Interval Analysis – Basics

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Interval Arithmetic

Function Evaluation

Centered Forms

Systems of Equations - general case

Systems of Equations - linear case

Introduction

- **Interval analysis** is one of the tools for global optimization.
- It combines **interval arithmetic** with analytic estimation techniques to obtain global information that is otherwise inaccessible.
- It can also be used for computer–assisted proofs using finite precision calculations, since it correctly accounts for rounding errors.
- Implementations: INTLAB, SUN Fortran

History

- 1960 developed by **Moore** for error control
- ≈1970 **McCormick** used interval arithmetic for optimization (a posteriori enclosures)
- ≈1980 **Hansen, Evtushenko** first global optimization application.
- since 1985 computer assisted proofs: Feigenbaum conjecture, chaos in molecules
- 1999 **Hales** solved Kepler's 300 years old conjecture on the densest packing of equal spheres using linear programming and interval analysis.

Interval Analysis in Global Optimization

- In the last few years several groups started to use interval analysis for deterministic global optimization.
- The most important developments are
  - Jansson/Knüppel (only for bound constraints)
  - INTOPT 90, GLOBSOL (Kearfott)
  - BARON (Sahinidis)
  - Numerica (Van Hentenryck)
  - αBB (Floudas)
  - GLOPT–2 (Neumaier)

Overview

- Interval Arithmetic
- Function Evaluation
- Centered Forms
- Systems of Equations − general case
- Systems of Equations − linear case

Intervals

- **Intervals** $[x]=[x,x]=[\check{x}-\mathrm{rad}[x],\check{x}+\mathrm{rad}[x]]$, where $\check{x}=\mathrm{mid}(x)=\frac{1}{2}(x+x)$ and $\mathrm{rad}[x]=\frac{1}{2}(x-x)$ can e.g. be interpreted as numbers not exactly known: $|x-\check{x}|\leq\mathrm{rad}[x]$
- The higher dimensional generalization is a **box** (interval vector) $[x]=\{x\in\mathbb{R}|x_i\in[x_i],i=1,\ldots,n\}$
- Point intervals (radius zero) will be identified with the unique number they contain $x\equiv[x,x]$

Interval Operations

- The arithmetic operations $+,-,*,/,\wedge$ are extended to intervals $[x]\circ[y]:=[\,]\{x\circ y|x\in[x],y\in[y]\}$, where $[\,]S$ denotes the smallest box containing the set S.
- Examples:
  - $[4,8]+[-3,2]=[1,10]$
  - $[-2,3]*[-1,2]=[-4,6]$
  - $[1,3]^{[2,4]}=[1,81]$
  - $[1,3]/[-1,2]=[-\infty,\infty]$

Elementary functions

- Elementary functions are extended to intervals using the same idea. $\varphi([x]) := [\,]\{\varphi(x) | x \in [x]\}$
- Examples:
  - $\sin([0, \frac{\pi}{2}]) = [0, 1]$
  - $[-2, 3]^4 = [0, 81]$
- The absolute value of an interval is defined by $|[x]| = \max(x, -x)$ and it has to be distinguished from the interval extension of the function abs.

Rounded interval operations

- In a computer system intervals are represented as pairs of floating point numbers, the bounding points of the interval.
- The rounding of the bounds after every interval operation has to be performed in such a way that the rounded interval **contains** the original interval.
- Hence, the bounds must be rounded **outward** (the lower towards –∞, the upper towards +∞).
- Example (3 significant digits)

$$\left[-1.15, 2.21\right]+\left[12.2, 13.1\right]=\left[11.0, 15.4\right]$$

Algebraic Properties

- The algebraic properties of intervals differ considerably from the properties of real numbers.
- Many algebraic laws are weakened. E.g.
  - $[x]-[x] \ni 0$ e.g. $[0,1]-[0,1]=[-1,1]$
  - $[a]([b]+[c]) \subseteq [a][b]+[a][c]$ (**subdistributivity**)
- One has to be careful in theoretical arguments involving interval arithmetic.

Interval Evaluation of Expressions (1)

- The simplest way to compute bounds for the range of a function *f* over an interval [*x*] is using interval arithmetic.
- Using an arithmetic formula for *f*, one replaces all variable occurrencies by intervals and evaluates the expression using interval arithmetic.
- Note that in general different expressions for the same function give different results.
- Example:

$$\mathrm{f}(x) = x + 1 = \frac{x^2 - 1}{x - 1}$$

$$\mathrm{f}([1.5, 2.5]) = [2.5, 3.5] \subset [1.5, 12.5]$$

Interval Evaluation of Expressions (2)

- Interval arithmetic has **linear approximation order**. $\operatorname{rad} f([x_1],\ldots,[x_n]) = O(\max_i \operatorname{rad}[x_i])$
- If every variable appears only once inside an arithmetic expression, no overestimation occurs.
- Interval arithmetic is memoryless $\Rightarrow$ dependence results in **overestimation** of the range. $[-1,1]^2 = [0,1] \subset [-1,1] = [-1,1] * [-1,1]$
- Caution: $[x] = [-2,2]$, $f(x) = 1/(1 - x + x^2)$

  $\Rightarrow \quad f([x]) = [-\infty, +\infty]$

Computing Estimates by Interval Analysis

- Range estimates obtained by interval arithmetic are usually **better than** those computed by **analytical estimates**, if in both cases estimation techniques are equally careful applied.
- Example:
  - analytic: $|x-1|\leq 1,\ |y+2|\leq 2 \ \Rightarrow\ |xy+2|\leq 2+2+2=6$

$$|x-\check{x}|\leq r,\ |y-\check{y}|\leq s \ \Rightarrow\ |xy-\check{x}\check{y}|\leq r|\check{y}|+s|\check{x}|+rs$$

  - interval: $[0,2]*[-4,0]=[-8,0]=-4\pm 4$

$$x\in[x],\ \ y\in[y] \ \Rightarrow\ |x\,y-\mathrm{mid}[x][y]|<r|\check{y}|+s|\check{x}|+rs \quad \text{in gen.}$$

The Mean Value Form

- Evaluation of functions can be improved by using Taylor expansions. E.g. the mean value theorem states that

$$\begin{aligned} \mathrm{f}(x) &= \mathrm{f}(z) + \mathrm{f}'(\xi)(x - z), \quad \xi \in x\, z \\ &\in \mathrm{f}(z) + \mathrm{f}'([x])([x] - z), \quad \text{if } x, z \in [x] \end{aligned}$$

- The **approximation order is quadratic**:

$$\operatorname{rad} \mathrm{f}([x]) = \operatorname{rad} \operatorname{range} \mathrm{f} + O(\operatorname{rad}[x]^2)$$

- For wide boxes the estimate may be bad, but for narrow boxes it is much better than interval evaluation.

Centered Forms, Slopes (1)

- Decompositions of the form

$$\mathrm{f}(x)=\mathrm{f}(z)+f[z,x](x-z)$$

lead to **centered forms** $\mathrm{f}([x])\in\mathrm{f}(z)+[s]([x]-z)$.

- The **slopes** $\mathrm{f}[z,x]$ can be computed recursively in the same way as in automatic differentiation;

$$\mathrm{f}'(x)=\mathrm{f}[x,x]$$

- In dimension one, the slope is a divided differ− ence: $\mathrm{f}[z,x]=(\mathrm{f}(x)-\mathrm{f}(z))/(x-z)$
- In higher dimensions slopes are not unique.

Centered Forms, Slopes (2)

- In general, slopes yield enclose the range of a function by a factor 2 better than the mean value form.
- Example: $\mathrm{f}(x)=x^2,\ [x]=[z-r,z+r]$

  derivative evaluation: $\mathrm{f'}(x)=2x,\ \ \mathrm{rad}\,\mathrm{f'}([x])=2r$

  slope evaluation: $\mathrm{f}[z,x]=x+z,\ \ \mathrm{rad}\,\mathrm{f}[z,[x]]=r$
- Further improvement by recursive intersection of interval evaluation and slope form.

Interval Linear Algebra

- An m×n **interval matrix** $[A]=[A, A]$ is an m×n array of intervals.
- Interval matrix addition is defined component−wise, and interval matrix multiplication is defined like ordinary matrix multiplication generalized to interval arithmetic.
- Again, many algebraic laws are weakened. In particular, associativity of multiplication fails.

Nonlinear Equations

- Find Enclosure $[x_l]$ for all solutions x_l^* of $\mathrm{F}(x)=0$ in a box [x].
- Using the mean value form, we can linearize this problem to

$$\mathrm{F}(x_0)+\mathrm{F'}([x_0])(x-x_0)\ni 0$$

An analogous formula holds for slopes.

- A **Newton operator** $\mathrm{N}(x_{0,}[x])$ is an enclosure of the solution set of the above linear equation in [x].

Properties of Newton Operators

- The Newton operator has the following important properties:
  - Reduction: $[x'] = [x] \cap \mathrm{N}([x])$ is usually smaller
  - Elimination: $[x'] \cap [x] = \emptyset \;\Rightarrow\;$ no solution
  - Existence: $\mathrm{N}([x]) \subseteq \mathrm{int}([x]) \;\Rightarrow\;$ existence
- Uniqueness:

  $\mathrm{F}'([x])$ regular $\Rightarrow$ unique solution

  $\mathrm{F}[[x],[x^*]]$ regular is sufficient

Existence proofs

- Existence proofs for the Newton operator normally use one of the following techniques:
  - **Brouwer's fixed point theorem**
  - Other fixed point theorems (Leray − Schauder,...)
  - **Implicit function theorem**
  - **Topological degree**
- Gives no improvement compared to the previous slide, if only linearized information is used.

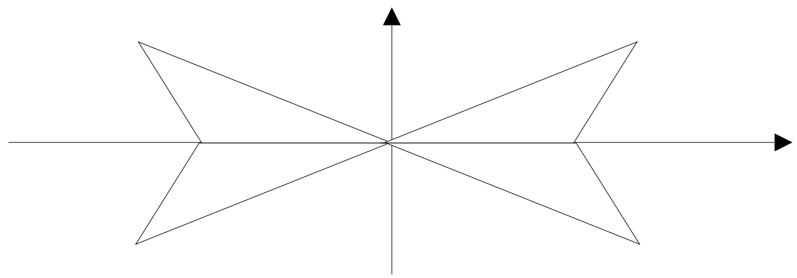
Linear Equations (1)

- The **solution set** for $[A]x=[b]$ is defined as

$$\sum([A],[b]):=\{x\in\mathbb{R}^n \mid Ax=b \text{ for some } A\in[A], b\in[b]\}$$

- It is connected and piecewise convex with up to 2^n pieces.
- Example: $[A]=\begin{pmatrix}[2,4] & [-1,1]\\ [-1,1] & [2,4]\end{pmatrix}$, $[b]=\begin{pmatrix}[-3,3]\\ 0\end{pmatrix}$

$\sum([A],[b])$



Linear Equations (2)

- In order that $\sum([A],[b])$ is bounded, all matrices in [A] have to be nonsingular. Then [A] is called **regular**.
- Computing optimal enclosures is NP–hard.
- Nearly optimal enclosures are obtained by **preconditioning**.
- Preconditioning with a matrix C changes the linear interval system to C[A] x = C[b].
- This step increases the solution set.

$$\sum([A],[b]) \subseteq \sum(C[A],C[b])$$

Linear Equations (3)

- The **midpoint inverse** is the best choice.
- After preconditioning with $C = \check{A}^{-1}$ we have C[A] = [I –*R*, I + *R*] with small R.
- If for any preconditioning matrix C we have $\| I - C[A] \| = \beta < 1$ then [A] is (strongly) regular.
- The overestimation in preconditioning is $O(\beta^2)$.

Krawczyk's Method

- The simplest method of improving an enclosure [x] for the solution set.
- The relation

$$A^{-1}b = Cb - (CA - \mathrm{I})(A^{-1}b) \in C[b] - (C[A] - \mathrm{I})[x]$$

leads to the **Krawczyk iteration**

$$[z^0] := [x], \; [z^{l+1}] := (C[b] - (C[A] - \mathrm{I})[z^l]) \cap [z^l]$$

- The first iteration is the most useful one:

$[z^1]$ has the **quadratic approximation property**, if $[z^0]$ has the linear approximation property.

Gauss – Seidel, Hansen – Bliek

- Krawczyk’s method can be improved significantly without much extra work.

- The interval **Gauss–Seidel** method produces better enclosures with $O(n^2)$ operations (after preconditioning), where $n=\dim(A)$.

- The **Hansen–Bliek** method is optimal after preconditioning but takes $O(n^3)$ operations.

References

- Further information can e.g. be found in

A. Neumaier, ***Interval Methods for Systems of Equations***, Encyclopedia of Mathematics and its Applications, 1990, Cambridge University Press

B. Kearfott, ***Rigorous Global Search***, 1996, Kluwer Academic Press

The **COCONUT homepage**

http://www.mat.univie.ac.at/~neum/glopt/coconut.html