Mathematical Programming: Modelling and Software

Leo Liberti

LIX, École Polytechnique, France

The course

Title:	**Mathematical Programming: Modelling and Software**
Code:	INF572 (DIX)
Teacher:	Leo Liberti (`liberti@lix.polytechnique.fr`)
Timetable INF572:	wed 22,29/9, 6,13,20/10, 3,10,24/11, 15/12 0815-1000 (PC20), 1015-1230 (SI34)
URL INF572:	`http://www.lix.polytechnique.fr/~liberti/teaching/inf572-10`

Contents

1. Introduction
2. AMPL basics
3. AMPL grammar
4. Solvers
5. Mathematical Programming
6. Sudoku
7. Kissing Number Problem
8. Some useful MP theory
9. Reformulations
10. Symmetry
11. The final attack on the KNP

Introduction

Example: Set covering

There are 12 possible geographical positions $A_1, \ldots, A_{12}$ where some discharge water filtering plants can be built. These plants are supposed to service 5 cities $C_1, \ldots, C_5$; building a plant at site j ($j \in \{1, \ldots, 12\}$) has cost c_j and filtering capacity (in kg/year) f_j; the total amount of discharge water produced by all cities is 1.2×10^{11} kg/year. A plant built on site j can serve city i if the corresponding (i, j)-th entry is marked by a '*' in the table below.

	A_1	A_2	A_3	A_4	A_5	A_6	A_7	A_8	A_9	A_{10}	A_{11}	A_{12}
C_1	*		*		*		*	*				*
C_2		*	*			*			*		*	*
C_3	*	*				*	*			*		
C_4		*		*			*	*		*		*
C_5				*	*	*			*	*	*	*
c_j	7	9	12	3	4	4	5	11	8	6	7	16
f_j	15	39	26	31	34	24	51	19	18	36	41	34

What is the best placement for the plants?

Example: Sudoku

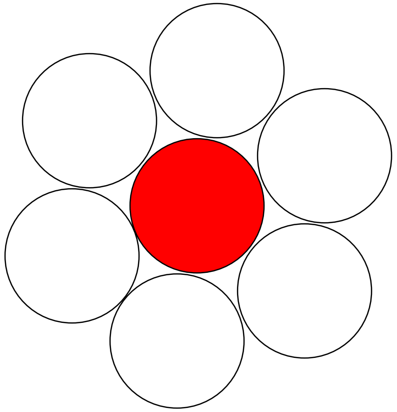
Given the Sudoku grid below, find a solution or prove that no solution exists

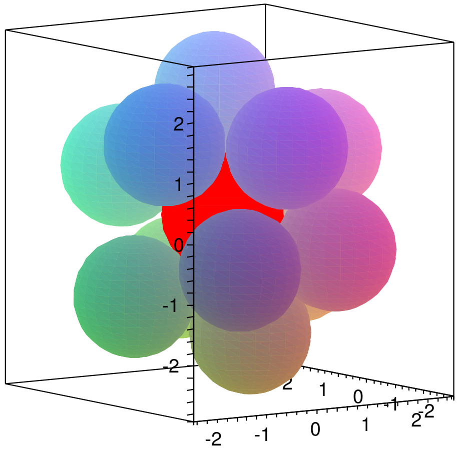
2								1
	4	1	9		2	8	6	
5	8						2	7
			5	1	3			
				9				
			7	8	6			
3	2	6					4	9
	1	9	4		5	2	8	
8								6

Example: Kissing Number

How many unit balls with disjoint interior can be placed adjacent to a central unit ball in $\mathbb{R}^d$?

In $\mathbb{R}^2$



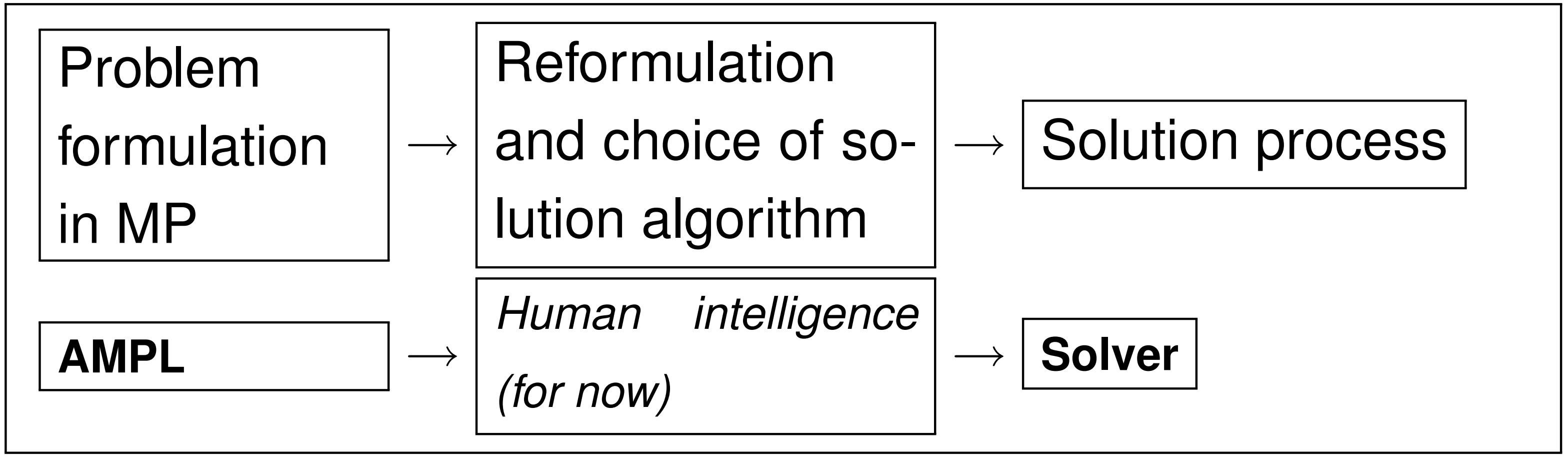


In $\mathbb{R}^3$

($D = 3$: problem proposed by Newton in 1694, settled by [Schütte and van der Waerden 1953] and [Leech 1956])

Mathematical programming

- The above three problems seemingly have *nothing* in common!
- Yet, there is a *formal language* that can be used to describe all three: **mathematical programming** (MP)
- Moreover, the MP language comes with a rich supply of solution algorithms so that problems can be solved right away



Problem formulation in MP → Reformulation and choice of solution algorithm → Solution process

AMPL → *Human intelligence (for now)* → **Solver**

MP language implementations

Software packages implementing (sub/supersets of the) MP language:

- **AMPL (our software of choice, mixture of MP and near-C language)**
  - commercial, but student version limited to 300 vars/constrs is available from `www.ampl.com`
  - quite a lot of solvers are hooked to AMPL
- GNU MathProg (subset of AMPL)
  - free, but only the GLPK solver (for LPs and MILPs) can be used
  - it is a significant subset of AMPL but not complete
- GAMS (can do everything AMPL can, but looks like COBOL — ugh!)
  - commercial, limited demo available from `www.gams.com`
  - quite a lot of solvers are hooked to GAMS
- Zimpl (free, C++ interface, linear modelling only)
- LINDO, MPL, . . . (other commercial modelling/solution packages)

How to model

Asking yourself the following questions should help you get started with your MP model

- The given problem is usually a particular *instance* of a *problem class*; you should model the whole class, not just the instance (replace given numbers by parameter symbols)
- What are the decisions to be taken? Are they logical, integer or continuous?
- What is the objective function? Is it to be minimized or maximized?
- What constraints are there in the problem? Beware — some constraints may be “hidden” in the problem text

If expressing objective and constraints is overly difficult, go back and change your variable definitions

Set covering 1

Let us now consider the Set Covering problem

What is the problem class?

- We replace the number 12 by the parameter symbol n, the number 5 by m and the number 1.2×10^{11} by d
- We already have symbols for costs (c_j) and capacities (f_j), where $j \leq n$ and $i \leq m$
- We represent the asterisks by a 0-1 matrix $A = (a_{ij})$ where $a_{ij} = 1$ if there is an asterisk at row i, column j of the table, and 0 otherwise

Set covering 2

What are the decisions to be taken?

- The crucial text in the problem is *what is the best placement for the plants?*; i.e. we need to **place each plant at some location**
  1. geographical placement on a plane? (continuous variables)
  2. yes/no placement? ("should the j-th plant be placed here?" — logical 0-1 variables)
- Because the text also says *there are n possible geographical positions...*, it means that for each position we have to decide **whether or not to build a plant** there
- For each of geographical position, introduce a **binary variable** (taking 0-1 values):

$$\forall j \leq n \quad x_j \in \{0, 1\}$$

Set covering 3

What is the objective function?

- In this case we only have the indication *best placement* in the text
- Given our data, two possibilities exist: cost (minimization) and filtering capacity (maximization)
- However, because of the presence of the parameter d, it wouldn't make sense to have more aggregated filtering capacity than d kg/year
- Hence, the objective function is the cost, which should be minimized:

$$\min \sum_{j \le n} c_j x_j$$

Set covering 4

What are the constraints?

- The total filtering capacity must be at least d:

$$\sum_{j \leq n} f_j x_j \geq d$$

- Each city must be served by at least one plant:

$$\forall i \leq m \quad \sum_{j \leq n} a_{ij} x_j \geq 1$$

- Because there are no more constraints in the text, this concludes the first modelling phase

Analysis

- What category does this mathematical program belong to?
  - Linear Programming (LP)
  - Mixed-Integer Linear Programming (MILP)
  - Nonlinear Programming (NLP)
  - Mixed-Integer Nonlinear Programming (MINLP)
- Does it have any notable mathematical property?
  - If an NLP, are the functions/constraints convex?
  - If a MILP, is the constraint matrix Totally Unimodular (TUM)?
  - Does it have any apparent symmetry?
- **Can it be reformulated to a form for which a fast solver is available?**

Set covering 5

- The objective function and all constraints are *linear forms*
- All the decision variables are *binary*
- Hence the problem is a MILP (actually, a BLP)
- **Good solutions** can be obtained via heuristics (e.g. local branching, feasibility pump, VNS, Tabu Search)
- **Exact solution** via Branch-and-Bound (solver: CPLEX)
- No need for reformulation: CPLEX is a fast enough solver
- CPLEX 11.0.1 solution: $x_4 = x_7 = x_{11} = 1$, all the rest 0 (i.e. build plants at positions 4,7,11)
- Notice the paradigm $\boxed{\text{model \& solver} \rightarrow \text{solution}}$

Since there are many solvers already available, $\boxed{\textit{solving the problem}}$ reduces to $\boxed{\textbf{modelling the problem}}$

AMPL Basics

AMPL

- AMPL means “A Mathematical Programming Language”
- AMPL is an implementation of the Mathematical Programming language
- Many solvers can work with AMPL
- AMPL works as follows:
  1. translates a user-defined model to a low-level formulation (called *flat form*) that can be understood by a solver
  2. passes the flat form to the solver
  3. reads a solution back from the solver and interprets it within the higher-level model (called *structured form*)

Model, data, run

- AMPL usually requires three files:
  - the *model* file (extension `.mod`) holding the MP formulation
  - the *data* file (extension `.dat`), which lists the values to be assigned to each parameter symbol
  - the *run* file (extension `.run`), which contains the (imperative) commands necessary to solve the problem
- The model file is written in the MP language
- The data file simply contains numerical data together with the corresponding parameter symbols
- The run file is written in an imperative C-like language (many notable differences from C, however)
- Sometimes, MP language and imperative language commands can be mixed in the same file (usually the run file)

To run AMPL, type `ampl < problem.run` from the command line

An elementary run file

- Consider the set covering problem, suppose we have coded the model file (`setcovering.mod`) and the data file (`setcovering.dat`), and that the CPLEX solver is installed on the system
- Then the following is a basic `setcovering.run` file

```
# basic run file for setcovering problem
model setcovering.mod; # specify model file
data setcovering.dat;  # specify data file
option solver cplex;   # specify solver
solve;                 # solve the problem
display cost;          # display opt. cost
display x;             # display opt. soln.
```

Set covering model file

```
# setcovering.mod
param m integer, >= 0;
param n integer, >= 0;
set M := 1..m;
set N := 1..n;

param c{N} >= 0;
param a{M,N} binary;
param f{N} >= 0;
param d >= 0;

var x{j in N} binary;

minimize cost: sum{j in N} c[j]*x[j];
subject to capacity: sum{j in N} f[j]*x[j] >= d;
subject to covering{i in M}: sum{j in N} a[i,j]*x[j] >= 1;
```

Set covering data file

```
param m := 5;
param n := 12;
param   :    c    f  :=
       1     7   15
       2     9   39
       3    12   26
       4     3   31
       5     4   34
       6     4   24
       7     5   51
       8    11   19
       9     8   18
      10     6   36
      11     7   41
      12    16   34  ;
param a:     1   2   3   4   5   6   7   8   9  10  11  12  :=
      1      1   0   1   0   1   0   1   1   0   0   0   0
      2      0   1   1   0   0   1   0   0   1   0   1   1
      3      1   1   0   0   0   1   1   0   0   1   0   0
      4      0   1   0   1   0   0   1   1   0   1   0   1
      5      0   0   0   1   1   1   0   0   1   1   1   1  ;
param d := 120;
```

AMPL+CPLEX solution

```
liberti@nox$ cat setcovering.run | ampl
ILOG CPLEX 11.010, options: e m b q use=2
CPLEX 11.0.1: optimal integer solution; objective 15
3 MIP simplex iterations
0 branch-and-bound nodes
cost = 15
x [*] :=
 1  0
 2  0
 3  0
 4  1
 5  0
 6  0
 7  1
 8  0
 9  0
10  0
11  1
12  0
;
```

AMPL Grammar

AMPL MP Language

- There are 5 main entities: sets, parameters, variables, objectives and constraints
- In AMPL, each entity has a name and can be quantified
  - `set` *name* [{*quantifier*}] *attributes* ;
  - `param` *name* [{*quantifier*}] *attributes* ;
  - `var` *name* [{*quantifier*}] *attributes* ;
  - `minimize` | `maximize` *name* [{*quantifier*}]`:` *iexpr* ;
  - `subject to` *name* [{*quantifier*}]`:` *iexpr* <= | = | >= *iexpr* ;
- Attributes on sets and parameters is used to validate values read from data files
- Attributes on vars specify integrality (`binary`, `integer`) and limit constraints (`>= lower`, `<= upper`)
- Entities indices: square brackets (e.g. `y[1]`, `x[i,k]`)
- The above is the basic syntax — there are some advanced options

AMPL data specification

In general, syntax is in map-like form; a

```
param p{i in S} integer;
```

is a map $S \to \mathbb{Z}$, and each pair (domain, codomain) must be specified:

```
param p :=
  1  4
  2 -3
  3  0;
```

The grammar is simple but tedious, best way is learning by example or trial and error

AMPL imperative language

- `model` *model_filename.mod* ;
- `data` *data_filename.dat* ;
- `option` *option_name literal_string*, ... ;
- `solve` ;
- `display` [{*quantifier*}] *iexpr* ; / `printf` (syntax similar to C)
- `let` [{*quantifier*}] *ivar* `:=`*number*;
- `if (`*condition_list*`) then {` *commands* `}` [`else {`*commands*`}`]
- `for {`*quantifier*`} {`*commands*`}` / `break;` / `continue;`
- `shell '` *command_line*`'` ; / `exit` *number*; / `quit;`
- `cd` *dir_name*; / `remove` *file_name*;
- In all output commands, screen output can be redirected to a file by appending > *output_filename.txt* before the semicolon
- These are basic commands, there are some advanced ones

Reformulation commands

- `fix` [{*quantifier*}] *ivar* [`:=`*number*]`;`
- `unfix` [{*quantifier*}] *ivar*`;`
- `delete` *entity_name*`;`
- `purge` *entity_name*`;`
- `redeclare` *entity_declaration*`;`
- `drop/restore` [{*quantifier*}] *constr_or_obj_name*`;`
- `problem` *name*[{*quantifier*}] [`:` *entity_name_list*] `;`
- This list is not exhaustive

Solvers

Solvers

In order of solver reliability / effectiveness:

1. **LPs**: use an LP solver ($O(10^6)$ vars/constrs, fast, e.g. CPLEX, CLP, GLPK)
2. **MILPs**: use a MILP solver ($O(10^4)$ vars/constrs, can be slow, e.g. CPLEX, Symphony, GLPK)
3. **NLPs**: use a local NLP solver to get a local optimum ($O(10^4)$ vars/constrs, quite fast, e.g. SNOPT, MINOS, IPOPT)
4. **NLPs/MINLPs**: use a heuristic solver to get a good local optimum ($O(10^3)$, quite fast, e.g. BONMIN, MINLP_BB)
5. **NLPs**: use a global NLP solver to get an (approximated) global optimum ($O(10^3)$ vars/constrs, can be slow, e.g. COUENNE, BARON)
6. **MINLPs**: use a global MINLP solver to get an (approximated) global optimum ($O(10^3)$ vars/constrs, can be slow, e.g. COUENNE, BARON)

Not all these solvers are available via AMPL

Solution algorithms (linear)

- **LPs**: *(convex)*
  1. simplex algorithm (non-polynomial complexity but very fast in practice, reliable)
  2. interior point algorithms (polynomial complexity, quite fast, fairly reliable)
- **MILPs**: *(nonconvex because of integrality)*
  1. *Local* (heuristics): Local Branching, Feasibility Pump [Fischetti&Lodi 05], VNS [Hansen et al. 06] (quite fast, reliable)
  2. *Global*: Branch-and-Bound (exact algorithm, non-polynomial complexity but often quite fast, heuristic if early termination, reliable)

Solution algorithms (nonlinear)

- **NLPs**: *(may be convex or nonconvex)*
  1. *Local*: Sequential Linear Programming (SLP), Sequential Quadratic Programming (SQP), interior point methods (linear/polynomial convergence, often quite fast, unreliable)
  2. *Global*: spatial Branch-and-Bound [Smith&Pantelides 99] (ε-approximate, nonpolynomial complexity, often quite slow, heuristic if early termination, unreliable)
- **MINLPs**: *(nonconvex because of integrality and terms)*
  1. *Local* (heuristics): Branching explorations [Fletcher&Leyffer 99], Outer approximation [Grossmann 86], Feasibility pump [Bonami et al. 06] (nonpolynomial complexity, often quite fast, unreliable)
  2. *Global*: spatial Branch-and-Bound [Sahinidis&Tawarmalani 05] (ε-approximate, nonpolynomial complexity, often quite slow, heuristic if early termination, unreliable)

Canonical MP formulation

$$\left.\begin{array}{rcccc} \min_x & f(x) & & & \\ \text{s.t.} & l \leq & g(x) & \leq u & \\ & x^L \leq & x & \leq x^U & \\ \forall i \in Z \subseteq \{1,\ldots,n\} & x_i & \in & \mathbb{Z} & \end{array}\right\} [P] \qquad (1)$$

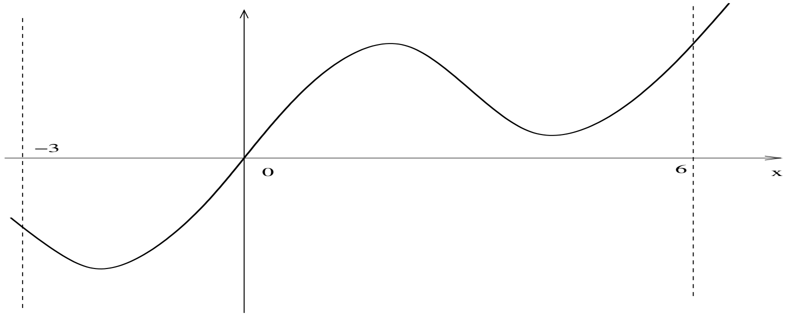
where $x, x^L, x^U \in \mathbb{R}^n$; $l, u \in \mathbb{R}^m$; $f : \mathbb{R}^n \to \mathbb{R}$; $g : \mathbb{R}^n \to \mathbb{R}^m$

- A point x^* is *feasible* in P if $l \leq g(x^*) \leq u$, $x^L \leq x^* \leq x^U$ and $\forall i \in Z$ $(x_i^* \in \mathbb{Z})$; $F(P) =$ set of feasible points of P
- If $g_i(x^*) = l$ or $= u$ for some i, g_i is *active at* x^*
- A feasible x^* is a *local minimum* if $\exists B(x^*, \varepsilon)$ s.t. $\forall x \in F(P) \cap B(x^*, \varepsilon)$ we have $f(x^*) \leq f(x)$
- A feasible x^* is a *global minimum* if $\forall x \in F(P)$ we have $f(x^*) \leq f(x)$

Feasibility and optimality

- $F(P) =$ feasible region of P, $L(P) =$ set of local optima, $G(P) =$ set of global optima
- Nonconvexity $\Rightarrow G(P) \subsetneq L(P)$

$$\min_{x\in[-3,6]} \frac{1}{4}x + \sin(x)$$

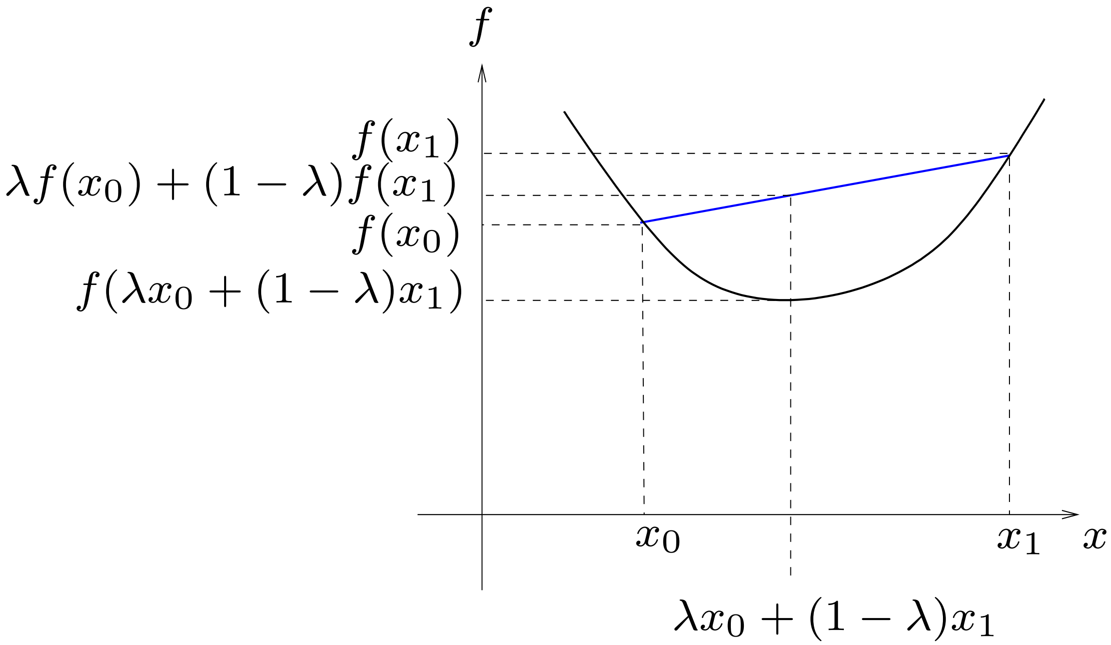


Convexity

- A function $f(x)$ is convex if the following holds:

$$\forall x_0, x_1 \in \text{dom}(f) \quad \forall \lambda \in [0,1]$$

$$f(\lambda x_0 + (1-\lambda)x_1) \quad \leq \quad \lambda f(x_0) + (1-\lambda) f(x_1)$$



f
$f(x_1)$
$\lambda f(x_0) + (1-\lambda) f(x_1)$
$f(x_0)$
$f(\lambda x_0 + (1-\lambda)x_1)$
x_0
x_1
x
$\lambda x_0 + (1-\lambda)x_1$

- A set $C \subseteq \mathbb{R}^n$ is convex if $\forall x_0, x_1 \in C, \lambda \in [0,1] \; (\lambda x_0 + (1-\lambda)x_1 \in C)$
- If $g : \mathbb{R}^m \to \mathbb{R}^n$ are convex, then $\{x \mid g(x) \leq 0\}$ is a convex set
- If f, g are convex, then every local optimum of $\min\limits_{g(x) \leq 0} f(x)$ is global
- **A local NLP solver suffices to solve the NLP to optimality**

Canonical form

- P is a *linear programming problem* (LP) if $f : \mathbb{R}^n \to \mathbb{R}$, $g : \mathbb{R}^n \to \mathbb{R}^m$ are **linear forms**
- LP in *canonical form*:

$$\left.\begin{array}{rl} \min_x & c^{\mathsf{T}} x \\ \text{s.t.} & Ax \le b \\ & x \ge 0 \end{array}\right\} [C] \qquad (2)$$

- Can reformulate inequalities to equations by adding a non-negative *slack variable* $x_{n+1} \ge 0$:

$$\sum_{j=1}^{n} a_j x_j \le b \;\Rightarrow\; \sum_{j=1}^{n} a_j x_j + x_{n+1} = b \;\wedge\; x_{n+1} \ge 0$$

Standard form

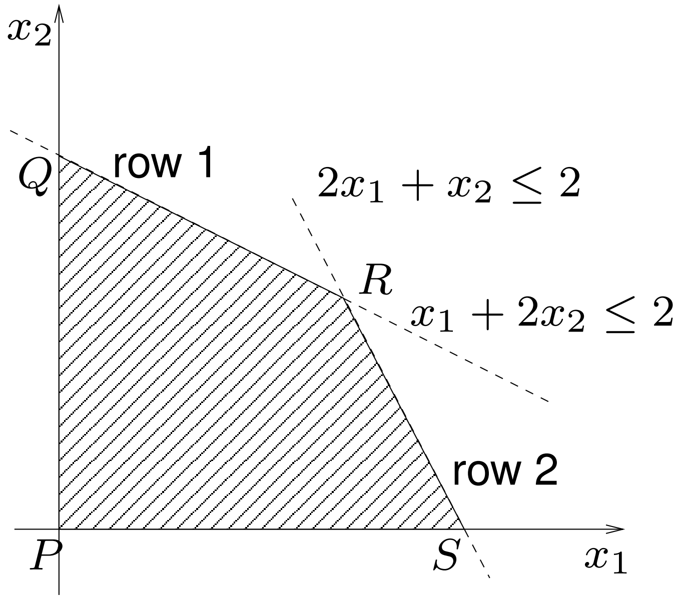
- LP in *standard form*: all inequalities transformed to equations

$$\left.\begin{array}{rl} \min_x & (c')^{\mathsf{T}} x \\ \text{s.t.} & A'x = b \\ & x \geq 0 \end{array}\right\} [S] \tag{3}$$

- where $x = (x_1, \ldots, x_n, x_{n+1}, \ldots, x_{n+m})$, $A' = (A, I_m)$, $c' = (c, \underbrace{0, \ldots, 0}_{m})$
- Standard form useful because linear systems of equations are computationally easier to deal with than systems of inequalities
- Used in simplex algorithm

Geometry of LP

- A *polyhedron* is the intersection of a finite number of closed halfspaces. A bounded, non-empty polyhedron is a *polytope*



Canonical feas. polyhedron: $F(C) = \{x \in \mathbb{R}^n \mid Ax \le b \ \wedge \ x \ge 0\}$

$A = \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix}$, $b^\mathsf{T} = (2,2)$

Standard feas. polyhedron: $F(S) = \{(x,y) \in \mathbb{R}^{n+m} \mid Ax + I_m y = b \ \wedge \ (x,y) \ge 0\}$

- $P = (0,0,2,2), Q = (0,1,0,1), R = (\frac{2}{3}, \frac{2}{3}, 0, 0), S = (1,0,1,0)$
- Each vertex corresponds to an intersection of at least n hyperplanes $\Rightarrow$ $\ge n$ coordinates are zero

Basic feasible solutions

- Consider polyhedron in “equation form” $K = \{x \in \mathbb{R}^n \mid Ax = b \wedge x \geq 0\}$. A is $m \times n$ of rank m **(N.B. n here is like $n + m$ in last slide!)**
- A subset of m linearly independent columns of A is a *basis* of A
- If β is the set of column indices of a basis of A, variables x_i are *basic* for $i \in \beta$ and *nonbasic* for $i \notin \beta$
- Partition A in a square $m \times m$ nonsingular matrix B (columns indexed by β) and an $(n - m) \times m$ matrix N
- Write $A = (B|N)$, $x_B \in \mathbb{R}^m$ basics, $x_N \in \mathbb{R}^{n-m}$ nonbasics
- Given a basis $(B|N)$ of A, the vector $x = (x_B, x_N)$ is a *basic feasible solution* (bfs) of K with respect to the given basis if $Ax = b$, $x_B \geq 0$ and $x_N = 0$

Fundamental Theorem of LP

- Given a non-empty polyhedron K in “equation form”, there is a surjective mapping between bfs and vertices of K
- For any $c \in \mathbb{R}^n$, either there is at least one bfs that solves the LP $\min\{c^{\mathsf{T}}x \,|x \in K\}$, or the problem is unbounded
- Proofs not difficult but long (see lecture notes or Papadimitriou and Steiglitz)
- Important correspondence between bfs’s and vertices suggests geometric solution method based on exploring vertices of K

Simplex Algorithm: Summary

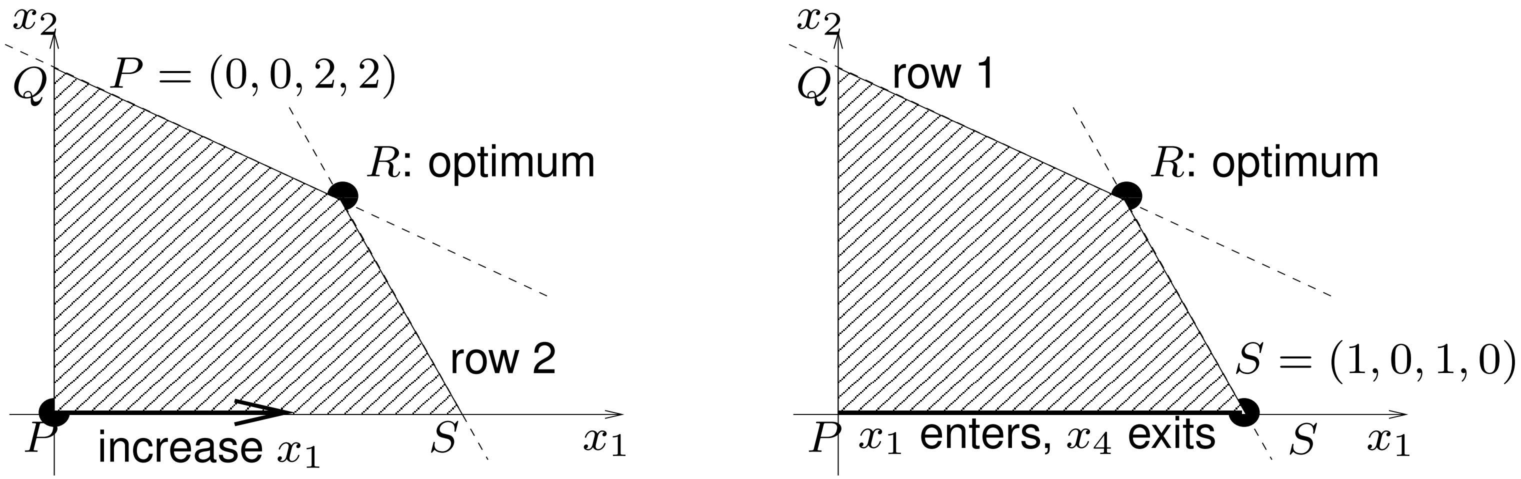
- Solves LPs in form $\min\limits_{x\in K} c^{\mathsf{T}}x$ where $K = \{Ax = b \wedge x \geq 0\}$
- Starts from any vertex x
- Moves to an adjacent improving vertex x'
(i.e. x' is s.t. $\exists$ edge $\{x, x'\}$ in K and $c^{\mathsf{T}}x' \leq c^{\mathsf{T}}x$)
- Two bfs's with basic vars indexed by sets β, β' correspond to adjacent vertices if $|\beta \cap \beta'| = m - 1$
- Stops when no such x' exists
- Detects unboundedness and prevents cycling $\Rightarrow$ convergence
- K convex $\Rightarrow$ global optimality follows from local optimality at termination

Simplex Algorithm I

- Let $x = (x_1, \ldots, x_n)$ be the current bfs, write $Ax = b$ as $Bx_B + Nx_N = b$
- Express basics in terms of nonbasics: $x_B = B^{-1}b - B^{-1}Nx_N$ (this system is a *dictionary*)
- Express objective function in terms of nonbasics: $c^\mathsf{T}x = c_B^\mathsf{T}x_B + c_N^\mathsf{T}x_N = c_B^\mathsf{T}(B^{-1}b - B^{-1}Nx_N) + c_N^\mathsf{T}x_N \Rightarrow$
  $\Rightarrow c^\mathsf{T}x = c_B^\mathsf{T}B^{-1}b + \bar{c}_N^\mathsf{T}x_N$
  ($\bar{c}_N^\mathsf{T} = c_N^\mathsf{T} - c_B^\mathsf{T}B^{-1}N$ are the *reduced costs*)
- Select an improving direction: choose a nonbasic variable x_h with negative reduced cost; increasing its value will decrease the objective function value
- If no such h exists, no improving direction, local minimum ⇒ global minimum ⇒ termination

Simplex Algorithm II

- Iteration start: x_h is out of basis $\Rightarrow$ its value is zero
- We want to increase its value to strictly positive to decrease objective function value
- ...corresponds to "moving along an edge"
- We stop when we reach another (improving) vertex
- ...corresponds to setting a basic variable x_l to zero



- x_h enters the basis, x_l exits the basis

Simplex Algorithm III

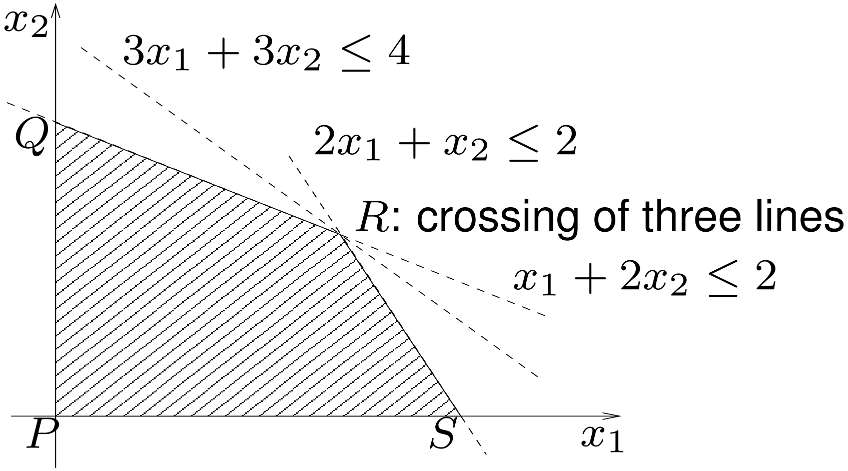
- How do we determine l and new positive value for x_h?
- Recall dictionary $x_B = B^{-1}b - B^{-1}Nx_N$,
  write $\bar{b} = B^{-1}b$ and $\bar{A} = (\bar{a}_{ij}) = B^{-1}N$
- For $i \in \beta$ (basics), $x_i = \bar{b}_i - \sum_{j\notin\beta} \bar{a}_{ij}x_j$
- Consider nonbasic index h of variable entering basis (all the other nonbasics stay at 0), get $x_i = \bar{b}_i - \bar{a}_{ih}x_h, \forall i \in \beta$
- Increasing x_h may make $x_i < 0$ (infeasible), to prevent this enforce $\forall i \in \beta\ (\bar{b}_i - \bar{a}_{ih}x_h \geq 0)$
- Require $x_h \leq \frac{\bar{b}_i}{\bar{a}_{ih}}$ for $i \in \beta$ and $\bar{a}_{ih} > 0$:

$$l = \text{argmin}\{\frac{\bar{b}_i}{\bar{a}_{ih}} \mid i \in \beta \wedge \bar{a}_{ih} > 0\}, \qquad x_h = \frac{\bar{b}_l}{\bar{a}_{lh}}$$

- If all $\bar{a}_{ih} \leq 0$, x_h can increase without limits: problem unbounded

Simplex Algorithm IV

- Suppose $> n$ hyperplanes cross at vtx R (*degenerate*)
- May get improving direction s.t. adjacent vertex is still R
- Objective function value does not change
- Seq. of improving dirs. may fail to move away from R
- $\Rightarrow$ simplex algorithm cycles indefinitely
- Use Bland's rule: among candidate entering / exiting variables, choose that with *least index*



Example: Formulation

- Consider problem:

$$\left.\begin{array}{rl}\max\limits_{x_1,x_2} & x_1+x_2 \\ \text{s.t.} & x_1+2x_2\le 2 \\ & 2x_1+x_2\le 2 \\ & x\ge 0\end{array}\right\}$$

- Standard form:

$$\left.\begin{array}{rl}-\min_x & -x_1-x_2 \\ \text{s.t.} & x_1+2x_2+x_3=2 \\ & 2x_1+x_2+x_4=2 \\ & x\ge 0\end{array}\right\}$$

- Obj. fun.: $\max f = -\min -f$, simply solve for $\min -f$

Example, itn 1: start

- Objective function vector $c^{\mathsf{T}} = (-1, -1, 0, 0)$
- Constraints in matrix form:

$$\begin{pmatrix} 1 & 2 & 1 & 0 \\ 2 & 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 2 \\ 2 \end{pmatrix}$$

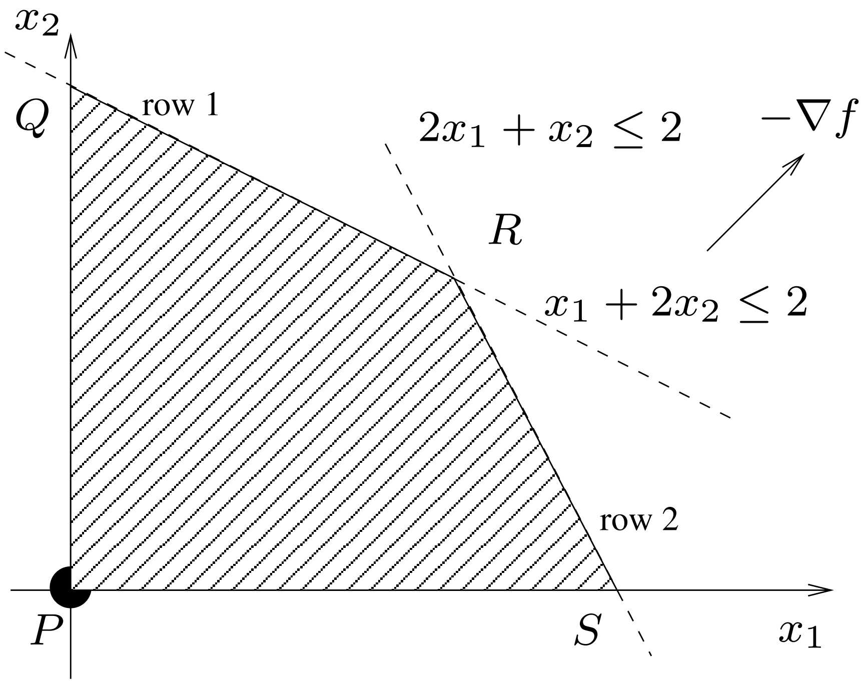
- Choose obvious starting basis with

$$B = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, N = \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix}, \beta = \{3, 4\}$$

- Corresponds to point $P = (0, 0, 2, 2)$

Example, itn 1: dictionary

- Start the simplex algorithm with basis in P



- Compute dictionary $x_B = B^{-1}b - B^{-1}Nx_N = \bar{b} - \bar{A}x_N$, where

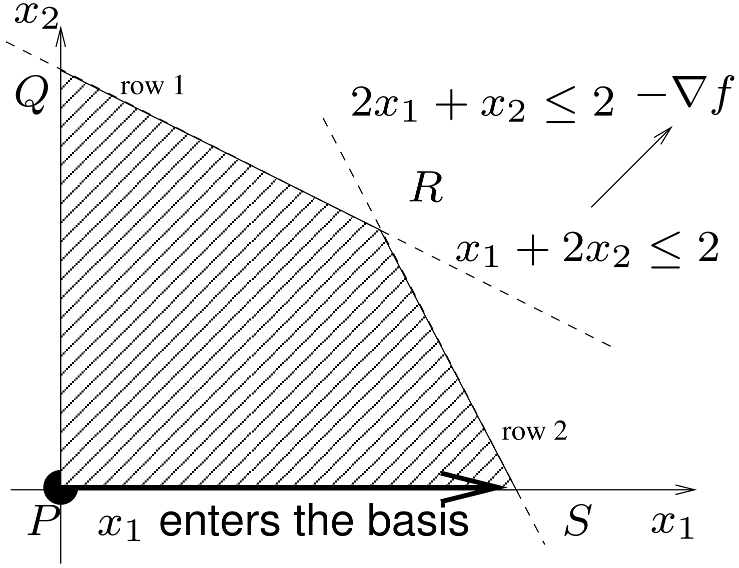
$$\bar{b} = \begin{pmatrix} 2 \\ 2 \end{pmatrix} \quad ; \quad \bar{A} = \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix}$$

Example, itn 1: entering var

- Compute reduced costs $\bar{c}_N = c_N^\top - c_B^\top \bar{A}$:

$$(\bar{c}_1, \bar{c}_2) = (-1, -1) - (0, 0)\bar{A} = (-1, -1)$$

- All nonbasic variables $\{x_1, x_2\}$ have negative reduced cost, can choose whichever to enter the basis
- Bland's rule: choose entering nonbasic with least index in $\{x_1, x_2\}$, i.e. pick $h = 1$ (move along edge $\overline{PS}$)



Example, itn 1: exiting var

- Select exiting basic index l

$$\begin{aligned} l &= \text{argmin}\{\frac{\bar{b}_i}{\bar{a}_{ih}} \mid i \in \beta \wedge \bar{a}_{ih} > 0\} = \text{argmin}\{\frac{\bar{b}_1}{\bar{a}_{11}}, \frac{\bar{b}_2}{\bar{a}_{21}}\} \\ &= \text{argmin}\{\frac{2}{1}, \frac{2}{2}\} = \text{argmin}\{2, 1\} = 2 \end{aligned}$$

- Means: “select second basic variable to exit the basis”, i.e. x_4
- Select new value $\frac{\bar{b}_l}{\bar{a}_{lh}}$ for x_h (recall $h = 1$ corrresponds to x_1):

$$\frac{\bar{b}_l}{\bar{a}_{lh}} = \frac{\bar{b}_2}{\bar{a}_{21}} = \frac{2}{2} = 1$$

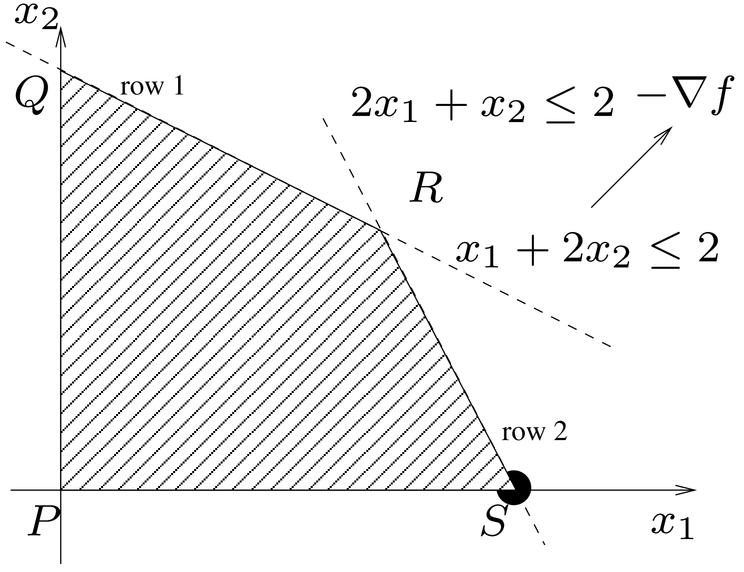
- x_1 enters, x_4 exits (apply swap $(1, 4)$ to β)

Example, itn 2: start

- Start of new iteration: basis is $\beta = \{1, 3\}$

$$B = \begin{pmatrix} 1 & 1 \\ 2 & 0 \end{pmatrix} \quad ; \quad B^{-1} = \begin{pmatrix} 0 & \frac{1}{2} \\ 1 & -\frac{1}{2} \end{pmatrix}$$

- $x_B = (x_1, x_3) = B^{-1}b = (1, 1)$, thus current bfs is $(1, 0, 1, 0) = S$

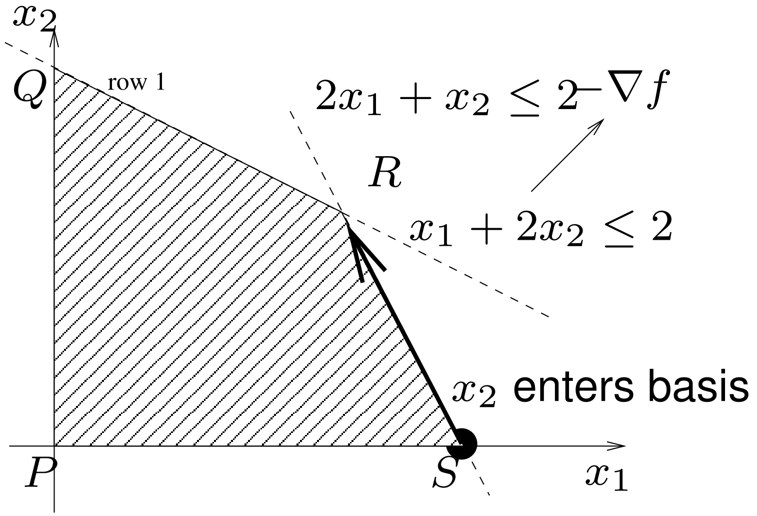


Example, itn 2: entering var

- Compute dictionary: $\bar{b} = B^{-1}b = (1,1)^\mathsf{T}$,

$$\bar{A} = B^{-1}N = \begin{pmatrix} 0 & \frac{1}{2} \\ 1 & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} 2 & 0 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{3}{2} & -\frac{1}{2} \end{pmatrix}$$

- Compute reduced costs:
  $(\bar{c}_2, \bar{c}_4) = (-1, 0) - (-1, 0)\bar{A} = (-1/2, 1/2)$
- Pick $h = 1$ (corresponds to x_2 entering the basis)



Example, itn 2: exiting var

- Compute l and new value for x_2:

$$\begin{aligned} l &= \text{argmin}\{\frac{\bar{b}_1}{\bar{a}_{11}}, \frac{\bar{b}_2}{\bar{a}_{21}}\} = \text{argmin}\{\frac{1}{1/2}, \frac{1}{3/2}\} = \\ &= \text{argmin}\{2, 2/3\} = 2 \end{aligned}$$

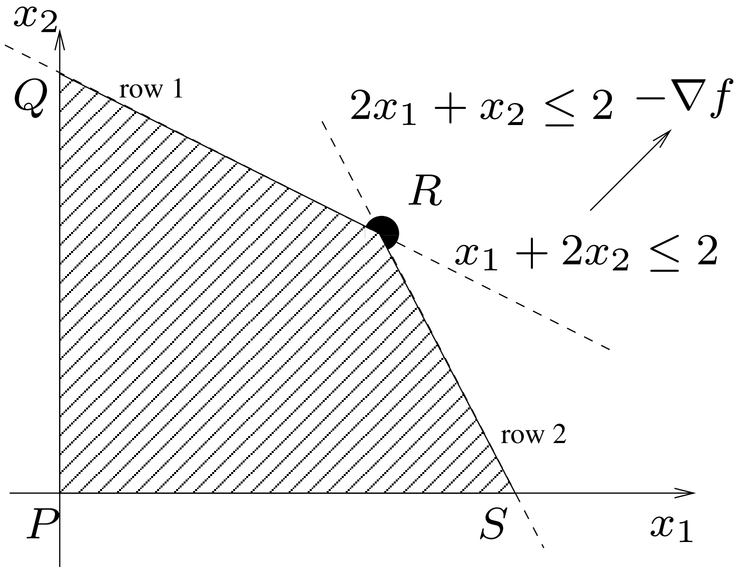
- $l = 2$ corresponds to second basic variable x_3
- New value for x_2 entering basis: $\frac{2}{3}$
- x_2 enters, x_3 exits (apply swap $(2, 3)$ to β)

Example, itn 3: start

- Start of new iteration: basis is $\beta = \{1, 2\}$

$$B = \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix} \quad ; \quad B^{-1} = \begin{pmatrix} -\frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & -\frac{1}{3} \end{pmatrix}$$

- $x_B = (x_1, x_2) = B^{-1}b = (\frac{2}{3}, \frac{2}{3})$, thus current bfs is $(\frac{2}{3}, \frac{2}{3}, 0, 0) = R$



Example, itn 3: termination

- Compute dictionary: $\bar{b} = B^{-1}b = (2/3, 2/3)^{\mathsf{T}}$,

$$\bar{A} = B^{-1}N = \begin{pmatrix} -\frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & -\frac{1}{3} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} -\frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & -\frac{1}{3} \end{pmatrix}$$

- Compute reduced costs:
  $(\bar{c}_3, \bar{c}_4) = (0, 0) - (-1, -1)\bar{A} = (1/3, 1/3)$
- No negative reduced cost: algorithm terminates
- Optimal basis: $\{1, 2\}$
- Optimal solution: $R = (\frac{2}{3}, \frac{2}{3})$
- Optimal objective function value $f(R) = -\frac{4}{3}$
- Permutation to apply to initial basis $\{3, 4\}$: $(1, 4)(2, 3)$

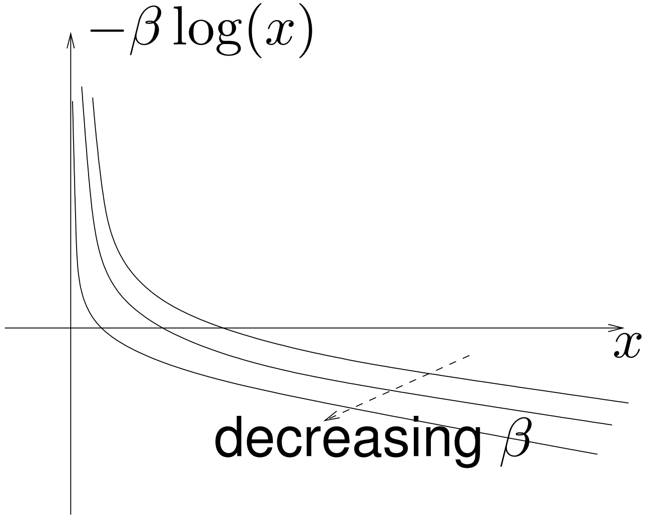
Interior point methods

- Simplex algorithm is practically efficient but nobody ever found a pivot choice rule that proves that it has polynomial worst-case running time
- Nobody ever managed to prove that such a rule does not exist
- With current pivoting rules, simplex worst-case running time is exponential
- Kachiyan managed to prove in 1979 that LP $\in$ **P** using a polynomial algorithm called *ellipsoid method* (`http://www.stanford.edu/class/msande310/ellip.pdf`)
- Ellipsoid method has polynomial worst-case running time but performs badly in practice
- Barrier interior point methods for LP have both polynomial running time and good practical performances

IPM I: Preliminaries

- Consider LP P in standard form: $\min\{c^{\mathsf{T}}x \mid Ax = b \wedge x \geq 0\}$.
- Reformulate by introducing "logarithmic barriers":

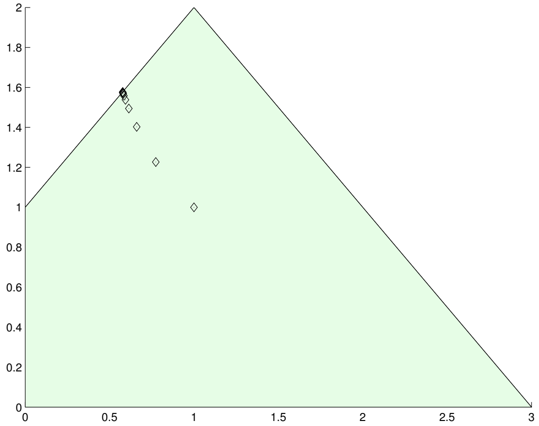
$$P(\beta) : \min\{c^{\mathsf{T}}x - \beta \sum_{j=1}^{n} \log x_j \mid Ax = b\}$$



- The term $-\beta \log(x_j)$ is a "penalty" that ensures that $x_j > 0$; the "limit" of this reformulation for $\beta \to 0$ should ensure that $x_j \geq 0$ as desired
- Notice $P(\beta)$ is convex $\forall \beta > 0$

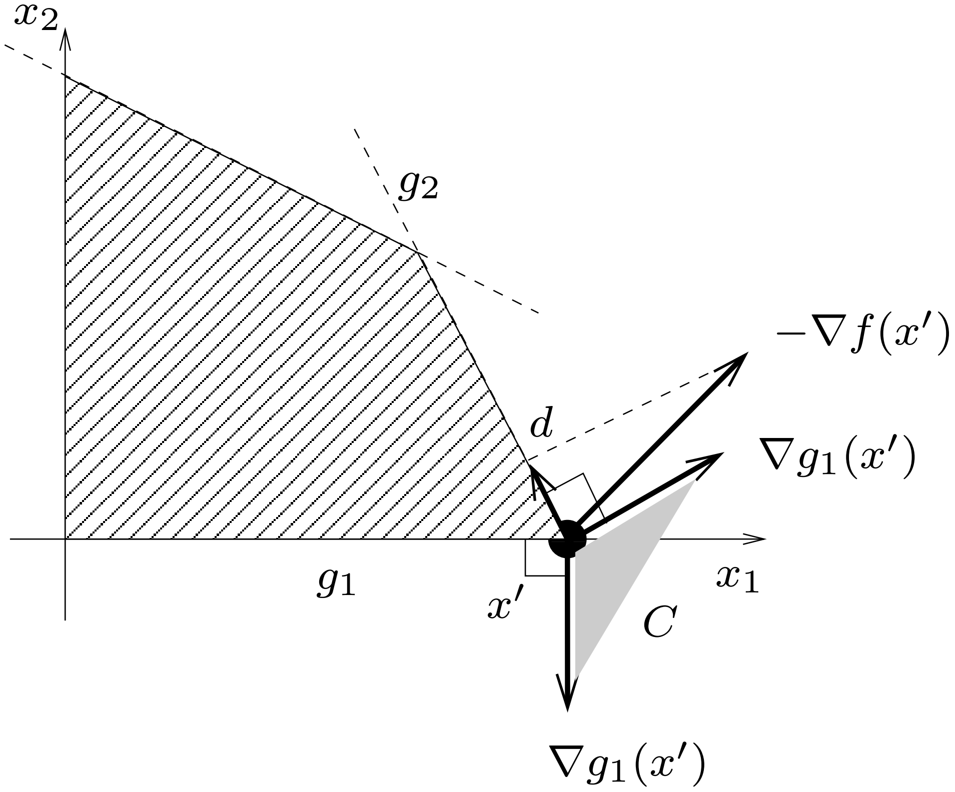
IPM II: Central path

- Let $x^*(\beta)$ the optimal solution of $P(\beta)$ and x^* the optimal solution of P
- The set $\{x^*(\beta) \mid \beta > 0\}$ is called the *central path*
- Idea: determine the central path by solving a sequence of convex problems $P(\beta)$ for some decreasing sequence of values of β and show that $x^*(\beta) \to x^*$ as $\beta \to 0$
- Since for $\beta > 0$, $-\beta \log(x_j) \to +\infty$ for $x_j \to 0$, $x^*(\beta)$ will never be on the boundary of the feasible polyhedron $\{x \geq 0 \mid Ax = b\}$; thus the name “interior point method”



Optimality Conditions I

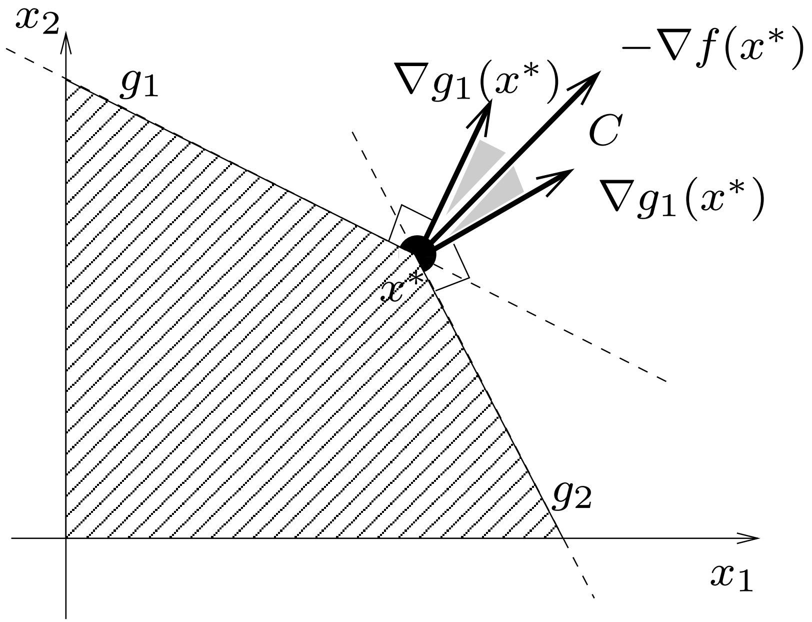
- If we can project improving direction $-\nabla f(x')$ on an active constraint g_2 and obtain a feasible direction d, point x' is not optimal



- Implies $-\nabla f(x') \notin C$ (*cone generated by active constraint gradients*)

Optimality Conditions II

- Geometric intuition: situation as above does not happen when $-\nabla f(x^*) \in C$, x^* optimum



- Projection of $-\nabla f(x^*)$ on active constraints is never a feasible direction

Optimality Conditions III

- If:

  1. x^* is a local minimum of problem $P \equiv \min\{f(x) \mid g(x) \leq 0\}$,
  2. I is the index set of the active constraints at x^*, i.e. $\forall i \in I \ (g_i(x^*) = 0)$
  3. $\nabla g_I(x^*) = \{\nabla g_i(x^*) \mid i \in I\}$ is a linearly independent set of vectors

- then $-\nabla f(x^*)$ is a conic combination of $\nabla g_I(x^*)$, i.e. $\exists y \in \mathbb{R}^{|I|}$ such that

$$\begin{aligned} \nabla f(x^*) + \sum_{i \in I} y_i \nabla g_i(x^*) &= 0 \\ \forall i \in I \ y_i &\geq 0 \end{aligned}$$

Karush-Kuhn-Tucker Conditions

- Define

$$L(x,y) = f(x) + \sum_{i=1}^{m} y_i g_i(x)$$

  as the *Lagrangian* of problem P

- KKT: If x^* is a local minimum of problem P and $\nabla g(x^*)$ is a linearly independent set of vectors, $\exists y \in \mathbb{R}^m$ s.t.

$$\begin{array}{rcl} \nabla_{x^*} L(x,y) & = & 0 \\ \forall i \le m \quad (y_i g_i(x^*) & = & 0) \\ \forall i \le m \quad (y_i & \ge & 0) \end{array}$$

Weak duality

Thm.

Let $\bar{L}(y) = \min\limits_{x \in F(P)} L(x,y)$ and x^* be the global optimum of P. Then $\forall y \geq 0 \quad \bar{L}(y) \leq f(x^*)$.

Proof

Since $y \geq 0$, if $x \in F(P)$ then $y_i g_i(x) \leq 0$, hence $L(x,y) \leq f(x)$; result follows as we are taking the minimum over all $x \in F(P)$.

- Important point: $\bar{L}(y)$ is a lower bound for P for all $y \geq 0$
- The problem of finding the tightest Lagrangian lower bound

$$\max_{y \geq 0} \min_{x \in F(P)} L(x,y)$$

is the *Lagrangian dual* of problem P

Dual of an LP I

- Consider LP P in form: $\min\{c^{\mathsf{T}}x \mid Ax \geq b \wedge x \geq 0\}$
- $L(x,s,y) = c^{\mathsf{T}}x - s^{\mathsf{T}}x + y^{\mathsf{T}}(b - Ax)$ where $s \in \mathbb{R}^n$, $y \in \mathbb{R}^m$
- Lagrangian dual:

$$\max_{s,y\geq 0} \min_{x \in F(P)} (yb + (c^{\mathsf{T}} - s - yA)x)$$

- KKT: for a point x to be optimal,

$$\begin{array}{rcl} c^{\mathsf{T}} - s - yA & = & 0 \text{ (KKT1)} \\ \forall j \leq n\ (s_j x_j = 0),\ \forall i \leq m\ (y_i(b_i - A_i x) & = & 0) \text{ (KKT2)} \\ s, y & \geq & 0 \text{ (KKT3)} \end{array}$$

- Consider Lagrangian dual s.t. (KKT1), (KKT3):

Dual of an LP II

- Obtain:

$$\left.\begin{array}{rrcl} \max\limits_{s,y} & yb & & \\ \text{s.t.} & yA+s & = & c^{\mathsf{T}} \\ & s,y & \geq & 0 \end{array}\right\}$$

- Interpret s as slack variables, get *dual of LP*:

$$\left.\begin{array}{rrcl} \min\limits_{x} & c^{\mathsf{T}}x & & \\ \text{s.t.} & Ax & \geq & b \\ & x & \geq & 0 \end{array}\right\}[P] \longrightarrow \left.\begin{array}{rrcl} \max\limits_{y} & yb & & \\ \text{s.t.} & yA & \leq & c^{\mathsf{T}} \\ & y & \geq & 0 \end{array}\right\}[D]$$

Alternative derivation of LP dual

- Lagrangian dual $\Rightarrow$ find tightest lower bound for LP $\min c^\mathsf{T} x$ s.t. $Ax \ge b$ and $x \ge 0$
- Multiply constraints $Ax \ge b$ by coefficients $y_1, \dots, y_m$ to obtain the inequalities $y_i Ax \ge y_i b$, valid provided $y \ge 0$
- Sum over i: $\sum_i y_i Ax \ge \sum_i y_i b = yAx \ge yb$
- Look for y such that obtained inequalities are as stringent as possible whilst still a lower bound for $c^\mathsf{T} x$
- $\Rightarrow yb \le yAx$ and $yb \le c^\mathsf{T} x$
- Suggests setting $yA = c^\mathsf{T}$ and maximizing yb
- Obtain LP dual: $\max yb$ s.t. $yA = c^\mathsf{T}$ and $y \ge 0$.

Strong Duality for LP

Thm.

If x is optimum of a linear problem and y is the optimum of its dual, primal and dual objective functions attain the same values at x and respectively y.

Proof

- Assume x optimum, KKT conditions hold
- Recall (KKT2) $\forall j \le n (s_i x_i = 0)$, $\forall i \le m \; (y_i(b_i - A_i x) = 0)$
- Get $y(b - Ax) = sx \Rightarrow yb = (yA + s)x$
- By (KKT1) $yA + s = c^{\mathsf{T}}$
- Obtain $yb = c^{\mathsf{T}} x$

Strong Duality for convex NLPs I

- Theory of KKT conditions derived for generic NLP $\min f(x)$ s.t. $g(x) \leq 0$, independent of linearity of f, g
- Derive strong duality results for convex NLPs
- Slater condition $\exists x' \in F(P)\ (g(x') < 0)$ requires non-empty interior of $F(P)$
- Let $f^* = \min_{x:g(x)\leq 0} f(x)$ be the optimal objective function value of the primal problem P
- Let $p^* = \max_{y\geq 0} \min_{x\in F(P)} L(x,y)$ be the optimal objective function value of the Lagrangian dual

Thm.

If f, g are convex functions and Slater's condition holds, then $f^* = p^*$.

Strong Duality for convex NLPs II

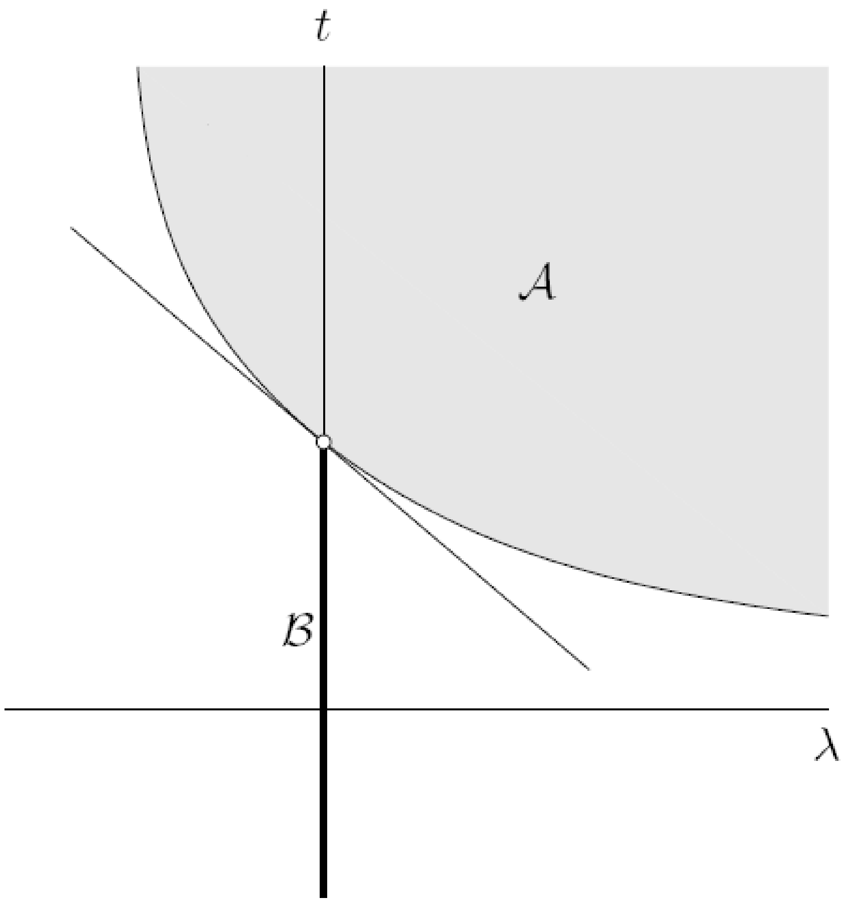
Proof

- Let $\mathcal{A} = \{(\lambda, t) \mid \exists x \ (\lambda \geq g(x) \wedge t \geq f(x))\}$, $\mathcal{B} = \{(0, t) \mid t < f^*\}$

  - $\mathcal{A} =$set of values taken by constraints and objectives
  - $\mathcal{A} \cap \mathcal{B} = \emptyset$ for otherwise f^* not optimal
  - P is convex $\Rightarrow \mathcal{A}, \mathcal{B}$ convex
  - $\Rightarrow \exists$ separating hyperplane $u\lambda + \mu t = \alpha$ s.t.

$$\forall (\lambda, t) \in \mathcal{A} \ (u\lambda + \mu t \geq \alpha) \quad (4)$$

$$\forall (\lambda, t) \in \mathcal{B} \ (u\lambda + \mu t \leq \alpha) \quad (5)$$



- Since λ, t may increase indefinitely, (4) bounded below $\Rightarrow u \geq 0, \mu \geq 0$

Strong Duality for convex NLPs III

Proof

- Since $\lambda = 0$ in $\mathcal{B}$, (5) $\Rightarrow \forall t < f^* \; (\mu t \leq \alpha)$
- Combining latter with (4) yields

$$\forall x \; (ug(x) + \mu f(x) \geq \mu f^*) \tag{6}$$

- Suppose $\mu = 0$: (6) becomes $ug(x) \geq 0$ for all feasible x; by Slater's condition $\exists x' \in F(P) \; (g(x') < 0)$, so $u \leq 0$, which together with $u \geq 0$ implies $u = 0$; hence $(u, \mu) = 0$ contradicting separating hyperplane theorem, thus $\mu > 0$
- Setting $\mu y = u$ in (6) yields $\forall x \in F(P) \; (f(x) + yg(x) \geq f^*)$
- Thus, for all feasible x we have $L(x, y) \geq f^*$
- In particular, $p^* = \max_y \min_x L(x, y) \geq f^*$
- Weak duality implies $p^* \leq f^*$
- Hence, $p^* = f^*$

Rules for LP dual

Primal	**Dual**
$\min$	$\max$
variables x	**constraints**
constraints	**variables** y
objective coefficients c	constraint right hand sides c
constraint right hand sides b	objective coefficients b
$A_i x \geq b_i$	$y_i \geq 0$
$A_i x \leq b_i$	$y_i \leq 0$
$A_i x = b_i$	y_i unconstrained
$x_j \geq 0$	$yA^j \leq c_j$
$x_j \leq 0$	$yA^j \geq c_j$
x_j unconstrained	$yA^j = c_j$

A_i**:** i**-th row of** A

A^j**:** j**-th column of** A

Examples: LP dual formulations

- Primal problem P and canonical form:

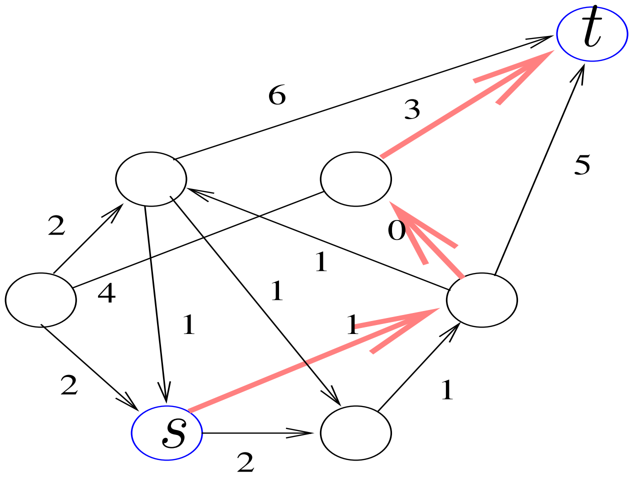
$$\left.\begin{array}{rl}\max\limits_{x_1,x_2} & x_1+x_2 \\ \text{s.t.} & x_1+2x_2\le 2 \\ & 2x_1+x_2\le 2 \\ & x\ge 0\end{array}\right\}\Rightarrow\left.\begin{array}{rl}-\min\limits_{x_1,x_2} & -x_1-x_2 \\ \text{s.t.} & -x_1-2x_2\ge -2 \\ & -2x_1-x_2\ge -2 \\ & x\ge 0\end{array}\right\}$$

- Dual problem D and reformulation:

$$\left.\begin{array}{rl}-\max\limits_{y_1,y_2} & -2y_1-2y_2 \\ \text{s.t.} & -y_1-2y_2\le -1 \\ & -2y_1-y_2\le -1 \\ & y\ge 0\end{array}\right\}\Rightarrow\left.\begin{array}{rl}\min\limits_{y_1,y_2} & 2y_1+2y_2 \\ \text{s.t.} & y_1+2y_2\ge 1 \\ & 2y_1+y_2\ge 1 \\ & y\ge 0\end{array}\right\}$$

Example: Shortest Path Problem

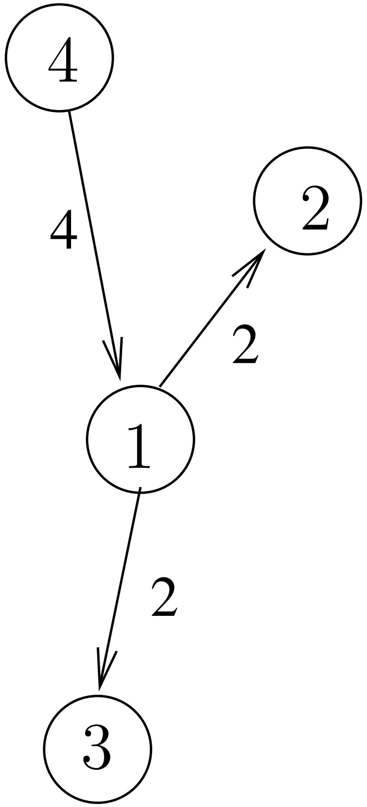
SHORTEST PATH PROBLEM.
Input: weighted digraph $G = (V, A, c)$, and $s, t \in V$.
Output: a minimum-weight path in G from s to t.



$$\left.\begin{array}{llll} \min\limits_{x\geq 0} & & \displaystyle\sum_{(u,v)\in A} c_{uv}x_{uv} & \\ \forall\ v \in V & \displaystyle\sum_{(v,u)\in A} x_{vu} - \sum_{(u,v)\in A} x_{uv} & = & \left\{\begin{array}{ll} 1 & v = s \\ -1 & v = t \\ 0 & \text{othw.} \end{array}\right. \end{array}\right\} [P]$$

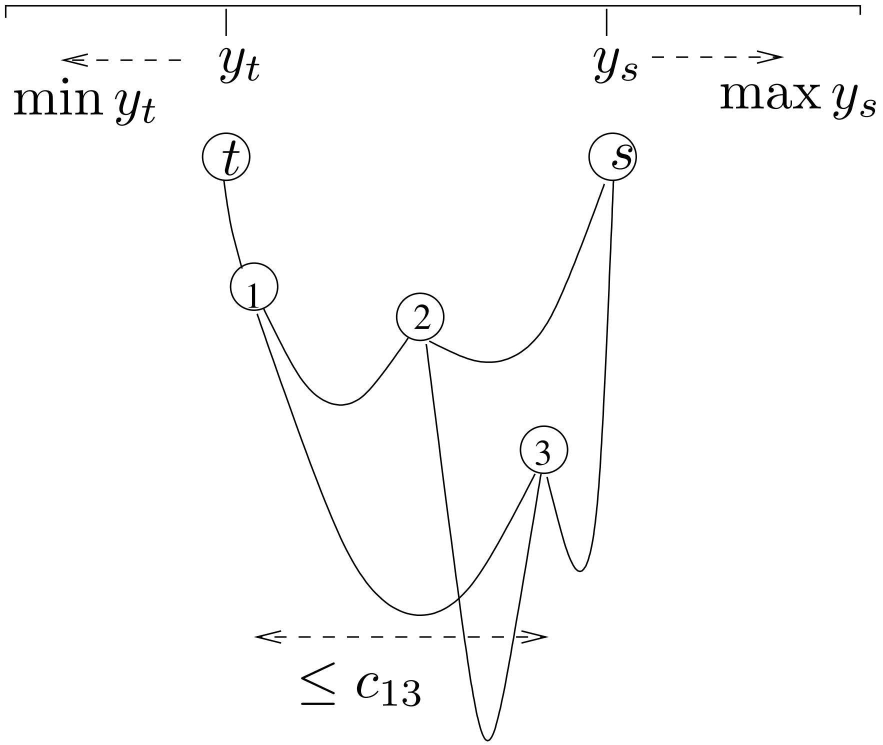
$$\left.\begin{array}{llll} \max\limits_{y} & y_s - y_t & & \\ \forall\ (u,v) \in A & y_v - y_u & \leq & c_{uv} \end{array}\right\} [D]$$

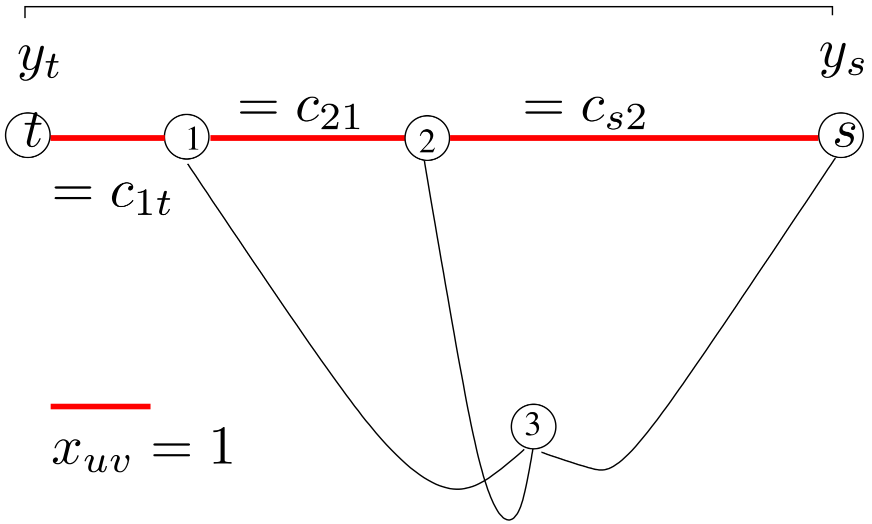
Shortest Path Dual



cols	(1,2)	(1,3)	…	(4,1)	…		
rows$\backslash c$	2	2	…	4	…	b	
1	1	1	…	-1	…	0	y_1
2	-1	0	…	0	…	0	y_2
3	0	-1	…	0	…	0	y_3
4	0	0	…	1	…	0	y_4
⋮	⋮	⋮		⋮		⋮	⋮
s	0	0	…	0	…	1	y_s
⋮	⋮	⋮		⋮		⋮	⋮
t	0	0	…	0	…	-1	y_t
⋮	⋮	⋮		⋮		⋮	⋮
	x_{12}	x_{13}	…	x_{41}	…		

SP Mechanical Algorithm





KKT2 on [D] $\Rightarrow \quad \forall (u,v) \in A \; (x_{uv}(y_v - y_u - c_{uv}) = 0) \Rightarrow$

$$\forall (u,v) \in A \; (x_{uv} = 1 \rightarrow y_v - y_u = c_{uv})$$

exAMPLes

LP example: `.mod`

```
# lp.mod
param n integer, default 3;
param m integer, default 4;
set N := 1..n;
set M := 1..m;
param a{M,N};
param b{M};
param c{N};

var x{N} >= 0;
minimize objective: sum{j in N} c[j]*x[j];
subject to constraints{i in M} :
  sum{j in N} a[i,j]*x[j] <= b[i];
```

LP example: .dat

```
# lp.dat
param n := 3; param m := 4;
param c                :=
            1  1
            2 -3
            3 -2.2 ;
param b                :=
            1 -1
            2  1.1
            3  2.4
            4  0.8 ;
param a : 1    2    3  :=
      1   0.1  0   -3.1
      2   2.7 -5.2  1.3
      3   1    0   -1
      4   1    1    0 ;
```

LP example: .run

```
# lp.run

model lp.mod;
data lp.dat;
option solver cplex;
solve;
display x;
```

LP example: output

```
CPLEX 11.0.1: optimal solution; objective -11.30153
0 dual simplex iterations (0 in phase I)
x [*] :=
1  0
2  0.8
3  4.04615
;
```

MILP example: .mod

```
# milp.mod
param n integer, default 3;
param m integer, default 4;
set N := 1..n;
set M := 1..m;
param a{M,N};
param b{M};
param c{N};

var x{N} >= 0, <= 3, integer;
var y >= 0;
minimize objective: sum{j in N} c[j]*x[j];
subject to constraints{i in M} :
  sum{j in N} a[i,j]*x[j] - y <= b[i];
```

MILP example: `.run`

```
# milp.run

model milp.mod;
data lp.dat;
option solver cplex;
solve;
display x;
display y;
```

MILP example: output

```
CPLEX 11.0.1: optimal integer solution; objective
0 MIP simplex iterations
0 branch-and-bound nodes
x [*] :=
1  0
2  3
3  3
;
y = 2.2
```

NLP example: `.mod`

```
# nlp.mod
param n integer, default 3;
param m integer, default 4;
set N := 1..n;
set M := 1..m;
param a{M,N};
param b{M};
param c{N};
var x{N} >= 0.1, <= 4;
minimize objective:
  c[1]*x[1]*x[2] + c[2]*x[3]^2 + c[3]*x[1]*x[2]/x[3];
subject to constraints{i in M diff {4}} :
  sum{j in N} a[i,j]*x[j] <= b[i]/x[i];
subject to constraint4 : prod{j in N} x[j] <= b[4];
```

NLP example: .run

```
# nlp.run
model nlp.mod;
data lp.dat;
## only enable one of the following methods
## 1: local solution
option solver minos;
# starting point
let x[1] := 0.1;
let x[2] := 0.1; # try 0.1, 0.4
let x[3] := 0.2;
## 2: global solution (heuristic)
#option solver bonmin;
## 3: global solution (guaranteed)
#option solver couenne;
solve;
display x;
```

NLP example: output

```
MINOS 5.51: optimal solution found.
140 iterations, objective -47.9955
Nonlin evals: obj = 358, grad = 357, constrs = 358,
x [*] :=
1   0.1
2   0.1
3   4
;
```

With $x_2 = 0.4$ we get 47 iterations, objective -38.03000929 and $x = (2.84106, 1.37232, 0.205189)$.

MINLP example: .mod

```
# minlp.mod
param n integer, default 3;
param m integer, default 4;
set N := 1..n;
set M := 1..m;
param a{M,N};
param b{M};
param c{N};
param epsilon := 0.1;
var x{N} >= 0, <= 4, integer;
minimize objective:
  c[1]*x[1]*x[2] + c[2]*x[3]^2 + c[3]*x[1]*x[2]/x[3] +
  x[1]*x[3]^3;
subject to constraints{i in M diff {4}} :
  sum{j in N} a[i,j]*x[j] <= b[i]/(x[i] + epsilon);
subject to constraint4 : prod{j in N} x[j] <= b[4];
```

MINLP example: .run

```
# minlp.run
model minlp.mod;
data lp.dat;

## only enable one of the following methods:
## 1: global solution (heuristic)
#option solver bonmin;
## 2: global solution (guaranteed)
option solver couenne;

solve;
display x;
```

MINLP example: output

```
bonmin: Optimal
x [*] :=
1   0
2   4
3   4
;
```

Sudoku

Sudoku: problem class

What is the problem class?

- The class of all sudoku grids
- Replace $\{1,\ldots,9\}$ with a set K
- Will need a set $H=\{1,2,3\}$ to define 3×3 sub-grids
- An “instance” is a partial assignment of integers to cases in the sudoku grid
- We model an empty sudoku grid, and then *fix* certain variables at the appropriate values

Modelling the Sudoku

- Q: *What are the decisions to be taken?*
- A: Whether to place an integer in $K = \{1, \ldots, 9\}$ in the case at coordinates (i, j) on the square grid ($i, j \in K$)
- **We might try integer variables** $y_{ij} \in K$
- Q: *What is the objective function?*
- A: There is no “natural” objective; we might wish to employ one if needed
- Q: *What are the constraints?*
- A: For example, the first row should contain all numbers in K; hence, we should express a constraint such as:
  - if $y_{11} = 1$ then $y_{1\ell} \neq 1$ for all $\ell \geq 1$;
  - if $y_{11} = 2$ then $y_{1\ell} \neq 2$ for all $\ell \geq 2$;
  - …(for all values, column and row indices)

Sudoku constraints 1

- In other words,

$$\forall i, j, k \in K, \ell \neq j \ (y_{ij} = k \to y_{i\ell} \neq k)$$

- *Put it another way*: a constraint that says “all values should be different”
- In *constraint programming* (a discipline related to MP) there is a constraint

$$\forall i \in K \ \text{AllDiff}(y_{ij} \mid j \in K)$$

that *asserts* that all variables in its argument take different values: **we can attempt to implement it in MP**

- A set of distinct values has the *pairwise distinctness property*: $\forall i, p, q \in K \ y_{ip} \neq y_{iq}$, which can also be written as:

$$\forall i, p < q \in K \quad |y_{ip} - y_{iq}| \geq 1$$

Sudoku constraints 2

- We also need the same constraints in each column:

$$\forall j, p < q \in K \quad |y_{pj} - y_{qj}| \geq 1$$

- ...and in some appropriate 3×3 sub-grids:
  1. let $H = \{1, \ldots, 3\}$ and $\alpha = |K|/|H|$; for all $h \in H$ define $R_h = \{i \in K \mid i > (h-1)\alpha \wedge i \leq h\alpha\}$ and $C_h = \{j \in K \mid j > (h-1)\alpha \wedge j \leq h\alpha\}$
  2. show that for all $(h, l) \in H \times H$, the set $R_h \times C_l$ contains the case coordinates of the (h, l)-th 3×3 sudoku sub-grid

- Thus, the following constraints must hold:

$$\forall h, l \in H, i < p \in R_h, j < q \in C_l \quad |y_{ij} - y_{pq}| \geq 1$$

The Sudoku MINLP

- The whole model is as follows:

$$\left.\begin{array}{rrcl} \min & 0 & & \\ \forall i, p < q \in K & |y_{ip} - y_{iq}| & \geq & 1 \\ \forall j, p < q \in K & |y_{pj} - y_{qj}| & \geq & 1 \\ \forall h, l \in H, i < p \in R_h, j < q \in C_l & |y_{ij} - y_{pq}| & \geq & 1 \\ \forall i \in K, j \in K & y_{ij} & \geq & 1 \\ \forall i \in K, j \in K & y_{ij} & \leq & 9 \\ \forall i \in K, j \in K & y_{ij} & \in & \mathbb{Z} \end{array}\right\}$$

- This is a nondifferentiable MINLP
- MINLP solvers (BonMin, MINLP_BB, Couenne) can't solve it

Absolute value reformulation

- This MINLP, however, can be linearized:

$$|a-b| >= 1 \iff a-b >= 1 \vee b-a >= 1$$

- For each $i,j,p,q \in K$ we introduce a binary variable $w_{ij}^{pq} = 1$ if $y_{ij} - y_{pq} \geq 1$ and 0 if $y_{pq} - y_{ij} \geq 1$
- For all $i,j,p,q \in K$ we add constraints
  1. $y_{ij} - y_{pq} \geq 1 - M(1 - w_{ij}^{pq})$
  2. $y_{pq} - y_{ij} \geq 1 - Mw_{ij}^{pq}$

  where $M = |K| + 1$
- This means: if $w_{ij}^{pq} = 1$ then constraint 1 is active and 2 is *always* inactive (as $y_{pq} - y_{ij}$ is always greater than $-|K|$); if $w_{ij}^{pq} = 0$ then 2 is active and 1 inactive
- Transforms problematic absolute value terms into added binary variables and linear constraints

The reformulated model

- The reformulated model is a MILP:

$$\left.\begin{array}{rrcl}
\min & 0 & & \\
\forall i, p < q \in K & y_{ip} - y_{iq} & \geq & 1 - M(1 - w_{ip}^{iq}) \\
\forall i, p < q \in K & y_{iq} - y_{ip} & \geq & 1 - M w_{ip}^{iq} \\
\forall j, p < q \in K & y_{pj} - y_{qj} & \geq & 1 - M(1 - w_{pj}^{qj}) \\
\forall j, p < q \in K & y_{qj} - y_{pj} & \geq & 1 - M w_{pj}^{qj} \\
\forall h, l \in H, i < p \in R_h, j < q \in C_l & y_{ij} - y_{pq} & \geq & 1 - M(1 - w_{ij}^{pq}) \\
\forall h, l \in H, i < p \in R_h, j < q \in C_l & y_{pq} - y_{ij} & \geq & 1 - M w_{ij}^{pq} \\
\forall i \in K, j \in K & y_{ij} & \geq & 1 \\
\forall i \in K, j \in K & y_{ij} & \leq & 9 \\
\forall i \in K, j \in K & y_{ij} & \in & \mathbb{Z}
\end{array}\right\}$$

- It can be solved by CPLEX; however, it has $O(|K|^4)$ binary variables on a $|K|^2$ cases grid with $|K|$ values per case ($O(|K|^3)$ in total) — often an effect of **bad modelling**

A better model

- *In such cases, we have to go back to variable definitions*
- One other possibility is to define **binary variables** $\forall i,j,k \in K\ (x_{ijk}=1)$ **if the** (i,j)**-th case has value** k, and 0 otherwise
- Each case must contain exactly one value

$$\forall i,j \in K \sum_{k\in K} x_{ijk} = 1$$

- For each row and value, there is precisely one row that contains that value, and likewise for cols

$$\forall i,k \in K \sum_{j\in K} x_{ijk} = 1 \quad \wedge \quad \forall j,k \in K \sum_{i\in K} x_{ijk} = 1$$

- Similarly for each $R_h \times C_h$ sub-square

$$\forall h,l \in H, k \in K \sum_{i\in R_h, j\in C_l} x_{ijk} = 1$$

The Sudoku MILP

- The whole model is as follows:

$$\left.\begin{array}{rrcl} \min & 0 & & \\ \forall i \in K, j \in K & \sum\limits_{k \in K} x_{ijk} & = & 1 \\ \forall i \in K, k \in K & \sum\limits_{j \in K} x_{ijk} & = & 1 \\ \forall j \in K, k \in K & \sum\limits_{i \in K} x_{ijk} & = & 1 \\ \forall h \in H, l \in H, k \in K & \sum\limits_{i \in R_h, j \in C_l} x_{ijk} & = & 1 \\ \forall i \in K, j \in K, k \in K & x_{ijk} & \in & \{0,1\} \end{array}\right\}$$

- This is a MILP with $O(|K|^3)$ variables
- Notice that there is a relation $\forall i,j \in K \; y_{ij} = \sum\limits_{k \in K} k x_{ijk}$ between the MINLP and the MILP
- *The MILP variables have been derived by the MINLP ones by “disaggregation”*

Sudoku model file

```
param Kcard integer, >= 1, default 9;
param Hcard integer, >= 1, default 3;
set K := 1..Kcard;
set H := 1..Hcard;
set R{H};
set C{H};
param alpha := card(K) / card(H);
param Instance {K,K} integer, >= 0, default 0;
let {h in H} R[h] := {i in K : i > (h-1) * alpha and i <= h * alpha};
let {h in H} C[h] := {j in K : j > (h-1) * alpha and j <= h * alpha};
var x{K,K,K} binary;

minimize nothing: 0;

subject to assignment {i in K, j in K} : sum{k in K} x[i,j,k] = 1;
subject to rows {i in K, k in K} : sum{j in K} x[i,j,k] = 1;
subject to columns {j in K, k in K} : sum{i in K} x[i,j,k] = 1;
subject to squares {h in H, l in H, k in K} :
  sum{i in R[h], j in C[l]} x[i,j,k] = 1;
```

Sudoku data file

```
param Instance :=
1 1 2         1 9 1        2 2 4        2 3 1        2 4 9
2 6 2         2 7 8        2 8 6        3 1 5        3 2 8
3 8 2         3 9 7        4 4 5        4 5 1        4 6 3
5 5 9         6 4 7        6 5 8        6 6 6        7 1 3
7 2 2         7 3 6        7 8 4        7 9 9        8 2 1
8 3 9         8 4 4        8 6 5        8 7 2        8 8 8
9 1 8         9 9 6 ;
```

Sudoku run file

```
# sudoku
# replace "/dev/null" with "nul" if using Windows
option randseed 0;
option presolve 0;
option solver_msg 0;
model sudoku.mod;
data sudoku-feas.dat;
let {i in K, j in K : Instance[i,j] > 0} x[i,j,Instance[i,j]] := 1;
fix {i in K, j in K : Instance[i,j] > 0} x[i,j,Instance[i,j]];
display Instance;
option solver cplex;
solve > /dev/null;
param Solution {K, K};
if (solve_result = "infeasible") then {
  printf "instance is infeasible\n";
} else {
  let {i in K, j in K} Solution[i,j] := sum{k in K} k * x[i,j,k];
  display Solution;
}
```

Sudoku AMPL output

```
liberti@nox$ cat sudoku.run | ampl
Instance [*,*]
:   1   2   3   4   5   6   7   8   9     :=
1   2   0   0   0   0   0   0   0   1
2   0   4   1   9   0   2   8   6   0
3   5   8   0   0   0   0   0   2   7
4   0   0   0   5   1   3   0   0   0
5   0   0   0   0   9   0   0   0   0
6   0   0   0   7   8   6   0   0   0
7   3   2   6   0   0   0   0   4   9
8   0   1   9   4   0   5   2   8   0
9   8   0   0   0   0   0   0   0   6
;
instance is infeasible
```

Sudoku data file 2

But with a different data file. . .

```
param Instance :=
1 1 2        1 9 1        2 2 4       2 3 1       2 4 9
2 6 2        2 7 8        2 8 6       3 1 5       3 2 8
3 8 2        3 9 7        4 4 5       4 5 1       4 6 3
5 5 9        6 4 7        6 5 8       6 6 6       7 1 3
7 2 2                     7 8 4       7 9 9       8 2 1
8 3 9        8 4 4        8 6 5       8 7 2       8 8 8
9 1 8        9 9 6 ;
```

Sudoku data file 2 grid

. . . corresponding to the grid below. . .

2								1
	4	1	9		2	8	6	
5	8						2	7
			5	1	3			
				9				
			7	8	6			
3	2						4	9
	1	9	4		5	2	8	
8								6

Sudoku AMPL output 2

. . . we find a solution!

```
liberti@nox$ cat sudoku.run | ampl
Solution [*,*]
:    1    2    3    4    5    6    7    8    9       :=
1    2    9    6    8    5    7    4    3    1
2    7    4    1    9    3    2    8    6    5
3    5    8    3    6    4    1    9    2    7
4    4    7    8    5    1    3    6    9    2
5    1    6    5    2    9    4    3    7    8
6    9    3    2    7    8    6    1    5    4
7    3    2    7    1    6    8    5    4    9
8    6    1    9    4    7    5    2    8    3
9    8    5    4    3    2    9    7    1    6
;
```

Kissing Number Problem

KNP: problem class

What is the problem class?

- There is no number in the problem definition:

  How many unit balls with disjoint interior can be placed adjacent to a central unit ball in $\mathbb{R}^d$*?*

- Hence the KNP is already defined as a problem class
- Instances are given by assigning a positive integer to the only parameter d

Modelling the KNP

- Q: *What are the decisions to be taken?*
- A: How many spheres to place, and where to place them
- **For each sphere, two types of variables**
  1. a logical one: $y_i = 1$ if sphere i is present, and 0 otherwise
  2. a d-vector of continuous ones: $x_i = (x_{i1}, \ldots, x_{id})$, position of i-th sphere center
- Q: *What is the objective function?*
- A: **Maximize the number of spheres**
- Q: *What are the constraints?*
- A: **Two types of constraints**
  1. the i-th center must be at distance 2 from the central sphere if the i-th sphere is placed (*center constraints*)
  2. for all distinct (and placed) spheres i, j, for their interior to be disjoint their centers must be at distance ≥ 2 (*distance constraints*)

Assumptions

1. **Logical variables** y
   - Since the objective function counts the number of placed spheres, it must be something like $\sum_i y_i$
   - What set N does the index i range over?
   - Denote $k^*(d)$ the optimal solution to the KNP in $\mathbb{R}^D$
   - Since $k^*(d)$ is unknown *a priori*, we cannot know N *a priori*; however, without N, we cannot express the objective function
   - *Assume* we know an **upper bound** $\bar{k}$ to $k^*(d)$; then we can define $N = \{1, \ldots, \bar{k}\}$ (and $D = \{1, \ldots, d\}$)
2. **Continuous variables** x
   - Since any sphere placement is invariant by translation, we *assume* that the central sphere is placed at the origin
   - Thus, each continuous variable x_{ik} ($i \in N, k \in D$) cannot attain values outside $[-2, 2]$ (why?)
   - Limit continuous variables: $-2 \leq x_{ik} \leq 2$

Problem restatement

- The above assumptions lead to a **problem restatement**

> *Given a positive integer $\bar{k}$, what is the maximum number (smaller than $\bar{k}$) of unit spheres with disjoint interior that can be placed adjacent to a unit sphere centered at the origin of $\mathbb{R}^d$?*

- *Each time assumptions are made for the sake of modelling, one must always keep track of the corresponding changes to the problem definition*
- The **Objective function** can now be written as:

$$\max \sum_{i \in N} y_i$$

Constraints

- *Center constraints*:

$$\forall i \in N \quad ||x_i|| = 2y_i$$

(if sphere i is placed then $y_i = 1$ and the constraint requires $||x_i|| = 2$, otherwise $||x_i|| = 0$, which implies $x_i = (0, \ldots, 0)$)

- *Distance constraints*:

$$\forall i \in N, j \in N \ : \ i \neq j \quad ||x_i - x_j|| \geq 2y_i y_j$$

(if spheres i, j are both are placed then $y_i y_j = 1$ and the constraint requires $||x_i - x_j|| \geq 2$, otherwise $||x_i - x_j|| \geq 0$ which is always by the definition of norm)

KNP model

$$\left.\begin{array}{rrcl}
\max & \sum\limits_{i\in N} y_i & & \\
\forall i \in N & \sqrt{\sum\limits_{k\in D} x_{ik}^2} & = & 2y_i \\
\forall i \in N, j \in N : i \neq j & \sqrt{\sum\limits_{k\in D} (x_{ik} - x_{jk})^2} & \geq & 2y_iy_j \\
\forall i \in N & y_i & \geq & 0 \\
\forall i \in N & y_i & \leq & 1 \\
\forall i \in N, k \in D & x_{ik} & \geq & -2 \\
\forall i \in N, k \in D & x_{ik} & \leq & 2 \\
\forall i \in N & y_i & \in & \mathbb{Z}
\end{array}\right\}$$

For brevity, we shall write $y_i \in \{0, 1\}$ and $x_{ik} \in [-2, 2]$

Reformulation 1

- Solution times for NLP/MINLP solvers often also depends on the number of nonlinear terms
- We square both sides of the nonlinear constraints, and notice that since y_i are binary variables, $y_i^2 = y_i$ for all $i \in N$; we get:

$$\begin{array}{rrcl} \forall i \in N & \sum\limits_{k \in D} x_{ik}^2 & = & 4y_i \\ \forall i \neq j \in N & \sum\limits_{k \in D} (x_{ik} - x_{jk})^2 & \geq & 4y_i y_j \end{array}$$

which has fewer nonlinear terms than the original problem

Reformulation 2

- Distance constraints are called *reverse convex* (because if we replace $\geq$ with $\leq$ the constraints become convex); these constraints often cause solution times to lengthen considerably
- Notice that distance constraints are repeated when i, j are swapped
- Change the quantifier to $i \in N, j \in N : i < j$ reduces the number of reverse convex constraints in the problem; get:

$$\begin{array}{rrcl} \forall i \in N & \sum_{k \in D} x_{ik}^2 & = & 4y_i \\ \forall i < j \in N & \sum_{k \in D} (x_{ik} - x_{jk})^2 & \geq & 4y_iy_j \end{array}$$

KNP model revisited

$$\left.\begin{array}{rrcl}
\max & \sum\limits_{i \in N} y_i & & \\
\forall i \in N & \sum\limits_{k \in D} x_{ik}^2 & = & 4y_i \\
\forall i \in N, j \in N : i < j & \sum\limits_{k \in D} (x_{ik} - x_{jk})^2 & \geq & 4y_i y_j \\
\forall i \in N, k \in D & x_{ik} & \in & [-2, 2] \\
\forall i \in N & y_i & \in & \{0, 1\}
\end{array}\right\}$$

This formulation is a (nonconvex) MINLP

KNP model file

```
# knp.mod
param d default 2;
param kbar default 7;
set D := 1..d;
set N := 1..kbar;

var y{i in N} binary;
var x{i in N, k in D} >= -2, <= 2;

maximize kstar : sum{i in N} y[i];

subject to center{i in N} : sum{k in D} x[i,k]^2 = 4*y[i];
subject to distance{i in N, j in N : i < j} :
   sum{k in D} (x[i,k] - x[j,k])^2 >= 4*y[i]*y[j];
```

KNP data file

Since the only data are the parameters d and $\bar{k}$ (two scalars), for simplicity we do not use a data file at all, and assign values in the model file instead

KNP run file

```
# knp.run
model knp.mod;
option solver couenne;
let kbar := 12;
let d := 3;
solve;
display x,y;
display kstar;
```

KNP solution (?)

- We tackle the easiest possible KNP instance ($d = 2$), and give it an upper bound $\bar{k} = 7$
- It is easy to see that $k^*(2) = 6$ (place 6 circles adjacent to another circle in an exagonal lattice)
- Yet, after *several minutes* of CPU time COUENNE has not made any progress from the trivial feasible solution $y = 0, x = 0$
- Likewise, heuristic solvers such as BONMIN and `MINLP_BB` only find the trivial zero solution and exit

What do we do next?

In order to solve the KNP and deal with other difficult MINLPs, we need more advanced techniques

Some useful MP theory

Open sets

- In general, MP cannot directly model problems involving sets which are not closed in the usual topology (such as e.g. open intervals)
- The reason is that the minimum/maximum of a non-closed set might not exist
- E.g. what is $\min\limits_{x\in(0,1)} x$? Since $(0,1)$ has no minimum (for each $\delta \in (0,1)$, $\frac{\delta}{2} < \delta$ and is in $(0,1)$), the question has no answer
- *This is why the MP language does not allow writing constraints that involve the $<, >$ and $\neq$ relations*
- Sometimes, problems involving open sets can be reformulated exactly to problems involving closed sets (e.g. $x > 0 \Leftrightarrow x \geq e^{-y}$)

Best fit hyperplane 1

- Consider the following problem:

  Given m points $p_1, \ldots, p_m \in \mathbb{R}^n$, find the hyperplane $w_1 x_1 + \cdots + w_n x_n = w_0$ minimizing the piecewise linear form $f(p, w) = \sum_{i \in P} |\sum_{j \in N} w_j p_{ij} - w_0|$

- Mathematical programming formulation:

1. **Sets**: $P = \{1, \ldots, m\}$, $N = \{1, \ldots, n\}$
2. **Parameters:** $\forall i \in P \; p_i \in \mathbb{R}^n$
3. **Decision variables**: $\forall j \in N \; w_j \in \mathbb{R}$, $w_0 \in \mathbb{R}$
4. **Objective**: $\min_w f(p, w)$
5. **Constraints**: none

- Trouble: $w = 0$ is the obvious, trivial solution of no interest
- We need to enforce a constraint $(w_1, \ldots, w_n, w_0) \neq (0, \ldots, 0)$
- *Bad news:* $\mathbb{R}^{n+1} \smallsetminus \{(0, \ldots, 0)\}$ *is not a closed set*

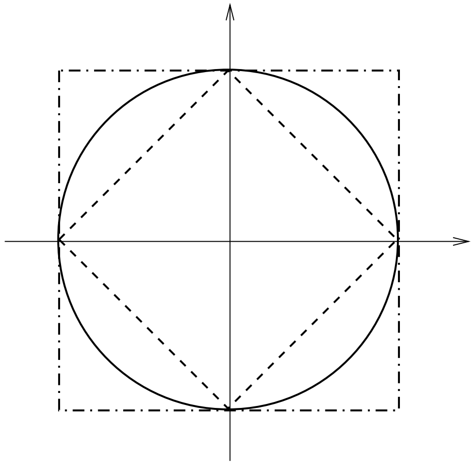
Best fit hyperplane 2

- We can implicitly impose such a constraint by transforming the objective function to $\min_w \frac{f(p,w)}{||w||}$ (for some norm $||\cdot||$)
- This implies that w is nonzero but the feasible region is $\mathbb{R}^{n+1}$, which is both open and closed
- **Obtain fractional objective — difficult to solve**
- Suppose $\mathbf{w}^* = (w^*, w_0^*) \in \mathbb{R}^{n+1}$ is an optimal solution to the above problem
- Then for all $d > 0$, $f(d\mathbf{w}^*, p) = df(\mathbf{w}^*, p)$
- Hence, it suffices to determine the optimal *direction* of $\mathbf{w}^*$, because the actual vector length simply scales the objective function value
- Can impose constraint $||w|| = 1$ and recover original objective
- *Solve reformulated problem*:

$$\min\{f(w,p) \mid ||w|| = 1\}$$

Best fit hyperplane 3

- The constraint $||w|| = 1$ is a *constraint schema*: we must specify the norm
- Some norms can be reformulated to linear constraints, some cannot
- max-norm (l_∞) 2-sphere (square), Euclidean norm (l_2) 2-sphere (circle), abs-norm (l_1) 2-sphere (rhombus)



- max- and abs-norms are piecewise linear, they can be linearized exactly by using binary variables (see later)

Convexity in practice

- Recognizing whether an arbitrary function is convex is an undecidable problem
- For some functions, however, this is possible
  - Certain functions are *known* to be convex (such as all affine functions, cx^{2n} for $n \in \mathbb{N}$ and $c \geq 0$, $\exp(x)$, $-\log(x)$)
  - Norms are convex functions
  - The sum of two convex functions is convex
- Application of the above rules repeatedly sometimes works (for more information, see Disciplined Convex Programming [Grant et al. 2006])
- *Warning*: problems involving integer variables are in general not convex; however, if the objective function and constraints are *convex forms*, we talk of *convex MINLPs*

Recognizing convexity 1

Consider the following mathematical program

$$\boxed{\begin{array}{rcl} \min\limits_{x,y\in[0,10]} & 8x^2 - 17xy + 10y^2 & \\ x - y & \geq & 1 \\ x^2 y & \geq & 1 \end{array}}$$

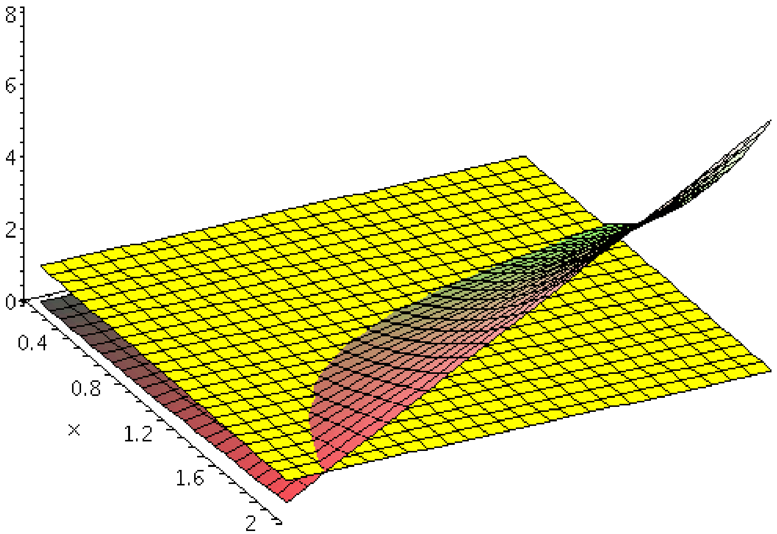
- Objective function and constraints contain nonconvex term xy
- There is no reason to believe that $x^2 y \geq 1$ might be convex
- Is this problem convex or not?

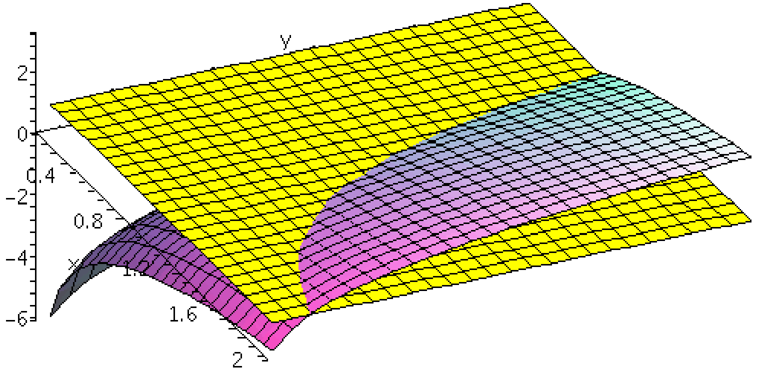
Recognizing convexity 2

- The objective function can be written as $(x,y)^\mathsf{T} Q(x,y)$ where $Q = \begin{pmatrix} 8 & -8 \\ -9 & 10 \end{pmatrix}$
- The eigenvalues of Q are $9 \pm \sqrt{73}$ (both positive), hence the Hessian of the objective is positive definite, hence **the objective function is convex**
- The affine constraint $x - y \geq 1$ is **convex by definition**
- $x^2 y \geq 1$ is not, but can be reformulated:
  1. Take logarithms of both sides: $\log x^2 y \geq \log 1$
  2. Implies $2\log x + \log y \geq 0 \Rightarrow -2\log x - \log y \leq 0$
  3. $-\log$ is a convex function, sum of convex functions is convex, *convex* $\leq$ *affine* is a convex constraint

Recognizing convexity 3

Indeed, the set $\{(x,y) \mid x^2y \geq 1\}$ is shown in yellow *below* the surface





Both pictures represent the *same set*

Recognizing convexity 4

```
model;
var x <= 10, >= 0.1;
var y <= 10, >= 0.1;
minimize f: 8*x^2 -17*x*y + 10*y^2;
subject to c1: x-y >= 1;
subject to c2: x^2*y >= 1;
option solver_msg 0;
printf "solving with sBB (couenne)\n";
option solver couenne;
solve > /dev/null;
display x,y;
printf "solving with local NLP solver (ipopt)\n";
option solver ipopt; let x := 0.1; let y := 0.1;
solve > /dev/null; display x,y;
```

Get approx. same solution $(1.5, 0.5)$ from COUENNE and IPOPT

Total Unimodularity

- A matrix A is Totally Unimodular (TUM) if all invertible square submatrices of A have determinant ± 1
  Thm.

  If A is TUM, then all vertices of the polyhedron

  $$\{x \ge 0 \mid Ax \le b\}$$

  have integral components

- *Consequence*: if the constraint matrix of a given MILP is TUM, then it suffices to solve the relaxed LP to get a solution for the original MILP

- **An LP solver suffices to solve the MILP to optimality**

TUM in practice 1

- If A is TUM, A^T and $(A|I)$ are TUM
- *TUM Sufficient conditions*. An $m \times n$ matrix A is TUM if:
  1. for all $i \le m$, $j \le n$ we have $a_{ij} \in \{0, 1, -1\}$;
  2. each column of A contains at most 2 nonzero coefficients;
  3. there is a partition R_1, R_2 of the set of rows such that for each column j, $\sum_{i \in R_1} a_{ij} - \sum_{i \in R_2} a_{ij} = 0$.
- Example: take $R_1 = \{1, 3, 4\}$, $R_2 = \{2\}$

$$\begin{pmatrix} 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 1 & -1 & 1 \\ -1 & -1 & 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 & -1 & 0 \end{pmatrix}$$

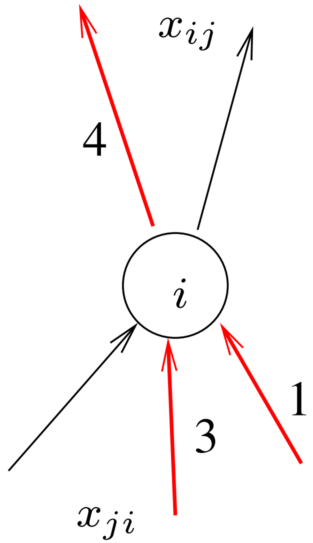
TUM in practice 2

- Consider digraph $G = (V, A)$ with nonnegative variables $x_{ij} \in \mathbb{R}_+$ defined on each arc
- *Flow constraints* $\boxed{\forall i \in V \quad \sum_{(i,j)\in A} x_{ij} - \sum_{(j,i)\in A} x_{ji} = b_i}$ yield a TUM matrix (partition: $R_1 =$ all rows, $R_2 = \emptyset$ — prove it)
- Maximum flow problems can be solved to integrality by simply solving the continuous relaxation with an LP solver
- *The constraints of the set covering problem do not form a TUM. To prove this, you just need to find a counterexample*

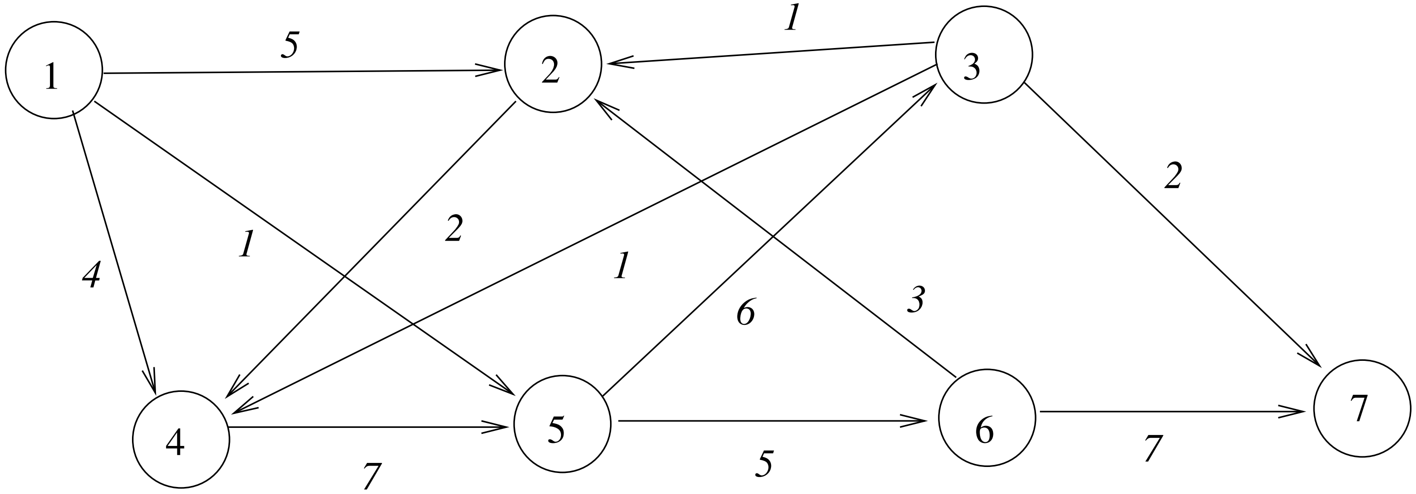
Maximum flow problem

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

$$\left.\begin{array}{rc}
\max_x & \displaystyle\sum_{(s,i)\in A} x_{si} \\
\forall\, i \leq V, \begin{array}{c} i \neq s \\ i \neq t \end{array} & \displaystyle\sum_{(i,j)\in A} x_{ij} = \sum_{(j,i)\in A} x_{ji} \\
\forall (i,j) \in A & 0 \leq x_{ij} \leq u_{ij} \\
\forall (i,j) \in A & x_{ij} \in \mathbb{Z}
\end{array}\right\}$$



Max Flow Example 1



arc capacities as shown in italics: find the maximum flow between node $s = 1$ and $t = 7$

Max Flow: MILP formulation

- **Sets**: $V = \{1, \ldots, n\}$, $A \subseteq V \times V$
- **Parameters**: $s, t \in V$, $u : A \to \mathbb{R}_+$
- **Variables**: $x : A \to \mathbb{Z}_+$
- **Objective**: $\max \sum\limits_{(s,i) \in A} x_{si}$
- **Constraints**: $\forall i \in V \smallsetminus \{s, t\} \quad \sum\limits_{(i,j) \in A} x_{ij} = \sum\limits_{(j,i) \in A} x_{ji}$

Max Flow: .mod file

```
# maxflow.mod
param n integer, > 0, default 7;
param s integer, > 0, default 1;
param t integer, > 0, default n;
set V := 1..n;
set A within {V,V};
param u{A} >= 0;

var x{(i,j) in A} >= 0, <= u[i,j], integer;

maximize flow : sum{(s,i) in A} x[s,i];

subject to flowcons{i in V diff {s,t}} :
  sum{(i,j) in A} x[i,j] = sum{(j,i) in A} x[j,i];
```

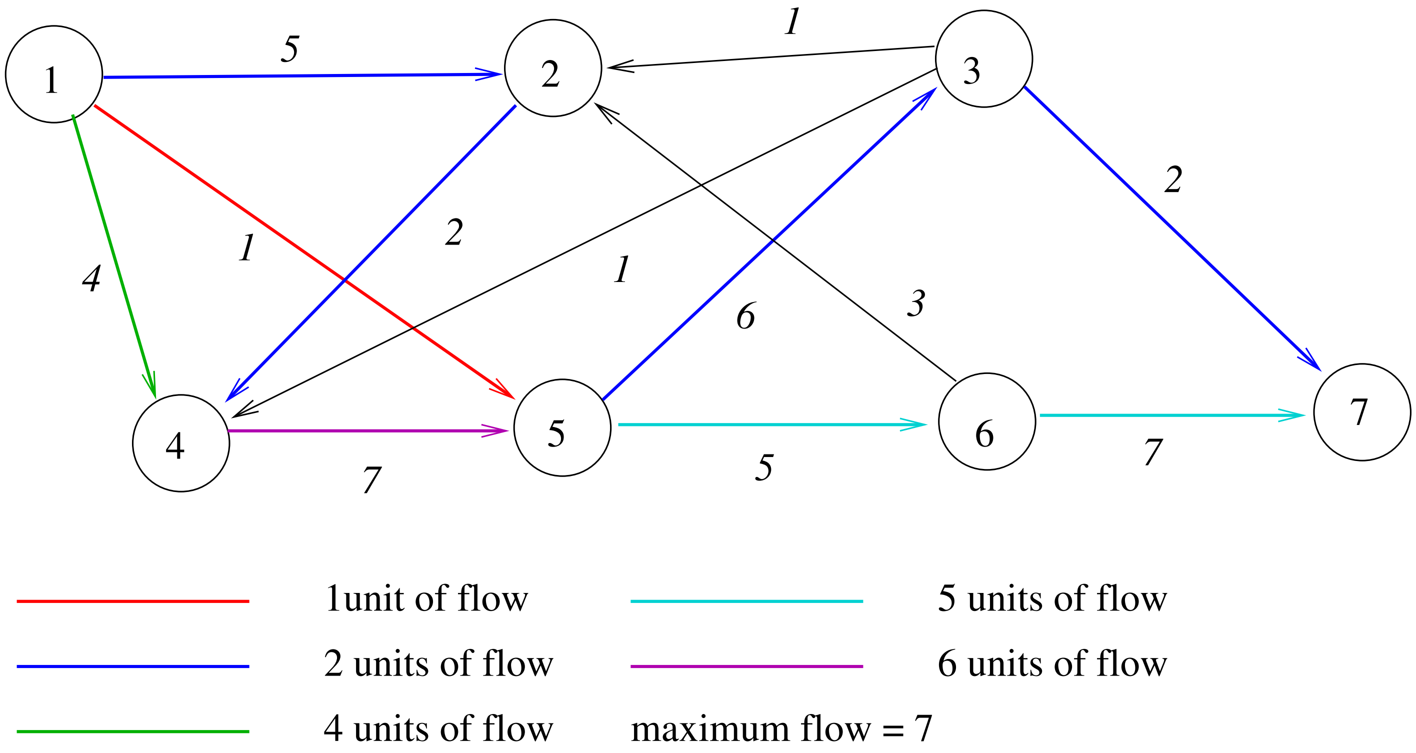
Max Flow: .dat file

```
# maxflow.dat
param : A     : u :=
        1  2    5
        1  4    4
        1  5    1
        2  4    2
        3  2    1
        3  4    1
        3  7    2
        4  5    7
        5  3    6
        5  6    5
        6  2    3
        6  7    7 ;
```

Max Flow: `.run` file

```
# maxflow.run
model maxflow.mod;
#model maxflow_constrained.mod;
data maxflow.dat;
option solver_msg 0;
option solver cplex;
solve;
for {(i,j) in A : x[i,j] > 0} {
  printf "x[%d,%d] = %g\n", i,j,x[i,j];
}
display flow;
```

Max Flow: MILP solution



1unit of flow

2 units of flow

4 units of flow

5 units of flow

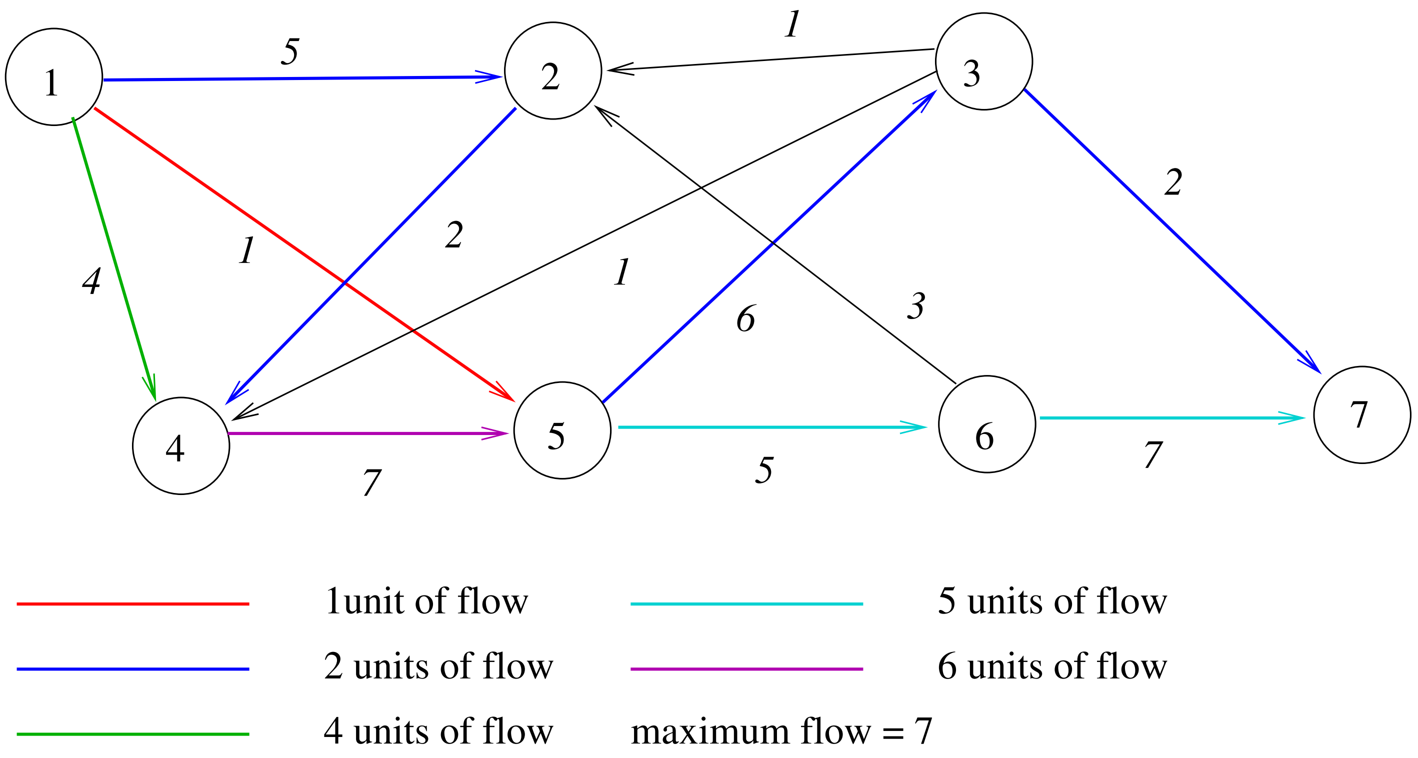
6 units of flow

maximum flow = 7

```
x[1,2] = 2          x[4,5] = 6
x[1,4] = 4          x[5,3] = 2
x[1,5] = 1          x[5,6] = 5
x[2,4] = 2          x[6,7] = 5
x[3,7] = 2          flow = 7
```

Max Flow: LP solution

Relax integrality constraints (take away `integer` keyword)



Get the same solution

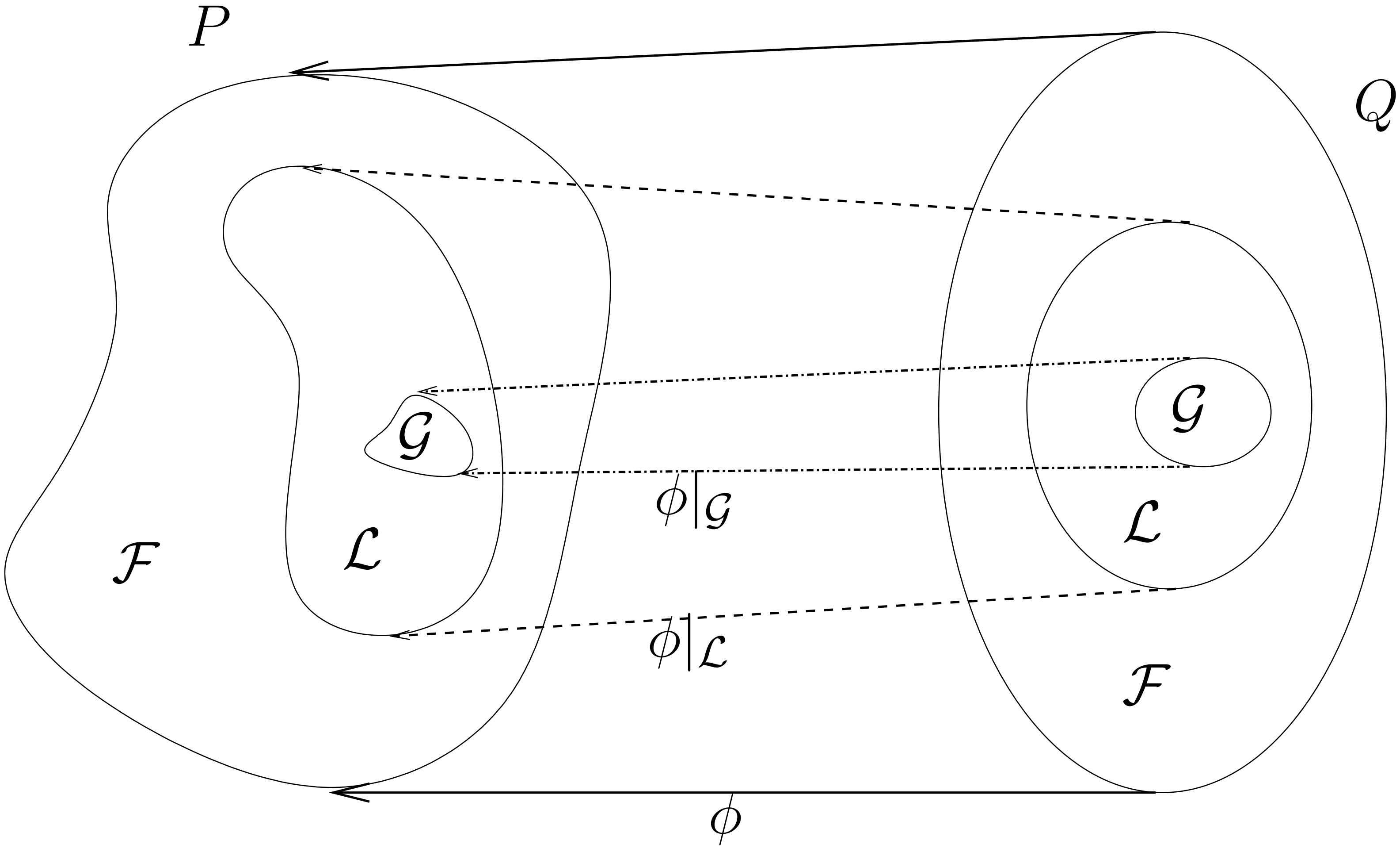
Reformulations

Reformulations

If problems P, Q are related by a computable function f through the relation $f(P, Q) = 0$, Q is an *auxiliary problem* with respect to P.

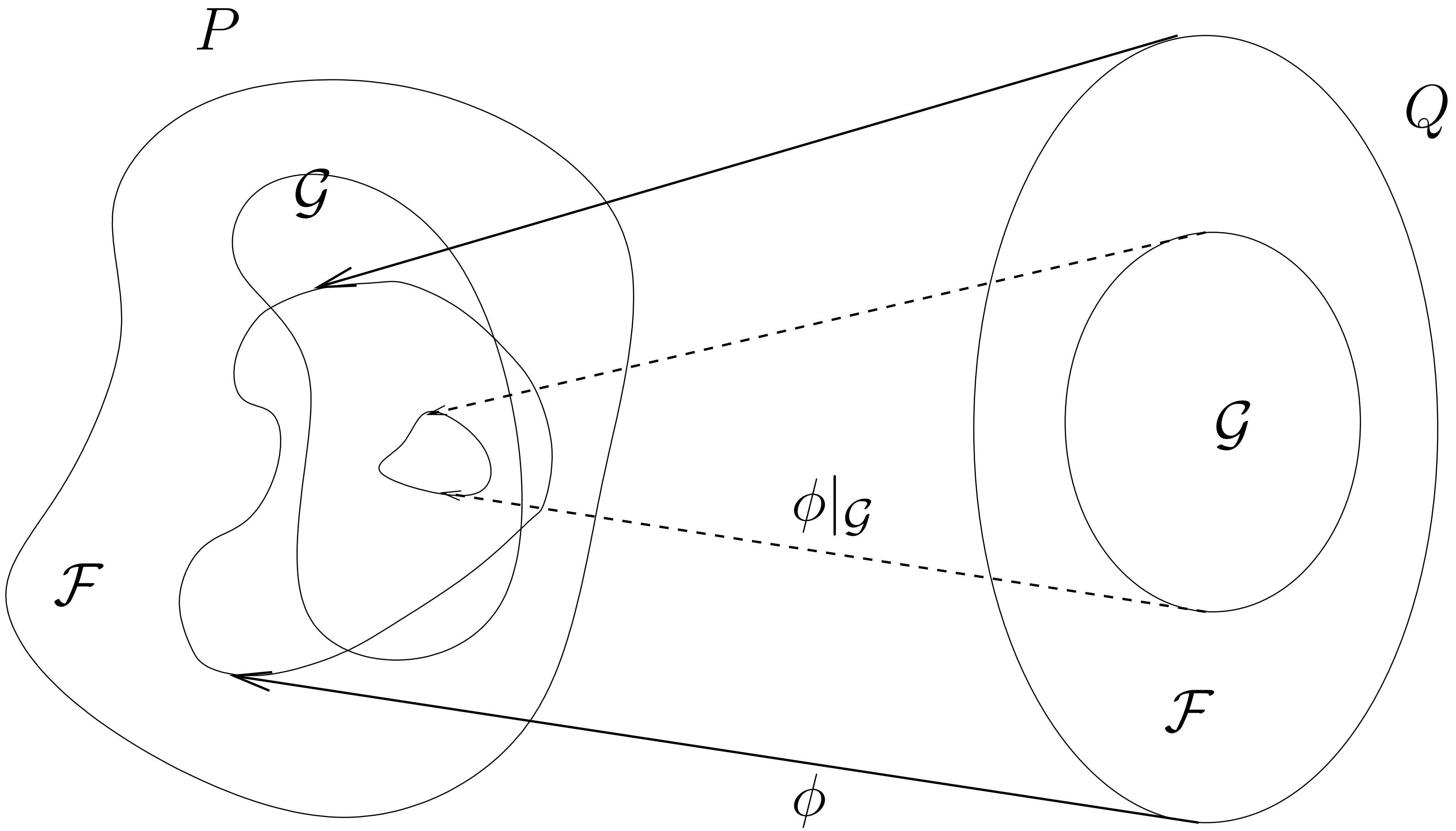
- **Exact reformulations**: preserve all optimality properties
- **Narrowings**: preserve some optimality properties
- **Relaxations**: provide bounds to the optimal objective function value
- **Approximations**: formulation Q depending on a parameter k such that "$\lim_{k\to\infty} Q(k)$" is an exact reformulation, narrowing or relaxation

Exact reformulations



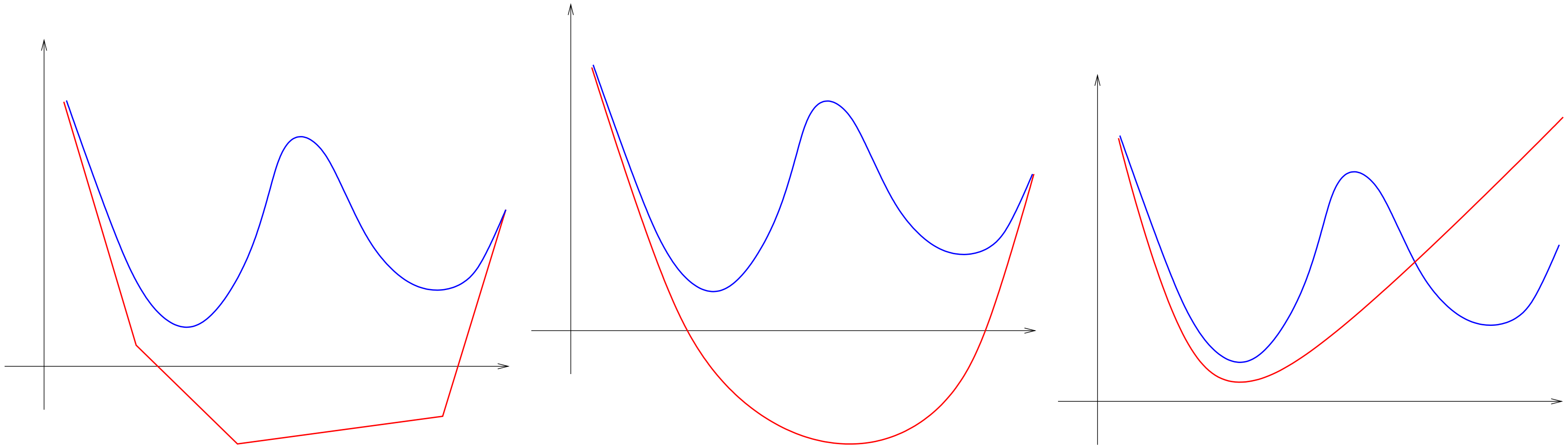
Main idea: if we find an optimum of Q, we can map it back to the same type of optimum of P, and for all optima of P, there is a corresponding optimum in Q. Also known as *exact reformulation*

Narrowings



Main idea: if we find a global optimum of Q, we can map it back to a global optimum of P. There may be optima of P without a corresponding optimum in Q.

Relaxations



A problem Q is a relaxation of P if the globally optimal value of the objective function $\min f_Q$ of Q is a lower bound to that of P.

Approximations

Q is an *approximation* of P if there exist: (a) an auxiliary problem Q^* of P; (b) a sequence $\{Q_k\}$ of problems; (c) an integer $\ell > 0$; such that:

1. $Q = Q_\ell$
2. $\forall$ objective f^* in Q^* there is a sequence of objectives f_k of Q_k converging uniformly to f^*;
3. $\forall$ constraint $l_i^* \leq g_i^*(x) \leq u_i^*$ of Q^* there is a sequence of constraints $l_i^k \leq g_i^k(x) \leq u_i^k$ of Q_k such that g_i^k converges uniformly to g_i^*, l_i^k converges to l_i^* and u_i^k to u_i^*

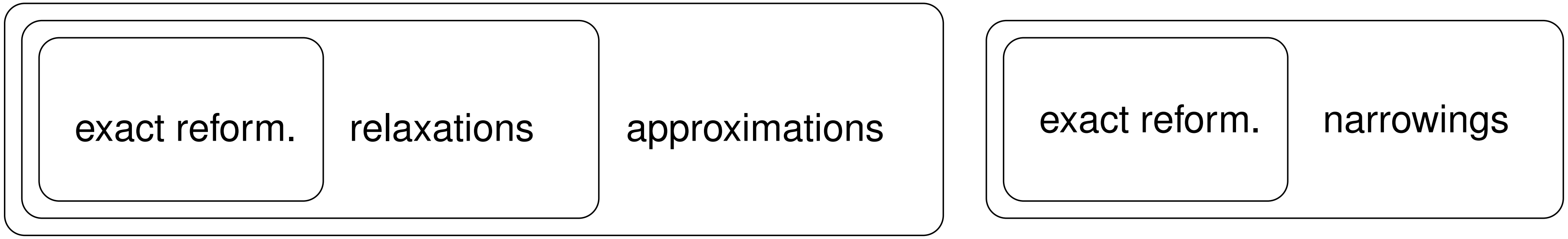
There can be approximations to exact reformulations, narrowings, relaxations.

$$Q_1,\ Q_2,\ Q_3, \ldots Q_\ell, \ldots \longrightarrow Q^* \ \langle\text{auxiliary problem of}\rangle\ \ P$$

approximation of P

Fundamental results

- Exact reformulation, narrowing, relaxation, approximation are all transitive relations
- *An approximation of any type of reformulation is an approximation*
- A reformulation consisting of exact reformulations, narrowings, relaxations is a relaxation
- *A reformulation consisting of exact reformulations and narrowings is a narrowing*
- A reformulation consisting of exact reformulations is an exact reformulation



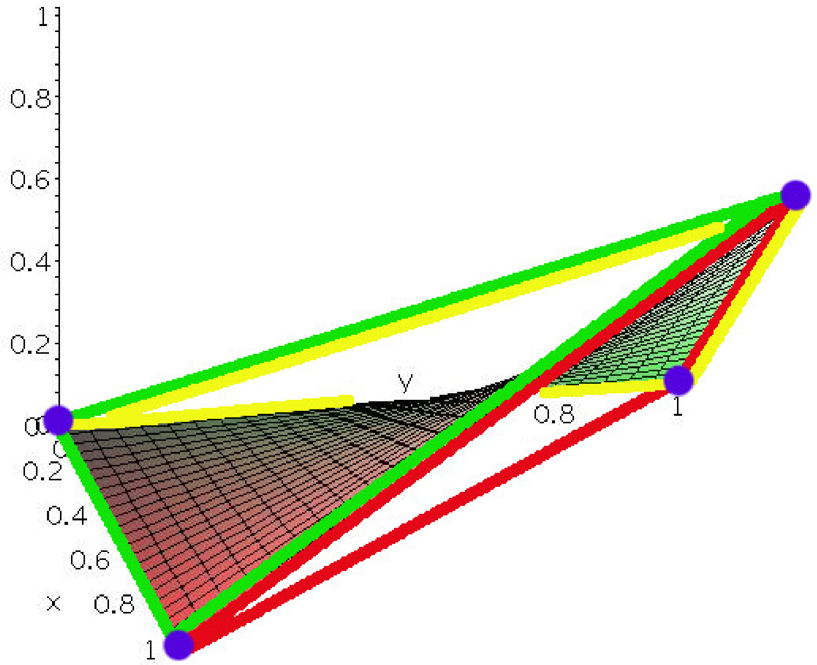
Reformulations in practice

- Reformulations are used to transform problems into equivalent (or related) formulations which are somehow “better”
- Basic reformulation operations:

1. change parameter values
2. add / remove variables
3. adjoin / remove constraints
4. replace a term with another term (e.g. a product xy with a new variable w)

Product of binary variables

- Consider binary variables x, y and a cost c to be added to the objective function only of $xy = 1$
- $\Rightarrow$ Add term cxy to objective
- Problem becomes mixed-integer (some variables are binary) and nonlinear
- Reformulate "xy" to MILP form (PRODBIN reform.):



- replace xy by z
- add $\boxed{z \le y}$, $\boxed{z \le x}$
  $z \ge 0$, $\boxed{z \ge x + y - 1}$
- $x, y \in \{0, 1\} \Rightarrow$
  $z = xy$

Application to the KNP

- In the RHS of the KNP's distance constraints we have $4y_iy_j$, where y_i, y_j are binary variables
- We apply ProdBin (call the added variable w_{ij}):

$$\left.\begin{array}{rrcl}
\min & \sum\limits_{i\in N} y_i & & \\
\forall i \in N & \sum\limits_{k\in D} x_{ik}^2 & = & 4y_i \\
\forall i \in N, j \in N : i < j & \sum\limits_{k\in D} (x_{ik} - x_{jk})^2 & \geq & 4w_{ij} \\
\forall i \in N, j \in N : i < j & w_{ij} & \leq & y_i \\
\forall i \in N, j \in N : i < j & w_{ij} & \leq & y_j \\
\forall i \in N, j \in N : i < j & w_{ij} & \geq & y_i + y_j - 1 \\
\forall i \in N, j \in N : i < j & w_{ij} & \in & [0,1] \\
\forall i \in N, k \in D & x_{ik} & \in & [-2,2] \\
\forall i \in N & y_i & \in & \{0,1\}
\end{array}\right\}$$

- Still a MINLP, but fewer nonlinear terms
- Still numerically difficult (2h CPU time to find $k^*(2) \geq 5$)

Product of bin. and cont. vars.

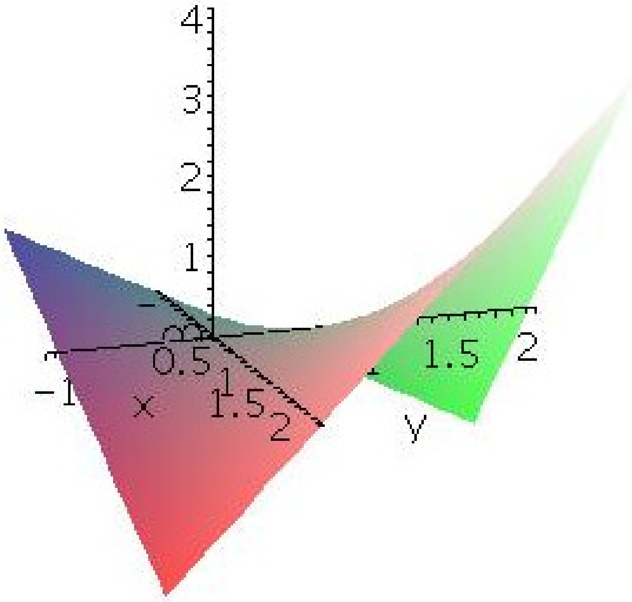
- PRODBINCONT reformulation
- Consider a binary variable x and a continuous variable $y \in [y^L, y^U]$, and assume product xy is in the problem
- Replace xy by an added variable w
- Add constraints:

$$\begin{array}{rcl} w & \leq & y^U x \\ w & \geq & y^L x \\ w & \leq & y + y^L(1-x) \\ w & \geq & y - y^U(1-x) \end{array}$$

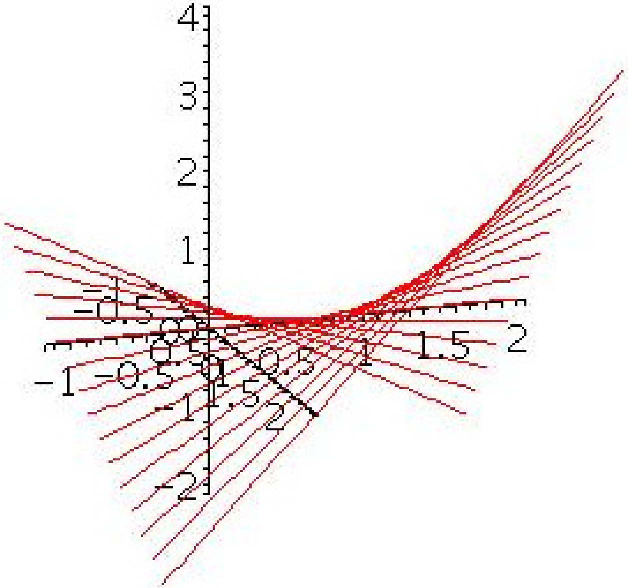
- Exercise 1: show that PRODBINCONT is an exact reformulation
- Exercise 2: show that if $y \in \{0,1\}$ then PRODBINCONT is equivalent to PRODBIN

Prod. cont. vars.: approximation

- BILINAPPROX approximation
- Consider $x \in [x^L, x^U], y \in [y^L, y^U]$ and product xy
- Suppose $x^U - x^L \leq y^U - y^L$, consider an integer $d > 0$
- Replace $[x^L, x^U]$ by a finite set $D = \{x^L + (i-1)\gamma \mid 1 \leq i \leq d\}$, where $\gamma = \frac{x^U - x^L}{d-1}$



→



BILINAPPROX

- Replace the product xy by a variable w
- Add binary variables z_i for $i \leq d$
- Add assignment constraint for z_i's

$$\sum_{i \leq d} z_i = 1$$

- Add definition constraint for x:

$$x = \sum_{i \leq d} (x^L + (i-1)\gamma) z_i$$

  (x takes exactly one value in D)

- Add definition constraint for w

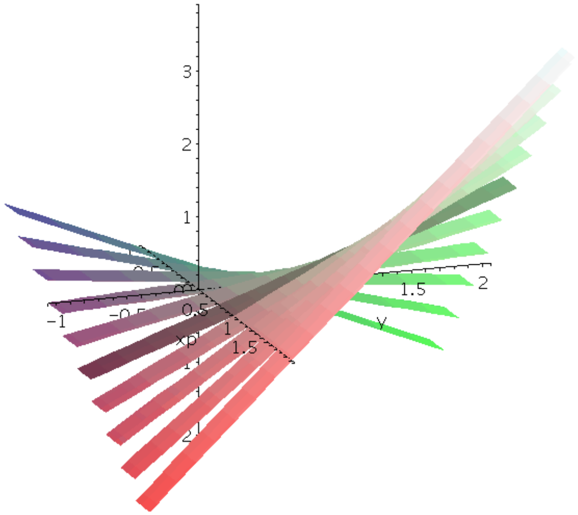
$$w = \sum_{i \leq d} (x^L + (i-1)\gamma) z_i y \tag{7}$$

- Reformulate the products $z_i y$ via PRODBINCONT

BilinApprox2

BilinApprox2: problem P has a term xy where $x \in [x^L, x^U], y \in [y^L, y^U]$ are continuous; assume $x^U - x^L \leq y^U - y^L$

1. choose integer $k > 0$; add $q = \{q_i \mid 0 \leq i \leq k\}$ to $\mathcal{P}$ so that $q_0 = x^L, q_k = x^U$, $q_i < q_{i+1}$ for all i
2. add continuous variable $w \in [w^L, w^U]$ (computed from ranges of x, y by interval arithmetic) and replace term xy by w
3. add binary variables z_i for $1 \leq i \leq k$ and constraint $\sum_{i \leq k} z_i = 1$
4. for all $1 \leq i \leq k$ add constraints:



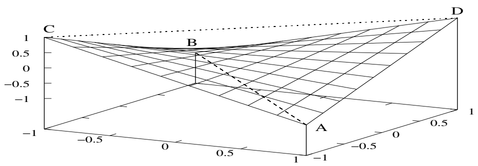
$k \to \infty$: get identity (exact) reformulation

$$\left.\begin{array}{c} \displaystyle\sum_{j=1}^{k} q_{j-1} z_j \leq x_i \leq \sum_{j=1}^{k} q_j z_j \\ \frac{q_i + q_{i-1}}{2} y - (w^U - w^L)(1 - z_i) \leq w \leq \frac{q_i + q_{i-1}}{2} y + (w^U - w^L)(1 - z_i), \end{array}\right\}$$

Relaxing bilinear terms

- RRLTRELAX: quadratic problem P with terms $x_i x_j$ ($i < j$) and constrs $Ax = b$ (x can be bin, int, cont); perform exact reformulation RRLT first:
  1. add continuous variables w_{ij} (let $w_i = (w_{i1}, \ldots, w_{1n})$)
  2. replace product $x_i x_j$ with w_{ij} (for all i, j)
  3. add the *reduced RLT* (RRLT) system $\forall k \; Aw_k - bx_k = 0$
  4. find a partition (B, N) of basic/nonbasic variables of $\forall k \; Aw_k = 0$ such that B corresponds to variables with smallest range
  5. for all $(i, j) \in N$ add constraints $w_{ij} = x_i x_j$ (†)
- then replace nonlinear constraints (†) with McCormick's envelopes

$$\begin{aligned} w_{ij} &\ge \max\{x_i^L x_j + x_j^L x_i - x_i^L x_j^L, x_i^U x_j + x_j^U x_i - x_i^U x_j^U\} \\ w_{ij} &\le \min\{x_i^U x_j + x_j^L x_i - x_i^U x_j^L, x_i^L x_j + x_j^U x_i - x_i^L x_j^U\} \end{aligned}$$



- The effect of RRLT is that of using information in $Ax = b$ to eliminate some of the problematic product terms (those with indices in B)

Linearizing the l_∞ norm

- INFNORM [Coniglio et al., MSc Thesis, 2007]. P has vars $x \in [-1,1]^d$ and constr. $||x||_\infty = 1$, s.t. $x^* \in \mathcal{F}(P) \leftrightarrow -x^* \in \mathcal{F}(P)$ and $f(x^*) = f(-x^*)$.
  1. $\forall k \le d$ add binary var u_k
  2. delete constraint $||x||_\infty = 1$
  3. add constraints:

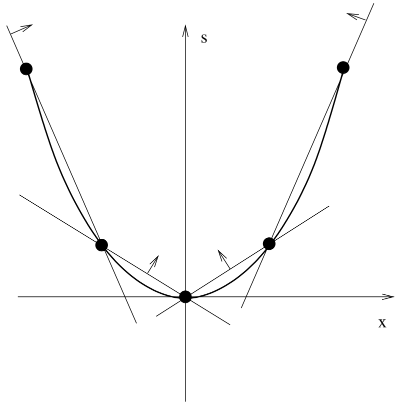
$$\begin{array}{rcl} \forall k \le d \quad x_k & \ge & 2u_k - 1 \\ \sum\limits_{k \le d} u_k & = & 1. \end{array}$$

- Narrowing INFNORM(P) cuts away all optima having $\max_k |x_k| = 1$ with $x_k < 1$ for all $k \le d$

Approximating squares

- INNERAPPROXSQ: P has a continuous variable $x \in [x^L, x^U]$ and a term x^2 appearing as a convex term in an objective or constraint

  1. add parameters $n \in \mathbb{N}$, $\varepsilon = \frac{x^U - x^L}{n-1}$, $\bar{x}_i = x^L + (i-1)\varepsilon$ for $i \leq n$
  2. add a continuous variable $w \in [w^L, w^U]$, where $w^L = 0$ if $x^L x^U \leq 0$ or $\min((x^L)^2, (x^U)^2)$ otherwise and $w^U = \max((x^L)^2, (x^U)^2)$
  3. replace all occurrences of term x^2 with w
  4. add constraints
  $$\forall i \leq n \quad w \geq (\bar{x}_i + \bar{x}_{i-1})x - \bar{x}_i \bar{x}_{i-1}.$$



$n \to \infty$: get identity (exact) reformulation

- Replace convex term by piecewise linear approximation

Conditional constraints

- Suppose $\exists$ a binary variable y and a constraint $g(x) \leq 0$ in the problem
- We want $g(x) \leq 0$ to be active iff $y = 1$
- Compute maximum value that $g(x)$ can take over all x, call this M
- Write the constraint as:

$$g(x) \leq M(1 - y)$$

- This sometimes called the “big M” modelling technique

Example:

Can replace constraint (7) in BILINAPPROX as follows:

$$\forall i \leq d \quad -M(1 - z_i) \leq w - (x^L + (i-1)\gamma)y \leq M(1 - z_i)$$

where M s.t. $w - (x^L + (i-1)\gamma)y \in [-M, M]$ for all w, x, y

Symmetry

Example

Consider the problem

$$\left.\begin{array}{rrcl} \min & x_1 + x_2 & & \\ & 3x_1 + 2x_2 & \geq & 1 \\ & 2x_1 + 3x_2 & \geq & 1 \\ & x_1, x_2 & \in & \{0, 1\} \end{array}\right\}$$

AMPL code:

```
set J := 1..2;
var x{J} binary;
minimize f: sum{j in J} x[j];
subject to c1: 3*x[1] + 2*x[2] >= 1;
subject to c2: 2*x[1] + 3*x[2] >= 1;
option solver cplex;
solve;
display x;
```

The solution (given by CPLEX) is $x_1 = 1$, $x_2 = 0$

If you swap x_1 with x_2, you obtain the same problem, with swapped constraints

Hence, $x_1 = 0$, $x_2 = 1$ is *also* an optimal solution!

Permutations

- We can represent permutations by maps $\mathbb{N} \to \mathbb{N}$
- The permutation of our example is $\begin{pmatrix} 1 & 2 \\ \downarrow & \downarrow \\ 2 & 1 \end{pmatrix}$
- Permutations are usually written as *cycles*: e.g. for a permutation $\begin{pmatrix} 1 & 2 & 3 \\ \downarrow & \downarrow & \downarrow \\ 3 & 1 & 2 \end{pmatrix}$, which sends $1 \to 3$, $3 \to 2$ and $2 \to 1$, we write $(1, 3, 2)$ to mean $1 \to 3 \to 2(\to 1)$
- The permutation of our example is $(1, 2)$ — a cycle of *length* 2 (also called a *transposition*, or *swap*)

Cycles

- Cycles can be multiplied together, but the multiplication is not commutative: $(1,2,3)(1,2) = (1,3)$ and $(1,2)(1,2,3) = (2,3)$
- The *identity* permutation e fixes all $\mathbb{N}$
- Notice $(1,2)(1,2) = e$ and $(1,2,3)(1,3,2) = e$, so $(1,2) = (1,2)^{-1}$ and $(1,3,2) = (1,2,3)^{-1}$
- Cycles are *disjoint* when they have no common element
- *Thm.* Disjoint cycles commute
- *Thm.* Every permutation can be written uniquely (up to order) as a product of disjoint cycles
- For each permutation π, let $\Gamma(\pi)$ be the set of its disjoint cycles

Groups

- A *group* is a set G together with a multiplication operation, an inverse operation, and an identity element $e \in G$, such that:
  1. $\forall g, h \in G \; (gh \in G)$ (multiplication closure)
  2. $\forall g \in G \; (g^{-1} \in G)$ (inverse closure)
  3. $\forall f, g, h \in G \; ((fg)h = f(gh))$ (associativity)
  4. $\forall g \in G \; (eg = g)$ (identity)
  5. $\forall g \in G \; (g^{-1}g = e)$ (inverse)
- The set $\{e\}$ is a group (denoted by 1) called the *trivial group*
- The set of all permutations over $\{1, \dots, n\}$ is a group, called the *symmetric group of order* n, and denoted by S_n
- For all $B \subseteq \{1, \dots, n\}$ define $\mathsf{Sym}(B)$ as the symmetric group over the symbols of B

Generators

- Given any subset $T \subseteq S_n$, the smallest group containing the permutations in T is the *group generated by* T, denoted by $\langle T \rangle$
- For example, if $T = \{(1,2),(1,2,3)\}$, then $\langle T \rangle$ is $\{(1),(1,2),(1,3),(2,3),(1,2,3),(1,3,2)\} = S_3$
- For any $n \in \mathbb{N}$, $\langle (1,\ldots,n) \rangle$ is the *cyclic group of order* n, denoted by C_n
- C_n is commutative, whereas S_n is not
- Commutative groups are also called *abelian*
- $\boxed{\textit{Thm. } \langle (1,2),(1,\ldots,n) \rangle = \langle (i,i+1) \mid 1 \leq i < n \rangle = S_n}$

Subgroups and homomorphisms

- A *subgroup* of a group G is a subset H of G which is also a group (denoted by $H \leq G$); e.g. $C_3 = \{e, (1,2,3), (1,3,2)\}$ is a subgroup of S_3
- Given two groups G, H, a map $\phi : G \to H$ such that $\forall f, g \in G \; (\; \phi(fg) = \phi(f)\phi(g) \;)$ is a *homomorphism*
- Ker$\phi = \{g \in G \mid \phi(g) = e\}$ is the *kernel* of ϕ (Ker$\phi \leq G$)
- Im$\phi = \{h \in H \mid \exists g \in G \; (h = \phi(g))\}$ is the *image* of ϕ (Im$\phi \leq H$)
- If ϕ is injective and surjective (i.e. if Ker$\phi = 1$ and Im$\phi = H$), then ϕ is an *isomorphism*, denoted by $G \cong H$
- *Thm.*[Lagrange] For all groups G and $H \leq G$, $|H|$ divides $|G|$
- *Thm.*[Cayley] Every finite group is isomorphic to a subgroup of S_n for some $n \in \mathbb{N}$

Normal subgroups

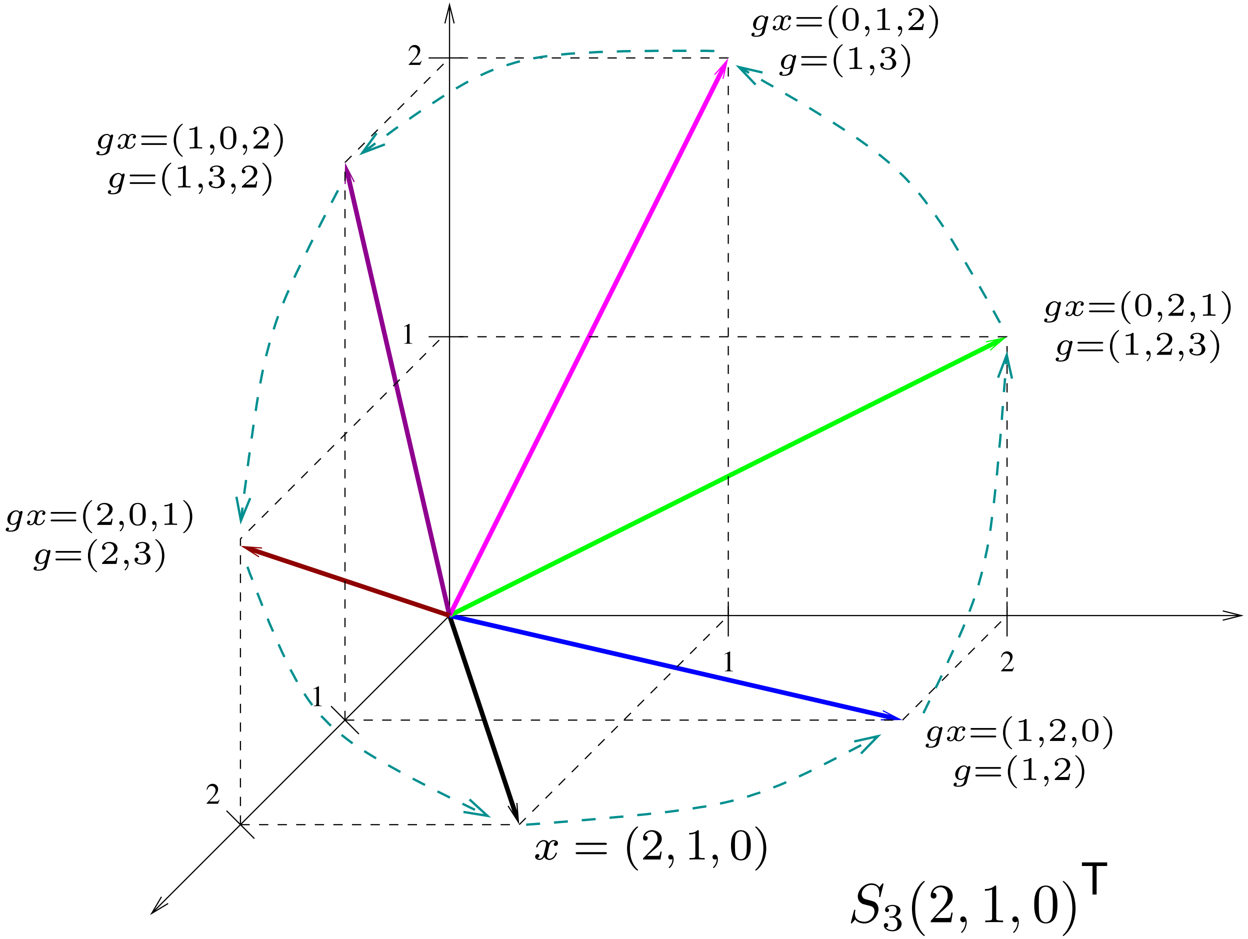
- Let $H \leq G$; for all $g \in G$, $gH = \{gh \mid h \in H\}$ and $Hg = \{hg \mid h \in H\}$ are in general *subsets* (not necessarily subgroups) of G, and in general $gH \neq Hg$
- If $\forall g \in G\ (gH = Hg)$ then H is a *normal subgroup* of G, denoted by $H \lhd G$ (e.g. $C_3 \lhd S_3$)
- If $H \lhd G$, then $\{gH \mid g \in G\}$ is denoted by G/H and has a group structure with multiplication $(fH)(gH) = (fg)H$, inverse $(gH)^{-1} = (g^{-1})H$ and identity $eH = H$
- For every group homomorphism ϕ, Ker$\phi \lhd G$ and $G/$Ker$\phi \cong$ Imϕ

Group actions

- Given a group G and a set X, the *action* of G on X is a set of mappings $\alpha_g : X \to X$ for all $g \in G$, such that $\alpha_g(x) = (gx) \in X$ for all $x \in X$
- Essentially, the action of G on X is the definition of what happens to $x \in X$ when g is applied to it
- For example, if $X = \mathbb{R}^n$ and $G = S_n$, a possible action of G on X is given by gx being the vector x with components permuted according to g (e.g. if $x = (0.1, -2, \sqrt{2})$ and $g = (1, 2)$, then $gx = (-2, 0.1, \sqrt{2})$)
- *Convention*: left multiplication if x is a column vector ($\alpha_g(x) = gx$), right if x is a row vector ($\alpha_g(x) = xg$): treat g as a matrix

Orbits

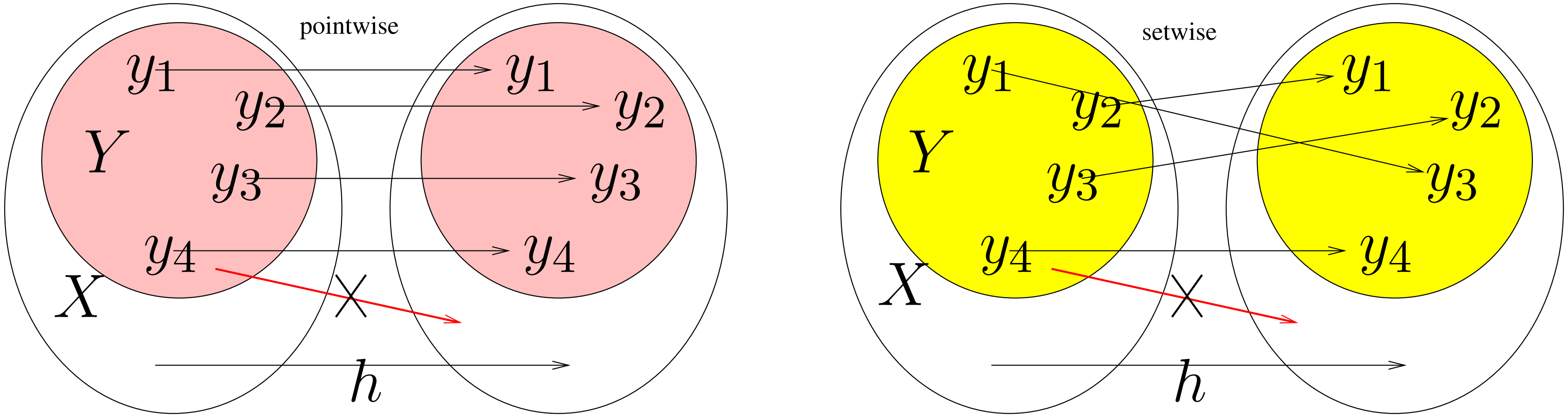
If G acts on $X \subseteq \mathbb{R}^n$, for all $x \in X$, $Gx = \{gx \mid g \in G\}$ is the *orbit* of x w.r.t. G



$S_3(2,1,0)^\mathsf{T}$

Stabilizers

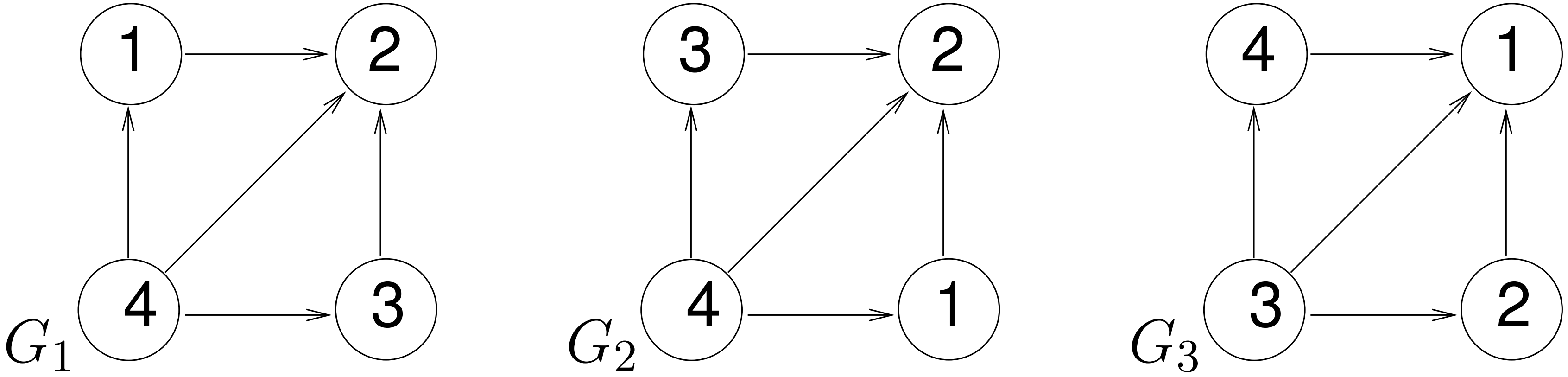
- Given $Y \subseteq X$, the *point-wise stabilizer* of Y w.r.t. G is a subgroup $H \leq G$ such that $hy = y$ for all $h \in H, y \in Y$



- The *set-wise stabilizer* of Y w.r.t. G is a subgroup $H \leq G$ such that $HY = Y$ (denote H by stab(Y, G))
- Let $\pi \in S_n$ with disjoint cycle product $\sigma_1 \cdots \sigma_k$ and $N \subseteq \{1 \ldots, n\}$
- $\pi[N] = \prod_{\sigma \in \Gamma(\pi) \cap \text{Sym}(N)} \sigma$: **restriction of π to N**

Groups and graphs

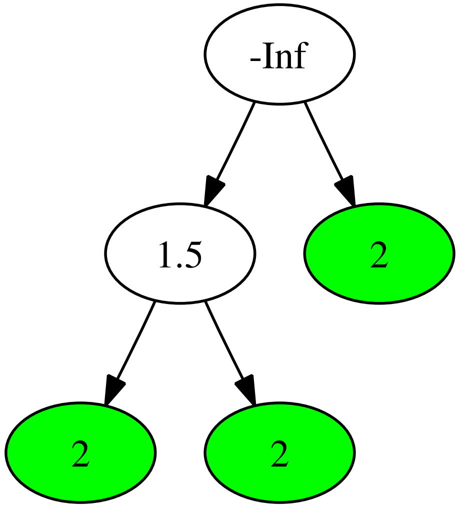
- Given a digraph $G = (V, A)$ with $V = \{v_1, \ldots, v_n\}$, the action of $\pi \in S_n$ on G is the natural action of π on V
- π is a *graph automorphism* if $\forall (i, j) \in A \; (\pi(i), \pi(j)) \in A$
- For example:



- $G_2 = (1, 3)G_1$ is a graph automorphism of G_1
- $G_3 = (1, 2, 3, 4)G_1$ is not an automorphism of G_1: e.g. $(4, 2) \in A$ but $(\pi(4), \pi(2)) = (1, 3) \not\in A$
- The *automorphism group* of G_1 is $\langle e, (1, 3) \rangle \cong C_2$ (denoted by Aut(G_1))

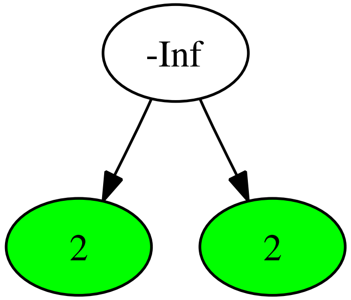
Back to MP: Symmetries and BB

- Symmetries are **bad** for Branch-and-Bound techniques: many branches will contain (symmetric) optimal solutions and therefore will not be pruned by bounding
  ⇒ *deep and large BB trees*



← *BB tree for symmetric problem*

BB tree for "problem modulo symmetries" →



- How do we write a "mathematical programming formulation modulo symmetries"?

Solution symmetries

- The set of solutions of the following problem:

$$\begin{array}{rrrrrrrcl} \min & x_{11} & +x_{12} & +x_{13} & +x_{21} & +x_{22} & +x_{23} & & \\ & x_{11} & +x_{12} & +x_{13} & & & & \geq & 1 \\ & & & & x_{21} & +x_{22} & +x_{23} & \geq & 1 \\ & x_{11} & & & +x_{21} & & & \geq & 1 \\ & & x_{12} & & & +x_{22} & & \geq & 1 \\ & & & x_{13} & & & +x_{23} & \geq & 1 \end{array}$$

  is $\mathcal{G}(P) = \begin{array}{l} \{(0,1,1,1,0,0),(1,0,0,0,1,1),(0,0,1,1,1,0), \\ \ (1,1,0,0,0,1),(1,0,1,0,1,0),(0,1,0,1,0,1)\} \end{array}$

- $G^* =$ stab$(\mathcal{G}(P), S_n)$ is the *solution group* **(variable permutations keeping $\mathcal{G}(P)$ fixed)**

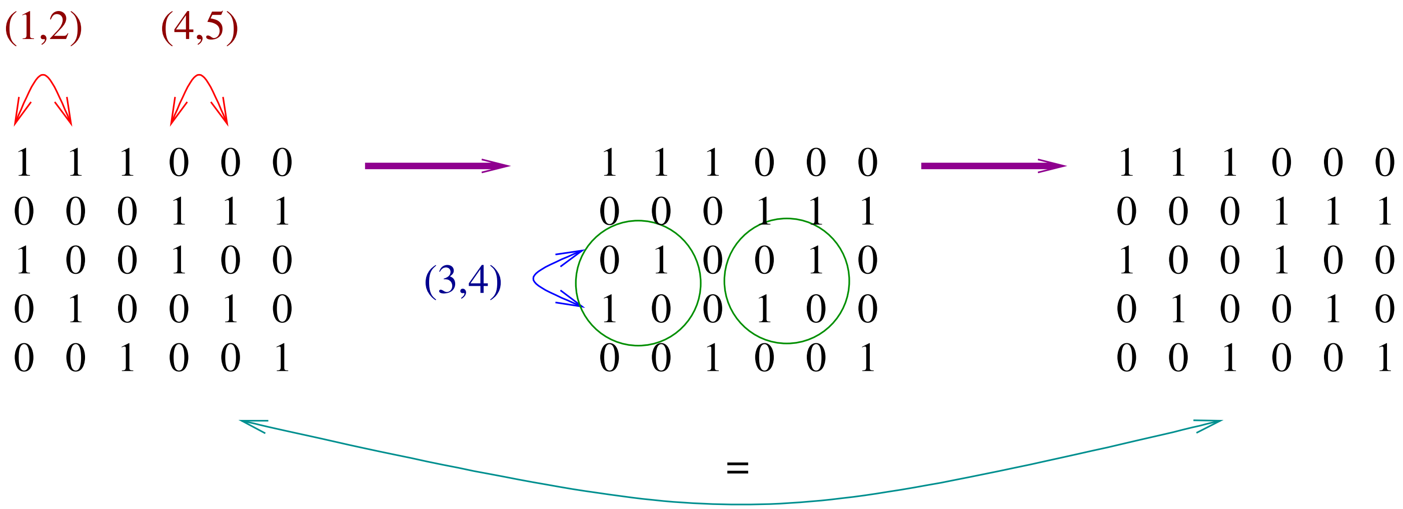
- For the above problem, G^* is $\langle(2,3)(5,6),(1,2)(4,5),(1,4)(2,5)(3,6)\rangle \cong D_{12}$

- For all $x^* \in \mathcal{G}(P)$, $G^* x^* = \mathcal{G}(P) \Rightarrow \exists$ only 1 orbit $\Rightarrow \exists$ only *one* solution in $\mathcal{G}(P)$ (modulo symmetries)

- How do we find G^* before solving P?

Formulation symmetries

- Cost vector $c = (1,1,1,1,1,1)$: $cS_6 = \{c\}$
- RHS vector $b = (1,1,1,1,1)$: $S_5 b = \{b\}$
- Constraint matrix A *(constraint order independence $\Rightarrow$ can always permute rows arbitrarily)*:



$$\begin{matrix}1&1&1&0&0&0\\0&0&0&1&1&1\\1&0&0&1&0&0\\0&1&0&0&1&0\\0&0&1&0&0&1\end{matrix} \longrightarrow \begin{matrix}1&1&1&0&0&0\\0&0&0&1&1&1\\0&1&0&0&1&0\\1&0&0&1&0&0\\0&0&1&0&0&1\end{matrix} \longrightarrow \begin{matrix}1&1&1&0&0&0\\0&0&0&1&1&1\\1&0&0&1&0&0\\0&1&0&0&1&0\\0&0&1&0&0&1\end{matrix}$$

$\Rightarrow (3,4)A(1,2)(4,5) = A$

- For general LPs with data A, b, c, if $\exists \pi \in S_n, \sigma \in S_m \; (c\pi = c \wedge \sigma b = b \wedge \sigma(A\pi) = A)$ then π *fixes the formulation* of the LP

The MILP formulation group

- If P is an LP with data A, b, c, then

$$G_P = \{\pi \in S_n \mid \exists \sigma \in S_m (c\pi = c \wedge \sigma b = b \wedge \sigma A \pi = A)\} \quad (8)$$

is the *formulation group* of P

- For the example, $G_{\texttt{example}} \cong D_{12} \cong G^*$

Thm.

$\boxed{\text{If } P \text{ is an LP, then } G_P \leq G^*_P.}$

- Result can be extended to all MILPs [Margot 2002, 2003, 2007]

Symmetries in MINLPs

- **Consider the following MINLP P:**

$$\left.\begin{array}{rrcl} \min & f(x) & & \\ & g(x) & \leq & 0 \\ & x & \in & X. \end{array}\right\} \qquad (9)$$

where X may contain integrality constraints on x

- For a row permutation $\sigma \in S_m$ and a column permutation $\pi \in S_n$, we define $\sigma P \pi$ as follows:

$$\left.\begin{array}{rrcl} \min & f(x\pi) & & \\ & \sigma g(x\pi) & \leq & 0 \\ & x\pi & \in & X. \end{array}\right\} \qquad (10)$$

- Define $\bar{G}_P = \{\pi \in S_n \mid \exists \sigma \in S_m \; (\sigma P \pi = P)\}$

A computable definition

- Establishing whether $\forall x\,(\sigma A x \pi = A x)$ is easy, just look at components of A and $\sigma A \pi$
- In general, the statement $\forall x\,(\sigma g(x\pi) = g(x) \wedge f(x\pi) = f(x))$ is undecidable
- Assume we have a computable "equality oracle" $\texttt{equal}(h_1, h_2)$ so that:

  if $\texttt{equal}(h_1, h_2) = \texttt{true}$, then $\forall x\,(h_1(x) = h_2(x))$

  The converse may not hold
- **Define G_P as $\bar{G}_P$ with $=$ replaced by $\texttt{equal}$ returning $\texttt{true}$**
- Can show $G_P \leq \bar{G}_P \leq G^*_P$

Decision problems:

FORMULATION SYMMETRY. Given formulations P, Q and the oracle $\texttt{equal}$, are there permutations σ, π such that $P = \sigma Q \pi$?

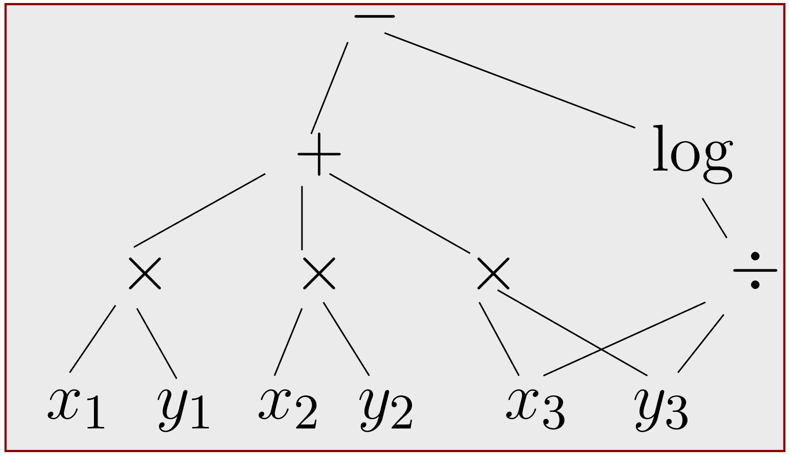
FORMULATION GROUP. Given P and $\texttt{equal}$, find generators for G_P

Equality oracle

- Consider the *expression DAG* representation of g

$$\sum_{i=1}^{3} x_i y_i - \log(x_3/y_3)$$

List of expressions $\equiv$ *expression DAG sharing variable leaf nodes*



- *Every function $g : \mathbb{R}^n \to \mathbb{R}^m$ is represented by a DAG whose leaf nodes are variables and constants and whose intermediate nodes are mathematical operators*

- `equal`$(g(x), \sigma g(x\pi))$ `=true` if and only if the DAGs representing $g(x)$ and $\sigma g(x\pi)$ are isomorphic

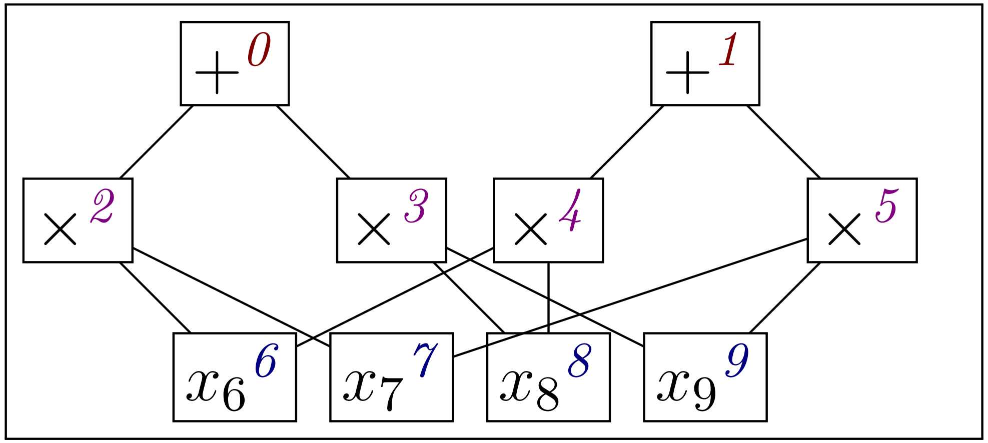
- Reduces the FORMULATION SYMMETRY problem to the GRAPH ISOMORPHISM problem

GRAPH ISOMORPHISM

- Citation: Babai, *Automorphism groups, ismorphism, reconstruction*, in Graham, Grötschel, Lovász (eds.), Handbook of Combinatorics, vol. 2
- GI is in **NP**
- It is unknown whether it is in **P** or **NP**-complete
- Solving GI on rooted DAGs is as hard as solving it on general graphs
- Solving GI on trees has linear complexity
- Our DAGs are "close" to trees, can hope they are not too hard for GI testing

Example

$$\begin{aligned} \mathsf{C}_0 &: x_6x_7 + x_8x_9 &= 1 \\ \mathsf{C}_1 &: x_6x_8 + x_7x_9 &= 1 \end{aligned}$$



- G_{DAG} = group of automorphisms of expression DAG fixing: (a) root node set having same constr. direction and coeff. (constraint permutations), (b) operators with same label and rank and (c) leaf node set (variable permutations)

$$G_{\mathsf{DAG}} = \langle (45)(67)(89),\ (23)(68)(79),\ (01)(24)(35)(78) \rangle$$

- G_P is the projection of G_{DAG} to variable indices $\langle (6,7)(8,9),(6,8)(7,9),(7,8) \rangle \cong D_8$

Node colors

- Let $D_P = (\mathcal{V}, \mathcal{A})$ be the union of all objective and constraint DAGs in the MINLP (a.k.a *the DAG of* P)
- *Colors on the DAG nodes* $\mathcal{V}$ *are used to identify those subsets of nodes which can be permuted* (e.g. variable and operator nodes can't be permuted)

1. **Root nodes (i.e. constraints) can be permuted if they have the same RHS**
2. **Operator nodes (including root nodes) can be permuted if they have the same DAG rank and label; if an operator node is non-commutative, then the order of the children node must be maintained**
3. **Constant nodes can be permuted if they have the same DAG rank level and value**
4. **Variable nodes can be permuted if they have the same bounds and integrality constraints**

- The relation $(u \sim v \iff u, v$ have the same color$)$ is an *equivalence relation* on V (reflexive, symmetric, transitive)
- $\sim$ partitions $\mathcal{V}$ into a disjoint union $\mathcal{V}/\sim$ of *equivalence classes* $V_1, \ldots, V_p$

MINLP formulation groups

- Let P be a MINLP and $D = (\mathcal{V}, \mathcal{A})$ be the DAG of P
- Let G_{DAG} be the group of automorphisms of D that fix each color class in $\mathcal{V}/\sim$
- Define $\phi : G_{\text{DAG}} \to S_n$ by $\phi(\pi) =$projection of π on variable indices; then
  Thm.
  ϕ is a group homomorphism and Im$\phi \cong G_P$
- Hence can find G_P by computing Imϕ
- Although the complexity status (**P**/**NP**-complete) of the GRAPH ISOMORPHISM problem is currently unknown, `nauty` is a practically efficient software for computing G_{DAG}
- **So now we have G_P, how do we write "P modulo G_P"?**

Symmetry-breaking reformulation

- Consider our first example P:

$$\left.\begin{array}{lrcl}\min & x_1+x_2 & & \\ & 3x_1+2x_2 & \ge & 1 \\ & 2x_1+3x_2 & \ge & 1 \\ & x_1,x_2 & \in & \{0,1\}\end{array}\right\}$$

- P has $\mathcal{G}(P)=\{(0,1),(1,0)\}$, $G^*=\langle(1,2)\rangle\cong C_2$ and $G_P=G^*$
- The orbit $G_P(0,1)$ is the whole of $\mathcal{G}(P)$
- We look for a reformulation of P where at least *one* representative of each orbit is feasible
- Let Q be the reformulation of P consisting of P with the added constraint $x_1\le x_2$
- We have $\mathcal{G}(Q)=\{(0,1)\}$ and $G^*=G_Q=1$

Breaking orbital symmetries 1

- Every group $G \leq S_n$ acting on the variable indices $N = \{1, \ldots, n\}$ partitions N into *disjoint orbits* (all subsets of N)
- *This follows from the equiv. rel.* $i \sim j \Leftrightarrow \exists g \in G\ (g(i) = j)$
- Let Ω be the set of *nontrivial* orbits ($\omega \in \Omega \iff |\omega| > 1$)
- $\boxed{\textit{Thm. } G \text{ acts transitively on each of its orbits}}$
- This means that $\forall \omega \in \Omega\ \forall i \neq j \in \omega\ \exists g \in G\ (g(i) = j)$
- **Applied to MP, if i, j are distinct variable indices belonging to the same orbit of G_P acting on N, then there is $\pi \in G_P$ sending x_i to x_j**
- Pick $x \in \mathcal{G}(P)$; if P is bounded, for all $\omega \in \Omega\ \exists i \in \omega$ s.t. x_i is a component having minimum value over all components of x
- By theorem above, $\exists \pi \in G_P$ sending x_i to $x_{\min \omega}$
- Hence $\bar{x} = x\pi$ is s.t. $\bar{x}_{\min \omega}$ is minimum over all other components of $\bar{x}$, and since $G_P \leq G^*$, $\bar{x} \in \mathcal{G}(P)$

Breaking orbital symmetries 2

- Thus, for all $\omega \in \Omega$ there is at least one optimal solution of P which is feasible w.r.t. the constraints $\forall j \in \omega \ (x_{\min \omega} \leq x_j)$
- Such constraints are called (orbit-based) *symmetry breaking constraints* (SBCs)
- Adding these SBCs to P yields a reformulation Q of P of the narrowing type (prove it!)
- *Thm.* If $g^\omega(x) \leq 0$ are SBCs for each orbit ω with "appropriate properties", then $\forall \omega \in \Lambda \ (g^\omega(x) \leq 0)$ are also SBCs
- Thus we can combine orbit-based SBCs for "appropriate properties"
- **Yields narrowings with fewer symmetric optima**

“Appropriate properties”

Notation: $g[B](x) \leq 0$ *if* $g(x)$ *only involve variable indices in* B

Conditions allowing adjunctions of many SBCs

Thm.

Let $\omega, \theta \subseteq \{1, \ldots, n\}$ be such that $\omega \cap \theta = \emptyset$. Consider $\rho, \sigma \in G_P$, and let $g[\omega](x) \leq 0$ be SBCs w.r.t. $\rho, \mathcal{G}(P)$ and $h[\theta](x) \leq 0$ be SBCs w.r.t. $\sigma, \mathcal{G}(P)$. If $\rho[\omega], \sigma[\theta] \in G_P[\omega \cup \theta]$ then the system of constraints $\{g[\omega](x) \leq 0, h[\theta](x) \leq 0\}$ is an SBC system for $\rho\sigma$.

Breaking the symmetric group

- The above SBCs work with any group G_P, but their extent is limited (they may not break all that many symmetries)
- If we find $\Lambda' \subseteq \Lambda$ such that $\forall \omega \in \Lambda'$ the action of G_P on ω is $\mathsf{Sym}(\omega)$, then there are much tighter SBCs
- For all $\omega \in \Lambda'$ let $\omega^- = \omega \smallsetminus \{\max \omega\}$ and for all $j \in \omega^-$ let j^+ be the successor of j in ω
- The following are valid SBCs:

$$\forall \omega \in \Lambda' \, \forall j \in \omega^- \quad x_j \leq x_{j^+}$$

which are likely to break many more symmetries

The final attack on the KNP

Decision KNP

- Recall the binary KNP variables are used to count the number of spheres
- Suggests simply considering whether a *fixed number of spheres* can be placed around a central sphere in a kissing configuration, or not
- This is the *decision version* of the KNP (dKNP):

  > *Given positive integers* n, d*, can* n *unit spheres with disjoint interior be placed adjacent to a unit sphere centered at the origin of* $\mathbb{R}^d$*?*

- Should eliminate binary variables, yielding a (nonconvex) NLP, simpler than the original MINLP
- In order to find the maximum value for n, we proceed by bisection on n and solve the dKNP repeatedly

The dKNP formulation

- Let $N = \{1, \ldots, n\}$; the following formulation P correctly models the dKNP:

$$\left.\begin{array}{rrcl}
\max & 0 & & \\
\forall i \in N & \sum\limits_{k\in D} x_{ik}^2 & = & 4 \\
\forall i \in N, j \in N : i < j & \sum\limits_{k\in D} (x_{ik} - x_{jk})^2 & \geq & 4 \\
\forall i \in N, k \in D & x_{ik} & \in & [-2, 2]
\end{array}\right\}$$

- If $\mathcal{F}(P) \neq \emptyset$ then the answer to the dKNP is YES, otherwise it is NO
- However, solving nonconvex feasibility NLPs is numerically *extremely difficult*

Feasibility tolerance

- We therefore add a *feasibility tolerance* variable α:

$$\left.\begin{array}{rrcl}
\max & \alpha & & \\
\forall i \in N & \sum\limits_{k\in D} x_{ik}^2 & = & 4 \\
\forall i \in N, j \in N : i < j & \sum\limits_{k\in D} (x_{ik} - x_{jk})^2 & \geq & 4\alpha \\
\forall i \in N, k \in D & x_{ik} & \in & [-2, 2] \\
 & \alpha & \geq & 0
\end{array}\right\}$$

- The above formulation Q is always feasible (why?)
- Much easier to solve than P, numerically
- Q also solves the dKNP: if the optimal α^* is ≥ 1 then the answer is YES, otherwise it is NO

The KNP group

- The dKNP turns out to have group S_d (i.e. each spatial dimension can be swapped with any other)
- Rewriting the distance constraints as follows:

$$\begin{aligned} ||x_i - x_j||^2 &= \sum_{k \in D} (x_{ik} - x_{jk})^2 \\ &= \sum_{k \in D} (x_{ik}^2 + x_{jk}^2 + 2x_{ik}x_{jk}) \\ &= 2(d + \sum_{k \in D} x_{ik}x_{jk}) \end{aligned}$$

(for $i < j \leq n$) yields an exact reformulation Q' of Q (prove it)

- The formulation group $G_{Q'}$ turns out to be $S_d \times S_n$ (pairs of distinct spatial dimensions can be swapped, and same for spheres), much larger than S_d
- Yields more effective SBC narrowings

Results

Instance		Solver	Without SBC				With SBC			
D	N		*Time*	*Nodes*	*OI*	*Gap*	*Time*	*Nodes*	*OI*	*Gap*
2	6	*Couenne*	4920.16	516000 **110150**	1	0.04%	100.19	14672	1	0%
2	6	*BARON*	1200*	45259 **6015**	1	10%	59.63	2785	131	0%
2	7	*Couenne*	7200†	465500 **127220**	1	41.8%	7200†	469780 **38693**	1	17.9%
2	7	*BARON*	10800	259800 **74419**	442	83.2%	16632	693162	208	0%

OI: *Iteration where optimum was found*

†: *default Couenne CPU time limit*

*: *default BARON CPU time limit*

nodes: $\frac{\textit{total nodes}}{\textbf{still on tree}}$

Thus, we finally established by MP that $k^*(2) = 6$

Actually, solutions for $k^*(3)$ and $k^*(4)$ can be found by using MINLP heuristics (VNS)

The end