Global Optimization with GAMS

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Agenda

- Global Optimization Introduction
- GAMS Global Solvers
- Performance & Quality
- Linking a new Code
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Algebraic Modeling Languages

- High-level programming languages for large scale mathematical optimization problems
- Algebraic formulation
  - Syntax similar to mathematical notation
  - Does not contain any hints how to process it
- Do not solve optimization problems directly but call appropriate external algorithms (solvers)

Goals

- Support of decision making process
- Efficient handling of mathematical optimization problems
- Simplify model building and solution process
- Increase productivity and support maintainable models
Global Optimization (GO)

- Practical optimization problems are often nonlinear and non-convex.
- 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
Relevance of GO
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

The solvers differ in the methods they use, in whether they find globally optimal solution with proven optimality, in the size of models they can handle, and in the characteristics of models they accept.
Optimization Methods

• **BARON**
  - Branch-and-bound algorithms
  - Range reduction techniques
  - Under-estimators for objective and constraints

• **LGO**
  - Branch-and-bound based global search
  - Stochastic sampling procedure

• **OQNLP**
  - Starts NLP solvers from a set of starting points chosen by the Scatter Search software OptQuest

• **LINDOGlobal**
  - Branch-and-cut methods
  - Breaks an NLP into a list of sub problems
Model Requirements

• BARON
  – LP and NLP solver for sub problems
  – Knowledge about model algebra

• LGO
  – Only Lipschitz-continuity of objective function
  – Black box models (external equations)

• OQNLP
  – Requirements of local solver used during search
  – Smooth problems

• LINDOGlobal
  – Local solver for nonlinear sub problems
  – Instruction list interface
Solution Quality Metrics

• **LGO**
  – Estimated statistical or Lipschitz lower bound
  – Stochastic convergence to global optimum

• **OQNLP**
  – Scatter Search ensures stochastic convergence towards the global optimum

• **BARON & LINDOGlobal**
  – Deterministic lower bound
  – Relative/absolute gap similar to MIP
  – Proven global optimum
BARON vs. LINDOGlobal

• Both find proven global optimum

• BARON
  - Requires finite bounds for all variables and nonlinear expressions to guarantee global optimum
  - Can return the $k$ best solutions
  - Not tied to one sub solver

• LINDOGlobal
  – Copes with trigonometric functions
  – Handles non-smooth functions directly
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MINLP Library

• Collection of Mixed Integer Nonlinear Programming models (~250 models)

• Large and varied set of both theoretical and practical models

• Helps algorithm developers to test their source

www.gamsworld.org/minlp/minlplib.htm
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

GAMS Models

Solve with “other” systems

Web

PAVER Server

Solve with GAMS

Web

II. Data Collection

III. Analysis & Visualization
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
Benchmarking 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)
GAMS/Bench Output

Primal constraints satisfied (tol = 1e-006)

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Solver Links

• Standardized Solver Interface
  – Return Codes, Limits, Interrupts, …
  – Common attributes (e.g. time) through GAMS options
  – Specific options through option file

  allows “hassle free” replacement of solvers:
  ```
  option minlp=lindoglobal;
  ```

• Open architecture assures seamless communication
  – IO Library (C, Fortran, Delphi) provides access to Matrix, Function/Derivative Evaluator, …
MODULE: NLP;
VARIABLES  x2,x3,x4,x5,x6;
EQUATIONS  e2,e3,e4;

e2: x3^2 + x4^3 + x2 == 6.24264068711929;
e3:  - x4^2 + x3 + x5 == 0.82842712474619;
e4:  x2*x6 == 2;

OBJ: minimize  (-1 + x2)^2 + (x2 - x3)^2 + (x3 - x4)^3 + (x4 - x5)^4 + (x5 - x6)^4;

STARTING_POINT{
x2: -1;
x3: 2;
x4: 1;
x5: -2;
x6: -2;
}
BEGINMODEL TEST
VARIABLES
x2 -1E30 -1 1E30 C
x3 -1E30 2 1E30 C
x4 -1E30 1 1E30 C
x5 -1E30 -2 1E30 C
x6 -1E30 -2 1E30 C
OBJECTIVES
OBJ MINIMIZE
EP_PUSH_NUM -1
EP_PUSH_VAR x2
EP_PLUS
EP_SQR
EP_PUSH_VAR x2
EP_PUSH_VAR x3
EP_MINUS
EP_SQR
EP_PLUS
EP_PUSH_VAR x3

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