Rigorous Global Search: Industrial Applications

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Outline:

1. Problem domain
2. When should I consider this technology?
3. How can this technology be applied?
4. Why is this technology effective?

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Reference: Kearfott, Rigorous Global Search:
Continuous Problems

Rigorous Global Search: Industrial Applications

We are currently working on several industrial applications of interval techniques for global optimization, including problems from

- Sun Microsystems (software development)
- MacNeal-Schwindler (finite element)
- Bank One (portfolio management)
- Swiss National Bank (currency trading)
- GE Medical Systems (control of NMR signals)
- Genome Thereputics (gene space search)

We suggest why rigorous techniques can be effective some of their limitations.

Problem Domain

$f : X \subset R^n \to R$ continuous,
differentiable objective function

$$\min_{x \in X} f(x),$$

possibly with linear or nonlinear constraints.
Seek validated, tight bounds for minimizer X^*,
optimum value f^*.

Linear systems $Ax = b$ and nonlinear systems $G(x) = 0$

Applications

Sun Microsystems - Global Solutions. Software and applications for interval techniques for global solutions of non-linear systems and optimization.
MacNeal-Schwindler - Stress analysis of rocket nozzle designs, finite element analysis
Bank One - Portfolio management using global optimization
Swiss National Bank - Modeling international currency trading
GE Medical Systems - Control of NMR signal, "black-box" optimization
Genome Thereputics - Genome search
Computer algebra - Inexact GCD

Enabling Component: Intervals

Fundamental Theorem of Interval Analysis:
If a function is evaluated using interval arithmetic instead of floating-point arithmetic, the resulting interval is guaranteed to enclose the range of function values.
Global minimum can never be discarded
We consider in turn

1. Enabling components: interval analysis, automatic differentiation
2. Branch and bound for exhaustive search
3. Discarding where the solution is not
4. Validation: Guarantee the existence of a unique local minimum in some box
5. Enclosing a local minimum: Find a small box in which a unique local minimum is rigorously guaranteed to lie

Enabling Component: Intervals

$\boldsymbol{x} \circ \boldsymbol{y} := \{x \circ y : x \in \boldsymbol{x}, y \in \boldsymbol{y}\}$
Rosenbrock function $f(x, y) := 100 * (y - x^2)^2 + (1 - x)^2$
$\boldsymbol{X} := (\boldsymbol{x}, \boldsymbol{y}) := ([0.7, 1], [0.0, 0.3])$
For $x \in \boldsymbol{x}$ and $y \in \boldsymbol{y}$,

$$\begin{aligned}
f(x, y) &= 100 * \left(y - x^2\right)^2 + (1 - x)^2 \\
&\in 100 * \left(\boldsymbol{y} - \boldsymbol{x}^2\right)^2 + (1 - \boldsymbol{x})^2 \\
&= 100 * \left([0.0, 0.3] - [0.7, 1]^2\right)^2 + (1 - [0.7, 1])^2 \\
&= 100 * ([0.0, 0.3] - [0.49, 1])^2 + [0.0, 0.3]^2 \\
&= 100 * [-1.0, -0.19]^2 + [0.0, 0.09] \\
&= [3.61, 100.09].
\end{aligned}$$

Guaranteed upper, lower bounds for range
over $[0.7, 1] \times [0.0, 0.3]$

$f(0,0) = 1$ box $[0.7, 1] \times [0.0, 0.3]$ cannot contain a global minimum

Enabling Components
Automatic Differentiation

Compute required gradients, Hessians
Fast, accurate propagation of numerical values of derivatives
Not subject to the expression swell of purely symbolic differentiation
Not subject to the numerical inaccuracies of divided difference approximations.
Interval arithmetic bounds derivatives, too

$$x := \boldsymbol{x} = [0.7, 1.0]; \qquad \nabla x := \left(\frac{\partial x}{\partial x}, \frac{\partial y}{\partial x} \right) = (1, 0)$$

$$y := \boldsymbol{y} = [0.0, 0.3]; \qquad \nabla y := \left(\frac{\partial x}{\partial y}, \frac{\partial y}{\partial y} \right) = (0, 1)$$

evaluate the code list using interval arithmetic

$$f = [3.61, 100.09]; \nabla f = ([52.6, 400], [-200, -38])$$

0 is not in either interval $[52.6, 400]$ or $[-200, -38]$
f has no critical point in the box $[0.7, 1] \times [0.0, 0.3]$

Branch and Bound

Maintain three lists of boxes:
- $\mathcal{L}$ not fully analyzed;
- $\mathcal{R}$ small boxes validated to enclose
  a unique local minimum; and
- $\mathcal{U}$ small boxes not validated either to enclose
  a minimum or *not* to enclose a minimum.

To find enclosures for f^* and X^* such that

$$f^* = f(X^*) \leq f(X),$$

for all $X \in \boldsymbol{X}_0 \subset R^n$:

Branch and Bound

```
Initialize L = {X_0}        // List of pending boxes
f̄ = +∞                      // f* ≤ f̄
DO WHILE L is not empty
    Get current box X^(c) from L
    IF f̄ < f(X^(c)) THEN
        // We can guarantee there is
            no global minimum in X^(c)
        Discard X^(c)
```

```
    ELSE
        Attempt to improve $\overline{f}$
    END IF
    IF we can otherwise guarantee that there
        is no global minimum in $X^{(c)}$ THEN
        Discard $X^{(c)}$
    ELSE IF we can validate the existence of
        a unique local minimum in $X^{(c)}$ THEN
        Shrink $X^{(c)}$, and add it to $\mathcal{R}$
    ELSE IF $X^{(c)}$ is small THEN
        Add $X^{(c)}$ to $\mathcal{U}$
    ELSE
        Split $X^{(c)}$ into sub-boxes, and add them to $\mathcal{L}$
    END IF
END DO
```

Discarding where the solution is NOT

Range on a sub-box > a known upper bound for f^*
Non-zero gradient
Hessian of f is not positive definite
Fritz-John or Kuhn-Tucker conditions
Feasibility of constraints

Validation

Neumaier: Purposes of validated scientific computation:

- Obtain rigorous verification of existence and uniqueness, and
- Find guaranteed enclosures with narrow bounds.

Three separate issues:

- validation
- guaranteed enclosures
- tight enclosures

For validation, **Banach Fixed-Point Theorem:**
Let $T : X \to X$ be defined on a complete metric space X with metric ρ. Let α satisfy $0 < \alpha < 1$, and let

$$\rho(T(x), T(y)) \leq \alpha\rho(x, y)$$

for all x and $y \in X$.
Then T has a unique fixed point $x^* \in X$.

Validation
Interval Newton Method

Univariate interval Newton method

$$\boldsymbol{N}(f;\boldsymbol{x},\check{x}) := \check{x} - f(\check{x})/\boldsymbol{f}'(\boldsymbol{x})$$
$$\boldsymbol{x}^{(k+1)} := \boldsymbol{x}^{(k)} \cap \boldsymbol{N}(f;\boldsymbol{x}^{(k)},\check{x}^{(k)})$$

Multi-dimensional version:
$G := \nabla f$; $\check{X}$ approximate minimizer; $||G(\check{X})||$ is small
$\boldsymbol{A}$ enclosure of Jacobian $\boldsymbol{G}'(\boldsymbol{X})$
(= the Hessian of f, computed by automatic differentiation).

DO
    $\boldsymbol{A} := \boldsymbol{G}'(\boldsymbol{X})$
    Bound solution set of $\boldsymbol{A}(X - \check{X}) = -\boldsymbol{G}(\check{X})$
        for $X - \check{X} \subset \boldsymbol{X1}$
    IF $\boldsymbol{X1} + \check{X} \subset$ Interior $(\boldsymbol{X1})$ THEN
        Have validated existence and uniqueness
        Done
    ELSE
        $\boldsymbol{X} := \boldsymbol{X} \cap \left(\boldsymbol{X1} + \check{X}\right)$
        $\check{X} :=$ midpoint $(\boldsymbol{X})$
    END IF
END DO

Box $\boldsymbol{X}$?

Where does the box $\boldsymbol{X}$ in which validation is attempted come from?

- Approximate optimizer $\check{X}$
- Verify existence in as small a box as possible
- Verify uniqueness in as large a box as possible

Enclosing the Solution

Runs until original box $\boldsymbol{X}$ is separated:

list $\mathcal{R}$	small boxes validated to enclose a unique local minimum; and
list $\mathcal{U}$	small boxes not validated either to enclose a minimum or NOT to enclose a minimum
discarded	regions where the global optimizer X^* cannot occur

or until time or memory resource limits are reached

Sensitivities

Learn more from you about sensitivities?
Tool: 1. Intervals. width $([x])$ cf width $(f([x]))$
Tool: 2. AD. $\dfrac{\partial \text{ output}}{\partial \text{ input}}$
Tool: Optimization. Max or Min #1 or #2
Super-sensitive: Narrow optima. Intervals don't miss
Insensitive: Broad, flat optima. Intervals enclose region

Optimization with Uncertainty
Noisy Measurements

Hard for interval techniques
What does it mean to evaluate with interval parameters?
Build statistical model of objective function based on sample points
Janos Pinter uses this to estimate Lipschitz constants, and uses these empirical Lipschitz constants in the same way we use interval values
Don Jones at GM also builds a statistical model of the function to estimate Lipschitz constants

Optimization with Uncertainty
Thick Parameters

Thick (uncertain) parameter values lead to thick objective values
Intervals give natural way to express
Validate technique does not miss anything
However, what is a Min?
Thick parameters lead to over-estimations leads to poor performance
Hard to throw anything away.

When should I consider this technology?

- Mission-critical problems or subproblems
- Feasibility
- Many local critical points
- Singular or near-singular solutions
- Uncertain parameters
- Bounded observation errors
- Model validation
- Speed

Limitations

- High dimensions
- Speed
- Recoding