Introduction to Linear Relaxations

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In this talk, we will

- define the global optimization problem;
- review interval branch and bound;
- describe the idea of linear relaxations;
- discuss obtaining linear relaxations;
- discuss validation of linear relaxations.

Interval Global Optimization

The General Nonlinear Programming Problem

Given a box

$$\boldsymbol{x} = ([\underline{x}_1, \overline{x}_1], \ldots [\underline{x}_n, \overline{x}_n]),$$

find small boxes

$$\boldsymbol{x}^* = ([\underline{x}_1^*, \overline{x}_1^*], \ldots [\underline{x}_n^*, \overline{x}_n]^*)$$

such that any solutions of

$$\boxed{\begin{array}{l} \text{minimize } \varphi(x) \\ \text{subject to } c_i(x) = 0, i = 1, \ldots, m_1, \\ \qquad\qquad\quad g_i(x) \le 0, i = 1, \ldots, m_2, \\ \text{where } \varphi : \mathbb{R}^n \to \mathbb{R} \text{ and } c_i, g_i : \mathbb{R}^n \to \mathbb{R} \end{array}}$$

are guaranteed to be within one of the $\boldsymbol{x}^*$ that has been found.

The Branch and Bound Structure

1. Start with an initial region $\boldsymbol{x}^{(0)}$.
2. Adaptively subdivide $\boldsymbol{x}^{(0)}$ into subregions $\boldsymbol{x}$.
3. Maintain an upper bound $\overline{\varphi}$ to the global optimum of φ (say, by evaluating φ at a succession of feasible points, as $\boldsymbol{x}^{(0)}$ is subdivided).
4. Compute a lower bound $\underline{\varphi}(\boldsymbol{x})$ on the optimum of φ over the subregion $\boldsymbol{x}$.
5. *IF* $\underline{\varphi}(\boldsymbol{x}) > \overline{\varphi}$

   THEN reject $\boldsymbol{x}$.

   ELSE use other techniques to reduce, eliminate, or subdivide $\boldsymbol{x}$.

   END IF

Effectiveness of the Branch and Bound Structure

- A "naive" but common way of obtaining $\underline{\varphi}(\boldsymbol{x})$ is to simply evaluate φ over $\boldsymbol{x}$ with interval arithmetic. However, this does not take account of the constraints; we'll give an example shortly.
- We can take account of constraints with interval Newton methods based on the Kuhn–Tucker (or Fritz–John) conditions.
  - However, the matrix tends to contain singular matrices in practice, or the interval Newton method tends to converge only for relatively small boxes.
  - Taylor arithmetic can help here, but is not the complete answer.

Sharpness of Underestimates on the Objective

The Nonlinear Minimax Problem

$$\min_x \max_{1\le i\le m} |f_i(x)|,$$

$$f_i : \mathbb{R}^n \to \mathbb{R}, \quad x \in \mathbb{R}^n, \quad m \ge n.$$

- To date, GlobSol's non-smooth slope extensions haven't adequately solved this.
- Alternately, we can convert the problem to a to a smooth problem with Lemaréchal's technique:

$$\min_{x\in\mathbb{R}^n} x_{n+1}$$

$$\text{such that } \left\{ \begin{array}{rcl} f_i(x) & \le & x_{n+1} \\ -f_i(x) & \le & x_{n+1} \end{array} \right\}, \quad 1 \le i \le m.$$

- Evaluation of φ with interval arithmetic gives a meaningless lower bound.

More Effectively Handling Constraints

The "Relaxation" Paradigm

1. If φ is replaced by a function ℓ_φ with $\ell_\varphi(x) \le \varphi(x)$ for $x \in \boldsymbol{x}$, then the resulting nonlinear programming problem (NLP) has optimum less than or equal to the optimum of the original NLP.
2. If each g_i is replaced by a function ℓ_i such that $\ell_i(x) \le g_i(x)$ for $x \in \boldsymbol{x}$, then the resulting NLP has feasible set containing the feasible set of the original NLP. Hence the resulting NLP has optimum less than or equal to the optimum of the original NLP.
3. The equality constraint $c_i(x) = 0$ can be replaced by $c_i(x) \le 0$ and $-c_i(x) \le 0$, and each of the resulting inequalities can be underestimated as in step 2.

Relaxations

Origin and Fundamentals

- Originally proposed by McCormick, in 1976.
- McCormick proposed an arithmetic to produce underestimators, very similar to automatic differentiation.
- Effective implementations within commercial-grade global optimization codes have appeared in the 1990's.

Obtaining Relaxations

- Relaxations can be obtained through any method; further work to compare different methods may be useful.
- We are presently thinking in terms of working with the intermediate expressions in evaluation of the objective and constraints; we'll give an example.

Consequences of Relaxations

Advantages

1. The ℓ_φ and ℓ_i can be chosen to be convex or even linear.
2. There are high-quality, fairly reliable point solvers for large linear programs and for convex programs.
3. The exact minimum of a resulting linear program is an underestimate for the minimum to the original NLP, and hence is a lower bound on φ over $\boldsymbol{x}$.
4. An LP solution takes full account of the constraints.

Consequences of Relaxations

Pitfalls

1. The approximation of the original NLP may not be sharp if the objective or constraints are highly non-convex.
2. Work to-date has been primarily non-validated.
3. Current proposed validation techniques (through post-processing) easily validate only the optimum, and not bounds on the optimizer.

Nonetheless, the technique has enjoyed great success in practice.

Work to Date with Relaxations

Non-Validated Codes

BARON (Nick Sahinidis's group)

- is commercially available through GAMS;
- is described in the 2002 book by Tawarmalani and Sahinidis (Kluwer);
- uses linearization and LP solvers.

α**BB** (A set of codes developed by Chris Floudas and his students)

- is a set of research codes, not publicly available but applied successfully;
- uses nonlinear convex terms and solves convex programs for relaxations;
- is described in the 2000 book by Floudas (Kluwer).

The above use interval arithmetic and constraint propagation in places to bound ranges, but are non-validated.

Non-Validated Codes

(continued)

from LINDO The LINDO company is presently developing a commercial-grade code.

- highly uses automatic differentiation technology;
- uses LINDO's own commercial LP solvers.

others such as the group at Colorado State with their large protein folding project.

On Validation

- Given an approximate solution to a linear program, rigorous bounds on the solution can be easily obtained by using the duality gap.
- Arnold Neumaier and Christian Jansson simultaneously discovered this.
- Neumaier's presentation is slightly simpler.
- Jansson describes how to obtain a lower bound on the optimum when the original LP has interval uncertainty.
- Both papers have been accepted and are soon to appear.

Refining the Accuracy of the Relaxation

- Some terms can be approximated more accurately by appending constraints to the relaxation.
- Other terms must be handled by subdividing the domain and solving relaxations on the subdomains.
- Such issues have been considered in the book by Tawarmalani / Sahinidis and elsewhere.
- We have recently proposed a novel way of determining the best ways of doing this.

More on Validation

- For the validation of an approximate solution to a relaxation to give a validated underestimate to the original NLP, the relaxation itself needs to be formed rigorously.
- This means that the coefficients of the linear underestimates must be rounded, such that the resulting machine representable linear expression is actually an underestimate.
- One approach: obtain machine representable relaxations with directed rounding, then validate the solution of the resulting point LP.
- Another approach: use interval arithmetic to produce a slightly "fuzzy" LP, then obtain a rigorous lower bound to the solution set of this set of LP's.