

Mixed Integer Nonlinear Programming (MINLP)

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Overview

- ① Introduction, Applications, and Formulations
- ② Classical Solution Methods
- ③ Modern Developments in MINLP
- ④ Implementation and Software



Part I

Introduction, Applications, and Formulations



The Problem of the Day

Mixed Integer Nonlinear Program (MINLP)

$$\left\{ \begin{array}{ll} \underset{x,y}{\text{minimize}} & f(x, y) \\ \text{subject to} & c(x, y) \leq 0 \\ & x \in X, y \in Y \text{ integer} \end{array} \right.$$



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- X, Y polyhedral sets, e.g. $Y = \{y \in [0, 1]^p \mid Ay \leq b\}$



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- f, c smooth (**convex**) functions
- X, Y polyhedral sets, e.g. $Y = \{y \in [0, 1]^p \mid Ay \leq b\}$
- $y \in Y$ integer \Rightarrow hard problem
- f, c not convex \Rightarrow **very** hard problem



Why the MI?

- We can use 0-1 (binary) variables for a variety of purposes
 - Modeling yes/no decisions
 - Enforcing disjunctions
 - Enforcing logical conditions
 - Modeling fixed costs
 - Modeling piecewise linear functions



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 - Modeling yes/no decisions
 - Enforcing disjunctions
 - Enforcing logical conditions
 - Modeling fixed costs
 - Modeling piecewise linear functions
- If the variable is associated with a physical entity that is indivisible, then it must be integer
 - Number of aircraft carriers to produce. Gomory's Initial Motivation



A Popular MINLP Method

Dantzig's Two-Phase Method for MINLP

Adapted by Leyffer and Linderoth



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- 1 Convince the user that he or she does not wish to solve a mixed integer nonlinear programming problem at all!



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- 2 Otherwise, solve the continuous relaxation (NLP) and round off the minimizer to the nearest integer.



A Popular MINLP Method

Dantzig's Two-Phase Method for MINLP

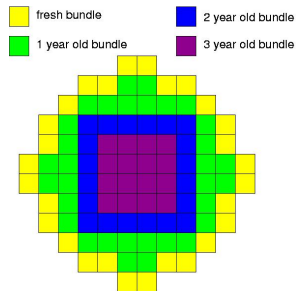
Adapted by Leyffer and Linderoth

- 1 Convince the user that he or she does not wish to solve a mixed integer nonlinear programming problem at all!
 - 2 Otherwise, solve the continuous relaxation (*NLP*) and round off the minimizer to the nearest integer.
- For **0 – 1 problems**, or those in which the $|y|$ is “small”, the continuous approximation to the discrete decision is **not** accurate enough for practical purposes.
 - **Conclusion:** MINLP methods must be studied!



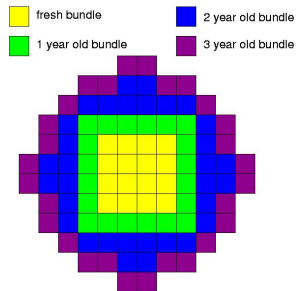
Example: Core Reload Operation (Quist, A.J., 2000)

- max. reactor efficiency after reload subject to diffusion PDE & safety
- diffusion PDE \simeq nonlinear equation
 \Rightarrow integer & nonlinear model
- avoid reactor becoming sub-critical



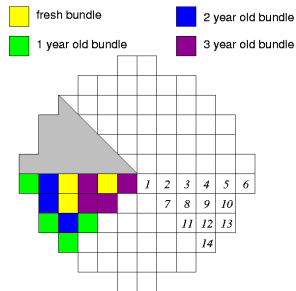
Example: Core Reload Operation (Quist, A.J., 2000)

- max. reactor efficiency after reload subject to diffusion PDE & safety
- diffusion PDE \simeq nonlinear equation
 \Rightarrow integer & nonlinear model
- avoid reactor becoming **overheated**



Example: Core Reload Operation (Quist, A.J., 2000)

- look for cycles for moving bundles:
e.g. $4 \rightarrow 6 \rightarrow 8 \rightarrow 10$
i.e. bundle moved from 4 to 6 ...
- model with binary $x_{ilm} \in \{0, 1\}$
 $x_{ilm} = 1$
 \Leftrightarrow node i has bundle l of cycle m



AMPL Model of Core Reload Operation

Exactly one bundle per node:

$$\sum_{l=1}^L \sum_{m=1}^M x_{ilm} = 1 \quad \forall i \in I$$

AMPL model:

```
var x {I,L,M} binary ;
```

```
Bundle {i in I}: sum{1 in L, m in M} x[i,1,m] = 1 ;
```

- **Multiple Choice:** One of the most common uses of IP
- Full AMPL model `c-reload.mod` at www.mcs.anl.gov/~leyffer/MacMINLP/



Gas Transmission Problem (De Wolf and Smeers, 2000)

- Belgium has no gas!



Gas Transmission Problem (De Wolf and Smeers, 2000)



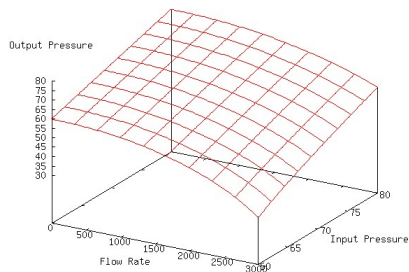
- Belgium has no gas!
- All natural gas is imported from Norway, Holland, or Algeria.
- Supply gas to all demand points in a network in a minimum cost fashion.

Gas Transmission Problem (De Wolf and Smeers, 2000)



- Belgium has no gas!
- All natural gas is imported from Norway, Holland, or Algeria.
- Supply gas to all demand points in a network in a minimum cost fashion.
- Gas is pumped through the network with a series of compressors
- There are constraints on the pressure of the gas within the pipe

Pressure Loss is Nonlinear



- Assume horizontal pipes and steady state flows
- Pressure loss p across a pipe is related to the flow rate f as

$$p_{in}^2 - p_{out}^2 = \frac{1}{\Psi} \text{sign}(f) f^2$$

- Ψ : “Friction Factor”



Gas Transmission: Problem Input

- Network (N, A) . $A = A_p \cup A_a$
 - A_a : **active** arcs have compressor. Flow rate can increase on arc
 - A_p : **passive** arcs simply conserve flow rate
- $N_s \subseteq N$: set of supply nodes
- $c_i, i \in N_s$: Purchase cost of gas
- $\underline{s}_i, \bar{s}_i$: Lower and upper bounds on gas “supply” at node i
- $\underline{p}_i, \bar{p}_i$: Lower and upper bounds on gas pressure at node i



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- $\underline{p}_i, \bar{p}_i$: Lower and upper bounds on gas pressure at node i
- $s_i, i \in N$: **supply** at node i .
 - $s_i > 0 \Rightarrow$ gas added to the network at node i
 - $s_i < 0 \Rightarrow$ gas removed from the network at node i to meet demand
- $f_{ij}, (i, j) \in A$: **flow** along arc (i, j)
 - $f(i, j) > 0 \Rightarrow$ gas flows $i \rightarrow j$
 - $f(i, j) < 0 \Rightarrow$ gas flows $j \rightarrow i$



Gas Transmission Model

$$\min \sum_{j \in N_s} c_j s_j$$

subject to

$$\begin{aligned} \sum_{j|(i,j) \in A} f_{ij} &= s_i & \forall i \in N \\ \text{sign}(f_{ij}) f_{ij}^2 - \Psi_{ij}(p_i^2 - p_j^2) &= 0 & \forall (i,j) \in A_p \\ \text{sign}(f_{ij}) f_{ij}^2 - \Psi_{ij}(p_i^2 - p_j^2) &\geq 0 & \forall (i,j) \in A_a \\ s_i &\in [\underline{s}_i, \bar{s}_i] & \forall i \in N \\ p_i &\in [\underline{p}_i, \bar{p}_i] & \forall i \in N \\ f_{ij} &\geq 0 & \forall (i,j) \in A_a \end{aligned}$$



Your First Modeling Trick

- Don't include nonlinearities or nonconvexities unless necessary!
- Replace $p_i^2 \leftarrow \rho_i$



Your First Modeling Trick

- Don't include nonlinearities or nonconvexities unless necessary!
- Replace $\rho_i^2 \leftarrow \rho_i$

$$\begin{aligned} \text{sign}(f_{ij})f_{ij}^2 - \Psi_{ij}(\rho_i - \rho_j) &= 0 & \forall (i,j) \in A_p \\ f_{ij}^2 - \Psi_{ij}(\rho_i - \rho_j) &\geq 0 & \forall (i,j) \in A_a \\ \rho_i &\in [\sqrt{\underline{p}_i}, \sqrt{\bar{p}_i}] & \forall i \in N \end{aligned}$$



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- This trick only works because
 - ① p_i^2 terms appear only in the bound constraints
 - ② Also $f_{ij} \geq 0 \forall (i,j) \in A_a$
- This model is nonconvex: $\text{sign}(f_{ij})f_{ij}^2$ is a nonconvex function
- Some solvers do not like sign



Dealing with $\text{sign}(\cdot)$: The NLP Way

- Use auxiliary binary variables to indicate direction of flow
- Let $|f_{ij}| \leq F \forall (i, j) \in A_p$

$$z_{ij} = \begin{cases} 1 & f_{ij} \geq 0 & f_{ij} \geq -F(1 - z_{ij}) \\ 0 & f_{ij} \leq 0 & f_{ij} \leq Fz_{ij} \end{cases}$$

- Note that

$$\text{sign}(f_{ij}) = 2z_{ij} - 1$$

- Write constraint as

$$(2z_{ij} - 1)f_{ij}^2 - \Psi_{ij}(\rho_i - \rho_j) = 0.$$



Special Ordered Sets

- Sven thinks this 'NLP trick' is pretty cool



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Special Ordered Sets

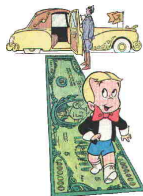
- Sven thinks this 'NLP trick' is pretty cool
- It is not how it is done in De Wolf and Smeers (2000).
- Heuristic for finding a good starting solution, then a local optimization approach based on a piecewise-linear simplex method
- Another (similar) approach involves approximating the nonlinear function by piecewise linear segments, but searching for the globally optimal solution: [Special Ordered Sets of Type 2](#)
- If the “multidimensional” nonlinearity cannot be removed, resort to [Special Ordered Sets of Type 3](#)

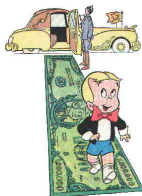


Portfolio Management

- N : Universe of asset to purchase
- x_i : Amount of asset i to hold
- B : Budget

$$\min_{x \in \mathbb{R}_+^{|N|}} \left\{ u(x) \mid \sum_{i \in N} x_i = B \right\}$$





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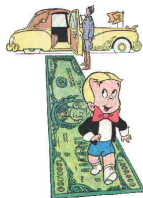
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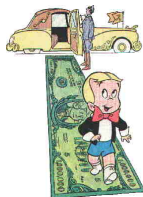
- **Markowitz:** $u(x) \stackrel{\text{def}}{=} -\alpha^T x + \lambda x^T Q x$
 - α : Expected returns
 - Q : Variance-covariance matrix of expected returns
 - λ : Risk aversion parameter



More Realistic Models

- $b \in \mathbb{R}^{|M|}$ of “benchmark” holdings
- **Benchmark Tracking:** $u(x) \stackrel{\text{def}}{=} (x - b)^T Q(x - b)$
 - **Constraint on $\mathbb{E}[\text{Return}]$:** $\alpha^T x \geq r$





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 - **Constraint on $\mathbb{E}[\text{Return}]$:** $\alpha^T x \geq r$
- **Limit Names:** $|i \in N : x_i > 0| \leq K$
 - Use binary indicator variables to model the implication $x_i > 0 \Rightarrow y_i = 1$
 - Implication modeled with **variable upper bounds:**

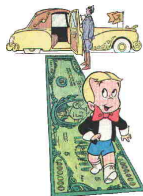
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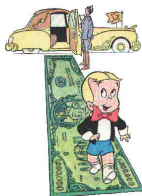
- $\sum_{i \in N} y_i \leq K$



Even More Models

- **Min Holdings:** $(x_i = 0) \vee (x_i \geq m)$
 - Model implication: $x_i > 0 \Rightarrow x_i \geq m$
 - $x_i > 0 \Rightarrow y_i = 1 \Rightarrow x_i \geq m$
 - $x_i \leq By_i, x_i \geq my_i \quad \forall i \in N$

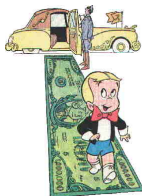




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- **Round Lots:** $x_i \in \{kL_i, k = 1, 2, \dots\}$
 - $x_i - z_iL_i = 0, z_i \in \mathbb{Z}_+ \quad \forall i \in N$





Even More Models

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 - $x_i - z_i L_i = 0, z_i \in \mathbb{Z}_+ \quad \forall i \in N$
- Vector h of initial holdings
- Transactions: $t_i = |x_i - h_i|$
- **Turnover:** $\sum_{i \in N} t_i \leq \Delta$
- **Transaction Costs:** $\sum_{i \in N} c_i t_i$ in objective
- **Market Impact:** $\sum_{i \in N} \gamma_i t_i^2$ in objective



Multiproduct Batch Plants (Kocis and Grossmann, 1988)



- M : Batch Processing Stages
 - N : Different Products
 - H : Horizon Time
 - Q_i : Required quantity of product i
 - t_{ij} : Processing time product i stage j
 - S_{ij} : "Size Factor" product i stage j
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 - S_{ij} : "Size Factor" product i stage j
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- B_i : Batch size of product $i \in N$
 - V_j : Stage j size: $V_j \geq S_{ij}B_i \forall i, j$
 - N_j : Number of machines at stage j
 - C_i : Longest stage time for product i : $C_i \geq t_{ij}/N_j \forall i, j$

Multiproduct Batch Plants



$$\min \sum_{j \in M} \alpha_j N_j V_j^{\beta_j}$$

s.t.

$$\begin{aligned} V_j - S_{ij} B_i &\geq 0 & \forall i \in N, \forall j \in M \\ C_i N_j &\geq t_{ij} & \forall i \in N, \forall j \in M \\ \sum_{i \in N} \frac{Q_i}{B_i} C_i &\leq H \end{aligned}$$

Bound Constraints on V_j, C_i, B_i, N_j

$$N_j \in \mathbb{Z} \quad \forall j \in M$$



Modeling Trick #2

- Horizon Time and Objective Function Nonconvex. :-)



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- Sometimes variable transformations work!

$$v_j = \ln(V_j), n_j = \ln(N_j), b_i = \ln(B_i), c_i = \ln C_i$$



Modeling Trick #2

- Horizon Time and Objective Function Nonconvex. :-)
- Sometimes variable transformations work!

$$v_j = \ln(V_j), n_j = \ln(N_j), b_i = \ln(B_i), c_i = \ln C_i$$

$$\min \sum_{j \in M} \alpha_j e^{N_j + \beta_j V_j}$$

$$\begin{aligned} \text{s.t. } v_j - \ln(S_{ij})b_i &\geq 0 && \forall i \in N, \forall j \in M \\ c_i + n_j &\geq \ln(\tau_{ij}) && \forall i \in N, \forall j \in M \\ \sum_{i \in N} Q_i e^{C_i - B_i} &\leq H \end{aligned}$$

(Transformed) Bound Constraints on V_j, C_i, B_i



How to Handle the Integrality?

- But what to do about the integrality?

$$1 \leq N_j \leq \bar{N}_j \quad \forall j \in M, N_j \in \mathbb{Z} \quad \forall j \in M$$

- $n_j \in \{0, \ln(2), \ln(3), \dots\}$

$$Y_{kj} = \begin{cases} 1 & n_j \text{ takes value } \ln(k) \\ 0 & \text{Otherwise} \end{cases}$$

$$n_j - \sum_{k=1}^K \ln(k) Y_{kj} = 0 \quad \forall j \in M$$

$$\sum_{k=1}^K Y_{kj} = 1 \quad \forall j \in M$$

- This model is available at <http://www-unix.mcs.anl.gov/~leyffer/macminlp/problems/batch.mod>

A Small Smattering of Other Applications

- Chemical Engineering Applications:
 - process synthesis (Kocis and Grossmann, 1988)
 - batch plant design (Grossmann and Sargent, 1979)
 - cyclic scheduling (Jain, V. and Grossmann, I.E., 1998)
 - design of distillation columns (Viswanathan and Grossmann, 1993)
 - pump configuration optimization (Westerlund, T., Pettersson, F. and Grossmann, I.E., 1994)
- Forestry/Paper
 - production (Westerlund, T., Isaksson, J. and Harjunkoski, I., 1995)
 - trimloss minimization (Harjunkoski, I., Westerlund, T., Pörn, R. and Skrifvars, H., 1998)
- Topology Optimization (Sigmund, 2001)



Part II

Classical Solution Methods



Classical Solution Methods for MINLP

- ① Classical Branch-and-Bound
- ② Outer Approximation & Benders Decomposition
- ③ Hybrid Methods
 - LP/NLP Based Branch-and-Bound
 - Integrating SQP with Branch-and-Bound

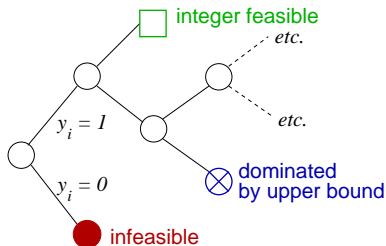


Branch-and-Bound

Solve relaxed NLP ($0 \leq y \leq 1$ continuous relaxation)

... solution value provides lower bound

- Branch on y_i non-integral
- Solve NLPs & branch until
 - 1 Node infeasible ... ●
 - 2 Node integer feasible ... □
⇒ get upper bound (U)
 - 3 Lower bound $\geq U$... ⊗



Search until no unexplored nodes on tree



Variable Selection for Branch-and-Bound

Assume $y_i \in \{0, 1\}$ for simplicity ...

(\hat{x}, \hat{y}) fractional solution to parent node; $\hat{f} = f(\hat{x}, \hat{y})$

- 1 **maximal fractional branching:** choose \hat{y}_i closest to $\frac{1}{2}$

$$\max_i \{ \min(1 - \hat{y}_i, \hat{y}_i) \}$$



Variable Selection for Branch-and-Bound

Assume $y_i \in \{0, 1\}$ for simplicity ...

(\hat{x}, \hat{y}) fractional solution to parent node; $\hat{f} = f(\hat{x}, \hat{y})$

- ① **maximal fractional branching:** choose \hat{y}_i closest to $\frac{1}{2}$

$$\max_i \{ \min(1 - \hat{y}_i, \hat{y}_i) \}$$

- ② **strong branching:** (approx) solve *all* NLP children:

$$f_i^{+/-} \leftarrow \begin{cases} \text{minimize} & f(x, y) \\ \text{subject to} & c(x, y) \leq 0 \\ & x \in X, y \in Y, y_i = 1/0 \end{cases}$$

branching variable y_i that changes objective the most:

$$\max_i \{ \min(f_i^+, f_i^-) \}$$



Node Selection for Branch-and-Bound

Which node n on tree \mathcal{T} should be solved next?

- ① **depth-first search:** select deepest node in tree
 - minimizes number of NLP nodes stored
 - exploit warm-starts (MILP/MIQP only)



Node Selection for Branch-and-Bound

Which node n on tree \mathcal{T} should be solved next?

- 1 **depth-first search:** select deepest node in tree
 - minimizes number of NLP nodes stored
 - exploit warm-starts (MILP/MIQP only)
- 2 **best estimate:** choose node with best expected integer soln

$$\min_{n \in \mathcal{T}} \left\{ f_{p(n)} + \sum_{i: y_i \text{ fractional}} \min \{ e_i^+ (1 - y_i), e_i^- y_i \} \right\}$$

where $f_{p(n)}$ = value of parent node, $e_i^{+/-}$ = pseudo-costs
summing pseudo-cost estimates for all integers in subtree



Outer Approximation (Duran and Grossmann, 1986)

Motivation: avoid solving huge number of NLPs

- Exploit MILP/NLP solvers: decompose integer/nonlinear part

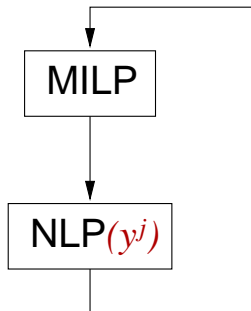
Key idea: reformulate MINLP as MILP (implicit)

- Solve alternating sequence of MILP & NLP

NLP subproblem y_j fixed:

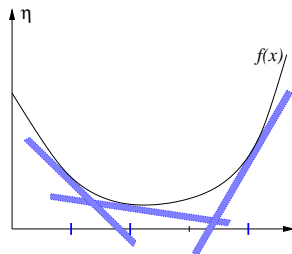
$$\text{NLP}(y_j) \begin{cases} \underset{x}{\text{minimize}} & f(x, y_j) \\ \text{subject to} & c(x, y_j) \leq 0 \\ & x \in X \end{cases}$$

Main Assumption: f, c are convex



Outer Approximation (Duran and Grossmann, 1986)

- let (x_j, y_j) solve $\text{NLP}(y_j)$
- linearize f, c about $(x_j, y_j) =: z_j$
- new objective variable $\eta \geq f(x, y)$
- $\text{MINLP}(P) \equiv \text{MILP}(M)$



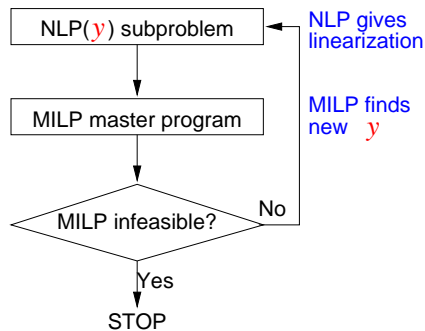
$$(M) \begin{cases} \text{minimize} & \eta \\ & z=(x,y),\eta \\ \text{subject to} & \eta \geq f_j + \nabla f_j^T (z - z_j) \quad \forall y_j \in Y \\ & 0 \geq c_j + \nabla c_j^T (z - z_j) \quad \forall y_j \in Y \\ & x \in X, y \in Y \text{ integer} \end{cases}$$

SNAG: need all $y_j \in Y$ linearizations

Outer Approximation (Duran and Grossmann, 1986)

(M_k) : lower bound (underestimate convex f, c)

$NLP(y_j)$: upper bound U (fixed y_j)



⇒ stop, if lower bound \geq upper bound

Outer Approximation & Benders Decomposition

Take OA cuts for $z_j := (x_j, y_j) \dots$ wlog $X = \mathbb{R}^n$

$$\eta \geq f_j + \nabla f_j^T (z - z_j) \quad \& \quad 0 \geq c_j + \nabla c_j^T (z - z_j)$$

sum with $(1, \lambda_j) \dots$ λ_j multipliers of $\text{NLP}(y_j)$

$$\eta \geq f_j + \lambda_j^T c_j + (\nabla f_j + \nabla c_j \lambda_j)^T (z - z_j)$$

KKT conditions of $\text{NLP}(y_j) \Rightarrow \nabla_x f_j + \nabla_x c_j \lambda_j = 0$
... eliminate x components from valid inequality in y

$$\Rightarrow \eta \geq f_j + (\nabla_y f_j + \nabla_y c_j \lambda_j)^T (y - y_j)$$

NB: $\mu_j = \nabla_y f_j + \nabla_y c_j \lambda_j$ multiplier of $y = y_j$ in $\text{NLP}(y_j)$

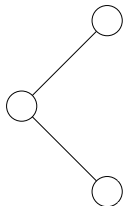
References: (Geoffrion, 1972)



LP/NLP Based Branch-and-Bound

AIM: avoid re-solving MILP master (M)

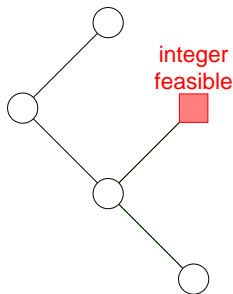
- Consider MILP branch-and-bound



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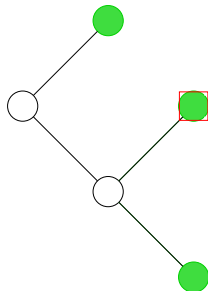
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- interrupt MILP, when y_j found
⇒ solve NLP(y_j) get x_j



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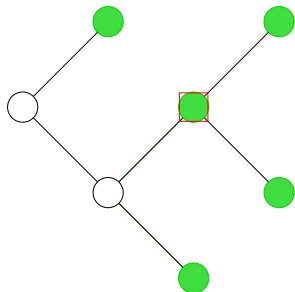
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- linearize f, c about (x_j, y_j)
⇒ add linearization to tree



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⇒ add linearization to tree
- continue MILP tree-search



... until lower bound \geq upper bound



LP/NLP Based Branch-and-Bound

- need access to MILP solver ... call back
 - exploit good MILP (branch-cut-price) solver
 - (Akrotirianakis et al., 2001) use Gomory cuts in tree-search

- preliminary results: order of magnitude faster than OA
 - same number of NLPs, but only one MILP
- similar ideas for Benders & Extended Cutting Plane methods
- recent implementation by CMU/IBM group

References: (Quesada and Grossmann, 1992)



Integrating SQP & Branch-and-Bound

AIM: Avoid solving NLP node to convergence.

Sequential Quadratic Programming (SQP)

→ solve sequence (QP_k) at every node

$$(QP_k) \begin{cases} \text{minimize}_d & f_k + \nabla f_k^T d + \frac{1}{2} d^T H_k d \\ \text{subject to} & c_k + \nabla c_k^T d \leq 0 \\ & x_k + d_x \in X \\ & y_k + d_y \in \hat{Y}. \end{cases}$$

Early branching:

After QP step choose non-integral y_i^{k+1} , branch & continue SQP

References: (Borchers and Mitchell, 1994; Leyffer, 2001)

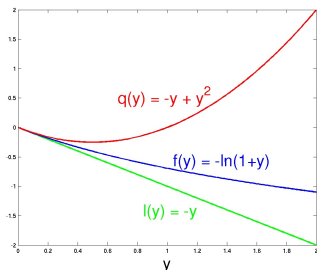


Integrating SQP & Branch-and-Bound

SNAG: (QP_k) not lower bound

\Rightarrow no fathoming from upper bound

$$\begin{aligned} & \underset{d}{\text{minimize}} && f_k + \nabla f_k^T d + \frac{1}{2} d^T H_k d \\ & \text{subject to} && c_k + \nabla c_k^T d \leq 0 \\ & && x_k + d_x \in X \\ & && y_k + d_y \in \hat{Y}. \end{aligned}$$



NB: (QP_k) inconsistent and trust-region active \Rightarrow do not fathom

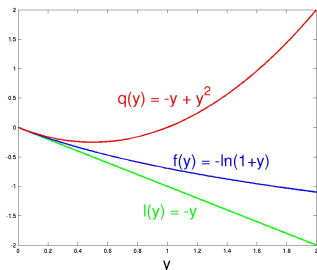


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Remedy: Exploit OA underestimating property (Leyffer, 2001):

- add objective cut $f_k + \nabla f_k^T d \leq U - \epsilon$ to (QP_k)
- fathom node, if (QP_k) inconsistent

NB: (QP_k) inconsistent and trust-region active \Rightarrow do not fathom



Comparison of Classical MINLP Techniques

Summary of numerical experience

- 1 Quadratic OA master: usually fewer iteration
MIQP harder to solve
- 2 NLP branch-and-bound faster than OA
... depends on MIP solver
- 3 LP/NLP-based-BB order of magnitude faster than OA
... also faster than B&B
- 4 Integrated SQP-B&B up to $3\times$ faster than B&B
 \simeq number of QPs per node
- 5 ECP works well, if function/gradient evals expensive



Part III

Modern Developments in MINLP



Modern Methods for MINLP

1 Formulations

- Relaxations
- Good formulations: big M 's and disaggregation

2 Cutting Planes

- Cuts from relaxations and special structures
- Cuts from integrality

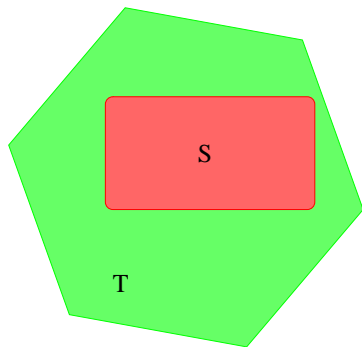
3 Handling Nonconvexity

- Envelopes
- Methods



Relaxations

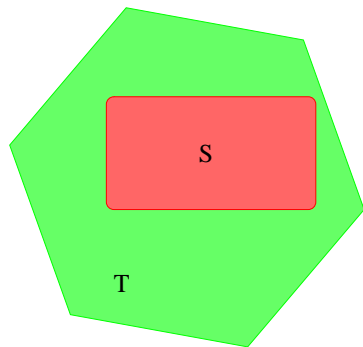
- $z(S) \stackrel{\text{def}}{=} \min_{x \in S} f(x)$
- $z(T) \stackrel{\text{def}}{=} \min_{x \in T} f(x)$



- Independent of f, S, T :
 $z(T) \leq z(S)$

Relaxations

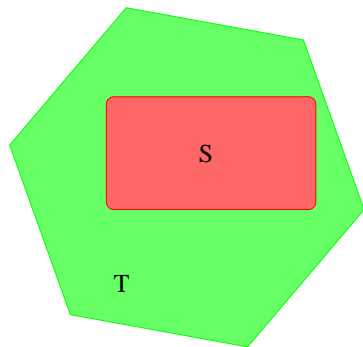
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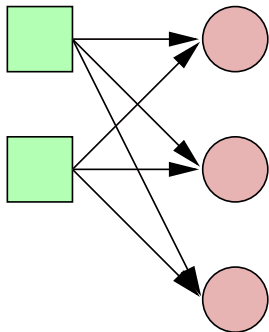
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UFL: Uncapacitated Facility Location

- Facilities: J
- Customers: I



$$\min \sum_{j \in J} f_j x_j + \sum_{i \in I} \sum_{j \in J} f_{ij} y_{ij}$$

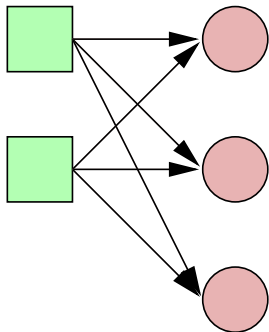
$$\sum_{j \in J} y_{ij} = 1 \quad \forall i \in I$$

$$\sum_{i \in I} y_{ij} \leq |I| x_j \quad \forall j \in J \quad (1)$$

$$\text{OR } y_{ij} \leq x_j \quad \forall i \in I, j \in J \quad (2)$$

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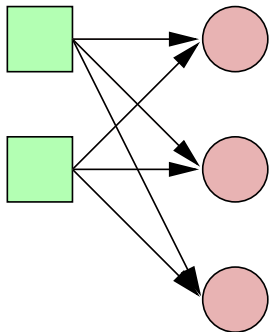
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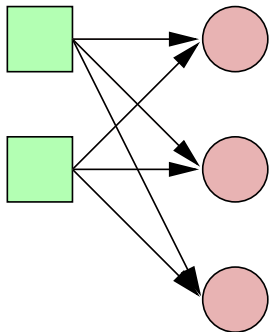
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- Which formulation is to be preferred?
- $I = J = 40$. Costs random.

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- Which formulation is to be preferred?
- $I = J = 40$. Costs random.
 - Formulation 1. 53,121 seconds, optimal solution.
 - Formulation 2. 2 seconds, optimal solution.



Valid Inequalities

- Sometimes we can get a better formulation by **dynamically** improving it.
-
- An inequality $\pi^T x \leq \pi_0$ is a **valid inequality** for S if $\pi^T x \leq \pi_0 \quad \forall x \in S$
 - Alternatively: $\max_{x \in S} \{\pi^T x\} \leq \pi_0$

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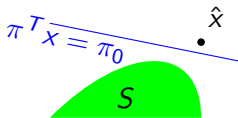
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- **Thm:** (Hahn-Banach). Let $S \subset \mathbb{R}^n$ be a closed, convex set, and let $\hat{x} \notin S$. Then there exists $\pi \in \mathbb{R}^n$ such that

$$\pi^T \hat{x} > \max_{x \in S} \{\pi^T x\}$$



Nonlinear Branch-and-Cut

Consider MINLP

$$\left\{ \begin{array}{l} \text{minimize}_{x,y} \quad f_x^T x + f_y^T y \\ \text{subject to} \quad c(x,y) \leq 0 \\ \quad \quad \quad y \in \{0,1\}^p, 0 \leq x \leq U \end{array} \right.$$

- Note the **Linear objective**
- This is WLOG:

$$\min f(x,y) \quad \Leftrightarrow \quad \min \eta \quad \text{s.t.} \quad \eta \geq f(x,y)$$

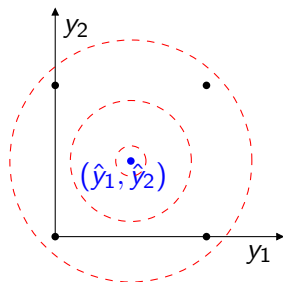


It's Actually Important!

- We want to approximate the convex hull of integer solutions, but without a linear objective function, the solution to the relaxation might occur in the interior.
- **No Separating Hyperplane!** :- (

$$\min(y_1 - 1/2)^2 + (y_2 - 1/2)^2$$

$$\text{s.t. } y_1 \in \{0, 1\}, y_2 \in \{0, 1\}$$



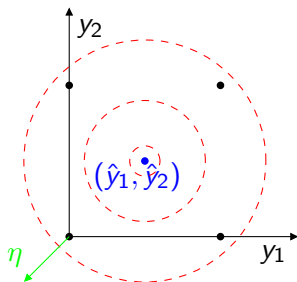
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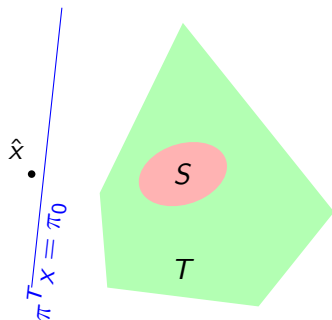
$$\text{s.t. } y_1 \in \{0, 1\}, y_2 \in \{0, 1\}$$

$$\eta \geq (y_1 - 1/2)^2 + (y_2 - 1/2)^2$$



Valid Inequalities From Relaxations

- **Idea:** Inequalities valid for a relaxation are valid for original 
- Generating valid inequalities for a relaxation is often easier.



- **Separation Problem** over T :
Given \hat{x} , T find (π, π_0) such
that $\pi^T \hat{x} > \pi_0$,
 $\pi^T x \leq \pi_0 \forall x \in T$

Simple Relaxations

- **Idea:** Consider **one row** relaxations 💡



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- If $P = \{x \in \{0, 1\}^n \mid Ax \leq b\}$, then for any row i ,
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- Crowder et al. (1983) is the seminal paper that shows this to be true for IP.
- **MINLP:** Single (linear) row relaxations are also valid \Rightarrow **same inequalities can also be used**



Knapsack Covers

$$K = \{x \in \{0, 1\}^n \mid a^T x \leq b\}$$

- A set $C \subseteq N$ is a **cover** if $\sum_{j \in C} a_j > b$
- A cover C is a **minimal cover** if $C \setminus j$ is not a cover $\forall j \in C$



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- A cover C is a **minimal cover** if $C \setminus j$ is not a cover $\forall j \in C$
- If $C \subseteq N$ is a cover, then the cover inequality

$$\sum_{j \in C} x_j \leq |C| - 1$$

is a valid inequality for S

- Sometimes (minimal) cover inequalities are **facets** of $\text{conv}(K)$



Other Substructures

- **Single node flow:** (Padberg et al., 1985)

$$S = \left\{ x \in \mathbb{R}_+^{|N|}, y \in \{0, 1\}^{|N|} \mid \sum_{j \in N} x_j \leq b, x_j \leq u_j y_j \quad \forall j \in N \right\}$$

- **Knapsack with single continuous variable:** (Marchand and Wolsey, 1999)

$$S = \left\{ x \in \mathbb{R}_+, y \in \{0, 1\}^{|N|} \mid \sum_{j \in N} a_j y_j \leq b + x \right\}$$

- **Set Packing:** (Borndörfer and Weismantel, 2000)

$$S = \left\{ y \in \{0, 1\}^{|M|} \mid Ay \leq e \right\}$$

$$A \in \{0, 1\}^{|M| \times |N|}, e = (1, 1, \dots, 1)^T$$

The Chvátal-Gomory Procedure

- A **general** procedure for generating valid inequalities for integer programs



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- Let the columns of $A \in \mathbb{R}^{m \times n}$ be denoted by $\{a_1, a_2, \dots, a_n\}$
- $S = \{y \in \mathbb{Z}_+^n \mid Ay \leq b\}$.
 - 1 Choose nonnegative multipliers $u \in \mathbb{R}_+^m$
 - 2 $u^T Ay \leq u^T b$ is a valid inequality ($\sum_{j \in N} u^T a_j y_j \leq u^T b$).
 - 3 $\sum_{j \in N} \lfloor u^T a_j \rfloor y_j \leq u^T b$ (Since $y \geq 0$).
 - 4 $\sum_{j \in N} \lfloor u^T a_j \rfloor y_j \leq \lfloor u^T b \rfloor$ is valid for S since $\lfloor u^T a_j \rfloor y_j$ is an integer



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 - ④ $\sum_{j \in N} \lfloor u^T a_j \rfloor y_j \leq \lfloor u^T b \rfloor$ is valid for S since $\lfloor u^T a_j \rfloor y_j$ is an integer
- **Simply Amazing:** This simple procedure **suffices** to generate every valid inequality for an integer program



Extension to MINLP (Çezik and Iyengar, 2005)

- This simple idea also extends to mixed 0-1 **conic** programming

$$\left\{ \begin{array}{ll} \text{minimize} & f^T z \\ z \stackrel{\text{def}}{=} (x, y) & \\ \text{subject to} & Az \succeq_{\mathcal{K}} b \\ & y \in \{0, 1\}^p, 0 \leq x \leq U \end{array} \right.$$

-
- \mathcal{K} : Homogeneous, self-dual, proper, convex cone
 - $x \succeq_{\mathcal{K}} y \Leftrightarrow (x - y) \in \mathcal{K}$



Gomory On Cones (Çezik and Iyengar, 2005)

- **LP:** $\mathcal{K}_l = \mathbb{R}_+^n$
- **SOCP:** $\mathcal{K}_q = \{(x_0, \bar{x}) \mid x_0 \geq \|\bar{x}\|\}$
- **SDP:** $\mathcal{K}_s = \{x = \text{vec}(X) \mid X = X^T, X \text{ p.s.d}\}$



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-
- Many classes of nonlinear inequalities can be represented as

$$Ax \succeq_{\mathcal{K}_q} b \text{ or } Ax \succeq_{\mathcal{K}_s} b$$



Using Gomory Cuts in MINLP (Akrotirianakis et al., 2001)

- LP/NLP Based Branch-and-Bound solves MILP instances:

$$\left\{ \begin{array}{ll} \text{minimize} & \eta \\ z \stackrel{\text{def}}{=} (x, y), \eta & \\ \text{subject to} & \eta \geq f_j + \nabla f_j^T (z - z_j) \quad \forall y_j \in Y^k \\ & 0 \geq c_j + \nabla c_j^T (z - z_j) \quad \forall y_j \in Y^k \\ & x \in X, y \in Y \text{ integer} \end{array} \right.$$



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- Create Gomory mixed integer cuts from

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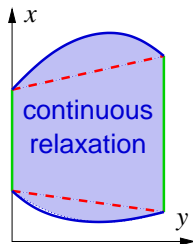
- Akrotirianakis et al. (2001) shows modest improvements
- Research Question: Other cut classes?
- Research Question: Exploit “outer approximation” property?

Disjunctive Cuts for MINLP (Stubbs and Mehrotra, 1999)

Extension of Disjunctive Cuts for MILP: (Balas, 1979; Balas et al., 1993)

Continuous relaxation ($z \stackrel{\text{def}}{=} (x, y)$)

- $C \stackrel{\text{def}}{=} \{z | c(z) \leq 0, 0 \leq y \leq 1, 0 \leq x \leq U\}$

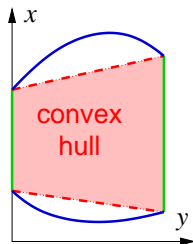


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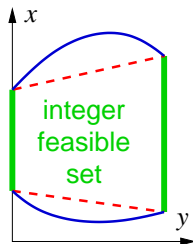
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- $C \stackrel{\text{def}}{=} \text{conv}(\{x \in C \mid y \in \{0, 1\}^p\})$
- $C_j^{0/1} \stackrel{\text{def}}{=} \{z \in C \mid y_j = 0/1\}$

$$\text{let } \mathcal{M}_j(C) \stackrel{\text{def}}{=} \left\{ \begin{array}{l} z = \lambda_0 u_0 + \lambda_1 u_1 \\ \lambda_0 + \lambda_1 = 1, \lambda_0, \lambda_1 \geq 0 \\ u_0 \in C_j^0, u_1 \in C_j^1 \end{array} \right\}$$

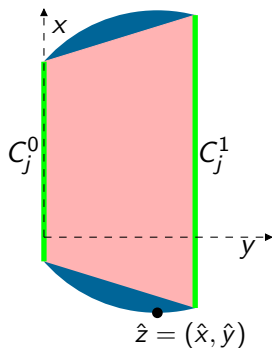
$\Rightarrow \mathcal{P}_j(C) := \text{projection of } \mathcal{M}_j(C) \text{ onto } z$

$\Rightarrow \mathcal{P}_j(C) = \text{conv}(C \cap y_j \in \{0, 1\})$ and $\mathcal{P}_{1\dots p}(C) = C$



Disjunctive Cuts: Example

$$\underset{x,y}{\text{minimize}} \{x \mid (x - 1/2)^2 + (y - 3/4)^2 \leq 1, -2 \leq x \leq 2, y \in \{0, 1\}\}$$

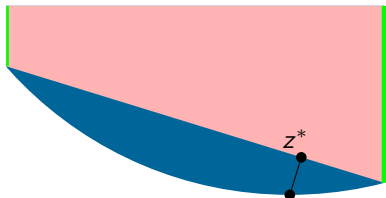


Given \hat{z} with $\hat{y}_j \notin \{0, 1\}$ find separating hyperplane

$$\Rightarrow \begin{cases} \underset{z}{\text{minimize}} & \|z - \hat{z}\| \\ \text{subject to} & z \in \mathcal{P}_j(C) \end{cases}$$

Disjunctive Cuts Example

$$z^* \stackrel{\text{def}}{=} \arg \min \|z - \hat{z}\|$$



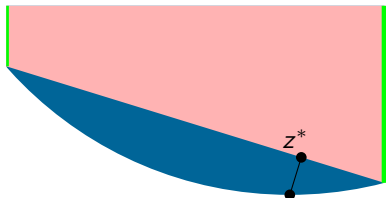
$$\hat{z} = (\hat{x}, \hat{y})$$

$$\begin{aligned} \text{s.t. } \lambda_0 u_0 + \lambda_1 u_1 &= z \\ \lambda_0 + \lambda_1 &= 1 \\ \begin{pmatrix} -0.16 \\ 0 \end{pmatrix} &\leq u_0 \leq \begin{pmatrix} 0.66 \\ 1 \end{pmatrix} \\ \begin{pmatrix} -0.47 \\ 0 \end{pmatrix} &\leq u_1 \leq \begin{pmatrix} 1.47 \\ 1 \end{pmatrix} \\ \lambda_0, \lambda_1 &\geq 0 \end{aligned}$$



Disjunctive Cuts Example

$$z^* \stackrel{\text{def}}{=} \arg \min \|z - \hat{z}\|_2^2$$



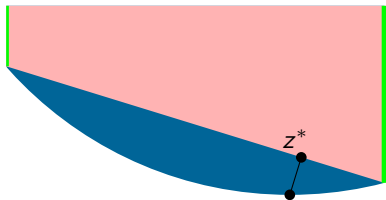
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Disjunctive Cuts Example

$$z^* \stackrel{\text{def}}{=} \arg \min \|z - \hat{z}\|_{\infty}$$



$$\hat{z} = (\hat{x}, \hat{y})$$

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Disjunctive Cuts Example

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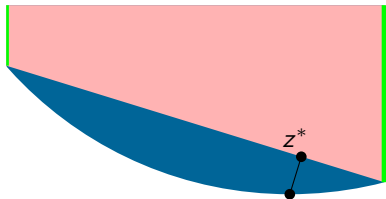
$$\text{s.t. } \lambda_0 u_0 + \lambda_1 u_1 = z$$

$$\lambda_0 + \lambda_1 = 1$$

$$\begin{pmatrix} -0.16 \\ 0 \end{pmatrix} \leq u_0 \leq \begin{pmatrix} 0.66 \\ 1 \end{pmatrix}$$

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$$\lambda_0, \lambda_1 \geq 0$$



$$\hat{z} = (\hat{x}, \hat{y})$$

NONCONVEX



What to do? (Stubbs and Mehrotra, 1999)

- Look at the **perspective** of $c(z)$

$$\mathcal{P}(c(\tilde{z}), \mu) = \mu c(\tilde{z}/\mu)$$

- Think of $\tilde{z} = \mu z$



What to do? (Stubbs and Mehrotra, 1999)

- Look at the **perspective** of $c(z)$

$$\mathcal{P}(c(\tilde{z}), \mu) = \mu c(\tilde{z}/\mu)$$

- Think of $\tilde{z} = \mu z$
- Perspective gives a **convex reformulation** of $\mathcal{M}_j(C)$: $\mathcal{M}_j(\tilde{C})$, where

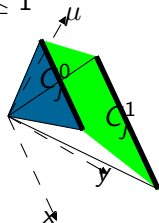
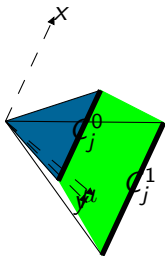
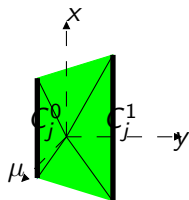
$$\tilde{C} := \left\{ (z, \mu) \left| \begin{array}{l} \mu c_i(z/\mu) \leq 0 \\ 0 \leq \mu \leq 1 \\ 0 \leq x \leq \mu U, 0 \leq y \leq \mu \end{array} \right. \right\}$$

- $c(0/0) = 0 \Rightarrow$ convex representation



Disjunctive Cuts Example

$$\tilde{C} = \left\{ \begin{array}{l} \begin{pmatrix} x \\ y \\ \mu \end{pmatrix} \mid \begin{array}{l} \mu [(x/\mu - 1/2)^2 + (y/\mu - 3/4)^2 - 1] \leq 0 \\ -2\mu \leq x \leq 2\mu \\ 0 \leq y \leq \mu \\ 0 \leq \mu \leq 1 \end{array} \end{array} \right\}$$



Example, cont.

$$\tilde{C}_j^0 = \{(z, \mu) \mid y_j = 0\} \quad \tilde{C}_j^1 = \{(z, \mu) \mid y_j = \mu\}$$



Example, cont.

$$\tilde{C}_j^0 = \{(z, \mu) \mid y_j = 0\} \quad \tilde{C}_j^1 = \{(z, \mu) \mid y_j = \mu\}$$

- Take $v_0 \leftarrow \mu_0 u_0$ $v_1 \leftarrow \mu_1 u_1$

$$\min \|z - \hat{z}\|$$

Solution to example:

$$\text{s.t. } v_0 + v_1 = z$$

$$\mu_0 + \mu_1 = 1$$

$$(v_0, \mu_0) \in \tilde{C}_j^0$$

$$(v_1, \mu_1) \in \tilde{C}_j^1$$

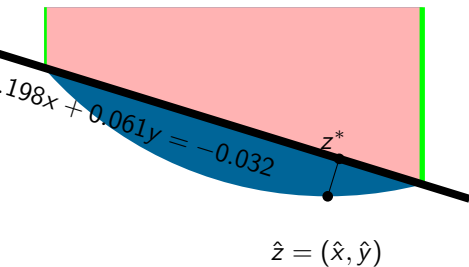
$$\mu_0, \mu_1 \geq 0$$

$$\begin{pmatrix} x^* \\ y^* \end{pmatrix} = \begin{pmatrix} -0.401 \\ 0.780 \end{pmatrix}$$

- separating hyperplane: $\psi^T(z - \hat{z})$, where $\psi \in \partial\|z - \hat{z}\|$



Example, Cont.



$$\psi = \begin{pmatrix} 2x^* + 0.5 \\ 2y^* - 0.75 \end{pmatrix}$$
$$0.198x + 0.061y \geq -0.032$$

Nonlinear Branch-and-Cut (Stubbs and Mehrotra, 1999)

- Can do this at all nodes of the branch-and-bound tree
- Generalize disjunctive approach from MILP
 - solve **one convex NLP per cut**
- Generalizes Sherali and Adams (1990) and Lovász and Schrijver (1991)
 - tighten cuts by adding semi-definite constraint
- Stubbs and Mehrotra (2002) also show how to generate convex quadratic inequalities, but computational results are not that promising



Generalized Disjunctive Programming (Raman and Grossmann, 1994; Lee and Grossmann, 2000)

Consider disjunctive NLP

$$\left\{ \begin{array}{l} \text{minimize}_{x, Y} \quad \sum f_i + f(x) \\ \text{subject to} \quad \left[\begin{array}{c} Y_i \\ c_i(x) \leq 0 \\ f_i = \gamma_i \end{array} \right] \vee \left[\begin{array}{c} \neg Y_i \\ B_i x = 0 \\ f_i = 0 \end{array} \right] \forall i \in I \\ 0 \leq x \leq U, \Omega(Y) = \text{true}, Y \in \{\text{true}, \text{false}\}^p \end{array} \right.$$

Application: process synthesis

- Y_i represents presence/absence of units
- $B_i x = 0$ eliminates variables if unit absent

Exploit disjunctive structure

- special branching ... OA/GBD algorithms



Generalized Disjunctive Programming (Raman and Grossmann, 1994; Lee and Grossmann, 2000)

Consider **disjunctive NLP**

$$\left\{ \begin{array}{l} \text{minimize}_{x, Y} \quad \sum f_i + f(x) \\ \text{subject to} \quad \begin{bmatrix} Y_i \\ c_i(x) \leq 0 \\ f_i = \gamma_i \end{bmatrix} \vee \begin{bmatrix} \neg Y_i \\ B_i x = 0 \\ f_i = 0 \end{bmatrix} \quad \forall i \in I \\ 0 \leq x \leq U, \quad \Omega(Y) = \text{true}, \quad Y \in \{\text{true}, \text{false}\}^p \end{array} \right.$$

Big-M formulation (**notoriously bad**), $M > 0$:

$$c_i(x) \leq M(1 - y_i)$$

$$-My_i \leq B_i x \leq My_i$$

$$f_i = y_i \gamma_i \quad \Omega(Y) \text{ converted to linear inequalities}$$



Generalized Disjunctive Programming (Raman and Grossmann, 1994; Lee and Grossmann, 2000)

Consider disjunctive NLP

Consider disjunctive NLP

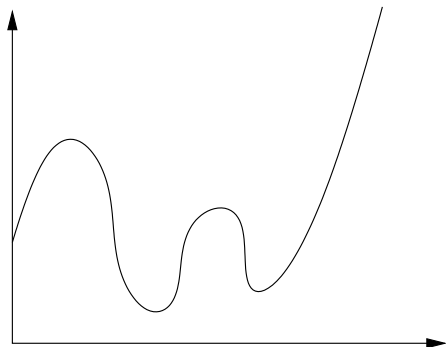
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convex hull representation ...

$$\begin{aligned} x &= v_{i1} + v_{i0}, & \lambda_{i1} + \lambda_{i0} &= 1 \\ \lambda_{i1} c_i(v_{i1}/\lambda_{i1}) &\leq 0, & B_i v_{i0} &= 0 \\ 0 \leq v_{ij} &\leq \lambda_{ij} U, & 0 \leq \lambda_{ij} &\leq 1, & f_i &= \lambda_{i1} \gamma_i \end{aligned}$$



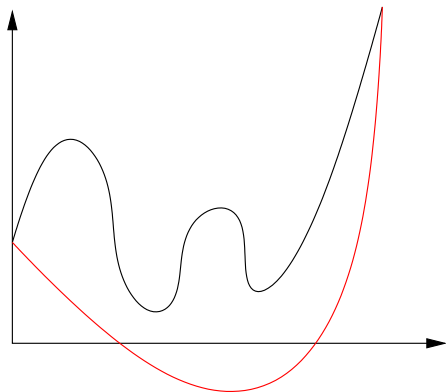
Dealing with Nonconvexities



- Functional nonconvexity causes serious problems.
 - Branch and bound must have **true** lower bound (**global solution**)

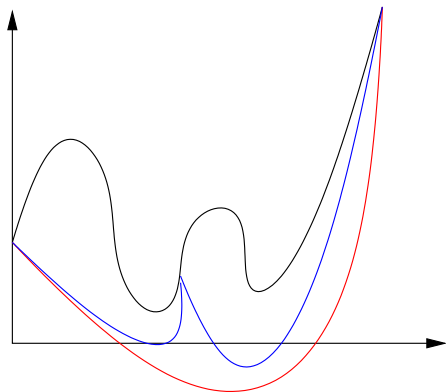


Dealing with Nonconvexities



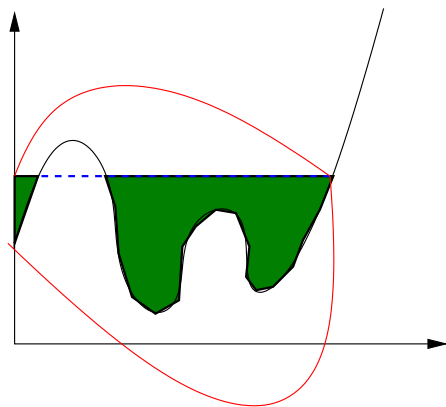
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- Underestimate nonconvex functions. Solve relaxation. Provides lower bound.

Dealing with Nonconvexities



- Functional nonconvexity causes serious problems.
 - Branch and bound must have **true** lower bound (**global solution**)
- Underestimate nonconvex functions. Solve relaxation. Provides lower bound.
- If relaxation is not exact, then branch

Dealing with Nonconvex Constraints



- If nonconvexity in constraints, may need to overestimate and underestimate the function to get a convex region

Envelopes

$$f : \Omega \rightarrow \mathbb{R}$$

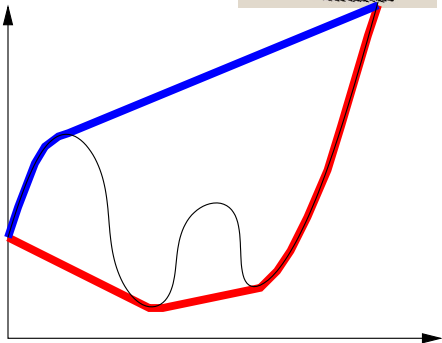
- **Convex Envelope** ($\text{vex}_{\Omega}(f)$):
Pointwise supremum of convex underestimators of f over Ω .



Envelopes

$$f : \Omega \rightarrow \mathbb{R}$$

- **Convex Envelope** ($\text{vex}_{\Omega}(f)$):
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- **Concave Envelope** ($\text{cav}_{\Omega}(f)$):
Pointwise infimum of concave overestimators of f over Ω .



Branch-and-Bound Global Optimization Methods

- Under/Overestimate “simple” parts of (Factorable) Functions individually
 - Bilinear Terms
 - Trilinear Terms
 - Fractional Terms
 - Univariate convex/concave terms



Branch-and-Bound Global Optimization Methods

- Under/Overestimate “simple” parts of (Factorable) Functions individually
 - Bilinear Terms
 - Trilinear Terms
 - Fractional Terms
 - Univariate convex/concave terms
- General nonconvex functions $f(x)$ can be underestimated over a region $[l, u]$ “overpowering” the function with a quadratic function that is ≤ 0 on the region of interest

$$\mathcal{L}(x) = f(x) + \sum_{i=1}^n \alpha_i (l_i - x_i)(u_i - x_i)$$

Refs: (McCormick, 1976; Adjiman et al., 1998; Tawarmalani and Sahinidis, 2002)



Bilinear Terms

The convex and concave envelopes of the bilinear function xy over a rectangular region

$$R \stackrel{\text{def}}{=} \{(x, y) \in \mathbb{R}^2 \mid l_x \leq x \leq u_x, l_y \leq y \leq u_y\}$$

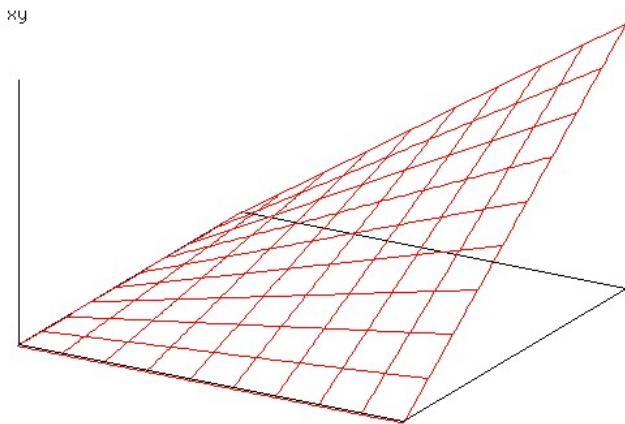
are given by the expressions

$$\begin{aligned} \text{vex}_{xy_R}(x, y) &= \max\{l_y x + l_x y - l_x l_y, u_y x + u_x y - u_x u_y\} \\ \text{cav}_{xy_R}(x, y) &= \min\{u_y x + l_x y - l_x u_y, l_y x + u_x y - u_x l_y\} \end{aligned}$$



Worth 1000 Words?

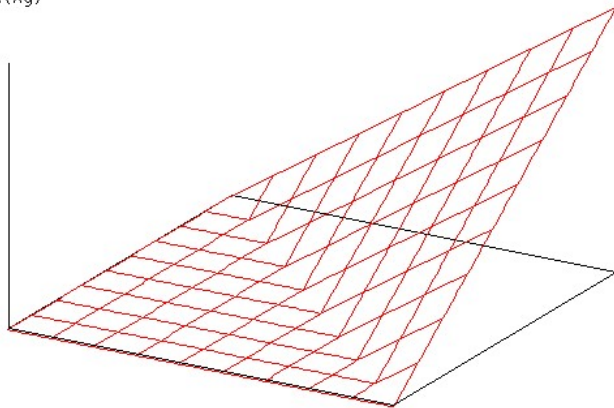
xy



Worth 1000 Words?

$vex_R(xy)$

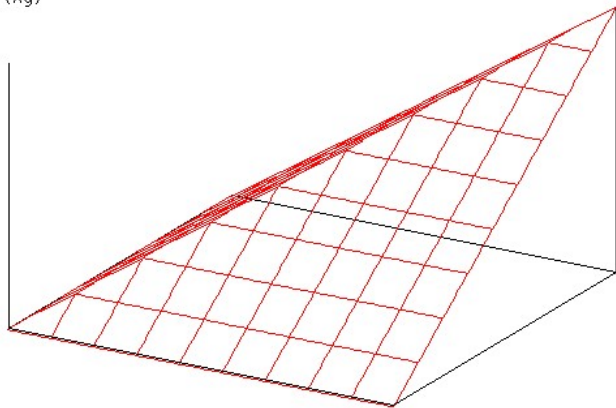
$vex(xy)$



Worth 1000 Words?

$$\text{cav}_R(xy)$$

$\text{cav}(xy)$



Summary

- MINLP: **Good** relaxations are important
- Relaxations can be improved
 - **Statically**: Better formulation/preprocessing
 - **Dynamically**: Cutting planes
- Nonconvex MINLP:
 - Methods exist, again based on relaxations
- Tight relaxations is an active area of research
- **Lots** of empirical questions remain



Part IV

Implementation and Software



Implementation and Software for MINLP

- ① Special Ordered Sets
- ② Implementation & Software Issues



Special Ordered Sets of Type 1

SOS1: $\sum \lambda_i = 1$ & at most one λ_i is nonzero

Example 1: $d \in \{d_1, \dots, d_p\}$ discrete diameters

$\Leftrightarrow d = \sum \lambda_i d_i$ and $\{\lambda_1, \dots, \lambda_p\}$ is SOS1

$\Leftrightarrow d = \sum \lambda_i d_i$ and $\sum \lambda_i = 1$ and $\lambda_i \in \{0, 1\}$

... d is convex combination with coefficients λ_i

Example 2: nonlinear function $c(y)$ of single integer

$\Leftrightarrow y = \sum i \lambda_i$ and $c = \sum c(i) \lambda_i$ and $\{\lambda_1, \dots, \lambda_p\}$ is SOS1

References: (Beale, 1979; Nemhauser, G.L. and Wolsey, L.A., 1988; Williams, 1993) ...

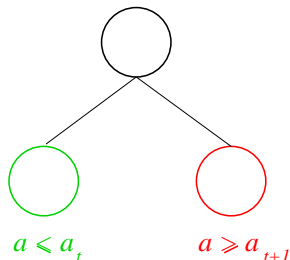


Special Ordered Sets of Type 1

SOS1: $\sum \lambda_i = 1$ & at most one λ_i is nonzero

Branching on SOS1

- 1 reference row $a_1 < \dots < a_p$
e.g. diameters
- 2 fractionality: $a := \sum a_i \lambda_i$

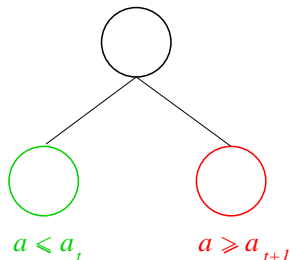


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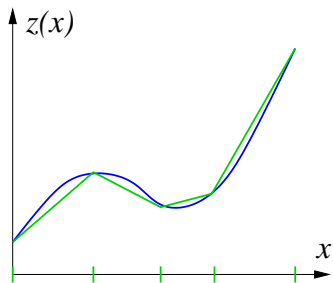
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e.g. diameters
- 2 fractionality: $a := \sum a_i \lambda_i$
- 3 find $t : a_t < a \leq a_{t+1}$
- 4 branch: $\{\lambda_{t+1}, \dots, \lambda_p\} = 0$
or $\{\lambda_1, \dots, \lambda_t\} = 0$



Special Ordered Sets of Type 2

SOS2: $\sum \lambda_i = 1$ & at most **two adjacent** λ_i nonzero

Example: Approximation of nonlinear function $z = z(x)$

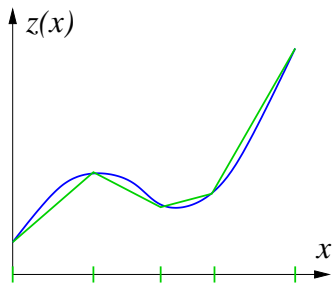


- breakpoints $x_1 < \dots < x_p$
- function values $z_i = z(x_i)$
- piece-wise linear

Special Ordered Sets of Type 2

SOS2: $\sum \lambda_i = 1$ & at most **two adjacent** λ_i nonzero

Example: Approximation of nonlinear function $z = z(x)$



- breakpoints $x_1 < \dots < x_p$
- function values $z_i = z(x_i)$
- piece-wise linear
- $x = \sum \lambda_i x_i$
- $z = \sum \lambda_i z_i$
- $\{\lambda_1, \dots, \lambda_p\}$ is SOS2

... convex combination of two breakpoints ...

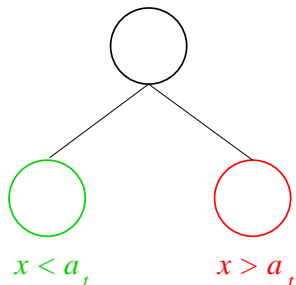


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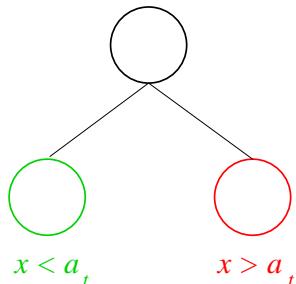


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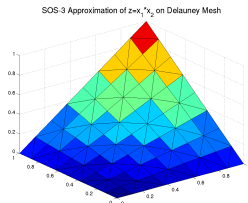


Special Ordered Sets of Type 3

Example: Approximation of 2D function $u = g(v, w)$

Triangularization of $[v_L, v_U] \times [w_L, w_U]$ domain

- 1 $v_L = v_1 < \dots < v_k = v_U$
- 2 $w_L = w_1 < \dots < w_l = w_U$
- 3 function $u_{ij} := g(v_i, w_j)$
- 4 λ_{ij} weight of vertex (i, j)

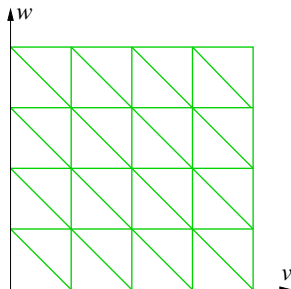


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 - 4 λ_{ij} weight of vertex (i, j)
- $v = \sum \lambda_{ij} v_i$
 - $w = \sum \lambda_{ij} w_j$
 - $u = \sum \lambda_{ij} u_{ij}$

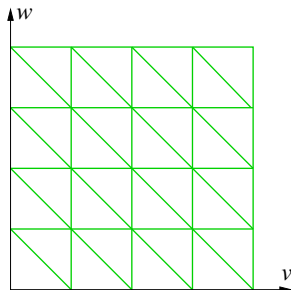


Special Ordered Sets of Type 3

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 - 4 λ_{ij} weight of vertex (i, j)
- $v = \sum \lambda_{ij} v_i$
 - $w = \sum \lambda_{ij} w_j$
 - $u = \sum \lambda_{ij} u_{ij}$



$1 = \sum \lambda_{ij}$ is SOS3 ...



Special Ordered Sets of Type 3

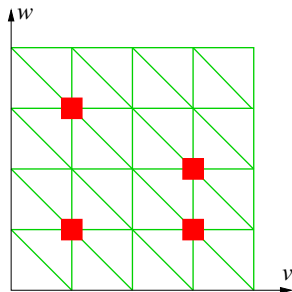
SOS3: $\sum \lambda_{ij} = 1$ & set condition holds

- 1 $v = \sum \lambda_{ij} v_i$... convex combinations
- 2 $w = \sum \lambda_{ij} w_j$
- 3 $u = \sum \lambda_{ij} u_{ij}$

$\{\lambda_{11}, \dots, \lambda_{kl}\}$ satisfies **set condition**

$\Leftrightarrow \exists$ triangle $\Delta : \{(i, j) : \lambda_{ij} > 0\} \subset \Delta$

i.e. nonzeros in single triangle Δ

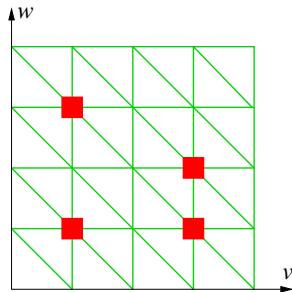


violates set condn

Branching on SOS3

λ violates set condition

- compute centers:
 $\hat{v} = \sum \lambda_{ij} v_i$ &
 $\hat{w} = \sum \lambda_{ij} w_i$
- find s, t such that
 $v_s \leq \hat{v} < v_{s+1}$ &
 $w_s \leq \hat{w} < w_{s+1}$
- branch on v or w

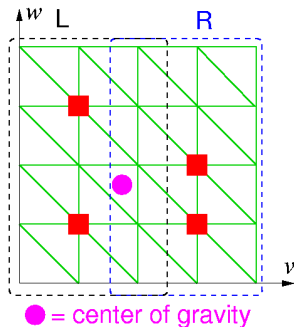


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vertical branching:

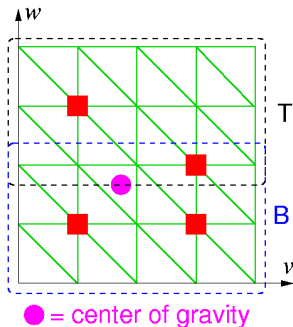
$$\sum_L \lambda_{ij} = 1$$

$$\sum_R \lambda_{ij} = 1$$

Branching on SOS3

λ violates set condition

- compute centers:
 $\hat{v} = \sum \lambda_{ij} v_i$ &
 $\hat{w} = \sum \lambda_{ij} w_i$
- find s, t such that
 $v_s \leq \hat{v} < v_{s+1}$ &
 $w_s \leq \hat{w} < w_{s+1}$
- branch on v or w



horizontal branching:

$$\sum_T \lambda_{ij} = 1$$

$$\sum_B \lambda_{ij} = 1$$

Extension to SOS- k

Example: electricity transmission network:

$$c(x) = 4x_1 - x_2^2 - 0.2 \cdot x_2 x_4 \sin(x_3)$$

(Martin et al., 2005) extend SOS3 to SOS k models for any k
 \Rightarrow function with p variables on N grid needs N^p λ 's



Extension to SOS- k

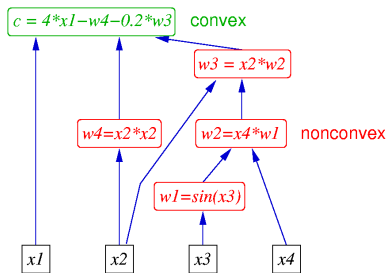
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- exploit computational graph
 \simeq automatic differentiation



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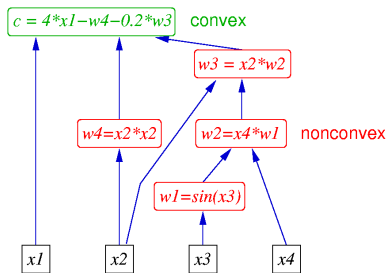
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- only need SOS2 & SOS3 ...
replace **nonconvex** parts



Extension to SOS- k

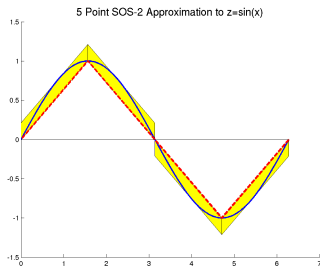
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 \Rightarrow function with p variables on N grid needs N^p λ 's

Alternative (Gatzke, 2005):

- exploit computational graph
 \simeq automatic differentiation
- only need SOS2 & SOS3 ...
replace **nonconvex** parts
- piece-wise polyhedral approx.



Software for MINLP

- **Outer Approximation:** DICOPT++ (& AIMMS)
NLP solvers: CONOPT, MINOS, SNOPT
MILP solvers: CPLEX, OSL2
- **Branch-and-Bound Solvers:** SBB & MINLP
NLP solvers: CONOPT, MINOS, SNOPT & FilterSQP
variable & node selection; SOS1 & SOS2 support
- **Global MINLP:** BARON & MINOPT underestimators & branching
CPLEX, MINOS, SNOPT, OSL
- **Online Tools:** MINLP World, MacMINLP & NEOS MINLP World
www.gamsworld.org/minlp/
NEOS server www-neos.mcs.anl.gov/



<http://www.coin-or.org>

- **CO**mputational **IN**frastructure for **O**perations **R**esearch
- A **library** of (interoperable) software tools for optimization
- A **development platform** for open source projects in the OR community
- Possibly Relevant Modules:
 - OSI: **O**pen **S**olver **I**nterface
 - CGL: **C**ut **G**eneration **L**ibrary
 - CLP: **C**oin **L**inear **P**rogramming Toolkit
 - CBC: **C**oin **B**ranch and **C**ut
 - IPOPT: **I**nterior **P**oint **OPT**imizer for NLP
 - NLPAPI: **N**on**L**inear **P**rogramming **API**



MINLP with COIN-OR

New implementation of LP/NLP based BB

- MIP branch-and-cut: CBC & CGL
- NLPs: IPOPT **interior point** ... OK for NLP(y_i)
- New hybrid method:
 - solve more NLPs at non-integer y_i
⇒ better outer approximation
 - allow complete MIP at some nodes
⇒ generate new integer assignment

... faster than DICOPT++, SBB

- simplifies to OA and BB at extremes ... less efficient

... see Bonami et al. (2005) ... coming in 2006.



Conclusions

MINLP rich modeling paradigm

- most popular solver on NEOS

Algorithms for MINLP:

- Branch-and-bound (branch-and-cut)
- Outer approximation et al.



Conclusions

MINLP rich modeling paradigm

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“MINLP solvers lag 15 years behind MIP solvers”

⇒ many research opportunities!!!



Part V

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