Global Optimization with GAMS

Alex Meeraus
Michael R. Bussieck
Steven P. Dirkse

GAMS Development Corp.
GAMS Software GmbH

ameeraus@gams.com
mbussieck@gams.com
sdirkse@gams.com

www.gams.com
www.gams.de

October 18th 2007
Relevance of GO
## Agenda

| 1 | Global Optimization Introduction |
| 2 | GAMS Global Solvers |
| 3 | Exotic Application of GO |
| 4 | Performance & Quality |
Global Optimization (GO)

- Practical optimization problems are often nonlinear and non-convex, with discrete variables

- They may contain disconnected feasible regions with multiple local optima

- The aim of Global Optimization is to find the best solution of all local optima
Examples for GO Applications

- Chemotherapy and radiotherapy design
- Chemical data and process analysis
- Differential equations
- Engineering design
- Environmental engineering
- Financial model development
- Laser design
- Packing and loading configuration design
- Staff scheduling
- Vehicle routing and scheduling
Algebraic Modeling System and GO

- AMS perfect platform to promote GO
  - Separation of problem formulation and solution technology
  - Model in mathematical algebra (not black box)
  - Experience with (local) nonlinear optimization

- GO Solvers benefit from GAMS:
  - Search algorithms have difficulties with equalities
    Defining equation elimination by GAMS
  - Dual solution unavailable, approximate solution
    Optional cleanup up call (CONOPT) from solution found
  - Currently, no MINLP capability (LGO, MSNLP)
    B&B code SBB uses GAMS NLP sub-solvers
Introduction of New Technology (GO)

• Cover large portion of existing algorithmic approaches
  – Deterministic
  – Stochastic
  – Heuristic/Meta-Heuristic

• Have fallback mechanisms
  – Variety of local solvers (program your own multi-start)
  – Multiple solvers implementing same algorithm

• Demonstrate the maturity of the technology
  – Reproducible Examples
  – Books focusing on GO Applications
  – Software Quality Assurance
GAMS Global Solvers

- **BARON**  
  Branch-and-Reduce Optimization Navigator for proven global solutions by The Optimization Firm, USA

- **LGO**  
  Lipschitz Global Optimizer by Pintér Consulting Services, Canada

- **OQNLP**  
  OptQuest/NLP Multi-start Solver by OptTek Systems/Optimal Methods, USA

- **LINDOGlobal**  
  MINLP solver for proven global solutions by LINDO Systems, USA
BARON and LINDOGlobal (MINLP)

• Algorithm
  – Branch-and-bound plus range reduction
  – Under-estimators for objective and constraints requires knowledge of algebra

• Deterministic global solution/bounds
  – Relative/absolute gap similar to MIP

• Differences BARON/LINDOGlobal
  – BARON:
    • Can returns the $k$ best solutions
    • Multiple LP/NLP solvers to solve subproblems
  – LINDOGlobal
    • Handles models with trig-functions (sin, cos, …)
    • Handles some non-smooth functions directly (abs, min, …)
OQNLP (MINLP) / MSNLP (NLP)

• Automates starting point selection
  – Starts local solvers from a set of starting points chosen by the Scatter Search software OptQuest and other point generators
  – Distance and merit filter limit the number of NLP calls
  – Works with any GAMS NLP solver

• Problem size similar to problem size limitation of local NLP solvers

• Scatter Search ensures stochastic convergence towards the global optimum
LGO (NLP)

• Integrates several global search algorithms
  – Partition and search (branch-and-bound)
  – Adaptive global random search, enhanced with a statistical bound estimation technique
  – Random local search/Multi-start

• Stochastic convergence to global optimum
  – Assumes only Lipschitz-continuity of objective
  – Black box models (external equations)
  – No requirement for other subsolvers
## Agenda

- Global Optimization Introduction
- GAMS Global Solvers
- Exotic Application of GO
- Performance & Quality
Linear Fixed-Charge Network Flow Problem

- Single-commodity, uncapacitated, fixed-charge network flow problem

\[
\begin{align*}
\min & \sum_{(i,j) \in A} (f_{ij}y_{ij} + c_{ij}x_{ij}), \text{ s.t. } \sum_{j \in \delta^{-}(i)} x_{ji} - \sum_{i \in \delta^{+}(j)} x_{ij} = b_i, 0 \leq x_{ij} \leq My_{ij}, y \in \{0,1\} \\
\end{align*}
\]

- Problem class includes Steiner Tree Problem


- 83 instances (including 24 not proven optimal)
Dicut Inequalities

- Dicut: \( \sum_{(i,j) \in \delta^-(S)} y_{ij} \geq 1 \quad \text{if} \quad S \subset V \quad \text{and} \quad b(S) > 0. \)

- Separation problem:
  \[ \xi = \min \left\{ \sum_{(i,j) \in A} \bar{y}_{ij}z_j(1 - z_i) : \sum_{i \in V} b_iz_i > 0, \quad z_i \in \{0, 1\} \quad \forall \quad i \in V \right\} \]

- Non-convex quadratic binary program:
  - Ortega/Wolsey: Greedy algorithm
  - Let’s solve this exactly (small #variables |V|)
Branch-and-Cut-and-Heuristic (BCH) Facility

- **Cut Generator and Heuristic**
  - Represented in terms of original GAMS problem formulation
  - Independent of the specific MIP solver
  - Use any other model type and solver available in GAMS

- **Design Principle:**

  ![Diagram showing the GAMS System with connections to GAMS Solver Link, BCH Facility, MIP Solver (e.g., CPLEX), and User Cut Generator & Heuristics.]
Local versus Global

- Berlin52 – from SteinLib
  - 52 nodes (1 source, n’=15 sinks), 1326 edges

<table>
<thead>
<tr>
<th></th>
<th>CPLEX 9 (no BCH)</th>
<th>BCH + SBB (local)</th>
<th>BCH + BARON (global)</th>
</tr>
</thead>
<tbody>
<tr>
<td># cuts</td>
<td>0</td>
<td>139</td>
<td>610</td>
</tr>
<tr>
<td># nodes</td>
<td>168449</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Time</td>
<td>1000</td>
<td>1000</td>
<td>223</td>
</tr>
<tr>
<td>Gap</td>
<td>45%</td>
<td>39%</td>
<td>0%</td>
</tr>
</tbody>
</table>
Unsolved Instances - Gap

[Graph showing instances vs. relative gap and log relative gap for different solvers: CPLEX, XPRESS, CPLEX+C, CPLEX+C+H]
Agenda

- Global Optimization Introduction
- GAMS Global Solvers
- Exotic Application of GO
- Performance & Quality
## LP vs. Global, Then vs. Now

<table>
<thead>
<tr>
<th>LP</th>
<th>Global</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simple certificate of optimality</td>
<td>Solutions, deterministic bounds, stochastic bounds, optimality gap</td>
</tr>
<tr>
<td>Established solvers, proven track record, 1-2 releases/year</td>
<td>Emerging technology, cutting/bleeding edge research, frequent software updates</td>
</tr>
<tr>
<td>Links all look quite similar</td>
<td>Libraries, shared source, “captive” links</td>
</tr>
<tr>
<td>Then: users were specialists, expert in modeling and solving</td>
<td>Now: users may be domain experts with little solver knowledge</td>
</tr>
</tbody>
</table>

• **Good motivation for increased performance testing (PT) and quality assurance (QA)**
Challenges in PT & QA

- QA is not glamorous – where’s the novelty & publications?
  - Make the tools used public - “open-source” them
  - Make it a group project with high priority

- QA & PT are time-consuming
  - Create standard libraries of test problems, categorized for convenient access
  - Automate the creation of test scripts, the collection of data, and the creation and display of statistics

- Results can be subjective, misleading, wrong, or useless
  - Test libraries, automation, and validation reduce subjective element and make results reproducible, hence believable
  - Automate the creation and display of useful statistics
GAMSWorld Libraries

- Collections of all kinds of models (~1e3 models)
- Large and varied set of both theoretical and practical models
- Helps algorithm developers to test their source
- Helps users do PT

www.gamsworld.org
PAVER

- **Performance Analysis and Visualization for Effortless Reproducibility**

- Online server to facilitate performance testing and analysis/visualization

- Results sent via e-mail in HTML format
  - System independent

www.gamsworld.org/performance/paver
Open Testing Architecture

I. Models

 Translate: GAMS/Convert

 Solve with "other" systems

 GAMS Models

 Solve with GAMS

 PAVER Server

 II. Data Collection

 III. Analysis & Visualization

 Web

 Web
PT/QA pitfalls

• Solvers may contain bugs – really!
  – Wrong solution returned
  – Wrong objective returned
  – False claims of feasibility/optimality

• Solvers will use different termination checks/tolerances
  – Difficult to compare “quality” of solutions
  – Common standard of comparison is lacking

• PAVER does not check validity of input data
GAMS/Examiner

- Purpose: to make an unbiased, independent report on the merit of points
- Points may come from GAMS or a solver
  - GAMS passes the previous solution as initial iterate
  - Solvers pass solutions back to GAMS
- Useful during solver debugging – helps pinpoint problems
  - Most checks are obvious
- Does checks on the scaled and unscaled (original) model
- All solution tolerances can be adjusted, default is tight
- Different points can be checked
- Examiner only reports, it doesn’t fix
GAMS/Bench

- Tool to help facilitate benchmarking of GAMS solvers
- Compares resource usage of solvers selected by the user
- Creates problem matrix once and spawns it to all solvers
- Can create trace files used by PAVER
- Can call GAMS/Examiner for every tested solver
- Comes free with every GAMS system (depends on licensed solvers)
PAVER: LINDOGlobal vs. BARON

- Tested complete MINLP Library (250 models)
- Time limit: 600 sec per model
- Optimality tolerance: 0

- BARON can solve 125 models to optimality, found a feasible solution for additional 40 model
- LINDOGlobal solved 131 models to optimality, found a feasible solution for 60 more models
- Both together: 141 optimal and 53 feasible models
Contacting GAMS

Europe

GAMS Software GmbH
Eupener Str. 135-137
50933 Cologne
Germany
Phone: +49 221 949 9170
Fax: +49 221 949 9171
http://www.gams.de
info@gams.de
support@gams-software.com

USA

GAMS Development Corp.
1217 Potomac Street, NW
Washington, DC 20007
USA
Phone: +1 202 342 0180
Fax: +1 202 342 0181
http://www.gams.com
sales@gams.com
support@gams.com