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/

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Outline

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

Interval Computations

Notation

An interval matrix

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

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 $\mathbf{x} \in \mathbb{IR}^n$. Determine the image

$$f(\mathbf{x}) = \{f(x) : x \in \mathbf{x}\}.$$

Interval Arithmetic

Interval Arithmetic

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

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

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

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

Example

$$\begin{aligned}
\mathbf{x}^2 - \mathbf{x} &= [-1, 2]^2 - [-1, 2] = [-2, 5],\\
\mathbf{x}(\mathbf{x} - 1) &= [-1, 2]([-1, 2] - 1) = [-4, 2],\\
(\mathbf{x} - \tfrac{1}{2})^2 - \tfrac{1}{4} &= ([-1, 2] - \tfrac{1}{2})^2 - \tfrac{1}{4} = [-\tfrac{1}{4}, 2].
\end{aligned}$$

Mean value form

Theorem

Let $f : \mathbb{R}^n \mapsto \mathbb{R}$, $\mathbf{x} \in \mathbb{IR}^n$ and $a \in \mathbf{x}$. Then

$$f(\mathbf{x}) \subseteq f(a) + \nabla f(\mathbf{x})^T(\mathbf{x} - a),$$

Proof.

By the mean value theorem, for any $x \in \mathbf{x}$ there is $c \in \mathbf{x}$ such that

$$f(x) = f(a) + \nabla f(c)^T(x - a) \in f(a) + \nabla f(\mathbf{x})^T(\mathbf{x} - a). \qquad \square$$

Improvements

- successive mean value form

$$\begin{aligned} f(\mathbf{x}) \subseteq f(a) &+ f'_{x_1}(\mathbf{x}_1, a_2, \dots, a_n)(\mathbf{x}_1 - a_1) \\ &+ f'_{x_2}(\mathbf{x}_1, \mathbf{x}_2, a_3 \dots, a_n)(\mathbf{x}_2 - a_2) + \dots \\ &+ f'_{x_n}(\mathbf{x}_1, \dots, \mathbf{x}_{n-1}, \mathbf{x}_n)(\mathbf{x}_n - a_n). \end{aligned}$$

- replace derivatives by slopes

Interval Linear Equations

Interval linear equations

Let $\mathbf{A} \in \mathbb{IR}^{m \times n}$ and $\mathbf{b} \in \mathbb{IR}^m$. The family of systems

$$Ax = b, \quad A \in \mathbf{A}, \; b \in \mathbf{b}.$$

is called interval linear equations and abbreviated as $\mathbf{A}x = \mathbf{b}$.

Solution set

The solution set is defined

$$\Sigma := \{x \in \mathbb{R}^n : \exists A \in \mathbf{A} \exists b \in \mathbf{b} : Ax = b\}.$$

Theorem (Oettli–Prager, 1964)

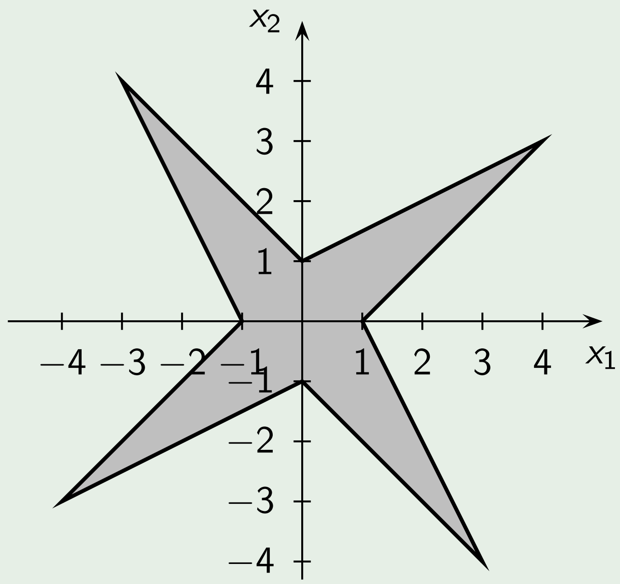
The solution set Σ is a non-convex polyhedral set described by

$$|A^c x - b^c| \le A^\Delta |x| + b^\Delta.$$

Interval Linear Equations

Example (Barth & Nuding, 1974))

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



Interval Linear Equations

Enclosure

Since Σ is hard to determine and deal with, we seek for enclosures

$$\mathbf{x} \in \mathbb{IR}^n \text{ such that } \Sigma \subseteq \mathbf{x}.$$

Many methods for enclosures exists, usually employ preconditioning.

Preconditioning (Hansen, 1965)

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

$$(R\mathbf{A})x = R\mathbf{b}.$$

Remark

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

Interval Linear Equations

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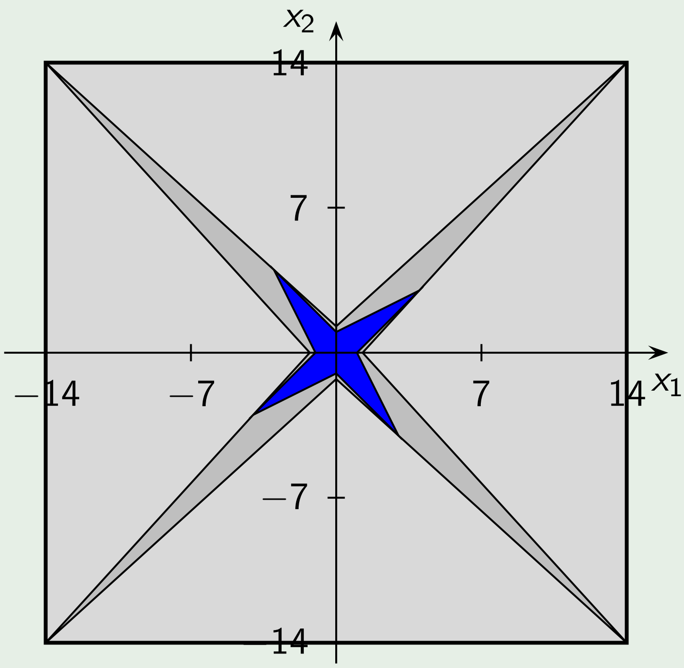
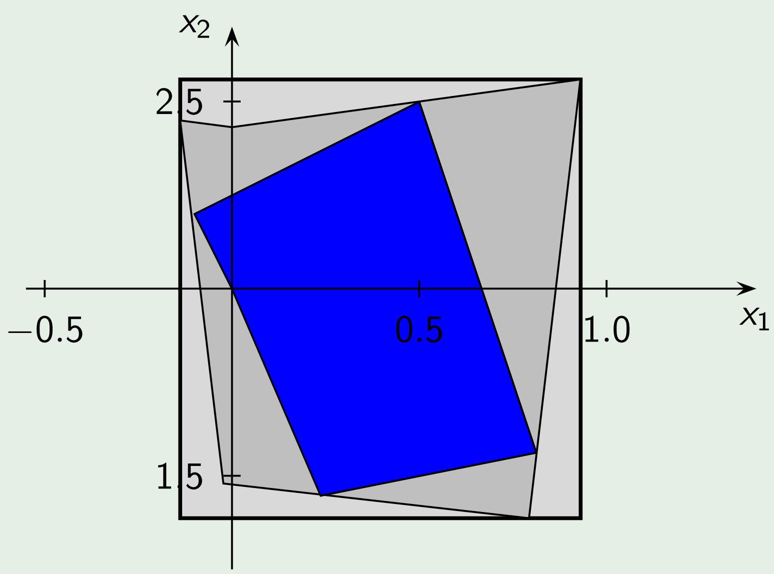


Interval Linear Equations

Example (typical case)

$$\begin{pmatrix} [6,7] & [2,3] \\ [1,2] & -[4,5] \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} [6,8] \\ -[7,9] \end{pmatrix}$$



Nonlinear Equations

System of nonlinear equations

Let $f : \mathbb{R}^n \mapsto \mathbb{R}^n$. Solve

$$f(x) = 0, \quad x \in \mathbf{x},$$

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

Interval Newton method (Moore, 1966)

- letting $x^0 \in \mathbf{x}$, the Interval Newton operator reads

$$N(\mathbf{x}) := x^0 - \nabla f(\mathbf{x})^{-1} f(x^0)$$

- $N(\mathbf{x})$ is computed from interval linear equations

$$\nabla f(\mathbf{x})\big(x^0 - N(\mathbf{x})\big) = f(x^0).$$

- iterations: $\quad \mathbf{x} := \mathbf{x} \cap N(\mathbf{x})$
- fast (loc. quadratically convergent) and rigorous (omits no root in $\mathbf{x}$)
- if $N(\mathbf{x}) \subseteq \operatorname{int} \mathbf{x}$, then there is a unique root in $\mathbf{x}$

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 $\mathbf{A} \in \mathbb{IR}^{n \times n}$, denote its eigenvalue sets

$$\boldsymbol{\lambda}_i(\mathbf{A}) = \{\lambda_i(A) \colon A \in \mathbf{A},\ A = A^T\}, \quad i = 1, \dots, n.$$

Theorem

- *Checking whether* $0 \in \boldsymbol{\lambda}_i(\mathbf{A})$ *for some* $i = 1, \dots, n$ *is NP-hard.*
- *We have the following enclosures for the eigenvalue sets*

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

- *By Hertz (1992)*

$$\overline{\lambda}_1(\mathbf{A}) = \max_{z \in \{\pm 1\}^n} \lambda_1(A^c + \operatorname{diag}(z)\, A^\Delta \operatorname{diag}(z)),$$

$$\underline{\lambda}_n(\mathbf{A}) = \min_{z \in \{\pm 1\}^n} \lambda_n(A^c - \operatorname{diag}(z)\, A^\Delta \operatorname{diag}(z)).$$

Global Optimization

Global optimization problem

Compute global (not just local!) optima to

$$\min f(x) \quad \text{subject to} \quad g(x) \le 0,\ \ h(x) = 0,\ \ x \in \mathbf{x}^0,$$

where $\mathbf{x}^0 \in \mathbb{IR}^n$ 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

```
L := {x^0},                                       [set of boxes]
c* := ∞,                       [upper bound on the minimal value]
while L ≠ ∅ do
   choose x ∈ L and remove x from L,
   contract x,
   find a feasible point x ∈ x and update c*,
   if max_i x_i^Δ > ε then
      split x into sub-boxes and put them into L,
   else
      give x to the output boxes,
   end if
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 $\underline{f}(\mathbf{x})$.

Division Directions

How to divide the box?

1. Take the widest edge of $\mathbf{x}$, that is
$$k := \arg \max_{i=1,\dots,n} x_i^\Delta.$$
2. (Walster, 1992) Choose a coordinate in which f varies possibly mostly
$$k := \arg \max_{i=1,\dots,n} f'_{x_i}(\mathbf{x})^\Delta x_i^\Delta.$$
3. (Ratz, 1992) It is similar to the previous one, but uses
$$k := \arg \max_{i=1,\dots,n} (f'_{x_i}(\mathbf{x})\mathbf{x}_i)^\Delta.$$

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

Optimality conditions

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

$$u_0 \nabla f(x) + u^T \nabla h(x) + v^T \nabla g(x) = 0,$$
$$h(x) = 0, \quad v_\ell g_\ell(x) = 0 \ \forall \ell, \quad \|(u_0, u, v)\| = 1.$$

- solve by the Interval Newton method

Contracting and Pruning

Inside the feasible region

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

- (monotonicity test) if $0 \notin f'_{x_i}(\mathbf{x})$ for some i, then remove $\mathbf{x}$
- apply the Interval Newton method to the additional constraint $\nabla f(x) = 0$
- (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

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

- 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

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

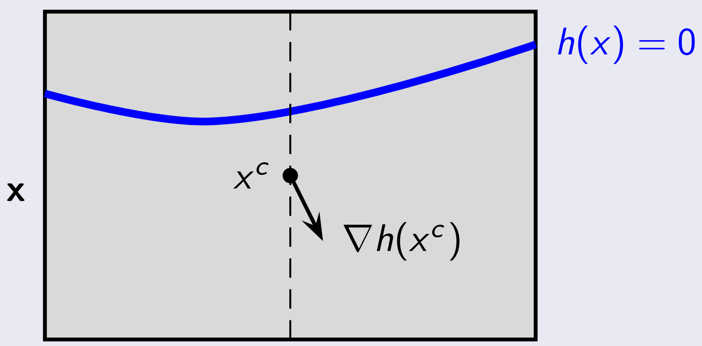
  thus, the domain for y is $[3, 5] \cap [1.5,\ 3.5] = [3,\ 3.5]$

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

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- 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 $f(x) \le c^*$ to the constraints

Lower Bounds

Aim

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

Why?

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

Methods

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

Lower Bounds: αBB algorithm

Special cases: bilinear terms

For every $y \in \mathbf{y} \in \mathbb{IR}$ and $z \in \mathbf{z} \in \mathbb{IR}$ 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 $\underline{g}(\mathbf{x}) \leq \underline{f}(\mathbf{x})$.
- 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 $x \in \mathbf{x}$. Thus we put

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

Examples

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

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

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

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

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

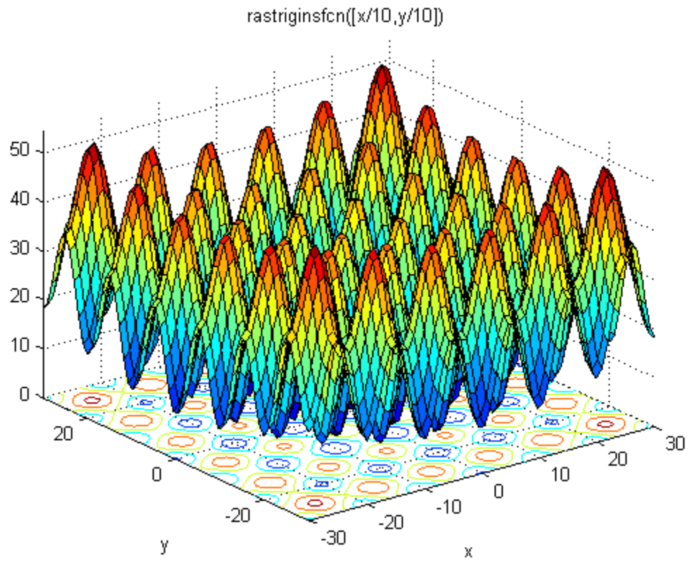
$$\begin{aligned} \text{s.t.}\quad -0.0022053x_3x_5 + 0.0056858x_2x_5 + 0.0006262x_1x_4 - 6.665593 &\leq 0, \\ -0.0022053x_3x_5 - 0.0056858x_2x_5 - 0.0006262x_1x_4 - 85.334407 &\leq 0, \\ 0.0071317x_2x_5 + 0.0021813x_3^2 + 0.0029955x_1x_2 - 29.48751 &\leq 0, \\ -0.0071317x_2x_5 - 0.0021813x_3^2 - 0.0029955x_1x_2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

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

Examples



One of the Rastrigin functions.

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Software

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`)