Relaxations and Probing – Highly Successful Techniques for Branch and Bound Search

by
R. Baker Kearfott
Department of Mathematics
University of Louisiana at Lafayette
rbk@louisiana.edu

Two techniques have been used quite successfully in non-validated software, but are new to the "interval" community:

1. Linear relaxations to compute lower bounds on ranges and approximate optima.
2. "Probing" to reduce the size of regions in which solutions (or optima) must lie.

Probing and Linear Relaxations

Significance in Global Optimization Software

- These techniques are very different from interval evaluation for ranges and interval Newton methods.
- Use of these techniques compares favorably with traditional interval techniques (for example, with the BARON software and the Neumaier benchmarking tests).
- The techniques *can* be used in a validated context. (This is the subject of current research.)
- We are in the process of developing validated versions and studying them in the GlobSol environment.

General Problem

minimize $\varphi(x)$
subject to:

$$c_i(x) = 0,\ i = 1, \ldots, m_1,$$
$$g_i(x) \leq 0,\ i = 1, \ldots, m_2,$$

where $\varphi : \boldsymbol{x} \rightarrow \mathbb{R}$ and $c_i, g_i : \boldsymbol{x} \rightarrow \mathbb{R}$, and where $\boldsymbol{x} \subset \mathbb{R}^n$ is the hyperrectangle (box) defined by

$$\underline{x}_i \leq x_i \leq \overline{x}_{i_j},\ 1 \leq j \leq m_3,$$

i_j between 1 and n, where the $\underline{x}_{i_j}$ and $\overline{x}_{i_j}$ are constant bounds.

If φ is constant or absent, this problem becomes a general constraint problem; if, in addition $m_2 = m_3 = 0$, this problem becomes a nonlinear system of equations.

The General Context

GlobSol's Overall Algorithm

(routine `f90intbi/rigorous_global_search.f90`)

INPUT: A list $\mathcal{L}$ of boxes $\boldsymbol{x}$ to be searched.
OUTPUT: A list $\mathcal{U}$ of small boxes and a list $\mathcal{C}$ of boxes verified to contain feasible points, such that any global mimimizer must lie in a box in $\mathcal{U}$ or $\mathcal{C}$.
DO WHILE ($\mathcal{L}$ is non-empty)

1. Remove a box $\boldsymbol{x}$ from the list $\mathcal{L}$.
2. *IF* $\boldsymbol{x}$ is sufficiently small *THEN*
   (a) Analyze $\boldsymbol{x}$ to validate feasible points, possibly widening the coordinate widths (ϵ-inflation) to a wider box within which uniqueness of a critical point can be proven.
   (b) Place $\boldsymbol{x}$ on either $\mathcal{U}$ or $\mathcal{C}$.
   (c) Apply the complementation process of p. 152 of *Rigorous Global Search: Continuous Problems.*
   (d) *CYCLE*

   END IF

GlobSol's Overall Algorithm

(Continued)

3. (Constraint Propagation)
   (a) Use constraint propagation to possibly narrow the coordinate widths of the box $\boldsymbol{x}$.
   (b) *IF* constraint propagation has shown that $\boldsymbol{x}$ cannot contain solutions *THEN CYCLE*
4. (Interval Newton)
   (a) Perform an interval Newton method to possibly narrow the coordinate widths of the box $\boldsymbol{x}$.
   (b) *IF* the interval Newton method has shown that $\boldsymbol{x}$ cannot contain solutions *THEN CYCLE*
5. *IF* the coordinate widths of $\boldsymbol{x}$ are now sufficiently narrow *THEN*
   (a) Analyze $\boldsymbol{x}$ to validate feasible points, possibly widening the coordinate widths (ϵ-inflation) to a wider box within which uniqueness of a critical point can be proven.
   (b) Place $\boldsymbol{x}$ on either $\mathcal{U}$ or $\mathcal{C}$.
   (c) Apply the box complementation process of [**?**, p. 154].
   (d) *CYCLE*

GlobSol's Overall Algorithm

(Continued)

6. (Subdivide)
   (a) Choose a coordinate index k to bisect (i.e. to replace $[\underline{x}_k, \overline{x}_k]$ by $[\underline{x}_k, (\underline{x}_k + \overline{x}_k)/2]$ and $[(\underline{x}_k + \overline{x}_k)/2, \overline{x}_k]$).
   (b) Bisect $\boldsymbol{x}$ along its k-th coordinate, forming two new boxes; place these boxes on the list $\mathcal{L}$.
   (c) *CYCLE*

END DO

A Weakness in the Current GlobSol Version

- During the interval Newton method and at various other places, a box $\boldsymbol{x}$ is rejected based upon the "lower bound test," that is, if the lower bound on the range of the function is less than or equal to the upper bound on the global optimum obtained by evaluating the objective over a box containing a feasible point.
- For many problems, the structural information is not in the objective, but in the constraints.

A Weakness in GlobSol

Example

$$\min_x \max_{1\le i\le m} |f_i(x)|, \quad f_i : \mathbb{R}^n \to \mathbb{R},$$
$$x \in \mathbb{R}^n, \quad m \ge n.$$

To date, we have had limited success in solving realistic problems of this type directly using GlobSol's non-smooth slope extensions. Alternately, we can convert the problem to a to a smooth problem with Lemaréchal's technique as follows:

$$\min_{x\in\mathbb{R}^n} v$$
$$\text{such that } \left\{ \begin{array}{rcl} f_i(x) & \le & v \\ -f_i(x) & \le & v \end{array} \right\}, \quad 1 \le i \le m.$$

Example of a GlobSol Weakness

(Continued)

- In the Lemaréchal formulation, we have introduced a single additional slack variable v, which becomes the value of the objective function.
- GlobSol presently tries to use constraint propagation to narrow the range of the new variable v.
- However, this process does not take account of the coupling between the constraints, and has not enabled GlobSol to solve minimax problems efficiently.
- Furthermore, interval Newton methods applied to the Lagrange multiplier (or Fritz–John) system associated with the Lemaréchal formulation over large regions are unsuccessful, due to singularities in the interval matrix.

Linear Relaxations

The basic idea

- If the objective φ is replaced by linear function $\varphi^{(\ell)}$ such that $\varphi^{(\ell)}(x) \leq \varphi(x)$ for $x \in \boldsymbol{x}$, then the resulting problem has global optimum less than or equal to the global optimum of the original problem.
- If each inequality constraint g_i replaced by a linear function $g_i^{(\ell)}$ such that $g_i^{(\ell)}(x) \leq g_i(x)$ for $x \in \boldsymbol{x}$, then the resulting problem has optimum that is less than or equal to the optimum of the original problem.
- If there are equality constraints, then each equality constraint can be replaced by two linear inequality constraints, and these inequality constraints can be replaced as above by linear inequality constraints.
- The resulting linear program is termed a *linear relaxation*.

Linear Relaxations

An Example

(An equality constraint and an inequality constraint – no objective):

$c_1(x) = x_1^2 - x_2 = 0, \quad g_1(x) = x_2 - x_1 \le 0,$
$x_1 \in [0, 1], \quad x_2 \in [0, 1].$

- Lower bounds of a convex function are tangent lines and upper bounds are secant lines.
- A corresponding linear program for computing an upper bound on x_2, using two underestimators for the convex function $x_2 = x_1^2$, is:

  minimize $-x_2$
  subject to
  $x_2 \le x_1$ (the overestimator),
  $x_2 \ge .125 + .5(x_1 - .25)$,
  $x_2 \le x_1$ (the original constraint),
  $x_1 \in [0, 1]$, $x_2 \in [0, 1]$.

Linear Relaxation Example

(continued)

- The exact minimum to this linear program is $\varphi = -.5$, corresponding to $x_2 \le 0.5$.
- Thus, we have narrowed x_2 to $x_2 \in [0, 0.5] \subset [0, 1]$.
- Basic constraint propagation now converges.

Rigor in Linear Relaxations

1. Typical procedures have been to compute the coefficients of the linear relaxation with floating point arithmetic, then to solve the relaxation with a state-of-the-art LP solver.
2. With carefully considered directed rounding and interval arithmetic, we can form a machine-representable LP that is an actual relaxation of the original problem.
3. Neumaier and Shcherbina, as well as Jansson, have presented a simple technique to utilize the duality gap to obtain a rigorous lower bound on the solution to an LP, given approximate values of the dual variables.
4. Combining (2) and (3) gives a procedure for rigorous computations of lower bounds on the solution to the original problem.

Implementation in GlobSol

- We have implemented linear relaxations in GlobSol.
- Initial experiments indicate the technique makes possible solution of problems that were previously intractable within GlobSol.
- A preprint of experimental results is available.
- GlobSol still is not fully competitive with other packages using relaxations in a non-validated way (e.g. BARON).
- One possibility for improvement: Use a better LP solver. (GlobSol presently is using a free one from the SLATEC library.)

Probing

- Ryoo and Sahinidis introduced probing in a 1995 paper.
- Further explanation occurs in M. Tawarmalani and N. V. Sahinidis, *Convexification and Global Optimization in Continuous and Mixed-Integer Nonlinear Programming: Theory, Algorithms, Software, and Applications*, Kluwer, 2002.
- Probing is presently successfully implemented in Sahinidis' BARON software (available commercially through GAMS).
- We are presently working on a validated version of probing.

The Idea Behind Probing

1. Let L be any underestimate for the global optimum of the original nonlinear programming problem (such as a rigorous lower bound on the solution to a linear relaxation).
2. Let U be a known upper bound for the optimum of the original problem.
3. Suppose, for some i, either that the solution of the relaxed linear problem corresponds to an active lower bound constraint $x_i = \underline{x}_i$, or else x_i has been artificially set at $x_i = \underline{x}_i$ before solving the relaxed problem, suppose the corresponding Lagrange multiplier at the solution is $\underline{y}_i > 0$, and define

   $$x_i^{(\ell)} = \overline{x}_i - (U - L)/\underline{y}_i.$$

   If $\underline{x}_i < x_i^{(\ell)}$ Then all global optimizers in the original nonlinear problem are also optimizers of the problem obtained by replacing $[\underline{x}_i, \overline{x}_i]$ by $[x_i^{(\ell)}, \overline{x}_i]$.
4. A corresponding technique can also be used to reduce the upper bound.

Validated Probing?

- For a validated version of probing, we need validated lower and upper bounds on the dual variables (i.e. on the Lagrange multipliers) of the problem.
- We have devised a technique for such validation and are presently writing it up.
- We intend to implement this validated technique soon.