Modelling and solution of Nonlinear Programs

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The story so far

- **Mathematical program**: problem model consisting of *parameters*, *variables*, *objective function*, *constraints*
- Parameters: the **problem input**
- Variables: the **problem output**
- Variables may be continuous ($\in \mathbb{R}$), integer ($\in \mathbb{Z}$) or binary ($\in \{0, 1\}$); they may also be bounded ($\in [L, U]$)
- Objective and constraints are expressed as mathematical functions of parameters and variables
- **Assumption**: objective and constraints are *linear forms*
- Modelling software: AMPL
- Solution software: CPLEX
- Many application examples

Nonlinear Programming

- Mathematical methods for modelling and solving nonlinear problems
- $\Rightarrow$ NonLinear Programming (NLP)
  - Nonconvex NLPs (NLPs with at least one nonconvex objective and/or constraint)
  - Mixed-Integer NLPs (MINLPs — with at least one integer variable)
- In practice, it is much more difficult to solve (MI)NLPs than (MI)LPs
  - No truly standard software
  - In general, no guarantee of optimality for nonconvex MINLPs
  - Few successful general-purpose algorithms
  - *Can still use AMPL, though*

Nonlinear Modelling

Linear assumption is not always valid

- Logical "and" condition:
  1. cost associated to conjunctive occurrence of two conditions *(if x_i is 1 and x_j is 1 then add a cost c_{ij})*
  2. a constraint is valid iff a certain binary variable has value 1 *(if y is 1 then $g(x) \leq 0$)*
- Percentages and quantities: variables expressing percentage and variables expressing quantity must be multiplied together
- Economies of scale: unit costs decrease with quantity
- Problems involving 1-, 2- and ∞-norms
- Nonlinear models of natural phenomena expressed in constraints

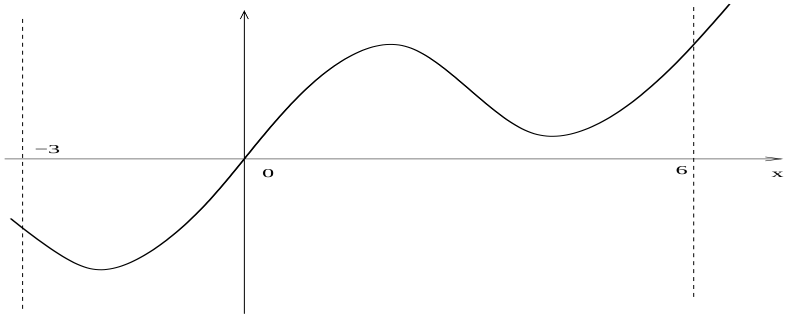
Canonical MINLP formulation

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

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

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

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



Reformulations

Defn.

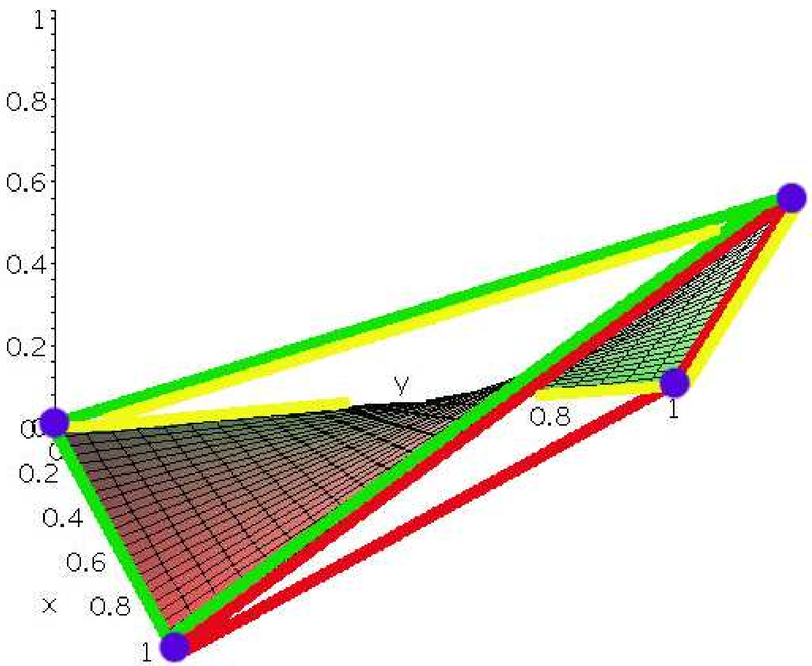
Given a formulation P and a formulation Q, Q is a *reformulation* of P if there is a mapping $\varphi : F(Q) \to F(P)$ such that $\varphi(L(Q)) = L(P)$ and $\varphi(G(Q)) = G(P)$

This means: φ restricted to $L(Q)$ is onto $L(P)$ and φ restricted to $G(Q)$ is onto $G(P)$

- Reformulations are used to transform problems into equivalent forms
- "Equivalence" here means a precise correspondence between local and global optima *via the same transformation*
- Basic reformulation operations:
  1. adding / deleting variables / constraints
  2. replacing 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 $z \leq y$, $z \leq x$
  $z \geq 0$, $z \geq x + y - 1$
- $x, y \in \{0, 1\} \Rightarrow$
  $z = xy$

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:

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

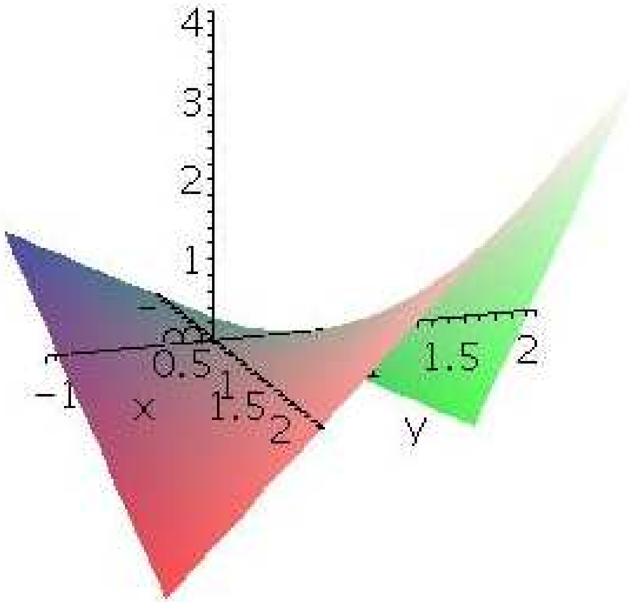
- Exercise 1: show that ProdBinCont is indeed a reformulation
- Exercise 2: show that if $y \in \{0,1\}$ then ProdBinCont is equivalent to ProdBin

Product of continuous variables

- Suppose a flow is composed by m different materials
- Let $x_i \in [0, 1]$ indicate the unknown fraction of material $i \leq m$ in the flow
- Let y be the unknown total flow
- Get terms $x_i y$ in the problem to indicate the amount of each material $i \leq m$ in the flow
- Constraint $\sum_{i \leq m} x_i = 1$: all fractions sum up to 1
- $\Rightarrow$ Nonconvex NLP
- No exact *linear* reformulation possible, but can be approximated by discretization
- Best way to solve it directly is by dedicated algorithm (e.g. SLP or SQP)

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 $\gamma = \frac{x^U - x^L}{d-1}$



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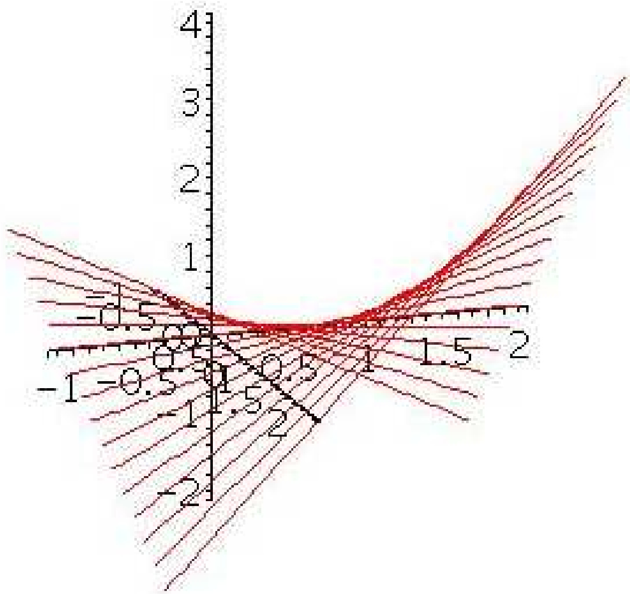


BilinApprox

- 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

$$w = \sum_{i \leq d} (x^L + (i-1)\gamma) z_i y \qquad (2)$$

- Reformulate the products $z_i y$ via ProdBinCont

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:

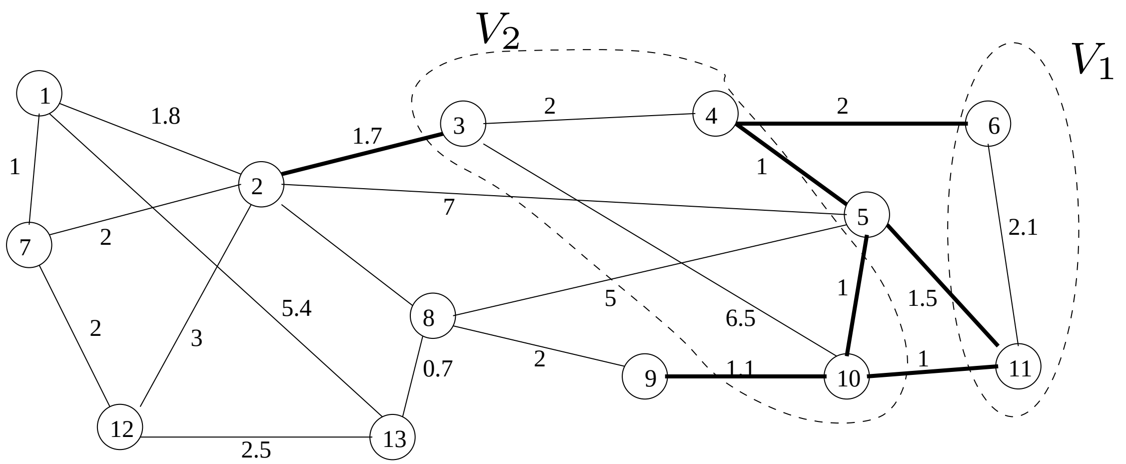
Can replace constraint (2) in BILINAPPROX as follows:

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

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

Graph Partitioning Problem I

- **GPP**: Given an undirected graph $G = (V, E)$ and an integer $k \leq |V|$, find a partition of V in k disjoint subsets $V_1, \ldots, V_k$ (called *clusters*) of minimal given cardinality M s.t. the number (weight) of edges with adjacent vertices in different clusters is minimized



$V_3 = V \setminus (V_1 \cup V_2)$

$k = 3$

min. clusters card. = 2

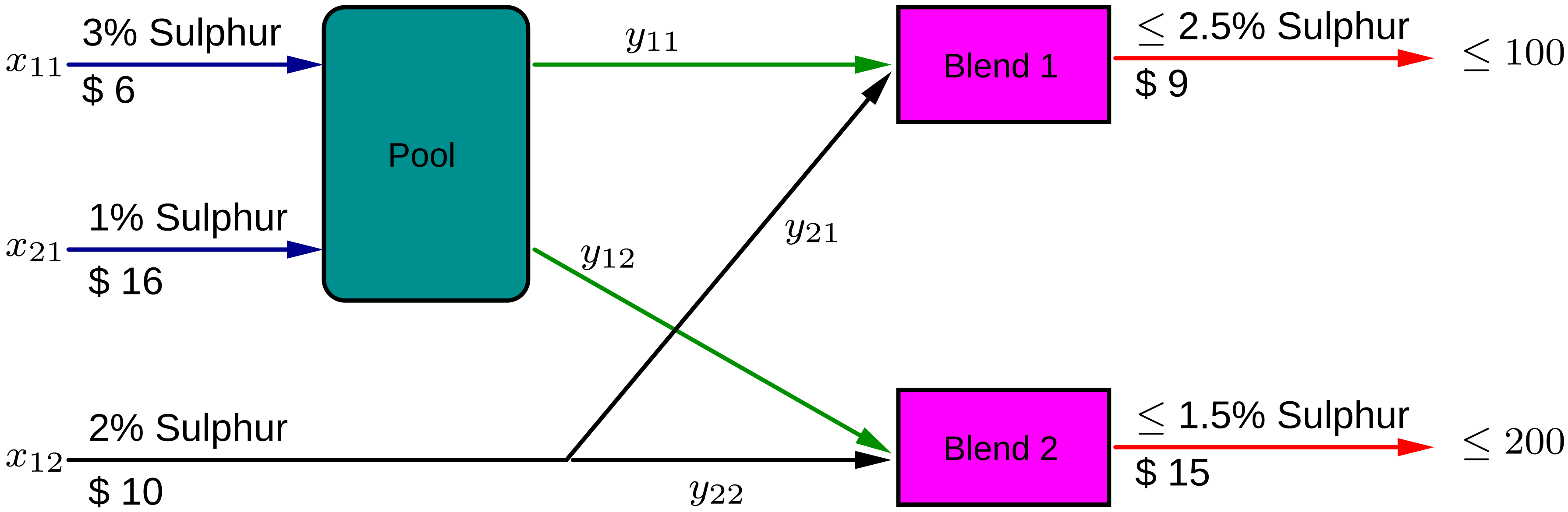
- **Applications**: telecom network planning, sparse matrix factorization, parallel computing, VLSI circuit placement
- **Minimal bibliography**: Battiti & Bertossi, *IEEE Trans. Comp.*, 1999 (heuristics); Boulle, *Opt. Eng.*, 2004 (formulations); Liberti *4OR*, 2007 (reformulations)

Graph Partitioning Problem II

- For all vertices $i \in V$, $h \leq k$:
  $x_{ih} = 1$ if vertex i in cluster h and 0 otherwise
- **Objective function**: $\min \frac{1}{2} \sum\limits_{h \neq l \leq k} \sum\limits_{\{i,j\} \in E} x_{ih} x_{jl}$
- Assignment: $\forall\, i \in V \;\; \sum\limits_{h \leq k} x_{ih} = 1$
- Cluster cardinality: $\forall\, h \leq k \;\; \sum_{i \in V} x_{ih} \leq M$
- nonconvex BQP: reformulate or linearize to MILP, then solve with CPLEX

Pooling and blending I

- Given an oil routing network with pools and blenders, unit prices, demands and quality requirements:



- Find the input quantities minimizing the costs and satisfying the constraints: mass balance, sulphur balance, quantity and quality demands

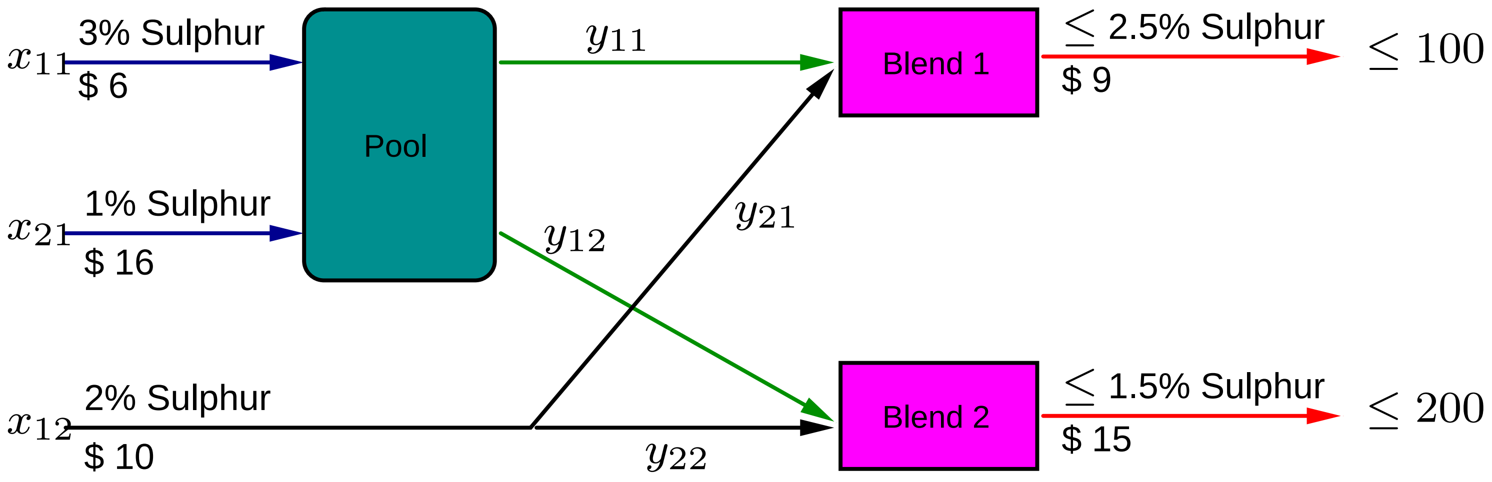
Pooling and blending II

- Variables: input quantities x, routed quantities y, percentage p of sulphur in pool
- Bilinear terms arise to express sulphur quantities in terms of p, y
- Sulphur balance constraint: $3x_{11} + x_{21} = p(y_{11} + y_{12})$
- Quality demands:

$$\begin{aligned} py_{11} + 2y_{21} &\leq 2.5(y_{11} + y_{21}) \\ py_{12} + 2y_{22} &\leq 1.5(y_{12} + y_{22}) \end{aligned}$$

- Continuous bilinear formulation $\Rightarrow$ nonconvex NLP

Haverly's pooling problem



$$\left\{\begin{array}{lll}
\min\limits_{x,y,p} & 6x_{11} + 16x_{21} + 10x_{12} - & \\
 & \quad -9(y_{11} + y_{21}) - 15(y_{12} + y_{22}) & \text{linear} \\
\text{s.t.} & x_{11} + x_{21} - y_{11} - y_{12} = 0 & \text{linear} \\
 & x_{12} - y_{21} - y_{22} = 0 & \text{linear} \\
 & y_{11} + y_{21} \leq 100 & \text{linear} \\
 & y_{12} + y_{22} \leq 200 & \text{linear} \\
 & 3x_{11} + x_{21} - p(y_{11} + y_{12}) = 0 & \text{bilinear} \\
 & py_{11} + 2y_{21} \leq 2.5(y_{11} + y_{21}) & \text{bilinear} \\
 & py_{12} + 2y_{22} \leq 1.5(y_{12} + y_{22}) & \text{bilinear}
\end{array}\right.$$

Successive Linear Programming

- Heuristic for solving bilinear programming problems
- Formulation includes bilinear terms $x_i y_j$ where $i \in I, j \in J$
- Problem is nonconvex $\Rightarrow$ many local optima
- Fact: fix $x_i, i \in I$, get LP$_1$; fix $y_j, j \in J$, get LP$_2$
- Algorithm: solve LP$_1$, get values for y, update and solve LP$_2$, get values for x, update and solve LP$_1$, and so on
- Iterate until no more improvement
- **Warning**: no convergence may be attained, and no guarantee to obtain global optimum

SLP applied to HPP

Problem LP$_1$: fixing p

$$
\begin{cases}
\min\limits_{x,y} & 6x_{11} + 16x_{21} + 10x_{12} - \\
 & \quad -9y_{11} - 9y_{21} - 15y_{12} - 15y_{22} \\
\text{s.t.} & x_{11} + x_{21} - y_{11} - y_{12} = 0 \\
 & x_{12} - y_{21} - y_{22} = 0 \\
 & y_{11} + y_{21} \leq 100 \\
 & y_{12} + y_{22} \leq 200 \\
 & 3x_{11} + x_{21} - \mathbf{p}y_{11} - \mathbf{p}y_{12} = 0 \\
 & (\mathbf{p} - 2.5)y_{11} - 0.5y_{21} \leq 0 \\
 & (\mathbf{p} - 1.5)y_{12} + 0.5y_{22} \leq 0
\end{cases}
$$

Problem LP$_2$: fixing y_{11}, y_{12}

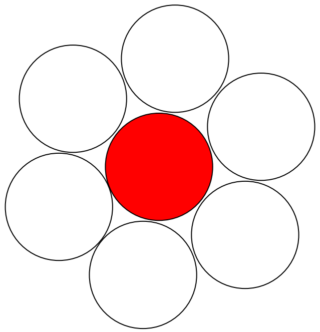
$$
\begin{cases}
\min\limits_{x,y_{21},y_{22},p} & 6x_{11} + 16x_{21} + 10x_{12} - \\
 & -(9(\mathbf{y_{11}} + \mathbf{y_{21}}) + 15(\mathbf{y_{12}} + \mathbf{y_{22}})) \\
\text{s.t.} & x_{11} + x_{21} = \mathbf{y_{11}} + \mathbf{y_{12}} \\
 & x_{12} - y_{21} - y_{22} = 0 \\
 & y_{21} \leq 100 - \mathbf{y_{11}} \\
 & y_{22} \leq 200 - \mathbf{y_{12}} \\
 & 3x_{11} + x_{21} - (\mathbf{y_{11}} + \mathbf{y_{12}})p = 0 \\
 & \mathbf{y_{11}}p - 0.5y_{21} \leq 2.5\mathbf{y_{11}} \\
 & \mathbf{y_{12}}p + 0.5y_{22} \leq 1.5\mathbf{y_{12}}
\end{cases}
$$

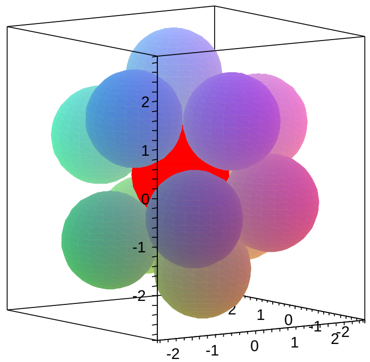
SLP Algorithm:

1. Solve LP$_1$, find value for y_{11}, y_{12}, update LP$_2$
2. Solve LP$_2$, find value for p, update LP$_1$
3. Repeat until solution does not change / iteration limit exceeded

Kissing Number Problem I

- Problem proposed by Newton
- Determine maximum number K of non-overlapping balls of radius 1 adjacent to a central ball of radius 1 in $\mathbb{R}^D$
- In $\mathbb{R}^2$: $K = 6$
- In $\mathbb{R}^3$: $K = 12$ (13 spheres prob.)





- In $\mathbb{R}^4$: $K = 24$ (recent result)
- Next open case: $D = 5$ ($40 \leq K \leq 45$)

Kissing Number Problem II

- Reduce to a decision problem (can N spheres be arranged in a kissing configuration?)
- Variables: let $x^i \in \mathbb{R}^D$ be the center of the i-th ball
- Continuous quadratic formulation:

$$\begin{array}{rl} \max & \alpha \\ \forall i \le N & ||x^i||^2 = 4 \\ \forall i < j \le N & ||x^i - x^j||^2 \ge 4\alpha \\ & \alpha \ge 0 \\ \forall i \le N & x^i \in \mathbb{R}^D, \end{array}$$

- If global optimum has $\alpha \ge 1$, then N balls can be arranged, otherwise they cannot
- [Kucherenko et al., DAM 2007]

The Hartree-Fock problem I

- Consider the time-independent non-relativistic Schrödinger equation $H_{el}\Psi = E_{el}\Psi$ for the electrons in a molecule
- Solution to Schrödinger equation are products of n molecular orbitals ψ_i
- Each ψ_i is composed of a spatial orbital $\bar{\varphi}_i$ and a spin orbital $\bar{\vartheta}_i$
- Spatial orbitals approximated by suitable bases $\{\chi_s\}_{s=1}^{b}$:

$$\varphi_i = \sum_{s=1}^{b} c_{si}\chi_s \qquad \forall i \leq n$$

where φ_i is the approximation of $\bar{\varphi}_i$

The Hartree-Fock problem II

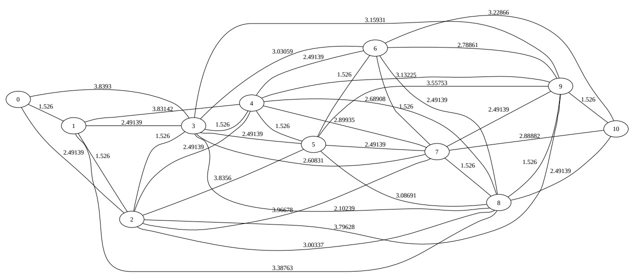
- Given b and $\{\chi_s\}_{s=1}^b$, determine the coefficients c_{si} such that the approximation is "best"
- Approximation is "best" when the energy $E(c)$ (quartic polynomial in c) of approximated spatial orbitals φ_i is minimum
- Orthogonality constraints on φ_i (to enforce lin. ind.)
- Coefficients c vary over a known range $c^L \leq c \leq c^U$
- Continuous quartic formulation:

$$\left.\begin{array}{rcl} \min_c & E(c) & \\ \text{s.t.} & \langle \varphi_i \mid \varphi_j \rangle = \delta_{ij} & \forall i \leq j \leq n \\ & c^L \leq c \leq c^U & \end{array}\right\}$$

- [Lavor et al., EPL 2007]

Molecular Distance Geometry

- Known set of atoms V, determine 3D structure
- Some inter-atomic distances d_{ij} known (NMR)
- Find atomic positions $x^i \in \mathbb{R}^3$ which preserve distances $\Rightarrow$ given weighted graph $G = (V, E, d)$, find immersion in $\mathbb{R}^3$



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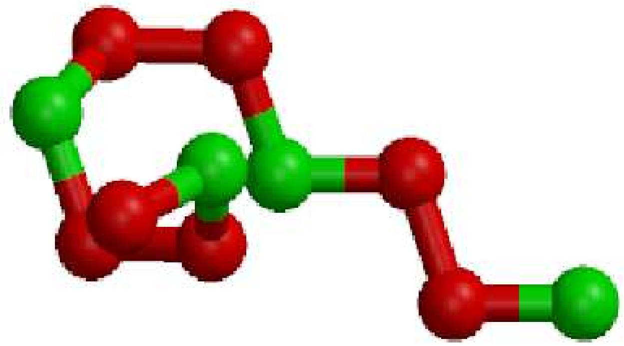


- Continuous quartic formulation:

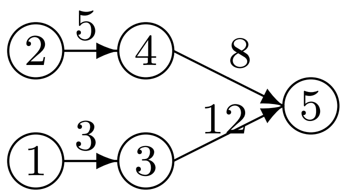
$$\min_x \sum_{\{i,j\} \in E} (||x^i - x^j||^2 - d_{ij}^2)^2 \quad (3)$$

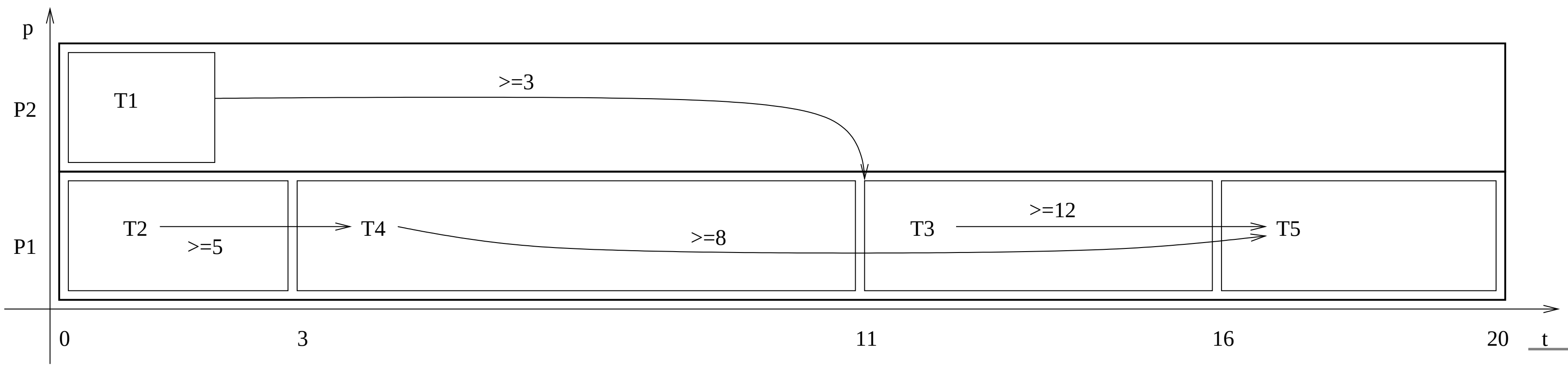
- [Lavor et al. 2006]

Scheduling with delays I

- T: tasks of length L_i with precedences given by DAG $G = (V, A, c)$, where c_{ij} = amount of data passed from i to j
- P: homogeneous processors with distance d_{kl} between processors k, l in architecture
- Delays γ_{ij}^{kl} occur if dependent tasks i, j are executed on different processors k, l

i	1	2	3	4	5
L_i	2	3	5	8	4





Scheduling with delays II

- Idea: pack $L_j \times 1$ “task rectangles” into a $T_{\text{max}} \times |P|$ “total time” rectangle
- Use binary assignment variables $z_{jk} = 1$ if task $j \in T$ is executed on processor $k \in P$
- Use continuous scheduling variables t_j = starting time of task j
- Model communication delays with quadratic constraints:

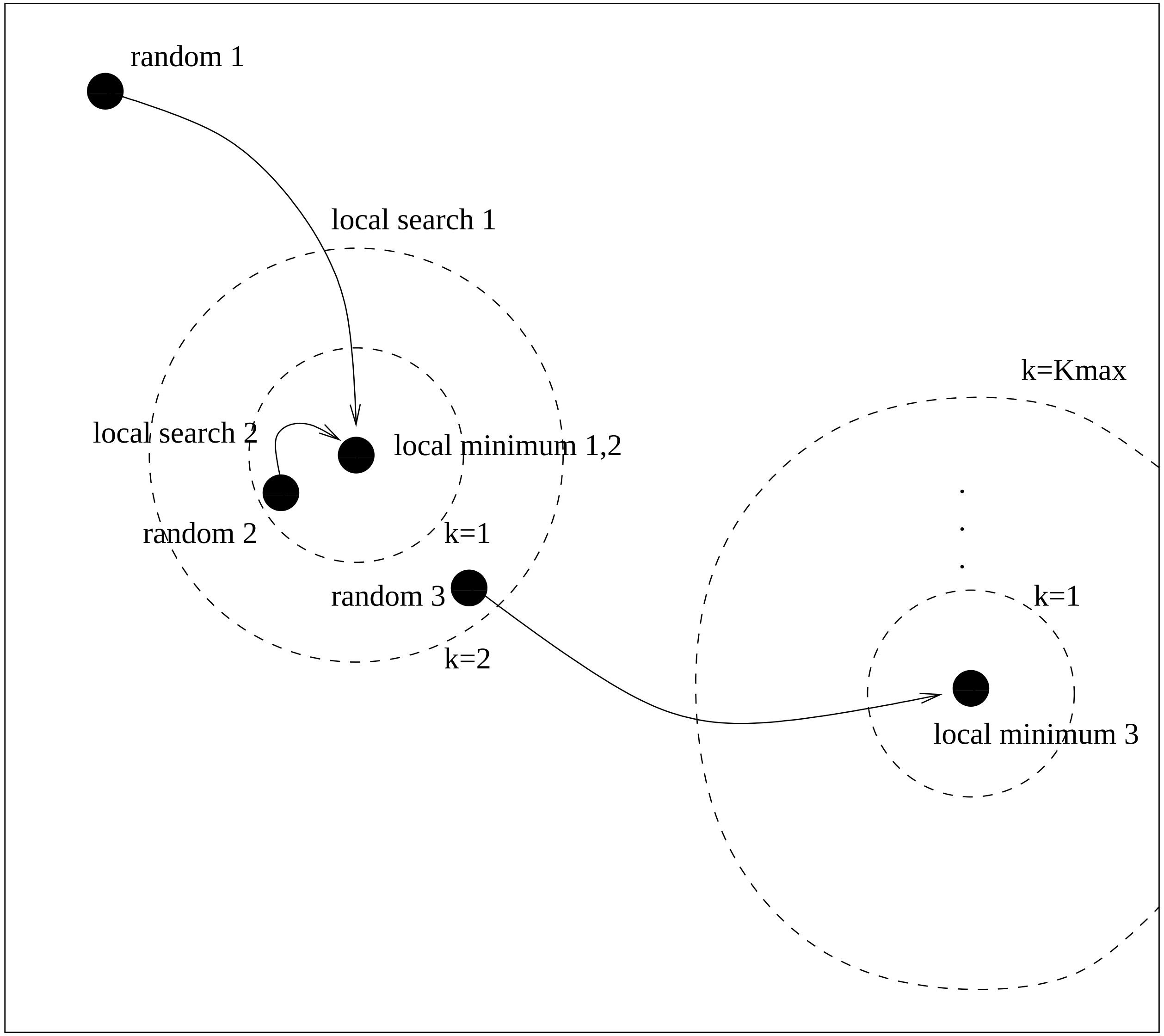
$$t_j \geq t_i + L_i + \sum_{k,l \in P} \gamma_{ij}^{kl} z_{ik} z_{jl} \quad \forall j \in V, i : (i,j) \in A$$

- Mixed-integer quadratic formulation
- [Davidović et al., MISTA Proc. 2007]

Variable Neighbourhood Search

- Applicable to discrete and continuous problems
- Uses any local search as a black-box
- In its basic form, easy to implement
- Few configurable parameters
- Structure of the problem dealt with by local search
- Few lines of code around LS black-box

VNS algorithm I



VNS algorithm II

Input: max no. k_{max} of neighbourhoods

loop

Set $k \leftarrow 1$, pick random point $\tilde{x}$, perform a local search to find a local minimum x^*.

while $k \leq k_{\text{max}}$ **do**

Let $N_k(x^*)$ neighb. of x^* s.t. $N_k(x^*) \supset N_{k-1}(x^*)$

Sample a random point $\tilde{x}$ from $N_k(x^*)$

Perform a local search from $\tilde{x}$ to find a local minimum x'

If x' is better than x^*, set $x^* \leftarrow x'$ and $k \leftarrow 0$

Set $k \leftarrow k + 1$

Verify termination condition; if true, exit

end while

end loop

Neighbourhoods in continuous space

- Use hyper-rectangular neighbourhoods $N_k(x')$ proportional to the region delimited by the variable ranges
- May also employ hyper-rectangular "shells" of size k/k_{max} of the original domain