Cyber-MINLP: A virtual environment for problem formulations and algorithmic developments

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General Goals of MINLP.org:

-Create a cyberinfrastructure environment for *virtual collaboration* for developing and collecting tools, and challenging MINLP test problems

- Develop basic algorithms, formulations for predicting tight lower bounds, and open-source software for solving *large-scale nonconvex MINLP problems*

(e.g. Couenne software for global optimization)

- Test software with challenge problems arising in real-world applications, mostly in engineering but also in biology and finance

Major component: Library of MINLP problems

Why if other MINLP Libraries?

GAMS World MINLP
http://www.gamsworld.org/minlp/index.htm

MacMINLP
http://www.mcs.anl.gov/~leyffer/macminlp/index.html

MINOPT Model Library
http://titan.princeton.edu/MINOPT/library.html

Major emphasis: problem formulation and collaborative environment

- provide high level description of problems
- one or several model formulations with their corresponding input file
- support multiple authors
- provide discussion forum

Motivation:

- Often several formulations for MINLP problem
- Current test problems are only input files
- Practitioners learn by example
- Promote reproducibility and discussion

Functionality website:

-Author submits problem with model (s), instance(s), results

-Other authors or same author can submit alternative models or instances for that problem

-Discussion with wiki forum

A possible scenario:

Version 1: Author X submits problem statement, models A & B, instances, results
(may submit only problem statement)

Author Y finds a better model C
Version 2: Author Y submits new model C, instances, results

Discussion between author X and Y

Author X finds can solve larger problems with his model
Version 3: Author X submits new instances, results for models A,B,C

Library of Optimization Problems

IBM Carnegie Mellon MINLP CYBER-INFRASTRUCTURE

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	Problem Title	Primary Author	Date Submitted	Date Last Modified	Application	Sessions	Model Types
1	A Deterministic Security Constrained Unit Commitment Model	Zondervan, Edwin	07/24/2009	10/06/2009 (Model Added)	Engineering	2	MINLP, MIQI
2	Close-Enough Vehicle Routing Problem	Mennell, William	01/09/2010	01/09/2010 (Problem Added)	Routing	1	MINLP
3	Design of Telecommunication Networks with Shared Protection	Belotti, Pietro	08/31/2009	08/31/2009 (Problem Added)	Engineering	1	MINLP, MILP
4	Extended Pooling Problem with the Summer Time (EPA) Complex Emissions Constraints	Misener, Ruth	03/04/2010	03/04/2010 (Problem Added)	Engineering	1	MINLP
5	Global multi-objective optimization of a nonconvex MINLP problem and its application on polygeneration energy systems design	Liu, Pei	07/30/2009	07/30/2009 (Problem Added)	Engineering	1	MINLP
6	MINLP & MPCC Strategies for Optimization of a Class of Hybrid Dynamic Systems	Baumrucker, Brian	05/21/2009	05/21/2009 (Problem Added)	Engineering	1	MINLP, NLP, MIQP
7	Mixed-Integer Nonlinear Programming Models and Algorithms for Supply Chain Design with Stochastic Inventory Management	You, Fengqi	06/10/2009	06/10/2009 (Problem Added)	Operations	1	MINLP
8	Mixed-Integer Nonlinear Programming Models for Optimal Simultaneous Synthesis of Heat Exchangers Network	Escobar, Marcelo	04/30/2010	04/30/2010 (Problem Added)	Engineering	1	MINLP
9	Mixed-Integer Nonlinear Programming Models for the Optimal Design of Multi-product Batch Plant	You, Fengqi	08/18/2009	08/18/2009 (Problem Added)	Engineering	1	MINLP
10	MPEC strategies for optimization of pipeline operations	Gopalakrishnan, Ajit	03/12/2010	03/12/2010 (Problem Added)	Engineering	1	NLP

Library of Optimization Problems

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	Problem Title	Primary Author	Date Submitted	Date Last Modified	Application	Sessions	Model Types
11	Optimal Scheduling of Refined Products Pipelines and Terminal Operations	Cafaro, Diego	04/06/2010	04/06/2010 (Problem Added)	Operations	1	MILP
12	Optimal Separation Sequences Based on Distillation: From Conventional to Fully Thermally Coupled Systems	Caballero, Jose	11/23/2009	11/23/2009 (Problem Added)	Engineering	1	MINLP
13	Optimization model for density modification based on single-crystal X-ray diffraction data	Sahinidis, Nick	06/13/2009	06/13/2009 (Problem Added)	Physics	1	MINLP, MILP
14	Optimization of metabolic networks in biotechnology	GUILLEN, GONZALO	02/19/2010	02/19/2010 (Problem Added)	Biology	1	MINLP
15	Periodic Scheduling of Continuous Multiproduct Plants	Castro, Pedro	06/25/2009	06/25/2009 (Problem Added)	Engineering	1	MINLP
16	Simultaneous Cyclic Scheduling and Control of a Multiproduct CSTR	Flores-Tlacuahuac, Antonio	12/24/2009	12/24/2009 (Problem Added)	Engineering	1	MINLP
17	Solving Mixed-Integer Linear Fractional Programming Problems with Dinkelbach's Algorithm and MINLP Methods	You, Fengqi	08/11/2009	08/11/2009 (Problem Added)	Algorithm	1	MINLP
18	Stabilizing controller design and the Belgian chocolate problem	Chang, YoungJung	09/26/2009	09/26/2009 (Problem Added)	Engineering	1	MINLP
19	Stochastic Portfolio Optimization with Round Lot Trading Constraints	Lejeune, Miguel	10/02/2009	10/02/2009 (Problem Added)	Finance	1	MINLP
20	The Close-Enough Traveling Salesman Problem	Mennell, William	11/15/2009	11/15/2009 (Problem Added)	Routing	1	MINLP

Library of Optimization Problems

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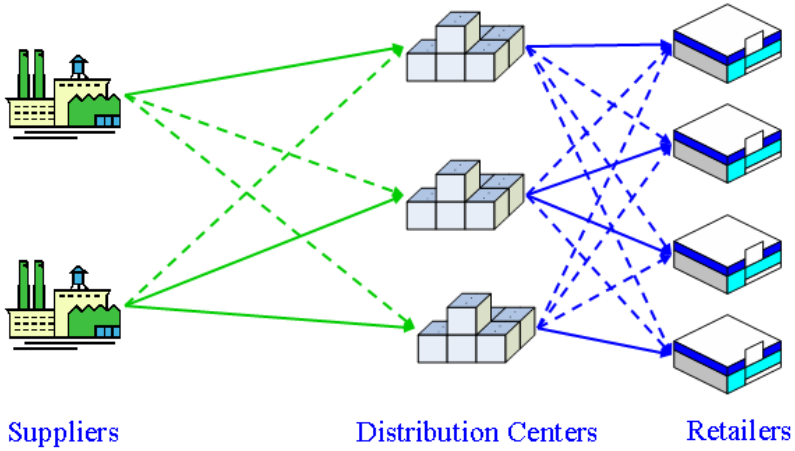
	Problem Title	Primary Author	Date Submitted	Date Last Modified	Application	Sessions	Model Types
21	The Delay Constrained Routing Problem (DCRP)	hijazi, hassan	11/10/2009	11/10/2009 (Problem Added)	Telecommunications	1	MINLP
22	Water Treatment Network Design	Ruiz, Juan	05/15/2009	05/15/2009 (Problem Added)	Engineering	1	MINLP

Supply Chain Design with Stochastic Inventory Management

Fengqi You, Ignacio Grossmann



Determine:

-how many distribution centers to locate & where to locate them

-which retailers to assign to each distribution center (DC)

-how often to reorder for replenishment at each DC

-what level of safety stock to maintain

Goal: minimize the total location, transportation, and inventory costs while ensuring a specified service level α.

Model 1:

Straightforward Model

Involves nonlinear 0-1 variables

X_j and Y_{ij} declared as 0-1 variables

$$\text{Min: } \sum_{j\in J} f_j X_j + \beta \sum_{j\in J}\sum_{i\in I} \chi d_{ij}\mu_i Y_{ij} + \sum_{j\in J} X_j \left[F_j n_j + \beta(g_j + a_j \frac{D_j}{n_j})n_j + \theta \frac{hD_j}{2n_j} \right] + \theta h z_\alpha \sum_{j\in J} \sqrt{\sum_{i\in I} L\sigma_i^2 Y_{ij}}$$

Linear in X and Y — **Bilinear in X and n; linear fractional in D and n** — **Nonlinear in Y**

$$\text{s.t.} \quad \sum_{j\in J} Y_{ij} = 1, \qquad \forall i \in I$$

$$Y_{ij} \le X_j, \qquad \forall i \in I,\ \forall j \in J$$

$$D_j = \sum_{i\in I} \chi \mu_i Y_{ij}, \qquad \forall j \in J$$

$$X_j \in \{0,1\}, \qquad \forall j \in J$$

$$Y_{ij} \in \{0,1\}, \qquad \forall i \in I,\ \forall j \in J$$

$$D_j \ge 0,\ n_j \ge 1, \qquad \forall j \in J$$

Model 2:

"Sophisticated" Model

Linear 0-1 variables

Only X_j declared as 0-1 variables; Y_{ij} as continuous

Min: $\sum_{j\in J}(f_j X_j + \sum_{i\in I}\hat{d}_{ij}Y_{ij} + K_j Z1_j + qZ2_j)$ **Linear**

s.t. $\sum_{j\in J} Y_{ij} = 1, \quad \forall i \in I.$

$Y_{ij} \le X_j, \quad \forall i \in I,\ \forall j \in J.$

Concave in Z

$-Z1_j^2 + \sum_{i\in I}\mu_i Y_{ij} \le 0, \quad \forall j \in J$

$-Z2_j^2 + \sum_{i\in I}\hat{\sigma}_i^2 Y_{ij} \le 0, \quad \forall j \in J$

$X_j \in \{0,1\}, \quad \forall j \in J$

$0 \le Y_{ij} \le 1, \quad \forall i \in I,\ \forall j \in J.$

$Z1_j \le \sqrt{\sum_{i\in I}\mu_i}, \quad \forall j \in J$

$Z2_j \le \sqrt{\sum_{i\in I}\hat{\sigma}_{iij}^2}, \quad \forall j \in J$

$Z1_j \ge 0,\ Z2_j \ge 0, \quad \forall j \in J$

where

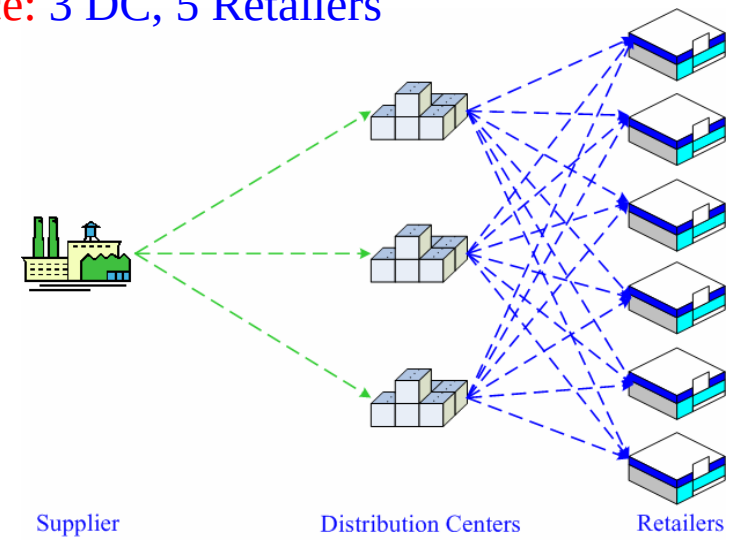
$\hat{d}_{ij} = \beta\chi\mu_i(d_{ij} + a_j)$

$K_j = \sqrt{2\theta h\chi(F_j + \beta g_j)}$

$q = \theta h z_\alpha$

$\hat{\sigma}_i^2 = L\sigma_i^2$

Small instance: 3 DC, 5 Retailers



Solution with BARON

Transportation cost (β)	Inventory cost (θ)	Model (**P1**)		Model (**P2**)	
		Obj. Fun	CPU (s)	Obj. Fun	CPU (s)
0.01	0.01	2260.26	7.940	2260.26	0.470
0.1	0.01	8122.93	28.610	8122.93	0.120
0.001	0.01	1099.25	2.720	1099.25	0.200
0.01	0.1	5359.18	9.300	5359.18	0.440
0.01	0.001	1341.04	7.450	1341.04	0.140

=> Model 2 solves much faster

Model 2 gets solved in root node!

Transportation cost weight factor (β)	Inventory cost weight factor (θ)	Model (P1) NLP Relaxation	Model (P1) # of Node	Model (P2) NLP Relaxation	Model (P2) # Nodes
0.01	0.01	2195.53	713	2260.26	1
0.1	0.01	8122.93	1162	8122.93	1
0.001	0.01	879.11	269	1099.25	1
0.01	0.1	5027.08	54	5359.18	1
0.01	0.001	1338.95	61	1341.04	1

Features in other problems

Optimal Periodic Scheduling of Continuous Multiproduct Plants

Pedro M. Castro, Augusto Q. Novais

Linear fractional objective: not solvable with any of standard codes (DICOPT, SBB, a-ECP, BARON)

MINLP and MPCC Strategies for Optimization of Hybrid Dynamic Systems

Brian Baumrucker, Larry Biegler

MPCC (continuous nonconvex NLP) much faster than MINLP model

Water Treatment Process Design Problem

Juan Pablo Ruiz, Ignacio Grossmann

Alternative models: (flow, composition), (individual flows, split fractions)
-Both cannot solved with proper lower, upper bounds on variables
-Flow, composition leads to fewer nodes

Optimization model for density modification based on single-crystal X-ray diffraction data

Alexander Smith, Nikolaos Sahinidis

Alternative models: MINLP and two MILPs (both huge in size)
None has been solved to optimality

Conclusions

1. **Proposed cyberinfrastructure: library of problems**
   - **Emphasis is on model formulation**
     Especially useful for practitioners who want to learn how to formulate problems
   - **Supports multiple authors**

2. **Site www.minlp.org is a source for:**
   - **Discussion forum about MINLP problems**
   - **Problems for research and teaching courses**

3. **Cybersite also has section on resources**

   Lectures, other libraries, solvers, modeling systems, bibliography, conferences