The Role of Interval Linear Algebra in Global Optimization

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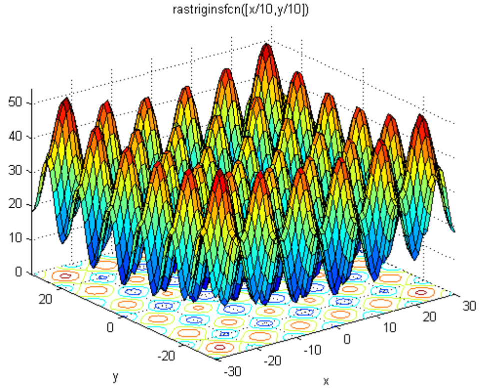
Example



One of the Rastrigin functions.

Global Optimization Questions

Questions

- Can we find global minimum?
- Can we prove that the found solution is optimal?
- Can we prove uniqueness?
- Can we handle roundoff errors?

Bad news

- **No**, there is no algorithm solving global optimization problems using operations $+, \times, \sin$. [Zhu, 2005]

  (From Matiyasevich's theorem solving the 10th Hilbert problem.)

Good news

- **Yes** (under certain assumption) by using *Interval Computations*.

Interval Computations

Notation

An interval matrix

$$\boldsymbol{A} := [\underline{A}, \overline{A}] = \{A \in \mathbb{R}^{m \times n} \mid \underline{A} \leq A \leq \overline{A}\}.$$

The center and radius matrices

$$A^c := \frac{1}{2}(\overline{A} + \underline{A}), \quad A^\Delta := \frac{1}{2}(\overline{A} - \underline{A}).$$

The set of all $m \times n$ interval matrices: $\mathbb{IR}^{m \times n}$.

Main Problem

Let $f : \mathbb{R}^n \mapsto \mathbb{R}^m$ and $\boldsymbol{x} \in \mathbb{IR}^n$. Determine the image

$$f(\boldsymbol{x}) = \{f(x) : x \in \boldsymbol{x}\},$$

or at least its tight interval enclosure.

Interval Arithmetic

Interval Arithmetic (proper rounding used when implemented)

For arithmetical operations $(+, -, \cdot, /)$, their images are readily computed

$$\boldsymbol{a} + \boldsymbol{b} = [\underline{a} + \underline{b}, \overline{a} + \overline{b}],$$

$$\boldsymbol{a} - \boldsymbol{b} = [\underline{a} - \overline{b}, \overline{a} - \underline{b}],$$

$$\boldsymbol{a} \cdot \boldsymbol{b} = [\min(\underline{a}\underline{b}, \underline{a}\overline{b}, \overline{a}\underline{b}, \overline{a}\overline{b}), \max(\underline{a}\underline{b}, \underline{a}\overline{b}, \overline{a}\underline{b}, \overline{a}\overline{b})],$$

$$\boldsymbol{a} / \boldsymbol{b} = [\min(\underline{a}/\underline{b}, \underline{a}/\overline{b}, \overline{a}/\underline{b}, \overline{a}/\overline{b}), \max(\underline{a}/\underline{b}, \underline{a}/\overline{b}, \overline{a}/\underline{b}, \overline{a}/\overline{b})], \quad 0 \notin \boldsymbol{b}.$$

Some basic functions $\boldsymbol{x}^2$, $\exp(\boldsymbol{x})$, $\sin(\boldsymbol{x})$, ..., too.

Can we evaluate every arithmetical expression on intervals?
Yes, but with overestimation in general due to dependencies.

Example (Evaluate $f(x) = x^2 - x$ on $\boldsymbol{x} = [-1, 2]$)

$$\boldsymbol{x}^2 - \boldsymbol{x} = [-1, 2]^2 - [-1, 2] = [-2, 5],$$

$$\boldsymbol{x}(\boldsymbol{x} - 1) = [-1, 2]([-1, 2] - 1) = [-4, 2],$$

$$(\boldsymbol{x} - \tfrac{1}{2})^2 - \tfrac{1}{4} = ([-1, 2] - \tfrac{1}{2})^2 - \tfrac{1}{4} = [-\tfrac{1}{4}, 2].$$

Global Optimization by Interval Techniques

Global optimization problem

Compute global (not just local!) optima to

$$\min \ f(x) \ \text{ subject to } \ g(x) \leq 0, \ h(x) = 0, \ x \in \boldsymbol{x}^0,$$

where $\boldsymbol{x}^0 \in \mathbb{IR}^n$ is an initial box.

Basic idea

- Split the initial box $\boldsymbol{x}^0$ into sub-boxes.
- If a sub-box does not contain an optimal solution, remove it. Otherwise split it into sub-boxes and repeat.

Interval Approach to Global Optimization

Branch & prune scheme

$\mathcal{L} := \{\boldsymbol{x}^0\}$, [set of boxes]
$c^* := \infty$, [upper bound on the minimal value]
while $\mathcal{L} \neq \emptyset$ **do**
  choose $\boldsymbol{x} \in \mathcal{L}$ and remove $\boldsymbol{x}$ from $\mathcal{L}$,
  contract $\boldsymbol{x}$,
  find a feasible point $x \in \boldsymbol{x}$ and update c^*,
  if $\max_i x_i^{\Delta} > \varepsilon$ **then**
    split $\boldsymbol{x}$ into sub-boxes and put them into $\mathcal{L}$,
  else
    give $\boldsymbol{x}$ to the output boxes,
  end if
end while

It is a rigorous method to enclose all global minima in a set of boxes.

Implementation Details

Which box to choose?

- the oldest one
- the one with the largest edge, i.e., for which $\max_i x_i^{\Delta}$ is maximal
- the one with minimal $\underline{f}(\boldsymbol{x})$.

How to divide the box?

- the widest edge
- the coordinate in which f varies possibly mostly (Walster, 1992; Ratz, 1992)

By Ratschek & Rokne (2009) there is no best strategy for splitting.

Contracting and Pruning $(\min f(x) \;\text{ s.t. }\; g(x) \le 0,\, h(x) = 0)$

Aim

Shrink $\boldsymbol{x}$ to a smaller box (or completely remove) such that no global minimum is removed.

Simple techniques

- if $0 \notin h_i(\boldsymbol{x})$ for some i, then remove $\boldsymbol{x}$
- if $0 < g_j(\boldsymbol{x})$ for some j, then remove $\boldsymbol{x}$
- if $0 < f'_{x_i}(\boldsymbol{x})$ for some i, then fix $\boldsymbol{x}_i := \underline{x}_i$
- if $0 > f'_{x_i}(\boldsymbol{x})$ for some i, then fix $\boldsymbol{x}_i := \overline{x}_i$

Optimality conditions

- employ the Fritz–John (or the Karush–Kuhn–Tucker) conditions

$$\begin{aligned} u_0 \nabla f(x) + u^T \nabla h(x) + v^T \nabla g(x) &= 0, \\ h(x) = 0, \quad v_\ell g_\ell(x) = 0 \;\forall \ell, \quad \|(u_0, u, v)\| &= 1. \end{aligned}$$

- solve by the Interval Newton method

Inside the feasible region

Suppose there are no equality constraints and $g_j(\boldsymbol{x}) < 0\ \forall j$.

- (monotonicity test) if $0 \notin f'_{x_i}(\boldsymbol{x})$ for some i, then remove $\boldsymbol{x}$
- apply the Interval Newton method to the additional constraint $\nabla f(x) = 0$
- (nonconvexity test) if the interval Hessian $\nabla^2 f(\boldsymbol{x})$ contains no positive semidefinite matrix, then remove $\boldsymbol{x}$

Contracting and Pruning

Constraint propagation

Iteratively reduce domains for variables such that no feasible solution is removed by handling the relations and the domains.

Example

Consider the constraint

$$x + yz = 7, \quad x \in [0, 3],\ y \in [3, 5],\ z \in [2, 4]$$

- express x

  $$x = 7 - yz \in 7 - [3, 5][2, 4] = [-13, 1]$$

  thus, the domain for x is $[0, 3] \cap [-13, 1] = [0, 1]$

- express y

  $$y = (7 - x)/z \in (7 - [0, 1])/[2, 4] = [1.5,\ 3.5]$$

  thus, the domain for y is $[3, 5] \cap [1.5,\ 3.5] = [3,\ 3.5]$

Lower and Upper Bounds

For each Branch & Bound algorithm are essential:

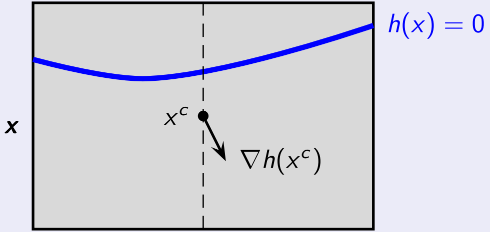
- tight upper bounds
- tight lower bounds

Upper Bounds – Feasibility Test

Aim

Find a feasible point x^*, and update $c^* := \min(c^*, f(x^*))$.

- if no equality constraints, take e.g. $x^* := x^c$
- if k equality constraints, fix $n - k$ variables $x_i := x_i^c$ and solve system of equations by the interval Newton method
- if $k = 1$, fix the variables corresponding to the smallest absolute values in $\nabla h(x^c)$



Upper Bounds – Feasibility Test

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- if k equality constraints, fix $n - k$ variables $x_i := x_i^c$ and solve system of equations by the interval Newton method
- if $k = 1$, fix the variables corresponding to the smallest absolute values in $\nabla h(x^c)$
- in general, if $k > 1$, transform the matrix $\nabla h(x^c)$ to a row echelon form by using a complete pivoting, and fix components corresponding to the right most columns
- we can include $f(x) \leq c^*$ to the constraints

Lower Bounds

Aim

Given a box $\boldsymbol{x} \in \mathbb{IR}^n$, determine a lower bound to $\underline{f}(\boldsymbol{x})$.

Why?

- if $\underline{f}(\boldsymbol{x}) > c^*$, we can remove $\boldsymbol{x}$
- minimum over all boxes gives a lower bound on the optimal value

Methods

- interval arithmetic
- mean value form
- Lipschitz constant approach
- αBB algorithm
- ...

Intermezzo – Eigenvalues of Symmetric Interval Matrices

A symmetric interval matrix

$$\boldsymbol{A}^S := \{A \in \boldsymbol{A} \colon A = A^T\}.$$

Without loss of generality assume that $\underline{A} = \underline{A}^T$, $\overline{A} = \overline{A}^T$, and $\boldsymbol{A}^S \neq \emptyset$.

Eigenvalues of a symmetric interval matrix

Eigenvalues of a symmetric $A \in \mathbb{R}^{n \times n}$: $\lambda_1(A) \geq \cdots \geq \lambda_n(A)$.

Eigenvalue sets of $\boldsymbol{A}^S$ are compact intervals

$$\boldsymbol{\lambda}_i(\boldsymbol{A}^S) := \left\{\lambda_i(A) \colon A \in \boldsymbol{A}^S\right\}, \quad i = 1, \ldots, n.$$

Theorem

Checking whether $0 \in \boldsymbol{\lambda}_i(\boldsymbol{A}^S)$ *for some* $i = 1, \ldots, n$ *is NP-hard.*

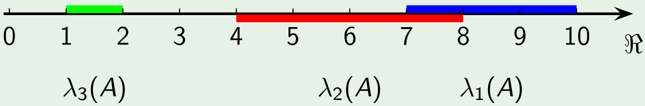
Eigenvalues – An Example

Example

Let

$$A \in \boldsymbol{A} = \begin{pmatrix} [1,2] & 0 & 0 \\ 0 & [7,8] & 0 \\ 0 & 0 & [4,10] \end{pmatrix}$$

What are the eigenvalue sets?
We have $\boldsymbol{\lambda}_1(\boldsymbol{A}^S) = [7,10]$, $\boldsymbol{\lambda}_2(\boldsymbol{A}^S) = [4,8]$ and $\boldsymbol{\lambda}_3(\boldsymbol{A}^S) = [1,2]$.



Eigenvalue sets are compact intervals. They may intersect or equal.

Eigenvalues – Some Exact Bounds

Theorem (Hertz, 1992)

We have

$$\overline{\lambda}_1(\boldsymbol{A}^S) = \max_{z \in \{\pm 1\}^n} \lambda_1(A^c + \operatorname{diag}(z) A^\Delta \operatorname{diag}(z)),$$
$$\underline{\lambda}_n(\boldsymbol{A}^S) = \min_{z \in \{\pm 1\}^n} \lambda_n(A^c - \operatorname{diag}(z) A^\Delta \operatorname{diag}(z)).$$

Theorem

$\underline{\lambda}_1(\boldsymbol{A}^S)$ *and* $\overline{\lambda}_n(\boldsymbol{A}^S)$ *are polynomially computable by semidefinite programming with arbitrary precision.*

Proof.

We have

$$\overline{\lambda}_n(\boldsymbol{A}^S) = \max\ \alpha \ \text{ subject to }\ A - \alpha I_n \text{ is positive semidefinite},\ A \in \boldsymbol{A}^S.$$

$\square$

Eigenvalues – Easy Cases and Enclosures

Theorem

1. *If A^c is essentially non-negative, i.e., $A^c_{ij} \geq 0 \ \forall i \neq j$, then*
$$\overline{\lambda}_1(\boldsymbol{A}^S) = \lambda_1(\overline{A}).$$
2. *If A^Δ is diagonal, then*
$$\overline{\lambda}_1(\boldsymbol{A}^S) = \lambda_1(\overline{A}), \quad \underline{\lambda}_n(\boldsymbol{A}^S) = \lambda_n(\underline{A}).$$

Theorem

We have
$$\boldsymbol{\lambda}_i(\boldsymbol{A}^S) \subseteq [\lambda_i(A^c) - \rho(A^\Delta), \lambda_i(A^c) + \rho(A^\Delta)], \quad i = 1, \ldots, n.$$

Lower Bounds: αBB algorithm

Special cases: bilinear terms

For every $y \in \boldsymbol{y} \in \mathbb{IR}$ and $z \in \boldsymbol{z} \in \mathbb{IR}$ we have

$$yz \geq \max\{\underline{y}z + \underline{z}y - \underline{y}\underline{z},\ \overline{y}z + \overline{z}y - \overline{y}\overline{z}\}.$$

αBB algorithm (Androulakis, Maranas & Floudas, 1995)

- Consider an underestimator $g(x) \leq f(x)$ in the form

$$g(x) := f(x) + \alpha(x - \underline{x})^T(x - \overline{x}), \quad \text{where } \alpha \geq 0.$$

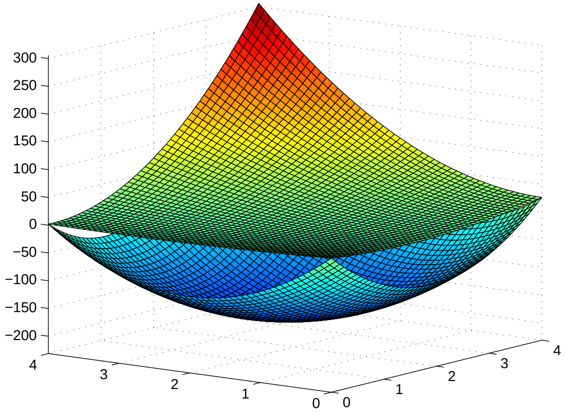
- We want $g(x)$ to be convex to easily determine $\underline{g}(\boldsymbol{x}) \leq \underline{f}(\boldsymbol{x})$.
- In order that $g(x)$ is convex, its Hessian

$$\nabla^2 g(x) = \nabla^2 f(x) + 2\alpha I_n$$

must be positive semidefinite on $x \in \boldsymbol{x}$. Thus we put

$$\alpha := -\tfrac{1}{2} \cdot \underline{\lambda}_{\min}(\nabla^2 f(\boldsymbol{x})).$$

Illustration of a Convex Underestimator



Function $f(x)$ and its convex underestimator $g(x)$.

Examples

Example (The COPRIN examples, 2007, precision $\sim 10^{-6}$)

- tf12 (origin: COCONUT, solutions: 1, computation time: 60 s)

$$\begin{aligned} \min\ & x_1 + \tfrac{1}{2}x_2 + \tfrac{1}{3}x_3 \\ \text{s.t.}\ & -x_1 - \tfrac{i}{m}x_2 - (\tfrac{i}{m})^2 x_3 + \tan(\tfrac{i}{m}) \le 0, \quad i = 1, \dots, m \ (m = 101). \end{aligned}$$

- o32 (origin: COCONUT, solutions: 1, computation time: 2.04 s)

$$\min\ 37.293239x_1 + 0.8356891x_5x_1 + 5.3578547x_3^2 - 40792.141$$

$$\begin{aligned} \text{s.t.}\quad -0.0022053x_3x_5 + 0.0056858x_2x_5 + 0.0006262x_1x_4 - 6.665593 &\le 0, \\ -0.0022053x_3x_5 - 0.0056858x_2x_5 - 0.0006262x_1x_4 - 85.334407 &\le 0, \\ 0.0071317x_2x_5 + 0.0021813x_3^2 + 0.0029955x_1x_2 - 29.48751 &\le 0, \\ -0.0071317x_2x_5 - 0.0021813x_3^2 - 0.0029955x_1x_2 + 9.48751 &\le 0, \\ 0.0047026x_3x_5 + 0.0019085x_3x_4 + 0.0012547x_1x_3 - 15.699039 &\le 0, \\ -0.0047026x_3x_5 - 0.0019085x_3x_4 - 0.0012547x_1x_3 + 10.699039 &\le 0. \end{aligned}$$

- Rastrigin (origin: Myatt (2004), solutions: 1 (approx.), time: 2.07 s)

$$\min\ 10n + \textstyle\sum_{j=1}^{n}(x_j - 1)^2 - 10\cos(2\pi(x_j - 1))$$

where $n = 10$, $x_j \in [-5.12, 5.12]$.

References

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Complete search in continuous global optimization and constraint satisfaction.
Acta Numer., 13:271–369, 2004.

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Wiley, Chichester, 2007.

Rigorous Global Optimization Software

- *GlobSol* (by R. Baker Kearfott), written in Fortran 95, open-source
  `http://interval.louisiana.edu/`
- *Alias* (by COPRIN team), A C++ library with Maple interface,
  `http://www-sop.inria.fr/coprin/logiciels/ALIAS/`
- *IBEX* (by G. Chabert, B. Neveu, J. Ninin and others),
  an open-source interval C++ library, `http://www.ibex-lib.org/`
- *COCONUT Environment*, open-source C++ classes
  `http://www.mat.univie.ac.at/~coconut/coconut-environment/`
- *GLOBAL* (by Tibor Csendes), for Matlab / Intlab, free for academic
  `http://www.inf.u-szeged.hu/~csendes/linkek_en.html`
- *PROFIL / BIAS* (by O. Knüppel et al.), free C++ class
  `http://www.ti3.tu-harburg.de/Software/PROFILEnglisch.html`

See also

- *C.A. Floudas* (`http://titan.princeton.edu/tools/`)
- *A. Neumaier* (`http://www.mat.univie.ac.at/~neum/glopt.html`)