Mixed-Integer Nonlinear Optimization

Anecdotes on complexity, modeling, solvers and HPC

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Yorktown Heights, New York

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subject to:

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where, if you are lucky, the functions $f : \mathbb{R}^{n_{\mathbb{R}}} \times \mathbb{R}^{n_{\mathbb{Z}}} \mapsto \mathbb{R}$ and the $g_i : \mathbb{R}^{n_{\mathbb{R}}} \times \mathbb{R}^{n_{\mathbb{Z}}} \mapsto \mathbb{R}$ $(i = 1, \ldots, m)$ are convex and twice continuously differentiable

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- COIN-OR projects: Bonmin (P. Bonami), Couenne (P. Belotti), LaGO (S. Vigerske)
- New Cyber-Infrastructure website: `www.minlp.org`

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- regularity conditions (constraint qualifications)
- convex (nice case?)
- bilinear (nice case?)
- polynomial
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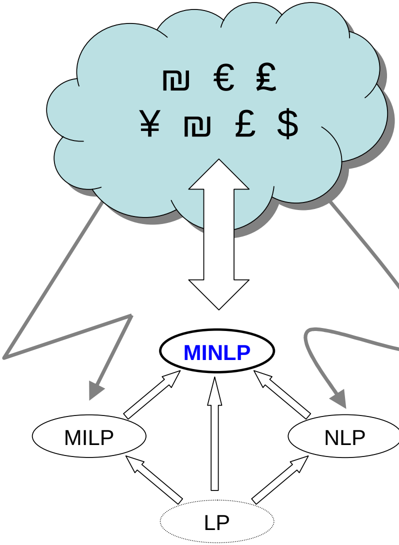
Formulation matters!

Balance tension between
Math/Algorithmic niceties $\Longleftrightarrow$ Modeling accuracy

Philosophy: Zen in the art of MINLP



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- De Loera, Hemmecke, Köppe, Weismantel: FPTAS for mixed-integer polynomial optimization with a fixed number of variables, *SODA 2006*.

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  - An NLP-based Branch-and-Bound
  - An Outer Approximation Decomposition Method
  - Quesada and Grossmann's branch-and-cut algorithm
  - a hybrid outer-approximation based branch-and-cut algorithm

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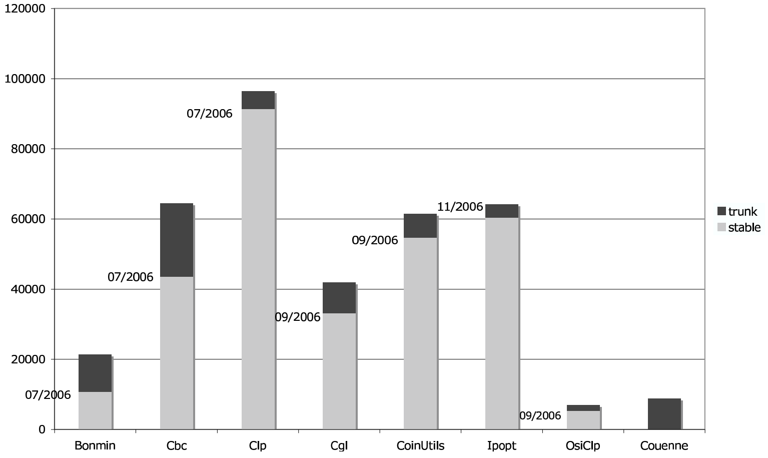
- The Branch-and-Bound algorithm has features aimed at dealing with non-convexity

Bonmin development



Water Network Optimization

Re-piping an aging water-distribution network. Pipe diameters are chosen from a discrete set supplied by a manufacturer. There are pressure constraints at pipe junctions. Pressure loss in a pipe due to friction is a nonlinear function of pipe diameter.

Model

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$$H(i) - H(j) = \underline{\underline{\mathrm{sgn}(Q(e))|Q(e)|^{1.852}}} \cdot \frac{10.7 \cdot len(e)}{k(e)^{1.852}} \underline{\underline{/D(e)^{4.87}}}$$

$$(\forall\ e = (i,j) \in E)$$

Techniques

- Branch-and-bound, but to not completely discriminate against a non-convex relaxation:
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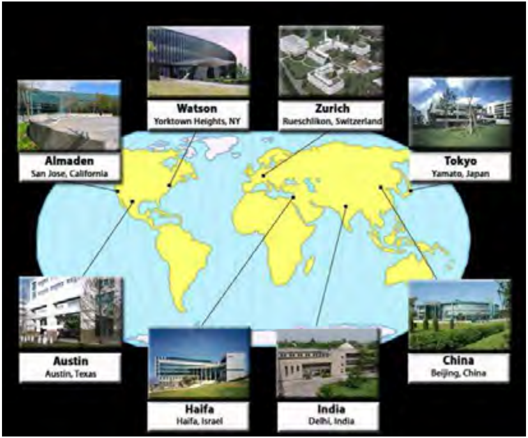
- Software challenges:
  - Hide complexity from the user — AMPL
  - Clear opportunities for parallelism (at different levels)

References

- Christiana Bragalli, Claudia D'Ambrosio, Jon Lee, Andrea Lodi, Paolo Toth. An MINLP model and solution method for a water-network optimization problem. Algorithms - ESA 2006 (14th Annual European Symposium. Zurich, Switzerland, September 2006, Proceedings), Y. Azar and T. Erlebach, Eds., pages 696-707. Springer, 2006.
- Cristiana Bragalli, Claudia D'Ambrosio, Jon Lee, Andrea Lodi, Paolo Toth. Water Network Design by MINLP, IBM Research Report RC24495, 02/2008.

Facility Location

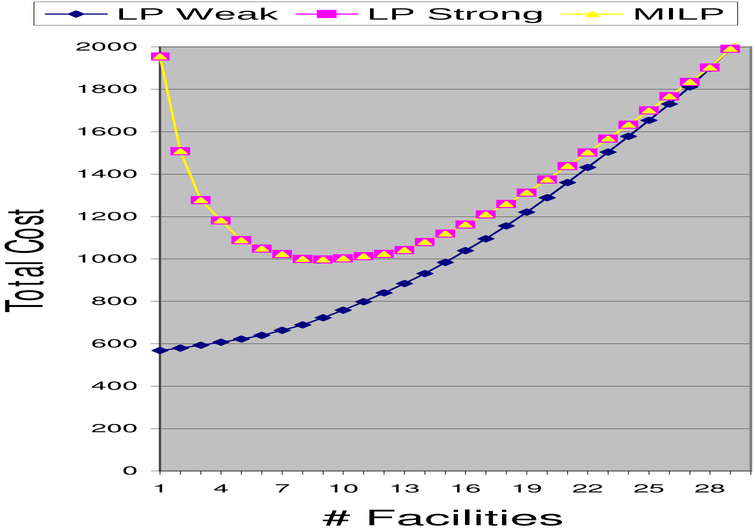
Locate facilities to serve customers. Model risk with costs that are nonlinear in shipment quantities.



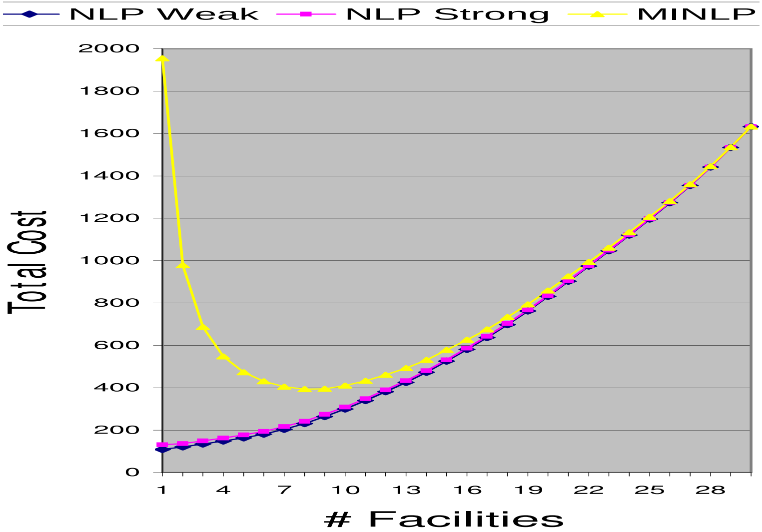
Basic models

$$
\begin{aligned}
& \min \ \sum_{i=1}^{n} c_i y_i + \sum_{i=1}^{m} \sum_{j=1}^{n} \underline{\underline{f(x_{ij})}} \\
& \text{subject to:} \\
& \qquad \sum_{i=1}^{m} x_{ij} = 1 \quad (j = 1, \ldots, n); \\
\textit{Strong}: & \qquad x_{ij} \le y_i \quad (i = 1, \ldots, m;\ j = 1, \ldots, n); \\
\textit{Weak}: & \qquad \sum_{j=1}^{n} x_{ij} \le n \cdot y_i \quad (i = 1, \ldots, m); \\
& \qquad x \in \mathbb{R}_{+}^{n},\ y \in \{0,1\}^m .
\end{aligned}
$$

Facility location: Linear objective vs. fixed number of facilities



Facility location: Separable quadratic objective: $f(x_{ij}) := q_{ij}x_{ij}^2$ vs. fixed number of facilities



Facility location: B&B

MILP	nodes	time
weak formulation	10,616	332.24
strong formulation	0	0.17
strong algorithmic	2	1.69

MINLP	nodes	time
weak formulation	45,901	16,697.46
strong formulation	29,277	21,206.56

HPC?

E.g., the Blue Gene/P supercomputer at the Jülich Research Centre in Germany is a petaflop machine of 294,912 ($= 72 \times 1024 \times 4$) processor cores (#3 on "List" as of June '09)

- BG/P architecture
  - Trade processor speed for lower power consumption
  - Four processors per node (1,2 or 4 active)
  - Large number of nodes (scalable in increments of 1024)
  - Three-dimensional torus interconnect with auxiliary network for global communication
- Super-computing trends
  - multi/many-core
  - green
  - same or less memory per core
  - non-homogeneous (e.g., IBM Roadrunner #1 on list)

Parallel Bonmin (Ladanyi, Lee, Wächter)

BlueGene

- Background
  - Bcp (a parallel COIN-OR MILP code)
  - (Cbc-)Bonmin (our serial MINLP code)
  - Nature of Branching methods
  - MINLP model size (small)
  - NLP re-solves (slow)
  - Architecture of BlueGene (little memory per node)
- Bcp-Bonmin
  - (Cbc-)Bonmin's B&B ported to Bcp framework
  - Running on BlueGene with access from AMPL

UFLX40.120

# Proc	Ramp up (sec)	Ramp down (sec)	Total (sec)[1]
32	0	43.55	6,597.72
64	0	16.82	3,402.07
128	31.25	40.12	1,741.07
256	36.24	64.85	959.89
512	43.26	73.36	570.86
1024	51.97	51.18	389.11
2048	64.18	100.47	316.32

[1] Times are elapsed wall time

UFLX50.150

# Proc	Ramp up (sec)	Ramp down (sec)	Total (sec)
64	0	113.56	24,810.06
128	48.43	112.43	11,768.07
256	56.48	145.31	6,203.34
512	68.03	122.77	3,169.80
1024	81.18	143.96	1,843.41
2048	100.34	159.91	1,080.57

UFLX60.180

# Proc	Ramp up (sec)	Ramp down (sec)	Total (sec)
256	89.77	298.22	24,329.60
512	108.93	315.78	12,585.37
1024	128.24	369.09	6,810.20
2048	156.08	398.89	3,882.95

UFLX70.210

# Proc	Ramp up (sec)	Ramp down (sec)	Total (sec)
2048			30,596.98 [2]

[2] 2-yr serial equivalent!

Can we strengthen the model?

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For $\emptyset \neq S \subseteq N := \{1, \ldots, n\}$ and $k \in \mathbb{Z}$ with $1 \leq k \leq m$, let

$$H_S^k := 1/\sum_{i=1}^{k} p_{iS} \ ,$$

where, for $i \in M := \{1, \ldots, m\}$, we let

$$p_{iS} := \sum_{j \in S} 1/q_{ij} \ .$$

and we assume that the p_{iS} are sorted (for a given S) so that

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H_S^k is exactly what it would cost to most cheaply serve the set of customers S, using k facilities, ignoring the fixed facility costs and the other customers.

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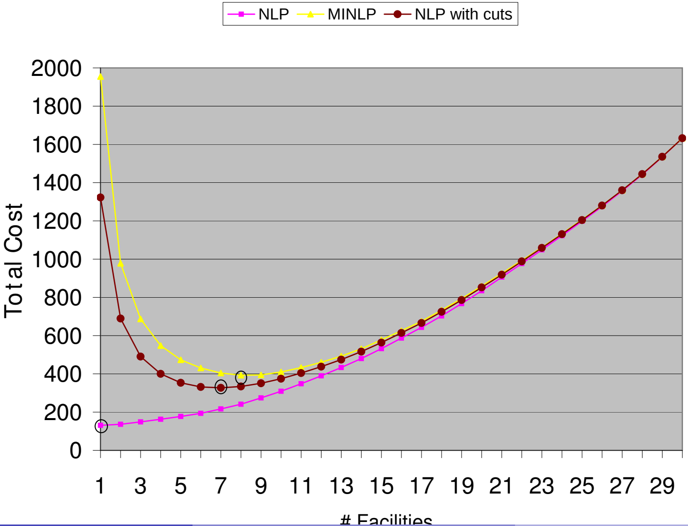
Convex! nonlinear cuts:

$$1/\sum_{j \in S} 1/\phi_j \ \geq \ H_S^k \left(k + 1 - \sum_{l \in M} y_l \right) + H_S^{k+1} \left(-k + \sum_{l \in M} y_l \right)$$

$$\left(\sum_{i \in M} q_{ij} x_{ij}^2 \leq \phi_j \right)$$

Quadratic objective with cuts vs. fixed number of facilities



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- Oktay Günlük and Jeff Linderoth. Perspective Relaxation of Mixed Integer Nonlinear Programs with Indicator Variables, to appear in Math. Programming. [a shorter version appeared in IPCO 2008].

Shameless advertising

- John Gunnels, Jon Lee, Susan Margulies. Efficient high-precision dense matrix algebra on parallel architectures for nonlinear discrete optimization, IBM Research Report RC24682, 10/2008. (talked about this work at MOPTA 2009)
- Forthcoming book "Nonlinear Discrete Optimization" (Lee, Onn, Weismantel). Preview is in the papers at my website.
- CMU/IBM Cyber-Infrastructure website: `www.minlp.org`