Global Optimization by Interval Analysis

Milan Hladík

Department of Applied Mathematics,
Faculty of Mathematics and Physics,
Charles University in Prague,
Czech Republic,
http://kam.mff.cuni.cz/~hladik/

Seminar on Stochastic Programming and Approximation
November 29, 2012

Outline

- Introduction to interval computation
  - interval arithmetic
  - interval functions
  - interval linear equations
  - nonlinear equations (the Interval Newton method)
  - eigenvalues of interval matrices
- Global optimization
  - interval approach (branch & prune scheme)
  - contracting and pruning boxes
  - lower and upper bounds
  - $\alpha$-BB algorithm
Interval Computations

Notation

An interval matrix

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

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: \( \mathbb{I} \mathbb{R}^{m \times n} \).

Main Problem

Let \( f : \mathbb{R}^n \mapsto \mathbb{R}^m \) and \( x \in \mathbb{I} \mathbb{R}^n \). Determine the image

\[ f(x) = \{ f(x) : x \in x \} . \]

Interval Arithmetic

For arithmetical operations (+, −, ·, ÷), their images are readily computed

\[
\begin{align*}
\mathbf{a} + \mathbf{b} &= [\underline{a} + \underline{b}, \overline{a} + \overline{b}], \\
\mathbf{a} - \mathbf{b} &= [\underline{a} - \overline{b}, \overline{a} - \underline{b}], \\
\mathbf{a} \cdot \mathbf{b} &= [\min(\underline{ab}, \underline{a}\overline{b}, \overline{a}b, \overline{a}\overline{b}), \max(\underline{ab}, \underline{a}\underline{b}, \overline{a}b, \overline{a}\overline{b})], \\
\mathbf{a} \div \mathbf{b} &= [\min(\underline{a} \div \underline{b}, \underline{a} \div \overline{b}, \overline{a} \div \underline{b}, \overline{a} \div \overline{b}), \max(\underline{a} \div \underline{b}, \underline{a} \div \overline{b}, \overline{a} \div \underline{b}, \overline{a} \div \overline{b})].
\end{align*}
\]

Some basic functions \( x^2, \exp(x), \sin(x), \ldots \), too.

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

Example

\[
\begin{align*}
x^2 - x &= [-1, 2]^2 - [-1, 2] = [-2, 5], \\
x(x - 1) &= [-1, 2][-1, 2] - 1 = [-4, 2], \\
(x - \frac{1}{2})^2 - \frac{1}{4} &= (([-1, 2] - \frac{1}{2})^2 - \frac{1}{4} = [-\frac{1}{4}, 2].
\end{align*}
\]
Mean value form

Theorem

Let \( f : \mathbb{R}^n \to \mathbb{R}, \ x \in \mathbb{R}^n \) and \( a \in x \). Then
\[
f(x) \subseteq f(a) + \nabla f(x)^T(x - a),
\]

Proof.

By the mean value theorem, for any \( x \in x \) there is \( c \in x \) such that
\[
f(x) = f(a) + \nabla f(c)^T(x - a) \in f(a) + \nabla f(x)^T(x - a).
\]

Improvements
- successive mean value form
\[
f(x) \subseteq f(a) + f'_{x_1}(x_1, a_2, \ldots, a_n)(x_1 - a_1) + f'_{x_2}(x_1, x_2, a_3 \ldots, a_n)(x_2 - a_2) + \ldots + f'_{x_n}(x_1, \ldots, x_{n-1}, x_n)(x_n - a_n).
\]
- replace derivatives by slopes

Interval Linear Equations

Interval linear equations

Let \( A \in \mathbb{IR}^{m \times n} \) and \( b \in \mathbb{IR}^m \). The family of systems
\[
Ax = b, \quad A \in A, \ b \in b.
\]
is called interval linear equations and abbreviated as \( Ax = b \).

Solution set

The solution set is defined
\[
\Sigma := \{ x \in \mathbb{R}^n : \exists A \in A \exists b \in b : Ax = b \}.
\]

Theorem (Oettli–Prager, 1964)

The solution set \( \Sigma \) is a non-convex polyhedral set described by
\[
|A^c x - b^c| \leq A^\Delta |x| + b^\Delta.
\]
Interval Linear Equations

Example (Barth & Nuding, 1974))

\[
\begin{pmatrix}
[2, 4] & [-2, 1] \\
[-1, 2] & [2, 4]
\end{pmatrix}
\begin{pmatrix}
x_1 \\
x_2
\end{pmatrix}
= 
\begin{pmatrix}
[-2, 2] \\
[-2, 2]
\end{pmatrix}
\]

Since \( \Sigma \) is hard to determine and deal with, we seek for enclosures \( x \in \mathbb{IR}^n \) such that \( \Sigma \subseteq x \).

Many methods for enclosures exists, usually employ preconditioning.

Preconditioning (Hansen, 1965)

Let \( R \in \mathbb{R}^{n \times n} \). The preconditioned system of equations:

\[
(RA)x = Rb.
\]

Remark

- the solution set of the preconditioned systems contains \( \Sigma \)
- usually, we use \( R \approx (A^c)^{-1} \)
- then we can compute the best enclosure (Hansen, 1992, Bliek, 1992, Rohn, 1993)
Interval Linear Equations

Example (Barth & Nuding, 1974))

\[
\begin{bmatrix}
  [2, 4] & [-2, 1] \\
  [-1, 2] & [2, 4]
\end{bmatrix}
\begin{bmatrix}
  x_1 \\
  x_2
\end{bmatrix}
= 
\begin{bmatrix}
  [-2, 2] \\
  [-2, 2]
\end{bmatrix}
\]

\[
\begin{bmatrix}
  x_1 \\
  x_2
\end{bmatrix}
= 
\begin{bmatrix}
  [6, 7] \\
  [1, 2]
\end{bmatrix}
\begin{bmatrix}
  [2, 3] \\
  [-4, 5]
\end{bmatrix}
= 
\begin{bmatrix}
  [6, 8] \\
  [-7, 9]
\end{bmatrix}
\]
Nonlinear Equations

System of nonlinear equations
Let \( f : \mathbb{R}^n \rightarrow \mathbb{R}^n \). Solve
\[ f(x) = 0, \quad x \in \mathbb{x}, \]
where \( \mathbb{x} \in \mathbb{IR}^n \) is an initial box.

Interval Newton method (Moore, 1966)
- letting \( x^0 \in \mathbb{x} \), the Interval Newton operator reads
  \[ N(x) := x^0 - \nabla f(x)^{-1} f(x^0) \]
- \( N(x) \) is computed from interval linear equations
  \[ \nabla f(x)(x^0 - N(x)) = f(x^0). \]
- iterations: \( x := x \cap N(x) \)
- fast (loc. quadratically convergent) and rigorous (omits no root in \( \mathbb{x} \))
- if \( N(x) \subseteq \text{int} \mathbb{x} \), then there is a unique root in \( \mathbb{x} \)

Eigenvalues of Interval Matrices

Eigenvalues
- For \( A \in \mathbb{R}^{n \times n} \), \( A = A^T \), denote its eigenvalues \( \lambda_1(A) \geq \cdots \geq \lambda_n(A) \).
- Let for \( A \in \mathbb{IR}^{n \times n} \), denote its eigenvalue sets
  \[ \lambda_i(A) = \{ \lambda_i(A) : A \in A, \ A = A^T \}, \quad i = 1, \ldots, n. \]

Theorem
- Checking whether \( 0 \in \lambda_i(A) \) for some \( i = 1, \ldots, n \) is NP-hard.
- We have the following enclosures for the eigenvalue sets
  \[ \lambda_i(A) \subseteq [\lambda_i(A^c) - \rho(A^\Delta), \lambda_i(A^c) + \rho(A^\Delta)], \quad i = 1, \ldots, n. \]
- By Hertz (1992)
  \[ \bar{\lambda}_1(A) = \max_{z \in \{\pm 1\}^n} \lambda_1(A^c + \text{diag}(z) A^\Delta \text{diag}(z)), \]
  \[ \underline{\lambda}_n(A) = \min_{z \in \{\pm 1\}^n} \lambda_n(A^c - \text{diag}(z) A^\Delta \text{diag}(z)). \]
Global Optimization

Global optimization problem

Compute global (not just local!) optima to

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

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

Theorem (Zhu, 2005)

There is no algorithm solving global optimization problems using operations +, \( \times \), \( \sin \).

Proof.

From Matiyasevich’s theorem solving the 10th Hilbert problem.

Remark

Using the arithmetical operations only, the problem is decidable by Tarski’s theorem (1951).

Interval Approach to Global Optimization

Branch & prune scheme

1: \( \mathcal{L} := \{x^0\} \), \quad \text{[set of boxes]}
2: \( c^* := \infty \), \quad \text{[upper bound on the minimal value]}
3: \textbf{while } \mathcal{L} \neq \emptyset \textbf{ do}
4: \quad \text{choose } x \in \mathcal{L} \text{ and remove } x \text{ from } \mathcal{L},
5: \quad \text{contract } x,
6: \quad \text{find a feasible point } x \in x \text{ and update } c^*,
7: \quad \textbf{if } \max_{i} x_i^A > \varepsilon \textbf{ then}
8: \quad \quad \text{split } x \text{ into sub-boxes and put them into } \mathcal{L},
9: \quad \textbf{else}
10: \quad \quad \text{give } x \text{ to the output boxes},
11: \quad \textbf{end if}
12: \textbf{end while}

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

### 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 \( f(x) \).

### Division Directions

#### How to divide the box?
- Take the widest edge of \( x \), that is
  \[
  k := \arg \max_{i=1,...,n} x_i^\Delta.
  \]
- (Walster, 1992) Choose a coordinate in which \( f \) varies possibly mostly
  \[
  k := \arg \max_{i=1,...,n} f'(x_i)(x)^\Delta x_i^\Delta.
  \]
- (Ratz, 1992) It is similar to the previous one, but uses
  \[
  k := \arg \max_{i=1,...,n} (f'(x) x_i)^\Delta.
  \]

#### Remarks
- by Ratschek & Rokne (2009) there is no best strategy for splitting
- combine several of them
- the splitting strategy influences the overall performance
## Contracting and Pruning

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

### Simple techniques
- if $0 \not\in h_i(\mathbf{x})$ for some $i$, then remove $\mathbf{x}$
- if $0 < g_j(\mathbf{x})$ for some $j$, then remove $\mathbf{x}$
- if $0 < f'_{x_i}(\mathbf{x})$ for some $i$, then fix $x_i := \overline{x}_i$
- if $0 > f'_{x_i}(\mathbf{x})$ for some $i$, then fix $x_i := \underline{x}_i$

### Optimality conditions
- employ the Fritz–John (or the Karush–Kuhn–Tucker) conditions
  \[ u_0 \nabla f(\mathbf{x}) + u^T \nabla h(\mathbf{x}) + v^T \nabla g(\mathbf{x}) = 0, \]
  \[ h(\mathbf{x}) = 0, \quad v_\ell g_\ell(\mathbf{x}) = 0 \quad \forall \ell, \quad \|(u_0, u, v)\| = 1. \]
- solve by the Interval Newton method

### Inside the feasible region
Suppose there are no equality constraints and $g_j(\mathbf{x}) < 0 \quad \forall j$.
- (monotonicity test) if $0 \not\in f'_{x_i}(\mathbf{x})$ for some $i$, then remove $\mathbf{x}$
- apply the Interval Newton method to the additional constraint $\nabla f(\mathbf{x}) = 0$
- (nonconvexity test) if the interval Hessian $\nabla^2 f(\mathbf{x})$ contains no positive semidefinite matrix, then remove $\mathbf{x}$
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
\[ x + yz = 7, \quad x \in [0, 3], \quad y \in [3, 5], \quad z \in [2, 4] \]

- eliminate \( x \)
  \[ x = 7 - yz \in 7 - [3, 5][2, 4] = [-13, 1] \]
  thus, the domain for \( x \) is \([0, 3] \cap [-13, 1] = [0, 1]\)

- eliminate \( y \)
  \[ y = (7 - x)/z \in (7 - [0, 1])/[2, 4] = [1.5, 3.5] \]
  thus, the domain for \( y \) is \([3, 5] \cap [1.5, 3.5] = [3, 3.5]\)

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 \( \nabla h(x^c) \)
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 $\nabla h(x^c)$
- 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 $x \in \mathbb{R}^n$, determine a lower bound to $f(x)$.

Why?
- if $f(x) > c^*$, we can remove $x$
- minimum over all boxes gives a lower bound on the optimal value

Methods
- interval arithmetic
- mean value form
- Lipschitz constant approach
- $\alpha$BB algorithm
- ...
Lower Bounds: $\alpha$BB algorithm

Special cases: bilinear terms

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

$$yz \geq \max\{yz + zy - yz, yz + zy - yz\}.$$

$\alpha$BB algorithm (Androulakis, Maranas & Floudas, 1995)

- Consider an underestimator $g(x) \leq f(x)$ in the form
  $$g(x) := f(x) + \alpha(x - \overline{x})^T(x - \overline{x}), \quad \text{where } \alpha \geq 0.$$

- We want $g(x)$ to be convex to easily determine $g(x) \leq f(x)$.

- 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 $x \in \mathbb{x}$. Thus we put

$$\alpha := -\frac{1}{2}\lambda_{\min}(\nabla^2 f(x)).$$

Examples

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

- **tf12** (origin: COCONUT, solutions: 1, computation time: 60 s)
  $$\min x_1 + \frac{1}{2}x_2 + \frac{1}{3}x_3$$
  $$\text{s.t. } -x_1 - \frac{i}{m}x_2 - (\frac{i}{m})^2x_3 + \tan(\frac{i}{m}) \leq 0, \quad i = 1, \ldots, m \quad (m = 101).$$

- **o32** (origin: COCONUT, solutions: 1, computation time: 2.04 s)
  $$\min 37.293239x_1 + 0.8356891x_5x_1 + 5.3578547x_3^2 - 40792.141$$
  $$\text{s.t. } -0.0022053x_3x_5 + 0.0056858x_2x_5 + 0.0006262x_1x_4 - 6.665593 \leq 0,$$
  $$-0.0022053x_3x_5 - 0.0056858x_2x_5 - 0.0006262x_1x_4 - 85.334407 \leq 0,$$
  $$0.0071317x_2x_5 + 0.0021813x_3^2 + 0.0029955x_1x_2 - 29.48751 \leq 0,$$
  $$-0.0071317x_2x_5 - 0.0021813x_3^2 - 0.0029955x_1x_2 + 9.48751 \leq 0,$$
  $$0.0047026x_3x_5 + 0.0019085x_3x_4 + 0.0012547x_1x_3 - 15.699039 \leq 0,$$
  $$-0.0047026x_3x_5 - 0.0019085x_3x_4 - 0.0012547x_1x_3 + 10.699039 \leq 0.$$

- **Rastrigin** (origin: Myatt (2004), solutions: 1 (approx.), time: 2.07 s)
  $$\min 10n + \sum_{j=1}^{n}(x_j - 1)^2 - 10\cos(2\pi(x_j - 1))$$
  where $n = 10$, $x_j \in [-5.12, 5.12]$. 
Examples

One of the Rastrigin functions.

References


Rigorous global optimization software

- *GlobSol* (by R. Baker Kearfott), written in Fortran 95, open-source exist conversions from AMPL and GAMS representations, http://interval.louisiana.edu/
- *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 purposes
  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)