, 17
negation, 33
negative, 85, 109, 110
neighbourhood, 35, 96, 140, 147
  incoming, 44
  size, 147
  structure, 146
net, 142, 143
  refinement, 142
  sequence, 142
network, 42
  flow, 112, 123
  topology, 48
network flow, 43
Newton
  descent, 120
  method, 120, 138
  step, 120
Newton's method, 88, 145
  one dimension, 144
NLP, 39, 47, 64, 78, 79, 82, 96, 100, 137–139, 144, 148
  continuous, 48
  convex, 39
  nonconvex, 40, 48, 137, 146, 147
  solver
    local, 146
  undecidable, 70
node, 32, 131
  contraction, 32
  current, 150
  incoming, 43
  leaf, 32
  outgoing, 43
  root, 149
non-differentiable, 134
non-empty, 98, 107
non-negative, 87, 127
non-overlapping, 29
non-positive, 85
nonbasic, 106, 111, 115
  column, 106
  index, 126
  variable, 106, 110, 121, 125
nonconvex, 39, 47, 48, 152
  set, 88
nonconvexity, 88
nondeterministic, 74
nonempty, 115
nonlinarity, 151
nonlinear, 39, 45, 152
  operator, 150
  part, 152
  programming, 137
  term, 37
nonlinear equation
  system, 70
nonlinearity, 22
nonnegative, 17
  constraint, 54
nonnegativity, 26, 27
nonsingular, 96, 106, 109
nonzero, 56, 108
norm, 81
normal, 96
NP, 74, 75, 78
NP-complete, 75
NP-complete, 75
NP-hard, 75, 121, 123, 124
NP-hardness, 77
NPO, 77
null
  space, 119
null space, 117
number
  finite, 93
  pseudo-random, 138
  rational, 114
numerator, 113

nutrient, 103

OBBT, 148, 149
  procedure, 149
objective, 48, 52, 117
  approximation, 114
  coefficient, 109
  convex, 101
  decrease, 109, 110
  direction, 27, 38, 97, 101, 113
  dual, 102
  function, 20, 22, 37, 44, 55, 107, 110, 111, 114, 117, 133, 137, 144, 151
    decrease, 111
    optimal, 111
    unbounded, 110
    value, 131, 144, 148
  Hessian, 138
  linearity, 117
  minimality, 27
  minimum, 107
  optimal, 101
    zero, 116
  primal, 102
  reduction, 117
  tangent, 144
  value, 102, 105, 109, 114, 141, 142
    best, 148
    better, 133
    current, 111
    lower, 110
    lower bounding, 143
    optimal, 143
objective function, 33, 34
  direction, 93
  globally optimal, 37
  min max, 45
  positive, 85
  value, 37
objective function value, 86
obstacle, 123
operation
  algebraic, 110
operator
  k-ary, 150
  binary, 32, 154
  implicit, 32
  minimum, 17
  nonlinear, 150
  precedence, 32
  primitive, 32
  scope, 32
  unary, 32, 154
OPTI toolbox, 42
optima, 93, 117, 123
  global, 131
optimal, 123, 128
  bfs, 119
  face, 119
  globally, 131
  Hamiltonian
    cycle, 124
  locally, 148
  objective, 113
    value, 117, 134
  partition, 119
  set, 37, 38
  solution, 119
  value
    known, 117
optimality, 33, 108, 111, 113
  certification, 37
  condition, 111
  first-order, 64
  global, 39, 40, 138
  local, 86, 137, 138, 143
    QP, 86
  properties, 116
  verification, 139
optimization, 33
  combinatorial, 114
  conic, 42
  direction, 48, 96, 124
  global, 47
  local, 137, 139
  problem, 13, 31
  procedure, 22
optimization direction, 34
optimization problem, 61
optimum, 35, 37, 110, 113, 144
  global, 35, 40, 63, 80, 82, 86, 88, 94, 131, 138, 139, 145, 146, 148
    putative, 139, 147
    region, 145
  improved, 140
  improving, 140
  local, 83, 85, 86, 88, 94, 95, 101, 109, 137, 138, 140, 145
    current, 140
  true, 143
oracle, 114, 115, 124
  algorithm, 113
  LI, 114
order
  index, 44
  linear, 21
  partial, 43
  precedence, 43
  total, 69
origin, 29, 106
original
  formulation, 134
  LP, 111
orthant, 88, 117
  non-negative, 88
orthogonal, 119
output, 33, 35
  format, 57
overestimator
  concave, 150

P
  P, 123
P, 73
packing, 28, 29
  circle, 29
pair
  unordered, 29, 36, 47
parabolic, 69
parameter, 18, 22, 33, 37, 48, 52, 53, 55, 76, 118, 120

configurable, 147
continuous, 37
formulation, 53
initialization, 54
input, 35, 45
integer, 54
scalar, 41
symbol, 18, 33, 35, 54
value, 55
vector, 19
parent
subproblem, 132
parser, 35, 150
part, 116
linear, 152
nonlinear, 152
partition, 46, 109, 122, 131
finite, 142
optimal, 119
unique, 119
path, 108, 118
central, 118, 119
default, 55
exponentially many, 112
primal-dual, 119
shortest, 44, 112
penalty
log-barrier, 117
performance
computational, 137
PFP, 64, 69
phase
global, 139, 140, 147
deterministic, 141
stochastic, 139, 140
local, 139, 140, 142, 146, 153, 154
PICOS, 41
piecewise
convex, 153
piecewise linear
curve, 84
pipe
filter, 51
pivot, 126, 128
element, 127
plane
cutting, 123
point, 94, 114, 118
branching, 145
critical, 97
current, 138
distinct, 94, 123
distinguished, 142, 143
dual
feasible, 118
feasible, 95, 108, 140
infeasible, 137
initial, 120
random, 147
returned, 139
saddle, 22
sample, 147
starting, 137
symmetric, 94
polyhedra, 129
union, 130
polyhedron, 93, 105–108, 111, 119
bounded, 108
closed, 115
feasible, 106, 107
open, 115
standardized, 123
unbounded, 108
vertex, 105, 108, 121, 122
polynomial, 73, 116
calls, 113
complexity, 112
convexity, 87
degree, 85
equation, 68
function, 73
integral, 67
minimal, 63
multivariate, 29, 63, 69
quartic, 29
system, 63, 65, 66
undecidable, 67
polynomial division, 63
polynomial feasibility, 64
polynomial programming, 64
polynomial reduction, 75
polynomial time, 35
polynomial-time, 73
polytime, 73, 74, 79, 81, 87, 88, 113, 121
analysis, 88
feasibility, 77
LP
algorithm, 112
strongly, 78, 82, 124
weakly, 78, 80, 124
polytope, 93, 108, 129, 130
pooling problem, 47
position
initiale, 75
vector, 29
positive, 110, 120
strictly, 99, 115
positive semidefinite, 34, 80
power, 151
PP, 64, 78
integer, 70
pre-processing, 141
precise
computation, 139
numerically, 143
precision, 138
premultiplication, 111
price, 103
retail, 19
pricing
problem, 112
primal
constraint, 102
feasible, 112, 119, 127
infeasible, 112, 126
objective, 102
problem, 102
simplex, 111
variable, 102
primal-dual

central
path, 119
optimal
solution, 119
pair, 119
prime, 77
priority
queue, 131
probability
1, 138–140
zero, 107
problem, 31, 73, 122
assignment, 22
decision, 31, 61, 62, 73, 77, 86, 113
diet, 103
dual, 102
fundamental, 22
hardest, 75
linear
optimization, 113
maximization, 103
MP, 34
nontrivial, 35
optimization, 31, 33, 34, 41, 61, 77, 113
original, 102
pair, 102
pricing, 112
primal, 102
recognition, 31
saddle, 101, 102
search, 61
unconstrained, 120
procedure, 105
efficient, 112
process
output, 36
terminate, 138
processor, 21, 43
product, 22, 76
binary variables, 45
Cartesian, 31
operator, 150
production, 24
level, 24
profit, 20
program variable, 35
programming
computer, 17
nonlinear, 137
quadratic
sequential, 137
project, 117
projection, 131
projective
transformation, 117
proof
by simulation, 73
property
integrality, 134
provability, 66
provable, 66
pruned, 131
pruning, 146, 148
PSD, 34, 80, 87, 116, 120
approximation, 138
cone, 88
PSD cone, 88
pseudo-convex, 87
pseudo-random
generator, 138
pseudocode, 36
pseudoconvex, 101
pseudopolynomial, 77
reduction, 78
push-relabel
algorithm, 124
PyOMO, 41
Python, 41, 57

QDE, 68
QKP
convex, 82
QP, 79, 80, 82–87, 138
NP-complete, 80
box-constrained, 80, 86
constrained, 86
convex, 80, 82
formulation, 83, 86
nonconvex, 83
QP1NE, 83, 84
QPLOC, 86
quadrant, 97
quadratic
DE, 68
form, 69, 79, 85, 87
integer programming, 69
knapsack, 81
objective, 47
programming, 79
structure, 40
quantifier, 18, 41, 44, 48
decision variable, 45
elimination, 65
existential, 67
universal, 67
bounded, 67
quantifier elimination, 65
quantile regression, 39
quartic, 29
quasi-convex, 87
quasiconvex, 101
queue
priority, 131, 132

radius, 49
random, 54
choice, 138
seed, 138
range, 19, 82, 87, 119, 132, 153
endpoint, 144
length, 146
midpoint, 154
partitioning, 154
smallest, 148
variable, 144, 148, 149
range constraint, 33
rank
one, 83
rational, 37, 62, 63, 77, 80
polynomial, 65

rational input, 61
ray
extreme, 89, 108
real, 62, 64, 65, 69
number, 138
real RAM model, 62
recognition algorithm, 32
rectangle, 29
boundary, 29
recursion, 36, 150
level, 65
recursive, 62
recursively enumerable, 62, 68, 69
reduced
cost, 110
negative, 110
nonnegative, 110, 112
reduction, 77, 80, 82, 84, 87, 113, 116
NP-hardness, 86
polynomial, 75, 115
pseudopolynomial, 78
strongly polytime, 78
redundant, 35
refinement, 142
reflection, 29
reformulation, 23, 39
exact, 45, 47, 76
standard form, 150, 151
symbolic, 150
reformulation-linearization
technique, 130
region, 124, 143–146, 148, 149
check, 148
choice, 148, 149
current, 143, 148, 150, 152, 153
discarding, 145
distinguished, 143
feasible, 37, 103, 108, 124, 131
relaxed, 124
original, 145
pruning, 146
qualified, 142
rejected, 143
remove, 148
selected, 148
selection, 149
unexamined, 145
register machine
universal, 68
relation, 32, 62
asymmetric, 77
decidable, 62
relational operator, 34
relational sign, 34
relaxation, 40, 101, 131, 148
continuous, 46, 121, 124, 125, 131–134
convex, 148–150, 152–154
Lagrangean, 121, 133, 134
reliability
algorithmic, 139
representation, 62
binary, 113
compact, 86
resource
allocation, 26
revenue, 17, 20
revised
simplex
method, 111
RHS, 22, 125, 149
vector, 53
rhs, 38
RLT
closure, 131
cut, 130
hierarchy, 131
robustness, 39
Roghozin, 61
root, 63, 138
rostering, 15
rotation, 29
invariant, 29
routing, 25
row, 122, 125, 134
additional, 127
bottom, 127
exiting, 128
first, 126
generation, 124
last, 125
permute, 122
tableau, 128
optimal, 126

saddle, 101
point, 96
saddle problem, 45
sales, 24
sampling, 139, 140, 146
approach, 140
point, 147
SAT, 75, 79, 80
SAT, 33
satisfiability, 75
sBB, 40, 62, 144, 147, 148
algorithm, 146, 148, 154
branching, 148
check
region, 148
choice
region, 148
initialization, 148
lower
bound, 148
node
root, 149
pruning, 148
upper
bound, 148
scalar, 54, 96, 106, 108
non-negative, 48
real, 48
schedule, 43
scheduling, 21, 26, 43
SDP, 34
SDP solver, 39
search
bisection, 114, 138
direction
vector, 137

finite, 105
local, 147
space, 131
variable neighbourhood, 140
search direction, 33
search problem, 61
segment, 93, 98, 137
selection
exact, 144
rule, 142, 148
exact, 143
self-concordant barrier, 88
self-dual, 88
semantics, 33
English, 33
format, 35
MP, 35
MP language, 35
semi-algebraic set, 65
semidefinite programming, 34
sensitivity, 111
senstivity
analysis, 111
sentence, 33, 75
logical, 65
separable, 82
separating
cutting
plane, 125
hyperplane, 99, 103, 124
separation, 124
polynomial, 124
problem, 124
sequence, 34, 137, 149, 150
conditional, 113
exponentially long, 39
finite, 124
nested
infinite, 144
step, 74
sequencing, 43
set, 103, 118, 129, 131, 146, 152
content, 55
convex, 93, 94, 103, 105
decidable, 62
description, 131
distinguished, 142
family, 142
feasible, 37, 115, 130, 132
relaxed, 124
finite, 93
index, 19, 22, 52, 54, 55, 131
infinite, 35
initialization, 54
instance, 35
label, 45
linear, 131
mixed-integer, 131
name, 45
optimal, 37
periodic, 26
polyhedral, 123
qualified, 142, 143
recursive, 62
sampling, 139
stable, 36
SET COVER, 43
Shannon, 61
shortest
path
problem, 112
shortest path, 78
side
length, 146
sign
opposite, 38
signal processing, 39
simplex, 117
algorithm, 110, 111, 125, 126
centre, 117
dual
iteration, 126
method, 105, 119, 123
dual, 111
revised, 111
two-phase, 111
tableau, 112, 125, 126
translated, 85
simplex method, 61, 64
simulated annealing, 140
simulation, 61
single-objective, 34
size, 123, 133
input, 75
instance, 113
maximum, 113
solution, 39
storage, 77
slack variable, 37
Slater constraint qualification, 103
small-sized
instance, 139
solution, 33, 37, 67, 108, 114, 115, 118, 120, 123, 133–135, 138, 144, 148, 153
basic
feasible, 106
best, 146
corresponding, 148
current, 109, 112, 124, 138
distinct, 107
feasible, 40, 77, 85, 102, 109, 115, 116, 124, 131
flat, 55
fractional, 85
fractionary, 132
global, 138
integer, 66, 123
feasible, 123
integral, 132, 133
local, 88, 143
lower
bounding, 132
lower bounding, 143
method, 137
not integral, 127
optimal, 35, 117, 119, 125, 127, 128, 138
unique
optimal, 106
upper
bounding, 154
vector, 86

solution algorithm, 33
solver, 18, 35, 36, 41, 55
  commercial, 35
  conic, 39
  efficient, 35
  free, 35
  global, 40
  input, 38
  local, 39
  LP, 39, 51
  MILP, 39, 51
  MP, 39
  NLP, 39
  off-the-shelf, 35
  open-source, 35
  robust, 39
  robust/efficient, 40
  SDP, 39
  state-of-the-art, 39
  status, 55
source, 25
space
  Euclidean, 29
  higher-dimensional, 130, 131, 137, 151
  projected, 117
  search, 131, 138, 144, 148
span, 93
sparse, 39
sphere, 49
  circumscribed
    smallest, 117
  inscribed
    largest, 117
SQP, 137
  algorithm, 139
square, 67, 81, 83, 106
  sum, 29
stable set, 36, 41
standard
  form, 125, 152
standard form, 151
standard quadratic programming, 87
starting
  point, 139, 140, 146
starting point, 40
state, 75
  initial, 75
  termination, 75, 76
statement
  logical, 36
step, 120, 125
  evaluation, 143
  length, 135, 137
  size, 117
steplength, 110
stochastic, 139
  algorithm, 138
stop, 114, 120
storage, 35, 48, 77, 111, 113
  balance, 24
  empty, 24
StQP, 87
strategy
  branching, 132
strict, 93, 94
string, 31
  constraint, 34
  decision variable, 34
  initial, 75
  objective, 34
  parameter, 34
strongly polytime, 78
structured
  format, 55
  formulation, 18
subexpression, 150
  complicated, 150
subfamily, 142
subgradient, 135
  method, 134
  vector, 135
subgraph
  enumeration, 36
submatrix, 110
  invertible, 121, 122
  square, 122
    smallest, 122
subnode, 150
suboptimal, 120
subproblem, 113, 120, 131–133, 139
  current, 131
  parent, 132
  unsolved, 132
subregion, 144, 148, 153, 154
  infeasible, 148
subsequence
  convergent, 98
  initial, 74
subset, 93
  disjoint, 46
  largest, 36
  minimality, 27
SUBSET-SUM, 79–81, 85
subtree, 150
symbol, 33, 76
symmetry, 107
syntax, 35, 41
  AMPL, 52
system, 111, 114
  linear, 121

tableau, 127, 128
  current, 125, 126
  modified, 127
  optimal, 126, 127
  sequence, 126
  simplex, 126
tabu
  list, 140
tabu search, 140
tangent, 144
tape, 75
  half-infinite, 73
  multiple, 73
  number, 73
target, 25
task, 21, 43
  index, 44
  order, 43
  starting time, 44

tautology, 65
tensor, 56
    form, 20
term
    bilinear, 47, 48
    linear, 152
    nonlinear, 35, 154
termination, 142
    artificial, 139
    condition, 120, 139, 140, 147
    failure, 62
    state, 76
test, 35, 36, 52
test branch, 74
text
    file, 51
theorem
    alternatives, 98
    convex analysis, 94
    duality, 101
        weak, 102
    Farkas, 99
    inverse function, 96
    KKT, 100
    Lagrange multiplier, 96
    strong duality, 103
    weak duality, 104
    Weierstraß, 98
theory, 65, 66, 69
    DE undecidability, 69
    decidable, 64
threshold, 80
time
    completion, 22
        maximum, 22
    current, 138
    index, 24
    infinite, 139
    infinity, 140
timetable, 26
TM, 61, 68, 74
    nondeterministic, 74, 75
    polytime, 75
    variant, 73
tolerance, 120, 138, 144, 147
    convergence, 148
TOMLAB, 42
trace, 74
    polynomially long, 88
tractable, 73
    case, 84
trade-off, 61
transcendental, 62
transformation
    projective, 117
    symbolic, 39
transition
    relation, 75, 76
translation, 29
    module, 41
translator, 41
    Matlab, 42
transportation, 15, 27, 123
    problem, 27
transportation problem, 42
travelling
    salesman, 124
tree, 133
    directed, 32, 141
    expression, 32, 150
    parsing, 32
    root, 141
    search, 131
    structure, 131
triangle, 98
triplet, 151
TRS, 81
trust region, 81
    radius, 81
TSP, 124
TUM, 122
    identity, 122
    matrix, 122
    property, 122
tunneling, 140
tuple, 34, 75
Turing, 61
    machine, 61
        universal, 61
Turing machine, 61
    universal, 36
Turing-complete, 36, 61
Turing-equivalent, 61
turning
    point, 153
two-phase
    simplex
        method, 111

UDE, 68
    complexity measure, 68
    degree, 68
unbounded, 37, 87, 102, 108, 113, 114
    direction, 108
    problem, 110
unboundedness, 69, 85, 105, 113, 114, 116
unconstrained
    problem, 120
uncountably many, 37
undecidable, 66–68, 78
    problem, 67
underestimating
    solution, 145
underestimation, 148
    convex, 146
underestimator
    convex, 144, 150
    tighter, 144
uniform
    distribution, 107
unimodular, 121, 123
unimodularity, 122
    total, 121
union, 131
unit, 19
univariate
    concave, 152
    convex, 153
    function, 137
universal

Turing machine, 61
Unix, 51
unquantified, 65
unreliability
inherent, 139
update, 111, 117, 120, 140
updated
current
point, 117
upper
bound, 145
UTM, 36, 68

valid, 130
cut, 112, 124, 133
globally, 131
hyperplane, 124
inequality, 112, 130
valid cut, 35
validation
input, 54
value, 52
current, 110
degenerate, 109
extremal, 149
maximum, 22
minimum, 112
primal, 111
negative, 86, 127
variable, 24, 27, 29, 52, 53, 65, 106, 109–112, 115, 127, 128, 131, 149, 150
additional, 23, 131, 150, 151, 153
basic, 106, 108–110, 121
binary, 22, 23, 27, 76, 78, 129, 131
bound, 151
branching, 132, 146, 153, 154
continuous, 33, 69, 78
decision, 18, 19, 22, 33, 76, 84, 86, 101, 151
dual, 102, 111, 118, 120
eliminated, 65
free, 65
index, 19, 125, 130, 151
integer, 67, 73, 132, 133
branching, 147
many, 146
new, 127
nonbasic, 106, 110, 113, 121
current, 109, 126
nonnegative, 110
number, 107, 116, 149
operand, 154
original, 151, 153
path, 112
primal, 102
product, 22, 129
program, 35, 53
range, 148, 154
ranges, 153
restriction, 17
scalar, 18, 137
scale, 116
slack, 37, 80, 116, 118, 125, 127
symbol, 35, 54
system, 55
unbounded, 69
value, 111
variable neighbourhood
search, 140
variation, 111
vector, 29, 33, 54, 55, 77, 99, 133
cost, 106
direction, 137
feasible, 37, 106, 123
function, 95
integer, 121, 123
parameter, 34
position, 29
rational, 112, 113
row, 102, 111
search
direction, 138
set, 29
unique, 106
variable, 18, 129
zero, 122
vertex, 36, 40, 94, 106, 107, 111, 123
adjacent, 40, 105, 109, 110
degenerate, 107, 109
feasible, 107
polyhedron, 105
fractional, 125
number, 108
optimal, 108
polyhedron, 105
single, 106, 107
vertices
exponentially many, 108
visualization, 52
VNS, 140, 146
algorithm, 146
volume, 115
smaller, 116
Von Neumann, 105

w.r.t., 35
weakly polytime, 78
weight, 124
well-defined, 150
Windows, 51
wlog, 37
worst case, 39, 40

XPress-MP, 35

YALMIP, 42