MINLP Short Course Overview

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

Today you will be "treated" to a draft of Part III.
(Maybe a little bit of II.)

Part I

Introduction, Applications, and Formulations

The Problem of the Day

Mixed Integer Nonlinear Program (MINLP)

$$\begin{cases} \underset{x,y}{\text{minimize}} & f(x,y) \\ \text{subject to} & c(x,y) \le 0 \\ & x \in X, \; y \in Y \text{ integer} \end{cases}$$

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

Why the N?

An anecdote: July, 1948. A young and frightened George Dantzig, presents his newfangled "linear programming" to a meeting of the Econometric Society of Wisconsin, attended by distinguished scientists like Hotelling, Koopmans, and Von Neumann. Following the lecture, Hotelling[a] pronounced to the audience:

> *But we all know the world is nonlinear!*

[a] in Dantzig's words "a huge whale of a man"

The world is indeed nonlinear

- Physical Processes and Properties
  - Equilibrium
  - Enthalpy
- Abstract Measures
  - Economies of Scale
  - Covariance
  - Utility of decisions

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
- If the variable is associated with a physical entity that is indivisible, then it must be integer
  1. Number of aircraft carriers to to produce. Gomory's Initial Motivation
  2. Yearly number of trees to harvest in Norrland

A Popular MINLP Method

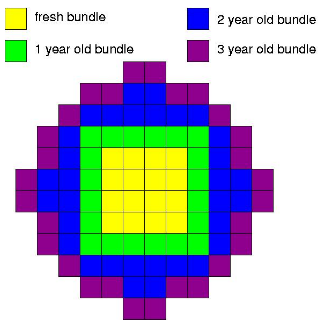
Dantzig's Two-Phase Method for MINLP Adapted by Leyffer and Linderoth

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.

- Sometimes a continuous approximation to the discrete (integer) decision is accurate enough for practical purposes.
  - Yearly tree harvest in Norrland
- 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!

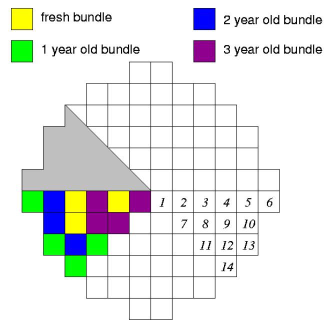
Example: Core Reload Operation (Quist, A.J., 2000)

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



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:

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

AMPL model:

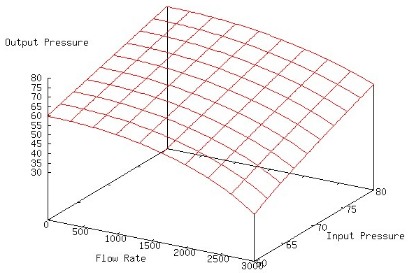
```
var x {I,L,M} binary ;
Bundle {i in I}:  sum{l in L, m in M} x[i,l,m] = 1 ;
```

- 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!
- 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
- $\underline{s}_i, \overline{s}_i$: Lower and upper bounds on gas "supply" at node i
- $\underline{p}_i, \overline{p}_i$: 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 $i \to j$
  - $f(i,j) < 0 \Rightarrow$ gas flows $j \to i$

Gas Transmission Model

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

subject to

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

Your First Modeling Trick

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

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

- 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

Dealing with sign(·): The NLP Way

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

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

- Note that

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

- Write constraint as

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

Dealing with sign(·): The MIP Way

Model

$$f_{ij} > 0 \Rightarrow \begin{cases} f_{ij}^2 \leq \Psi_{ij}(\rho_i - \rho_j) \\ f_{ij}^2 \geq \Psi_{ij}(\rho_i - \rho_j) \end{cases} \qquad f_{ij} < 0 \Rightarrow \begin{cases} f_{ij}^2 \leq \Psi_{ij}(\rho_j - \rho_i) \\ f_{ij}^2 \geq \Psi_{ij}(\rho_j - \rho_i) \end{cases}$$

$$m \leq f_{ij}^2 - \Psi(\rho_i - \rho_j) \leq M \qquad l \leq f_{ij}^2 - \Psi(\rho_j - \rho_i) \leq L$$

Example

$$f_{ij} > 0 \Rightarrow z_{ij} = 1 \Rightarrow f_{ij}^2 \leq \Psi(\rho_i - \rho_j)$$

$$f_{ij} > 0 \Rightarrow z_{ij} = 1 \Rightarrow f_{ij}^2 \leq \Psi(\rho_i - \rho_j)$$

$$f_{ij} > 0 \Rightarrow z_{ij} = 1 \Rightarrow f_{ij}^2 \leq \Psi(\rho_i - \rho_j)$$

Dealing with sign(·): The MIP Way

- Wonderful MIP Modeling reference is Williams (1993)
- If you put it all together you get...

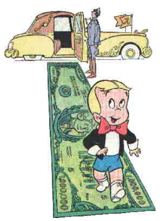
- $z_{ij} \in \{0, 1\}$: Indicator if flow is positive
- $y_{ij} \in \{0, 1\}$: Indicator if flow is negative

$$\begin{aligned}
f_{ij} &\leq F z_{ij} \\
f_{ij} &\geq -F y_{ij} \\
z_{ij} + y_{ij} &= 1 \\
f_{ij}^2 + M z_{ij} &\leq M + \Psi_{ij}(\rho_i - \rho_j) \\
f_{ij}^2 + m z_{ij} &\geq m + \Psi_{ij}(\rho_i - \rho_j) \\
f_{ij}^2 + L y_{ij} &\leq L + \Psi_{ij}(\rho_j - \rho_i) \\
f_{ij}^2 + l y_{ij} &\geq l + \Psi_{ij}(\rho_j - \rho_i)
\end{aligned}$$

Special Ordered Sets

- Sven thinks the NLP way is better
- Jeff thinks the MIP way is better
- Neither way is 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

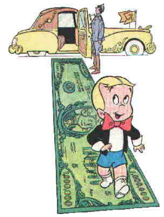


- N: Universe of asset to purchase
- x_i: Amount of asset i to hold
- B: Budget

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

- 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

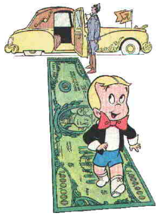
More Realistic Models



- $b \in \mathbb{R}^{|N|}$ of "benchmark" holdings
- Benchmark Tracking: $u(x) \stackrel{\text{def}}{=} (x - b)^T Q (x - b)$
  - Constraint on $\mathbb{E}$[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:

$$x_i \leq B y_i \qquad \forall i \in N$$

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



Even More Models

- Min Holdings: $(x_i = 0) \vee (x_i \geq m)$
  - Model implication: $x_i > 0 \Rightarrow x_i \geq m$
  - $x_i > 0 \Rightarrow y_i = 1 \Rightarrow x_i \geq m$
  - $x_i \leq By_i, x_i \geq my_i \; \forall i \in N$
- Round Lots: $x_i \in \{kL_i, k = 1, 2, \dots\}$
  - $x_i - z_i L_i = 0, z_i \in \mathbb{Z}_+ \; \forall i \in N$
- 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

Making "Plays"

- Suppose that the stocks are partitioned into sectors $S_1 \subseteq N, S_2 \subseteq N, \dots S_K \subseteq N$
- The Fund Manager wants to invest all money into one sector "play"
  - $\sum_{i \in S_k} x_i > 0 \Rightarrow \sum_{j \in N \setminus S_k} x_j = 0$
- Modeling Choices:
- Aggregated:

$$\sum_{i \in S_k} x_i \leq B z_k \qquad \sum_{j \in N \setminus S_k} x_j + B z_k \leq B$$

- Disaggregated:

$$x_i \leq u_i z_i \quad \forall i \in N \qquad x_j + u_j z_i \leq u_j \; \forall j \mid i \in S_k, j \notin S_k$$

Which is better?: Part III has the answer

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

- B_i: Batch size of product $i \in N$
- V_j: Stage j size: $V_j \geq S_{ij} B_i \forall i, j$
- C_i: Longest stage time for product i: $C_i \geq t_{ij}/N_j \forall i, j$
- N_j: Number of machines at stage j

Multiproduct Batch Plants

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

s.t.

$$\begin{array}{rcll} V_j - S_{ij} B_i & \geq & 0 & \forall i \in N, \forall j \in M \\ C_i N_j & \geq & t_{ij} & \forall i \in N, \forall j \in M \\ \sum_{i \in N} \frac{Q_i}{B_i} C_i & \leq & H & \\ \text{Bound Constraints} & \text{on} & V_j, C_i, B_i, N_j & \\ N_j & \in & \mathbb{Z} & \forall j \in M \end{array}$$

Modeling Trick #2

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

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

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

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

(Transformed) Bound Constraints on V_j, C_i, B_i

How to Handle the Integrality?

- But what to do about the integrality?

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

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

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

$$\begin{aligned} n_j - \sum_{k=1}^{K} \ln(k) Y_{kj} &= 0 \qquad \forall j \in M \\ \sum_{k=1}^{K} Y_{kj} &= 1 \qquad \forall j \in M \end{aligned}$$

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

MIQP: Modeling Tricks

- In 0-1 quadratic programming, we can always make quadratic forms convex.
- Key: If $y \in \{0,1\}$, then $y = y^2$, so add a "large enough" constant to the diagonal, and subtract it from the linear term:
- $y \in \{0,1\}^n$ consider any quadratic

$$\begin{aligned} q(y) &= y^T Q y + g^T y \\ &= y^T W y + c^T y \end{aligned}$$

where $W = Q + \lambda I$ and $c = g - \lambda e$ $(e = (1, \ldots, 1))$

- If $\lambda \geq$(smallest eigenvalue of Q), then $W \succeq 0$.

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

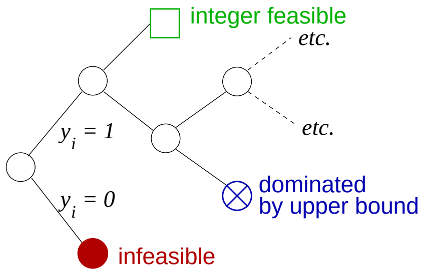
Classical Solution Methods for MINLP

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

Branch-and-Bound

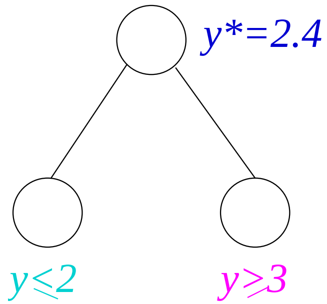
Solve relaxed NLP ($0 \le y \le 1$ continuous relaxation)
. . . solution value provides lower bound

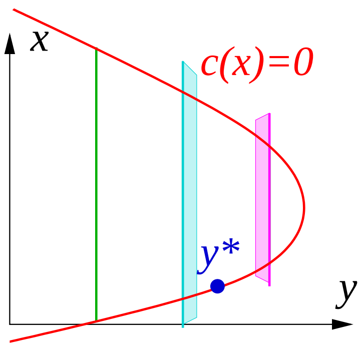
- Branch on y_i non-integral
- Solve NLPs & branch until
  1. Node infeasible ...
  2. Node integer feasible ...
     $\Rightarrow$ get upper bound (U)
  3. Lower bound $\ge U$ ... $\otimes$



Search until no unexplored nodes on tree

Convergence of Branch-and-Bound





All NLP problems solved globally & finite number of NLPs on tree
$\Rightarrow$ Branch-and-Bound converges

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. **user defined priorities**
   ... branch on most important variable first
2. **maximal fractional branching**

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

... find $\hat{y}_i$ closest to $\frac{1}{2}$ $\Rightarrow$ largest change in problem

Variable Selection for Branch-and-Bound

Assume $y_i \in \{0,1\}$ for simplicity ...
$(\hat{x}, \hat{y})$ fractional solution to parent node; $\hat{f} = f(\hat{x}, \hat{y})$

3. **pseudo-cost branching**
   estimates e_i^+, e_i^- of change in $f(x,y)$ after branching

$$\max_i \left\{ \min(\hat{f} + e_i^+(1-\hat{y}_i), \hat{f} + e_i^- \hat{y}_i) \right\}$$

... find y_i, whose expected change of objective is largest
... estimate e_i^+, e_i^- by keeping track of

$$e_i^+ = \frac{f_i^+ - \hat{f}}{1-\hat{y}_i} \quad \text{and} \quad e_i^- = \frac{f_i^- - \hat{f}}{\hat{y}_i}$$

where $f_i^{+/-}$ solution value after branching

Variable Selection for Branch-and-Bound

Assume $y_i \in \{0,1\}$ for simplicity ...
$(\hat{x}, \hat{y})$ fractional solution to parent node; $\hat{f} = f(\hat{x}, \hat{y})$

4. **strong branching**: solve *all* NLP child nodes:

$$f_i^{+/-} \leftarrow \left\{ \begin{array}{ll} \underset{x,y}{\text{minimize}} & f(x,y) \\ \text{subject to} & c(x,y) \le 0 \\ & x \in X,\ y \in Y,\ y_i = 1/0 \end{array} \right.$$

choose branching variable as

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

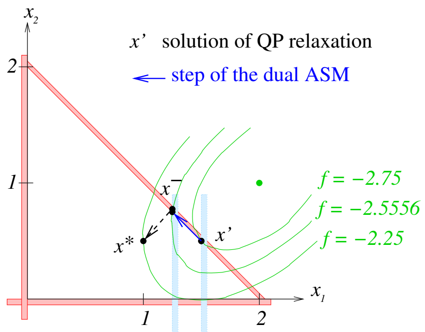
... find y_i that changes objective the most

Variable Selection for Branch-and-Bound

Assume $y_i \in \{0,1\}$ for simplicity ...
$(\hat{x}, \hat{y})$ fractional solution to parent node; $\hat{f} = f(\hat{x}, \hat{y})$

5. **MIQP strong branching**: (Fletcher and Leyffer, 1998)
   parametric solution of QPs ... much cheaper than re-solve

- step of dual active set method
- factorization of KKT matrix
- $\simeq$ multiple KKT solves
- generalizes old MILP ideas



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 lower bound**
   choose node with least value of parent node $f_{p(n)}$
   - minimizes number of NLPs solved

Node Selection for Branch-and-Bound

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

3. **best estimate**
   choose node leading to best expected integer solution

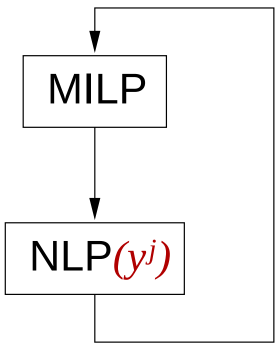
$$\max_{n \in \mathcal{T}} \left\{ f_{p(n)} + \sum_{i:y_i \text{fractional}} \min\left\{ e_i^+(1-y_i), e_i^- y_i \right\} \right\}$$

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



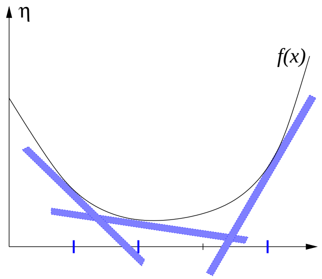
NLP subproblem y_j fixed:

$$\text{NLP}(y_j) \left\{ \begin{array}{ll} \underset{x}{\text{minimize}} & f(x, y_j) \\ \text{subject to} & c(x, y_j) \le 0 \\ & x \in X \end{array} \right.$$

Main Assumption: f, c are convex

Outer Approximation (Duran and Grossmann, 1986)

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

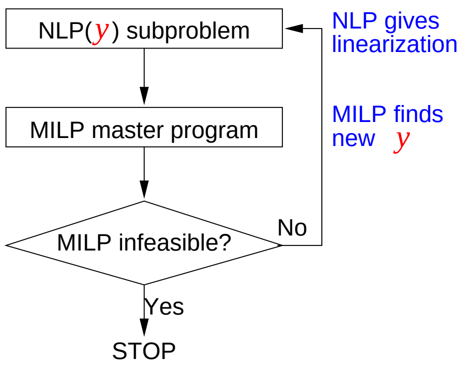


$$(M) \left\{ \begin{array}{lll} \underset{z=(x,y),\eta}{\text{minimize}} & \eta & \\ \text{subject to} & \eta \ge f_j + \nabla f_j^T (z - z_j) & \forall y_j \in Y \\ & 0 \ge c_j + \nabla c_j^T (z - z_j) & \forall y_j \in Y \\ & x \in X,\ y \in Y \text{ integer} & \end{array} \right.$$

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)



$\Rightarrow$ stop, if lower bound $\geq$ upper bound

Convergence of Outer Approximation

Lemma: Each $y_i \in Y$ generated at most once.

Proof: Assume $y_i \in Y$ generated again at iteration $j > i$
$\Rightarrow \exists\, \hat{x}$ such that $(\hat{x}, y_i)$ feasible in (M_j):

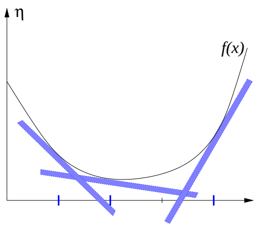
$$\eta \geq f_i + \nabla_x f_i^T (\hat{x} - x_i)$$
$$0 \geq c_i + \nabla_x c_i^T (\hat{x} - x_i)$$

... because $y_i - y_i = 0$
Now sum with $(1, \lambda_i)$ multipliers of NLP(y_i)
$\Rightarrow \eta \geq f_i + (\nabla_x f_i + \nabla_x c_i \lambda_i)^T (\hat{x} - x_i)$ ... KKT conditions
$\Rightarrow \eta \geq f_i$ contradicts $\eta < U \leq f_i$ upper bound
$\Rightarrow$ each $y_i \in Y$ generated at most once $\square$
Refs: (Duran and Grossmann, 1986; Fletcher and Leyffer, 1994)

Convergence of Outer Approximation

1. each $y_i \in Y$ generated at most once & $|Y| < \infty \Rightarrow$ finite termination
2. convexity $\Rightarrow$ outer approximation

$\Rightarrow$ convergence to global min



Convexity important!!!

Outer Approximation & Benders Decomposition

Take OA master ... $z := (x, y)$ ... wlog $X = \mathbb{R}^n$

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

sum constraints $0 \geq c_j$... weighted with multipliers λ_j $\forall j$

$$\Rightarrow \quad \eta \geq f_j + \lambda_j^T c_j + (\nabla f_j + \nabla c_j \lambda_j)^T (z - z_j) \qquad \forall y_j \in Y$$

... is a valid inequality.
References: (Geoffrion, 1972)

Outer Approximation & Benders Decomposition

Valid inequality from OA master; $z = (x, y)$:

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

use first order conditions of NLP(y_j) ...

$$\nabla_x f_j + \nabla_x c_j \lambda_j = 0$$

... to eliminate x components from valid inequality in y

$$\begin{aligned} &\Rightarrow \quad \eta \geq f_j + \lambda_j^T c_j + (\nabla_y f_j + \nabla_y c_j \lambda_j)^T (y - y_j) \\ &\Leftrightarrow \quad \eta \geq \mathcal{L}_j + (\mu_j)^T (y - y_j) \end{aligned}$$

where $\mathcal{L}_j = f(z_j) + \lambda_j^T c(z_j)$ Lagrangian ...
... $\mu_j = \nabla_y f_j + \nabla_y c_j \lambda_j$ multiplier of $y = y_j$ in NLP(y_j)

Outer Approximation & Benders Decomposition

$\Rightarrow$ remove x from master problem ... Benders master problem

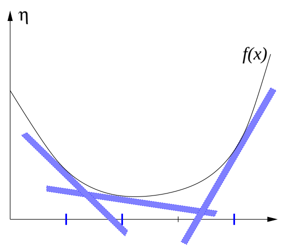
$$(M_B) \begin{cases} \underset{y,\eta}{\text{minimize}} & \eta \\ \text{subject to} & \eta \geq \mathcal{L}_j + (\mu_j)^T (y - y_j) \quad \forall y_j \in Y \\ & y \in Y \text{ integer} \end{cases}$$

where $\mathcal{L}_j$ Lagrangian & μ_j multiplier of $y = y_j$ in NLP(y_j)

- (M_B) has less constraints & variables (no x!)
- (M_B) almost ILP (except for η)
- (M_B) weaker than OA (from derivation)

Extended Cutting Plane Method

Replace NLP(y_i) solve in OA by linearization about solution of (M_j)
get cutting plane for violated constraint
$\Rightarrow$ no NLP(y_j) solves ...
... Kelley's cutting plane method instead
$\Rightarrow$ slow nonlinear convergence:
> 1 evaluation per y

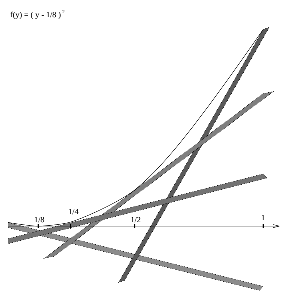


References: (Westerlund, T. and Pettersson, F., 1995)

Disadvantages of Outer Approximation

- MILP tree-search can be bottle-neck
- potentially large number of iterations

$$\begin{array}{ll} \text{minimize} & (y - \frac{1}{2^n})^2 \\ \text{subject to} & y \in \{0, \frac{1}{2^n}, \ldots 1\} \end{array}$$



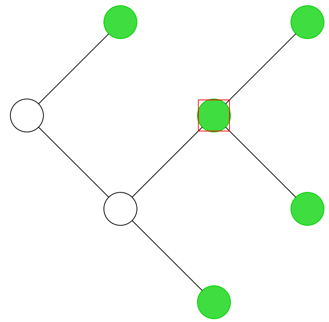
Second order master (MIQP): (Fletcher and Leyffer, 1994):
- add Hessian term to MILP (M_i) becomes MIQP:

$$\text{minimize} \quad \eta + \frac{1}{2}(z - z_i)^T W (z - z_i) \quad \text{subject to} \ldots$$

LP/NLP Based Branch-and-Bound

AIM: avoid re-solving MILP master (M)

- Consider MILP branch-and-bound
- interrupt MILP, when y_j found
  $\Rightarrow$ solve NLP(y_j) get x_j
- linearize f, c about (x_j, y_j)
  $\Rightarrow$ 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
- no commercial implementation of this idea
- preliminary results: order of magnitude faster than OA
  - ◦ same number of NLPs, but only one MILP
- similar ideas for Benders & Extended Cutting Plane methods

References: (Quesada and Grossmann, 1992)

Integrating SQP & Branch-and-Bound

AIM: Avoid solving NLP node to convergence.

Sequential Quadratic Programming (SQP)
$\rightarrow$ solve sequence (QP_k) at every node

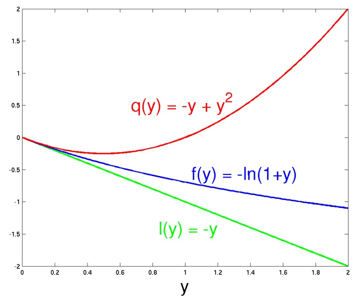
$$(QP_k) \left\{ \begin{array}{ll} \underset{d}{\text{minimize}} & f_k + \nabla f_k^T d + \frac{1}{2} d^T H_k d \\ \text{subject to} & c_k + \nabla c_k^T d \leq 0 \\ & x_k + d_x \in X \\ & y_k + d_y \in \hat{Y}. \end{array} \right.$$

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

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



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
  $\Rightarrow$ converge for *convex* MINLP

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× faster than B&B
   $\simeq$ number of QPs per node
5. ECP works well, if function/gradient evals expensive

Part III

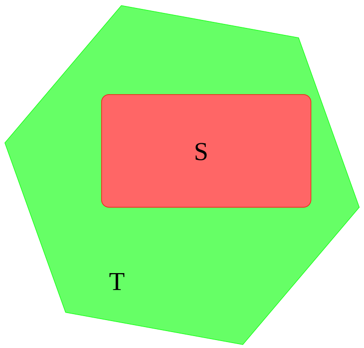
Modern Developments in MINLP

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. Global methods
   - Envelopes
   - Methods

Relaxations

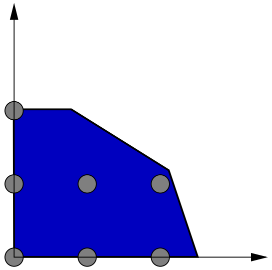
- $z(S) \stackrel{\text{def}}{=} \min_{x \in S} f(x)$
- $z(T) \stackrel{\text{def}}{=} \min_{x \in T} f(x)$



- Independent of f, S, T:
  $z(T) \leq z(S)$
- If $x_T^* = \arg\min_{x \in T} f(x)$
- And $x_T^* \in S$, then
- $x_T^* = \arg\min_{x \in S} f(x)$

A Pure Integer Program

$$z(S) = \min\{c^T x : x \in S\}, \qquad S = \{x \in \mathbb{Z}^n_+ : Ax \le b\}$$



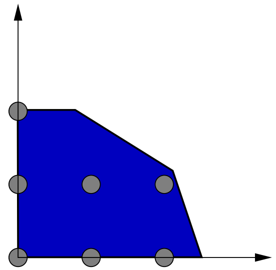
$$\begin{aligned} S &= \{(x_1, x_2) \in \mathbb{Z}^2_+ : 6x_1 + x_2 \le 15, \\ &\quad 5x_1 + 8x_2 \le 20, x_2 \le 2\} \\ &= \{(0,0), (0,1), (0,2), (1,0), \\ &\quad (1,1), (1,2), (2,0)\} \end{aligned}$$

How to Solve Integer Programs?

- Relaxations!
  - $T \supseteq S \Rightarrow z(T) \le z(S)$
  - People commonly use the linear programming relaxation:

$$z(LP(S)) = \min\{c^T x : x \in LP(S)\}$$

$$LP(S) = \{x \in \mathbb{R}^n_+ : Ax \le b\}$$



- If $LP(S) = \text{conv}(S)$, we are done.
- Minimum of any linear function over any convex set occurs on the boundary
- We need only know conv(S) in the direction of c.
- The "closer" $LP(S)$ is to conv(S) the better.

Small M's Good. Big M's Baaaaaaaaaaaaaaaaad!

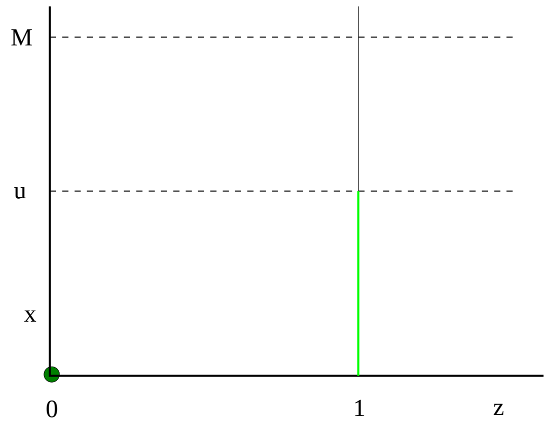
- Sometimes, we can get a better relaxation (make $LP(S)$ a closer approximation to conv(S)) through a different tighter formulation
- Let's look at the geometry

$$P = \{x \in \mathbb{R}_+, z \in \{0,1\} : x \le Mz, x \le u\}$$

$$LP(P) = \{x \in \mathbb{R}_+, z \in [0,1] : x \le Mz, x \le u\}$$

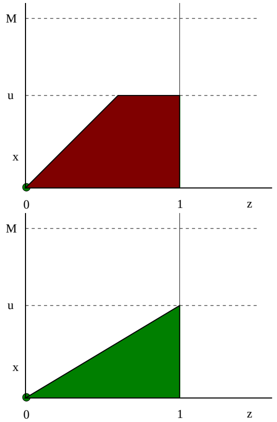
$$\text{conv}(P) = \{x \in \mathbb{R}_+, z \in \{0,1\} : x \le uz\}$$

P



$$P = \{x \in \mathbb{R}_+, z \in \{0,1\} : x \le Mz, x \le u\}$$

LP Versus Conv



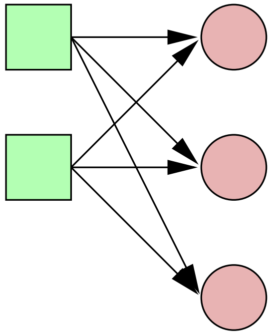
$$LP(P) = \{x \in \mathbb{R}_+, z \in [0,1] : x \le Mz, x \le u\}$$

$$\text{conv}(P) = \{x \in \mathbb{R}_+, z \in [0,1] : x \le uz\}$$

- KEY: If $M = u$, $LP(P) = \text{conv}(P)$
- Small M's good. Big M's baaaaaaaad.

UFL: Uncapacitated Facility Location

- Facilities: I
- Customers: J



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

$$\begin{aligned} \sum_{j \in N} y_{ij} &= 1 \quad \forall i \in I \\ \sum_{i \in I} y_{ij} &\le |I| x_j \quad \forall j \in J \qquad (1) \\ \text{OR } y_{ij} &\le x_j \quad \forall i \in I,\ j \in J \qquad (2) \end{aligned}$$

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

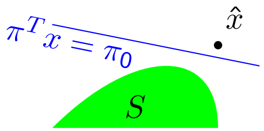
Valid Inequalities

- Sometimes we can get a better formulation by dynamically improving it.

- An inequality $\pi^T x \le \pi_0$ is a valid inequality for S if $\pi^T x \le \pi_0\ \forall x \in S$
- Alternatively: $\max_{x \in S}\{\pi^T x\} \le \pi_0$

- **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

$$\begin{cases} \underset{x,y}{\text{minimize}} & f_x^T x + f_y^T y \\ \text{subject to} & c(x,y) \le 0 \\ & y \in \{0,1\}^p,\ 0 \le x \le U \end{cases}$$

- Note the Linear objective
- This is WLOG:

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

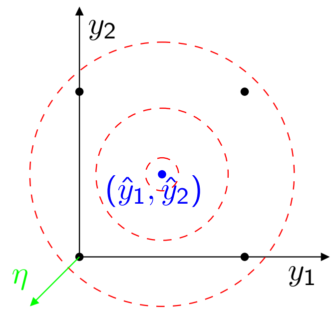
It's Actually Important!

- 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! :-(

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

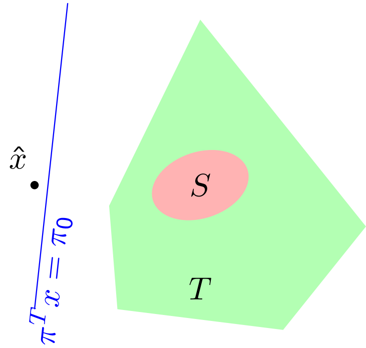
$$\text{s.t. } y_1 \in \{0,1\}, y_2 \in \{0,1\}$$

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



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
- If $P = \{x \in \{0,1\}^n \mid Ax \leq b\}$, then for any row i, $P_i = \{x \in \{0,1\}^n \mid a_i^T x \leq b_i\}$ is a relaxation of P.
- If the intersection of the relaxations is a good approximation to the true problem, then the inequalities will be quite useful.
- 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 $\forall j \in C$
- 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 conv(K)

Example

$$K = \{x \in \{0,1\}^7 \mid 11x_1 + 6x_2 + 6x_3 + 5x_4 + 5x_5 + 4x_6 + x_7 \leq 19\}$$

$$LP(K) = \{x \in [0,1]^7 \mid 11x_1 + 6x_2 + 6x_3 + 5x_4 + 5x_5 + 4x_6 + x_7 \leq 19\}$$

- $(1, 1, 1/3, 0, 0, 0, 0) \in LP(K)$
  - CHOPPED OFF BY $x_1 + x_2 + x_3 \leq 2$
- $(0, 0, 1, 1, 1, 3/4, 0) \in LP(K)$
  - CHOPPED OFF BY $x_3 + x_4 + x_5 + x_6 \leq 3$

The Chvátal-Gomory Procedure

- A general procedure for generating valid inequalities for integer programs
- Let the columns of $A \in \mathbb{R}^{m \times n}$ be denoted by $\{a_1, a_2, \ldots a_n\}$
- $S = \{x \in \mathbb{Z}_+^n \mid Ax \leq b\}$.
  1. Choose nonnegative multipliers $u \in \mathbb{R}_+^m$
  2. $u^T Ax \leq u^T b$ is a valid inequality ($\sum_{j \in N} u^T a_j x_j \leq u^T b$).
  3. $\sum_{j \in N} \lfloor u^T a_j \rfloor x_j \leq u^T b$ (Since $x \geq 0$).
  4. $\sum_{j \in N} \lfloor u^T a_j \rfloor x_j \leq \lfloor u^T b \rfloor$ is valid for X since $\lfloor u^T a_j \rfloor x_j$ is an integer
- Simply Amazing: This simple procedure suffices to generate every valid inequality for an integer program

Other Substructures

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

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

- 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)

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

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

Extension to MINLP (Çezik and Iyengar, 2005)

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

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

- $\mathcal{K}$: 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: $\mathcal{K}_s = \{x = \text{vec}(X) \mid X = X^T, X \text{ p.s.d}\}$
- Dual Cone: $\mathcal{K}^* \stackrel{\text{def}}{=} \{u \mid u^T z \geq 0 \ \forall z \in \mathcal{K}\}$
- Extension is clear from the following equivalence:

$$Az \succeq_{\mathcal{K}} b \quad \Leftrightarrow \quad u^T A z \geq u^T b \ \forall u \succeq_{\mathcal{K}^*} 0$$

- Many classes of nonlinear inequalities can be represented as

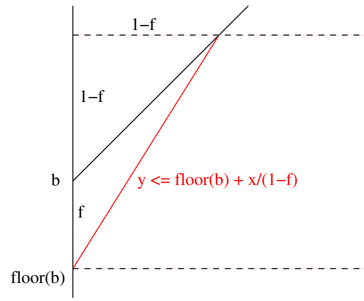
$$Ax \succeq_{\mathcal{K}_q} b \text{ or } Ax \succeq_{\mathcal{K}_s} b$$

- Go to other SIAM Short Course to find out about Semidefinite Programming

Mixed Integer Rounding—MIR

Almost everything comes from considering the following very simple set, and observation.

- $X = \{(x, y) \in \mathbb{R} \times \mathbb{Z} \mid y \leq b + x\}$
- $f = b - \lfloor b \rfloor$: fractional
  - NLP People are silly and use f for the objective function
- $LP(X)$
- $\text{conv}(X)$
- $y \leq \lfloor b \rfloor + \frac{1}{1-f} x$ is a valid inequality for X



Extension of MIR

$$X_2 = \left\{ (x^+, x^-, y) \in \mathbb{R}^2_+ \times \mathbb{Z}^{|N|} \mid \sum_{j \in N} a_j y_j + x^+ \leq b + x^- \right\}$$

- The inequality

$$\sum_{j \in N} \left(\lfloor (a_j) \rfloor + \frac{(f_j - f)^+}{1 - f} \right) y_j \leq \lfloor b \rfloor + \frac{x^-}{1 - f}$$

  is valid for X_2
- $f_j \stackrel{\text{def}}{=} a_j - \lfloor a_j \rfloor$, $(t)^+ \stackrel{\text{def}}{=} \max(t, 0)$
- X is a one-row relaxation of a general *mixed* integer program
  - Continuous variables aggregated into two: x^+, x^-

It's So Easy, Even I Can Do It

Proof:

- $N_1 = \{j \in N \mid f_j \leq f\}$
- $N_2 = N \setminus N_1$
- Let

$$P = \{(x, y) \in \mathbb{R}^2_+ \times \mathbb{Z}^{|N|} \mid \sum_{j \in N_1} \lfloor a_j \rfloor y_j + \sum_{j \in N_2} \lceil a_j \rceil y_y \leq b + x^- + \sum_{j \in N_2} (1 - f_j) y_j\}$$

1. Show $X \subseteq P$
2. Show simple (2-variable) MIR inequality is valid for P (with an appropriate variable substitution).
3. Collect the terms

Gomory Mixed Integer Cut is a MIR Inequality

- Consider the set

$$X^{=} = \left\{ (x^+, x^-, y_0, y) \in \mathbb{R}^2_+ \times \mathbb{Z} \times \mathbb{Z}^{|N|}_+ \mid y_0 + \sum_{j \in N} a_j y_j + x^+ - x^- \right.$$

which is essentially the row of an LP tableau

- Relax the equality to an inequality and apply MIR
- Gomory Mixed Integer Cut:

$$\sum_{j \in N_1} f_j y_j + x^+ + \frac{f}{1-f} x^- + \sum_{j \in N_2} (f_j - \frac{f_j - f}{1-f}) y_j \geq f$$

Formulations | Preliminaries
Inequalities | MILP Inequalities Applied to MINLP
Dealing with Nonconvexity | Disjunctive Inequalities

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

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

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

- Create Gomory mixed integer cuts from

$$\begin{array}{rcl} \eta & \geq & f_j + \nabla f_j^T z - z_j \\ 0 & \geq & c_j + \nabla c_j^T (z - z_j) \end{array}$$

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

Formulations | Preliminaries
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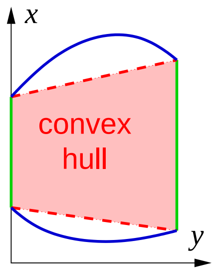
Disjunctive Cuts for MINLP (Stubbs and Mehrotra, 1999)

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

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

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



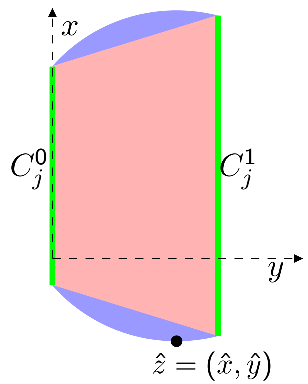
$$\text{let } \mathcal{M}_j(C) \stackrel{\text{def}}{=} \left\{ \begin{array}{l} z = \lambda_0 u_0 + \lambda_1 u_1 \\ \lambda_0 + \lambda_1 = 1, \ \lambda_0, \lambda_1 \geq 0 \\ u_0 \in C_j^0, \ u_1 \in C_j^1 \end{array} \right\}$$

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

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

Disjunctive Cuts: Example

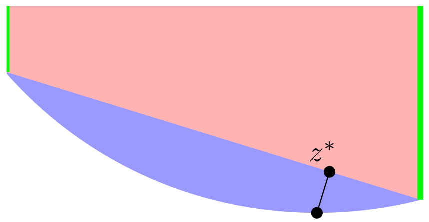
$$\underset{x,y}{\text{minimize}} \left\{ x \mid (x - 1/2)^2 + (y - 3/4)^2 \leq 1, -2 \leq x \leq 2, y \in \{0,1\} \right\}$$



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

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

Disjunctive Cuts Example



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

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

$$\begin{array}{rcl} \text{s.t. } \lambda_0 u_0 + \lambda_1 u_1 & = & z \\ \lambda_0 + \lambda_1 & = & 1 \\ \begin{pmatrix} -0.16 \\ 0 \end{pmatrix} \le u_0 & \le & \begin{pmatrix} 0.66 \\ 1 \end{pmatrix} \\ \begin{pmatrix} -0.47 \\ 0 \end{pmatrix} \le u_1 & \le & \begin{pmatrix} 1.47 \\ 1 \end{pmatrix} \\ \lambda_0, \lambda_1 & \ge & 0 \end{array}$$

NONCONVEX

What to do? (Stubbs and Mehrotra, 1999)

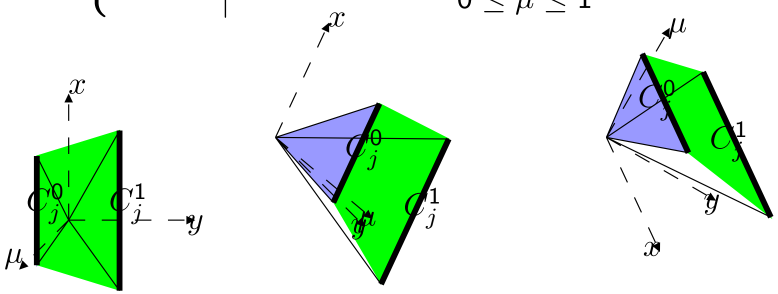
- Look at the perspective of $c(z)$, which gives a convex reformulation of $\mathcal{M}_j(C)$: $\mathcal{M}_j(\tilde{C})$, where

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

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

Disjunctive Cuts Example

$$\tilde{C} = \left\{ \begin{pmatrix} x \\ y \\ \mu \end{pmatrix} \;\middle|\; \begin{array}{c} \mu \left[(x/\mu - 1/2)^2 + (y/\mu - 3/4)^2 - 1 \right] \le 0 \\ -2\mu \le x \le 2\mu \\ 0 \le y \le \mu \\ 0 \le \mu \le 1 \end{array} \right\}$$



Example, cont.

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

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

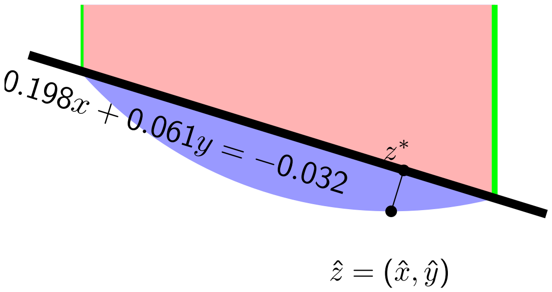
$$\begin{array}{rcl} \text{s.t. } v_0 + v_1 & = & z \\ \lambda_0 + \lambda_1 & = & 1 \\ (v_0, \lambda_0) & \in & \tilde{C}_j^0 \\ (v_0, \lambda_1) & \in & \tilde{C}_j^1 \\ \lambda_0, \lambda_1 & \ge & 1 \end{array}$$

Solution to example:

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

- 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 Mehrohtra (2002) also show how to generate convex quadratic inequalities, but computational results are not that promising

Disjunctive Programming [Grossmann]

Consider disjunctive NLP

$$\begin{cases} \underset{x,Y}{\text{minimize}} & \sum f_i \; + \; f(x) \\ \text{subject to} & \begin{bmatrix} Y_i \\ c_i(x) \leq 0 \\ f_i = \gamma_i \end{bmatrix} \bigvee \begin{bmatrix} \neg Y_i \\ B_i x = 0 \\ f_i = 0 \end{bmatrix} \forall i \in I \\ & 0 \leq x \leq U, \; \Omega(Y) = \text{true}, \; Y \in \{\text{true}, \text{false}\}^p \end{cases}$$

convex hull representation ...

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

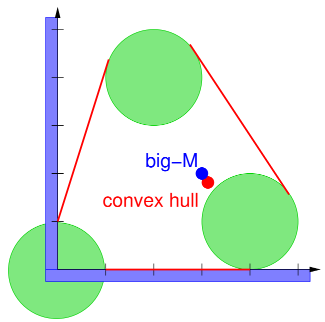
Disjunctive Programming: Example

$$\begin{bmatrix} Y_1 \\ x_1^2 + x_2^2 \leq 1 \end{bmatrix}$$

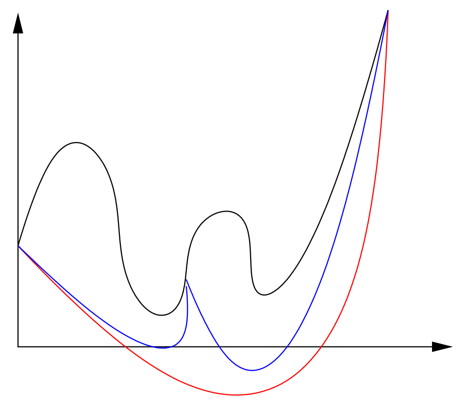
$$\vee \begin{bmatrix} Y_2 \\ (x_1 - 4)^2 + (x_2 - 1)^2 \leq 1 \end{bmatrix}$$

$$\vee \begin{bmatrix} Y_3 \\ (x_1 - 2)^2 + (x_2 - 4)^2 \leq 1 \end{bmatrix}$$

$\Rightarrow$

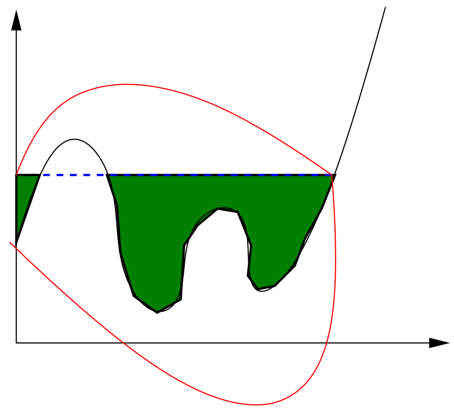


Dealing with Nonconvexities



- 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

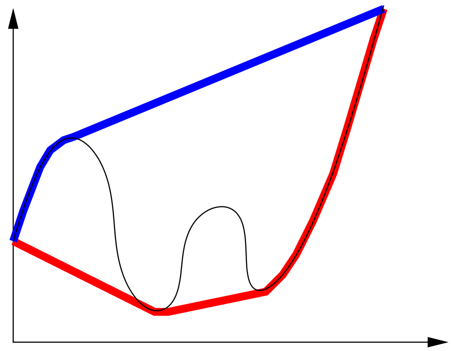


- If nonconvexity in constraints, may need to overestimate and underestimate the function to get a convex region

Envelopes

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

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



Bilinear Terms

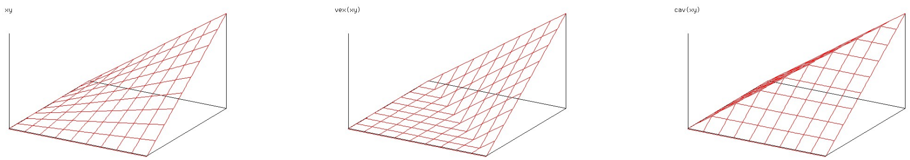
The convex and concave envelopes of the bilinear function xy over a rectangular region

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

are given by the expressions

$$\begin{aligned} \text{vexxy}_R(x,y) &= \max\{l_y x + l_x y - l_x l_y, u_y x + u_x y - u_x u_y\} \\ \text{cavxy}_R(x,y) &= \min\{u_y x + l_x y - l_x u_y, l_y x + u_x y - u_x l_y\} \end{aligned}$$

Worth 1000 Words?



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)

Disaggregation Tawarmalani et al. (2002)

Consider convex problem with bilinear objective

$$\begin{cases} \underset{w, x_1, \ldots, x_n}{\text{minimize}} & w \sum_{i=1}^{n} c_i x_i \\ \text{subject to} & (w, x) \in P \quad \text{Polyhedron} \\ & 0 \leq w \leq v \quad 0 \leq x \leq u \end{cases}$$

Formulation #1

$$\begin{aligned} \min\ & z \\ \text{s.t. } (w, x) & \in P \\ 0 & \leq z \\ (\sum_{i=1}^{n} c_i u_i) w + v (\sum_{i=1}^{n} c_i x_i) & \\ - v (\sum_{i=1}^{n} c_i u_i) & \leq 0 \end{aligned}$$

Formulation #2

$$\begin{aligned} \min \sum_{i=1}^{n} z_i & \\ \text{s.t. } (w, x) & \in P \\ 0 & \leq z_i \quad \forall i \\ c_i u_i w + v c_i x_i & \\ - v c_i u_i & \leq 0 \quad \forall i \end{aligned}$$

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. Parallel BB and Grid Computing
3. Implementation & Software Issues

Special Ordered Sets of Type 1

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

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

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

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

$\ldots d$ 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 $\{\lambda_1, \ldots, \lambda_p\}$ is SOS1

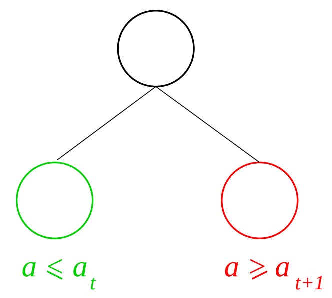
References: (Beale, 1979; Nemhauser, G.L. and Wolsey, L.A., 1988; Williams, 1993) ...

Special Ordered Sets of Type 1

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

Branching on SOS1

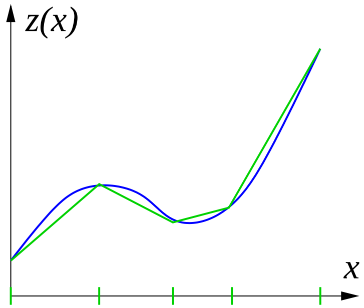
1. reference row $a_1 < \ldots < a_p$
   e.g. diameters
2. fractionality: $a := \sum a_i \lambda_i$
3. find $t: \; a_t < a \leq a_{t+1}$
4. branch: $\{\lambda_{t+1}, \ldots, \lambda_p\} = 0$
   or $\{\lambda_1, \ldots, \lambda_t\} = 0$



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

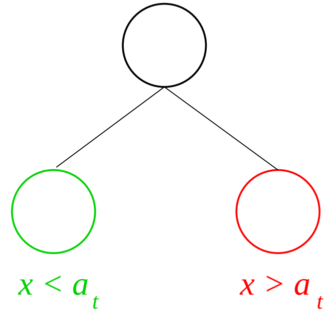
... convex combination of two breakpoints ...

Special Ordered Sets of Type 2

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

Branching on SOS2

1. reference row $a_1 < \ldots < a_p$
   e.g. $a_i = x_i$
2. fractionality: $a := \sum a_i \lambda_i$
3. find t : $a_t < a \leq a_{t+1}$
4. branch: $\{\lambda_{t+1}, \ldots, \lambda_p\} = 0$
   or $\{\lambda_1, \ldots, \lambda_{t-1}\}$



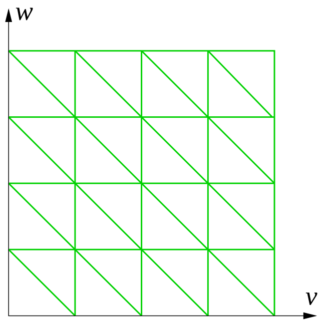
Special Ordered Sets of Type 3

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

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

1. $v_L = v_1 < \ldots < v_k = v_U$
2. $w_L = w_1 < \ldots < w_l = w_U$
3. function $u_{ij} := g(v_i, w_j)$
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

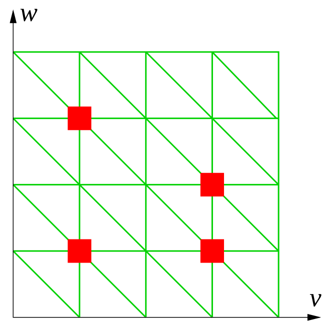
SOS3: $\sum \lambda_{ij} = 1$ & set condition holds

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

$\{\lambda_{11}, \ldots, \lambda_{kl}\}$ satisfies set condition

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

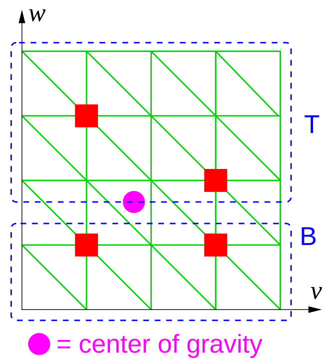
i.e. nonzeros in single triangle Δ



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 $v_s \le \hat{v} < v_{s+1}$ & $w_s \le \hat{w} < w_{s+1}$
- branch on v or w

vertical branching: $\sum_L \lambda_{ij} = 0$ $\sum_R \lambda_{ij} = 0$ **horizontal branching**: $\sum_T \lambda_{ij} = 0$ $\sum_B \lambda_{ij} = 0$

Special Ordered Sets | Special Ordered Sets of Type 1
Parallel BB and Grid Computing | Special Ordered Sets of Type 2
Implementation & Software Issues | Special Ordered Sets of Type 3

Branching on SOS3

Example: gas network from first lecture ...

- pressure loss p across pipe is related to flow rate f as

$$p_{in}^2 - p_{out}^2 = \Psi^{-1}\text{sign}(f)f \;\Leftrightarrow\; p_{in} = \sqrt{p_{out}^2 + \Psi^{-1}\text{sign}(f)f}$$

  where Ψ: "Friction Factor"
- nonconvex equation $u = g(v, w)$
  ... assume pressures needed elsewhere
- (Martin et al., 2005) use SOS3 model
  ... study polyhedral properties
  ... solve medium sized problem

Parallel Branch-and-Bound

meta-computing platforms:

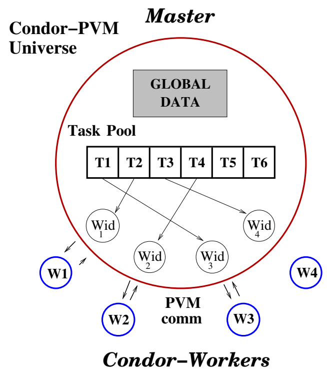
- set of distributed heterogeneous computers, e.g.
  - pool of workstations
  - group of supercomputers or anything
- low quality with respect to bandwidth, latency, availability
- low cost: *i*t's free!!! ... huge amount of resources

... use *Condor* to "build" MetaComputer
... high-throughput computing

Special Ordered Sets
Parallel BB and Grid Computing
Implementation & Software Issues

Parallel Branch-and-Bound

Master Worker Paradigm (`MWdriver`)
Object oriented C++ library on top of Condor-PVM

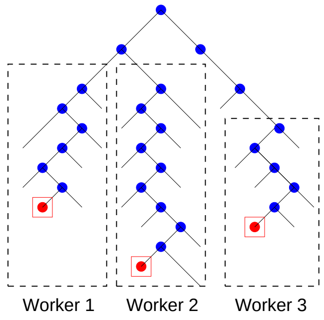


Fault tolerance via master *check-pointing*

Parallel Branch-and-Bound

First Strategy: 1 worker $\equiv$ 1 NLP
$\Rightarrow$ grain-size *too small*
... NLPs solve in seconds

New Strategy:
1 worker $\equiv$ 1 subtree (MINLP)
... "streamers" running down tree



Parallel Branch-and-Bound

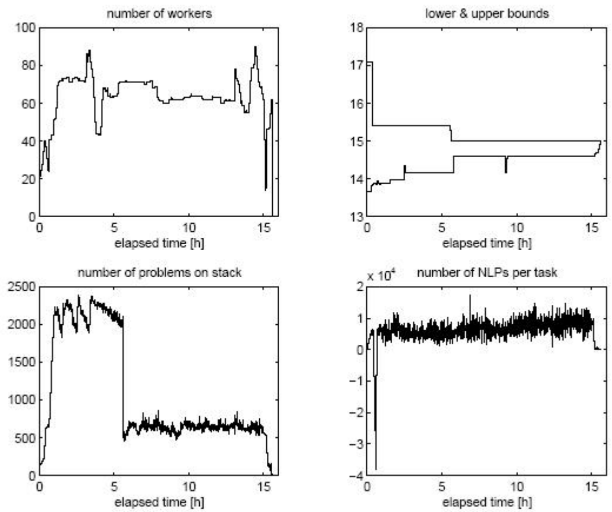
Trimloss optimization with 56 general integers
$\Rightarrow$ solve 96,408 MINLPs on 62.7 workers
$\Rightarrow$ 600,518,018 NLPs

Wall clock time = 15.5 hours
Cumulative worker CPU time = 752.7 hours $\simeq$ 31 days

$$\text{efficiency} := \frac{\text{work-time}}{\text{work} \times \text{job-time}} = \frac{752.7}{62.7 \times 15.5} = 80.5$$

... proportion of time workers were busy

Parallel Branch-and-Bound: Results



Detecting Infeasibility

NLP node inconsistent (BB, OA, GBD)
$\Rightarrow$ NLP solver must prove infeasibility
$\Rightarrow$ solve feasibility problem: restoration

$$(F) \left\{ \begin{array}{ll} \underset{x,y}{\text{minimize}} & \|c^+(x,y)\| \\ \text{subject to} & x \in X, \; y \in \hat{Y} \end{array} \right.$$

where $c^+(x,y) = \max\left(c(x,y), 0\right)$ and $\| \quad \|$ any norm

If $\exists$ solution $(\hat{x}, \hat{y})$ such that $\|c^+(\hat{x},\hat{y})\| > 0$
$\Rightarrow$ no feasible point (if convex) in neighborhood (if nonconvex)

Feasibility Cuts for OA et al.

$\hat{Y} = \{\hat{y}\}$ singleton & $c(c, y)$ convex

$(\hat{x}, \hat{y})$ solves $F(\hat{y})$ with $\|c^+(\hat{x}, \hat{y})\| > 0$
$\Rightarrow$ valid cut to eliminate $\hat{y}$ given by

$$0 \geq c^+(\hat{x}, \hat{y}) + \hat{\gamma}^T \begin{pmatrix} x - \hat{x} \\ y - \hat{y} \end{pmatrix}$$

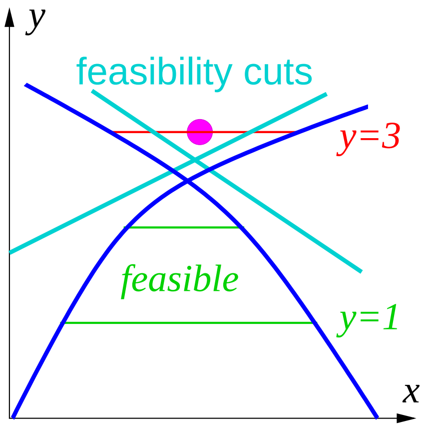
where $\hat{\gamma} \in \partial \|c^+(\hat{x}, \hat{y})\|$ subdifferential

Polyhedral norms: $\hat{\gamma} = \nabla \hat{c} \lambda$ where

1. ℓ_∞ norm: $\sum \lambda_i = 1$, and $0 \leq \lambda_i \perp \hat{c}_i \leq \|\hat{c}^+\|$
2. ℓ_1 norm: $0 \leq \lambda_i \leq 1 \perp \hat{c}_i$

... λ multipliers of equivalent smooth NLP ... easy exercise

Geometry of Feasibility Cuts



$y = 3$ infeasible
solution to feasibility problem
feasibility cuts for OA

Infeasibility in Branch-and-Bound

FilterSQP restoration phase

- satisfiable constraints: $J := \{j : c_j(\hat{x}, \hat{y}) \leq 0$
- violated constraints $J^\perp$ (complement of J)

$$\left\{ \begin{array}{lll} \underset{x,y}{\text{minimize}} & \sum_{j \in J^\perp} c_j(x, y) & \\ \text{subject to} & c_j(x, y) \leq 0 & \forall j \in J \\ & x \in X, \; y \in \hat{Y} & \end{array} \right.$$

- filter SQP algorithm on $\|c_J^+\|$ and $\|c_{J^\perp}^+\|$
  $\Rightarrow$ 2nd order convergence
- adaptively change J
- similar to ℓ_1-norm, but $\lambda_i \not\leq 1$

Choice of NLP Solver

MILP/MIQP branch-and-bound

- $(\hat{x}, \hat{y})$ solution to parent node
- new bound: $y_i \geq \lfloor \hat{y}_i \rfloor$ added to parent LP/QP

$\Rightarrow$ dual active set method; $(\hat{x}, \hat{y})$ dual feasible
$\Rightarrow$ fast re-optimization (MIQP 2-3 pivots!)

MILP exploit factorization of constraint basis
$\Rightarrow$ no re-factorization, just updates
... also works for MIQP (KKT matrix factorization)

$\Rightarrow$ interior-point methods not competitive
... how to check $\lambda_i > 0$ for SOS branching ???

Choice of NLP Solver

MINLP branch-and-bound

- $(\hat{x}, \hat{y})$ solution to parent node
- new bound: $y_i \geq \lceil \hat{y}_i \rceil$ added to parent NLP

Snag: $\nabla c(x, y)$, $\nabla^2 \mathcal{L}$ etc. change ...

- factorized KKT system at (x^k, y^k) to find step (d_x, d_y)
- NLP solution:
  $(\hat{x}, \hat{y}) = (x^{k+1}, y^{k+1}) = (x^k + \alpha d_x, y^k + \alpha d_y)$
  but KKT system at (x^{k+1}, y^{k+1}) never factorized

...SQP methods take 2-3 iterations (good active set)

Outer Approximation et al.

no good warm start (y changes too much)
$\Rightarrow$ interior-point methods or SQP can be used

Software for MINLP

- **Outer Approximation**: DICOPT++
- **Branch-and-Bound Solvers**: SBB & MINLP
- **Global MINLP**: BARON & MINOPT
- **Online Tools**: MINLP World, MacMINLP & NEOS

Outer Approximation: DICOPT++

Outer approximation with equality relaxation & penalty
Reference: (Kocis and Grossmann, 1989)
Features:

- GAMS interface
- NLP solvers: CONOPT, MINOS, SNOPT
- MILP solvers: CPLEX, OSL2
- solve root NLP, or NLP(y^0) initially
- relax linearizations of nonlinear equalities:
  λ_i multiplier of $c_i(z) = 0$ ...

$$c_i(\hat{z}) + \nabla c_i(\hat{z})^T (z - \hat{z}) \begin{cases} \geq 0 & \text{if } \lambda_i > 0 \\ \leq 0 & \text{if } \lambda_i < 0 \end{cases}$$

- heuristic stopping rule: STOP if NLP(y^j) gets worse

AIMMS has version of outer approximation

SBB: (Bussieck and Drud, 2000)

Features:

- GAMS branch-and-bound solver
- variable types: integer, binary, SOS1, SOS2, semi-integer
- variable selection: integrality, pseudo-costs
- node selection: depth-first, best bound, best estimate
- multiple NLP solvers: CONOPT, MINOS, SNOPT
  $\Rightarrow$ multiple solves if NLP fails

Comparison to DICOPT (OA):

- DICOPT better, if combinatorial part dominates
- SBB better, if difficult nonlinearities

MINLPBB: (Leyffer, 1998)

Features:

- AMPL branch-and-bound solver
- variable types: integer, binary, SOS1
- variable selection: integrality, priorities
- node selection: depth-first & best bound after infeasible node
- NLP solver: filterSQP ⇒ feasibility restoration
- CUTEr interface available

Global MINLP Solvers

α-BB & MINOPT: (Schweiger and Floudas, 1998)

- problem classes: MINLP, DAE, optimal control, etc
- multiple solvers: OA, GBD, MINOS, CPLEX
- own modeling language

BARON: (Sahinidis, 2000)

- global optimization from underestimators & branching
- range reduction important
- classes of underestimators & factorable NLP
  exception: cannot handle sin(x), cos(x)
- CPLEX, MINOS, SNOPT, OSL
- mixed integer semi-definite optimization: SDPA

Online Tools

Model Libraries

- MINLP World `www.gamsworld.org/minlp/`
  scalar GAMS models ... difficult to read
- GAMS library `www.gams.com/modlib/modlib.htm`
- MacMINLP `www.mcs.anl.gov/~leyffer/macminlp/`
  AMPL models

NEOS Server

- MINLP solvers: SBB (GAMS), MINLPBB (AMPL)
- MIQP solvers: FORTMP, XPRESS

COIN-OR

`http://www.coin-or.org`

- COmputational INfrastructure for Operations Research
- A library of (interoperable) software tools for optimization
- A development platform for open source projects in the OR community
- Possibly Relevant Modules:
  - OSI: Open Solver Interface
  - CGL: Cut Generation Library
  - CLP: Coin Linear Programming Toolkit
  - CBC: Coin Branch and Cut
  - IPOPT: Interior Point OPTimizer for NLP
  - NLPAPI: NonLinear Programming API

Conclusions

MINLP rich modeling paradigm
◦ most popular solver on NEOS

Algorithms for MINLP:
◦ Branch-and-bound (branch-and-cut)
◦ Outer approximation et al.

"MINLP solvers lag 15 years behind MIP solvers"

⇒ many research opportunities!!!

Part V

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