An Overview of the GlobSol Package for Verified Global Optimization

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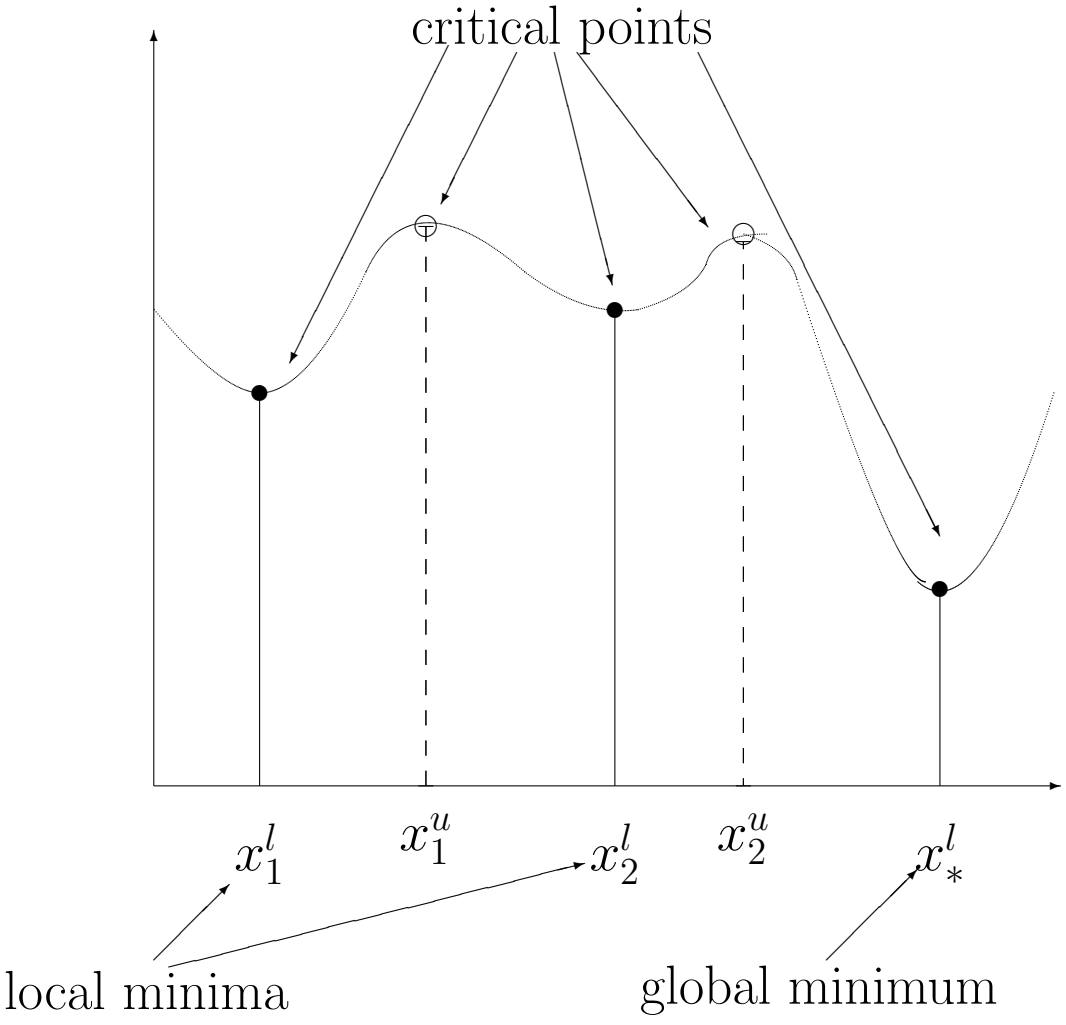
This talk will

- Contrast verified and non-verified global optimization
- Briefly discuss the underlying mathematics of verified global optimization
- Review capabilities of the GlobSol software package
- Review an example of how to use GlobSol
- Give an on-line demonstration.

Local Versus Global Optimization



Local Optimization Versus Global Optimization

Local Optimization

- The model is steepest descent with univariate line searches (for monotone decrease of the objective function). (Start a ball on a hill and let it roll to the bottom of the nearest valley.)
- Algorithm developers speak of "globalization," but mean only the design of algorithm variants that increase the domain of convergence. (See J. E. Dennis and R. B. Schnabel, *Numerical Methods for Unconstrained Optimization and Nonlinear Least Squares*, Prentice–Hall, 1983.)
- Algorithms contain many heuristics, and do not always work. However, many useful implementations exist.

Local Optimization Versus Global Optimization

Global Optimization

- is a much harder problem. Progress has accelerated with increases in computing power.
- Early milestones are L. C. W. Dixon and G. P. Szego, *Towards Global Optimization* (North–Holland, 1975), and *Towards Global Optimization 2* (North–Holland, 1977).
- Two types of algorithms: stochastic and deterministic.
- Deterministic algorithms can be either rigorous or heuristic.

Global Optimization

Stochastic Algorithms

Monte-Carlo search: Random points are generated in the search space. The point with lowest objective value is taken to be the global optimum.

Simulated annealing: is similar to a local optimization method, although larger objective values are accepted with a probability that decreases as the algorithm progresses.

Genetic algorithms: Attributes, such as values of a particular coordinate, correspond to particular "genes." "Chromosomes" of these genes are recombined randomly, and only the best results are kept. Random "mutations" are introduced.

Global Optimization

Deterministic Optimization

- involves some kind of systematic global search over the domain.
- The various algorithms rely on estimates of the range of the objective function over subdomains.
- Methods of bounding the ranges:
  - Heuristic estimation of Lipschitz constants (Schubert, Wood, Mladineo, Pinter, etc.)
  - Convex overestimators and underestimators of the objective and constraints (Sahinidis, Floudas et al)
  - Outwardly rounded interval arithmetic.

Global Optimization

Some Successful Non-Rigorous Deterministic Packages

- Janos Pinter uses a statistical model to estimate local approximations to Lipschitz constants in the the LGO software package. See `http://www.dal.ca/~jdpinter/l_s_d.html`
- Nikolaos Sahinidis et al, in the BARON package (available through GAMS), use convex over- and underestimators. See `http://archimedes.scs.uiuc.edu/baron.html`
- Christodoulos Floudas et al also use convex over- and underestimators in a different way in the software package alphaBB. See `http://titan.princeton.edu/soft.html`

On the State of the Art

- Minimizing a function over a compact set in $\mathbb{R}^n$ is an NP-complete problem.
- Thus, barring monumental discoveries, any *general* algorithm will fail for some high-dimensional problems.
- Some low-dimensional problems are difficult, while many practical low-dimensional problems can be solved.
- Advances in computer speed and algorithm construction have allowed more classes of higher-dimensional practical problems to be solved.
- The aforementioned packages of Pinter, Sahinidis and Floudas have been very successful. However, although they employ interval arithmetic in places, they are not rigorous, and they give incorrect conclusions for certain test problems.

Deterministic Global Optimization

Interval Methods

- Evaluation of an objective function $\phi(X)$ at an interval vector $\boldsymbol{X}$ gives bounds on the actual range of ϕ over $\boldsymbol{X}$.
  - If directed rounding is used, the bounds rigorously contain the mathematical range.
  - The bounds, in general, are overestimates.
- If the lower bound of $\phi(\boldsymbol{X})$ is greater than a previously computed objective value $\phi(X)$, then $\boldsymbol{X}$ can be discarded.
- Interval Newton Methods, combined with directed rounding, can *prove* existence and uniqueness of critical points, as well as reduce the size of regions $\boldsymbol{X}$.

Interval Methods

Advantages

easier to use: Obtaining bounds with interval methods involves programming the objective function, while using Lipschitz constant-based methods may require extensive preliminary analysis.

more efficient: Despite interval overestimation of ranges, the overestimation is often less than with a fixed Lipschitz constant. *(But keep in mind the success of the aforementioned non-rigorous algorithms.)*

more capable: With directed roundings, interval methods cannot lie. Also, interval Newton iteration results in quadratic convergence effects.

Underlying Mathematics

- Classical fixed point theory implies existence.
  - Contraction Mapping Theorem
  - Brouwer Fixed Point Theorem
  - Miranda's Theorem
- Regularity (non-singularity) implies uniqueness.
- Fundamental property of interval arithmetic allows *computational* existence and uniqueness.

What is GlobSol?

- A Fortran 90 package
  - well-tested.
  - self-contained.
- Solves constrained and unconstrained global optimization problems
- Separate program solves square algebraic systems of equations.
- Utility programs for interval and point evaluation, etc.
- Subroutine / module libraries for interval arithmetic, automatic differentiation, etc.
- Publicly available free of charge:
  `http://interval.louisiana.edu`
  `/GlobSol/download_GlobSol.html`

Elements of GlobSol

- automatic differentiation,
- constraint propagation,
- interval Newton methods,
- additional, specialized techniques.

Automatic Differentiation in GlobSol

- Designed originally for small problems.
- Implemented simply, to aid understanding of the code and minimize implementation effort.
- Serves its purpose, but certain inefficiencies are present.

Constraint Propagation in GlobSol

GlobSol applies constraint propagation at the level of individual operations.

- Allows simple, automatic constraint propagation connected with the automatic differentiation.
- Allows decoupling of interval dependencies in the "big system."
- *Usually* results in some savings in the overall algorithm, relative to not doing the propagation.
- *Sometimes* results in the difference between being able to solve a problem and not being able to solve it.

Interval Newton Methods in GlobSol

- Used with generalized Lagrange multiplier equations.
  - to narrow bounds;
  - *not* to verify critical points.
- Used to verify feasibility:
  - works with inequality and active equality constraints only;
  - works well, but only when the number of equality constraints is small.
- We have adopted this scheme from experimental observation of efficiencies on a number of problems.
- By not verifying critical points, we give up some strength in the statements we make about the answers.

Use of Already Found Approximate Optima

- Approximate feasible points are found with a generalized Newton method based on the Moore–Penrose pseudo-inverse.
- Boxes are constructed with diameters proportional to the square root of the tolerance to which the approximate feasible points are found.
- These boxes are placed on a list, then removed from the search space with a set complementation process.
- Boxes are later culled from the list as better upper bounds for the optimizer are found.
- This scheme avoids excessive clusters, even near singular roots;

History of GlobSol

(continued)

AD, algorithm improvements: `INTOPT_90`, *SIAM. J. Sci. Comput.* **18** (1997) and the book *Rigorous Global Search: Continuous Problems*, Kluwer, 1996.

The Sun Microsystems project: User interface, testing and bug removal, improvements, applications; first called "GlobSol"
`http://www.mscs.mu.edu/~globsol/`

INTBIS and INTLIB

- Emphasis is on simplicity and ability of user to modify the code and to port the code.
- There is no constraint propagation other than interval Newton methods, and algorithms are simple.
- Except for polynomial systems, the user inputs the equations by assembly-language-like programming.
- Nonetheless:
  - Evaluation of the equations (constraints) is significantly more efficient than in GlobSol.
  - Stadtherr et al have modified `INTBIS` / `INTLIB` for some of the most impressive application successes in the field.

Our Motivations for INTOPT_90 and Further Development

Motivation for AD: We were hampered by having to program many lengthy subroutines for even simple test functions for algorithm research.

Motivation for constraint propagation: This was one possible way of dealing with interval dependency and speeding up the overall global search process.

Motivation for restructuring, etc.: To make it easier

- for students, etc. to learn how to use the package, to pursue the applications in the SunSoft cooperative research project;
- to deliver and install;
- to support.

The Sun Microsystems Project

- GlobSol grew from `INTOPT_90`.
- Collaborative effort with George Corliss, under Bill Walster, with participation of graduate students
- Much improved distribution packaging (the build is automated)
- Improved package structuring (subroutine calling sequences, source directory structure, etc.)
- Removal of many bugs
- Improved capabilities:
  - both inequality and equality constraints
  - "thick" constants
  - subdivision stopping criteria
- Improved understanding of how to use in applications and of advice to give users

GlobSol's Overall Algorithm

- The GlobSol script
- The overall GlobSol optimization process
  - Initial I/O
  - The "peeling" process.
  - The actual global search routine
  - Final I/O.

The GlobSol Script

`globsol <source file> <data number>`

1. Compiles and runs the user-provided Fortran-90 program to produce the internal representation, or *codelist* for the objective, constraints, and gradients.
2. Runs an optimizing program that removes redundant operations from the code list.
3. Runs the overall GlobSol optimization process.
4. Cleans the directory and temporary files.

GlobSol's Global Search Routine

`rigorous_global_search.f90`

1. Remove a box $\boldsymbol{x}$ from a list of not-yet-examined boxes $\mathcal{L}$.
2. *IF* $\boldsymbol{x}$ is sufficiently small *THEN* store $\boldsymbol{x}$ and *CYCLE*.
3. Use constraint propagation to possibly narrow the coordinate widths of the box $\boldsymbol{x}$ and possibly reject the box $\boldsymbol{x}$.
4. Perform an interval Newton method to possibly narrow the coordinate widths of $\boldsymbol{x}$ and to possibly reject $\boldsymbol{x}$.
5. *IF* the coordinate widths of $\boldsymbol{x}$ are now sufficiently narrow *THEN* store $\boldsymbol{x}$ and *CYCLE*.
6. (Subdivide) Bisect $\boldsymbol{x}$ along a chosen coordinate, forming two new boxes; place these boxes on the list $\mathcal{L}$.

GlobSol's Algorithms

Some Complications

"Storing" a box $\boldsymbol{x}$ presently involves

- an attempt to verify existence of feasible points within the box, and to adjust the best upper bound for the global optimum;
- expansion to avoid clustering of solution boxes;
- examination of intersections with not-yet-processed boxes and already-stored boxes to avoid redundancy.

Use of GlobSol: Required Files

(How the user controls GlobSol)

`GlobSol.CFG:` The GlobSol configuration file. This is used to

- control printing,
- set tolerances,
- select algorithm components, such as choice of preconditioner, choice of interval Newton method, form of problem (nonlinear system optimization), etc.

`<`*`name`*`>.f90:` The user-supplied Fortran 90 source file defining the objective and constraints.

`<`*`name`*`>.DT#:` The "box data file." where the user supplies search limits, which coordinates are considered as bound constraints, and an initial guess for a global optimizer, if available.

The Configuration File
`GlobSol.CFG`

- Is largely self-documenting.
- Users should seldom need to change items other than level of printing, tolerances, and type of problem, and things such as the total CPU time to be allowed to solve a particular problem.
- GlobSol contains several algorithm variants of an experimental nature. Some variants are not presently supported at the level that more promising variants are; users should be wary of changing the configuration file to use these variants.

An Example Problem and Box Data file

$$\text{minimize} \quad \phi(X) = -2 * x_1^2 - x_2^2$$

subject to constraints

$$\begin{aligned} x_1^2 + x_2^2 - 1 &\leq 0 \\ x_1^2 - x_2 &\leq 0 \\ x_1^2 - x_2^2 &= 0 \end{aligned}$$

`mixed.DT1`

```
1D-5          ! General domain tolerance
 0   1        ! Bounds on the first variable
 0   1        ! Bounds on the second variable
F F           ! X(1) has no bound constraints
F F           ! X(2) has no bound constraints
```

Subsequent optional lines can give an initial guess point.

A Simple User-Supplied Function file `mixed.f90`

```
PROGRAM SIMPLE_MIXED_CONSTRAINTS
  USE CODELIST_CREATION
      PARAMETER (NN = 2)
      TYPE(CDLVAR), DIMENSION(NN) :: X
      TYPE(CDLLHS), DIMENSION(1):: PHI
      TYPE(CDLINEQ), DIMENSION(2) :: G
      TYPE(CDLEQ), DIMENSION(1)   :: C

      CALL INITIALIZE_CODELIST(X)

  PHI(1) = -2*X(1)**2 - X(2)**2
  G(1) = X(1)**2 + X(2)**2 - 1
  G(2) = X(1)**2 - X(2)
  C(1) = X(1)**2 - X(2)**2

      CALL FINISH_CODELIST
END PROGRAM SIMPLE_MIXED_CONSTRAINTS
```

GlobSol Output File

abridged first part

Typing "`globsol mixed 1`" gives `mixed.OT1`, containing:

```
Output from FIND_GLOBAL_MIN on  04/06/1999  at  08:03:52.
Version for the system is: March 20, 1999

Codelist file name is: MIXEDG.CDL
Box data file name is: MIXED.DT1

Initial box:
[    0.0000E+00,   0.1000E+01 ] [    0.0000E+00,   0.1000E+01 ]

BOUND_CONSTRAINT:
  F F   F F

---------------------------------------
CONFIGURATION VALUES:

EPS_DOMAIN:   0.1000E-04   MAXITR:   60000
DO_INTERVAL_NEWTON: T  QUADRATIC: T  FULL_SPACE: F
VERY_GOOD_INITIAL_GUESS:F
USE_SUBSIT:T
OUTPUT UNIT:7 PRINT_LENGTH:1
Default point optimizer was used.
```

Globsol Output File

abridged second part

```
 THERE WERE NO BOXES IN COMPLETED_LIST.

 LIST OF BOXES CONTAINING VERIFIED FEASIBLE POINTS:

 Box no.:1
Box coordinates:
 [    0.7071E+00,   0.7071E+00 ] [    0.7071E+00,   0.7071E+00 ]
PHI:
 [   -0.1500E+01,  -0.1500E+01 ]
 Level: 3
 Box contains the following approximate root:
    0.7071E+00   0.7071E+00
 OBJECTIVE ENCLOSURE AT APPROXIMATE ROOT:
 [   -0.1500E+01,  -0.1500E+01 ]
U0:
 [    0.3852E+00,   0.3852E+00 ]
U:
 [    0.5777E+00,   0.5777E+00 ] [    0.0000E+00,   0.1000E+01 ]
V:
 [    0.1926E+00,   0.1926E+00 ]
INEQ_CERT_FEASIBLE:
  F T
NIN_POSS_BINDING:1

Number of bisections: 1
BEST_ESTIMATE:   -0.1500E+01
 Total number of boxes processed in loop:            4
 Overall CPU time:    0.5000D-01
```

Advice on GlobSol's Use

Interpretation of Results

- The only guarantees (at present): Any global minimizers must lie within the boxes in the output list.
- A non-empty output list does not guarantee existence of global minima.
- An empty output list does not necessarily mean a bug. It usually means either an overconstrained or an underconstrained problem. (The search box does not correspond to bound constraints unless explicitly set.)

Advice on GlobSol's Use

Turning On and Off Constraint Propagation

- On average, and for most problems, constraint propagation gives a small but significant improvement in GlobSol's overall performance.
- Constraint propagation is indispensable for some problems.
- Because inverses are not implemented in extended arithmetic in GlobSol, constraint propagation does not work for some problems.
- Users can experiment with the switch `USE_SUBSIT` (use "substitution-iteration") in `GlobSol.CFG` to turn on and off constraint propagation.

Advice on Bound Constraints

- GlobSol solves unconstrained problems more efficiently than constrained problems.
  - Large numbers of bound constraints lead to excessive "peeling."
  - In practice, interval Newton methods do not seem to function well with the Fritz–John system for larger boxes.
- Suggestion:
  1. Start with an unconstrained system.
  2. Selectively add constraints until the problem has a solution.
  3. Experiment with which constraints are important.

On Equality Constraints, Data Fitting

- We have tried GlobSol with numerous test sets with nonlinear least squares problems and nonlinear minimax problems (which we reformulated as smooth problems with constraints using Lemaréchal's technique).
- GlobSol almost uniformly failed to solve these problems efficiently.
- Although the Fritz–John matrix is not necessarily singular at critical points, we believe the problems to be related to intrinsic properties of the Fritz–John matrix, in the case of minimax problems.
- We have also tried several variants for least squares, without success.
- Thus, GlobSol cannot presently handle overdetermined systems well.

Possibilities for Data Fitting Problems

- For the interval Newton method, reformulate the minimax problem as an uncertain linear programming problem, and solve with Jansson's techniques.
- Reformulate as a system of equations with tolerances (as Hansen / Walster explain).
  - We have experimented in some depth with this technique last summer.
  - Although hopeful, we don't have a final answer yet.
  - This technique will involve getting the user to accept a different interpretation of "solution". The solution will not be least-squares or minimax, but a set over which all residuals are within a tolerance. (See my talk on the linear case from Validated Computing 2002.)

GlobSol's Future

- Totally rewrite to simplify the structure more.
- Improve the user interface (better I/O) and low-level (more efficient code list interpretation, etc.)
- Include of additional good algorithms of others (the LP rejection technique of Nenov, van Hentenryck's univariate search, etc.)
- Do additional research on new algorithms (such as for nonlinear data fitting).

These items need to be prioritized, and time resources need to be found.

GlobSol's Future

- Make GlobSol available through a web interface (probably NEOS)
- Implement affine arithmetic, convex underestimators and overestimators
- Implement capabilities for mixed integer programming.

GlobSol References

- For the source, installation instructions, user guide, etc.:
  `http://www.mscs.mu.edu/~globsol/`
- *Rigorous Global Search: Continuous Problems*, R. B. Kearfott, Kluwer Academic Publishers, 1996. Contains
  - Most of the basic ideas underlying GlobSol.
  - Structure of the research code that eventually became GlobSol.
- For various preprints related to techniques in GlobSol and applications:
  `http://interval.louisiana.edu/preprints.html`
- For these transparencies:
  `http://interval.louisiana.edu/preprints/2003_McMaster.pdf`