Mainstream Contributions of Interval Computations in Engineering and Scientific Computing

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Outline

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Basic Tasks Intervals Might Accomplish

Account for uncertainty in measurements What range of outputs is expected from a range of inputs?

Account for roundoff error with mathematical rigor Provide numerical output with the certainty of a mathematical proof.

Compute bounds on ranges Lower bounds and upper bounds on quantities might be computed easily.

Handle multiple-valued quantities simply This includes direct computation with generalized gradients of non-smooth functions.

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Early Motivations for Interval Arithmetic

Prior to the Age of Digital Computation

The same basic interval operations were described in all of these works, but with somewhat different motivations. All of this early work is apparently independent.

Rosaline Cecily Young (*Mathematische Annalen*, 1931)

"The Algebra of Many-Valued Quantities." The focus is on an arithmetic on limits, where $\liminf_{x \to x_0} f(x)$ and $\limsup_{x \to x_0} f(x)$ are distinct[1]. Describing ranges and encompassing roundoff error does not seem to have been the primary motivation.

[1] Such limits might occur in generalized gradients of non-smooth functions.

Early Motivations for Interval Arithmetic

From the Onset of the Age of Digital Computers

Paul S. Dwyer (Chapter in *Linear Computations*, 1951)
"Computation with Approximate Numbers." Interval computations are introduced as an integral part of roundoff error analysis.

Mieczyslaw Warmus (*Calculus of Approximations*, 1956)
"Calculus of Approximations." The motivation is apparently to provide a sound theoretical backing to numerical computation.

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Early Motivations for Interval Arithmetic

From the Onset of the Age of Digital Computers (continued)

Teruro Sunaga (*RAAG Memoirs*, 1958) "Theory of an Interval Algebra and its Application to Numerical Analysis." The emphasis is on mathematical theory, but the motivation appears to be automatically accounting for uncertainty and error in measurement and computation.

Early Motivations for Interval Arithmetic

From the Onset of the Age of Digital Computers (continued)

Ray Moore (*Lockheed Technical Report*, 1959) "Automatic Error Analysis in Digital Computation." The motivation is given in the title. The basic operations are given in this monograph, and development of numerical solution of ODE's, numerical integration, etc. based on intervals is in Moore's 1962 dissertation. It is made clear that interval computations promise rigorous bounds on the exact result, even when finite (rounded) computer arithmetic is used.

References are from the interval computations website, at `http://www.cs.utep.edu/interval-comp`

The Basic Operations of Interval Arithmetic

- Each basic interval operation $\odot \in \{+, -, \times, \div, \text{etc.}\}$ is defined by

$$\boldsymbol{x} \odot \boldsymbol{y} = \{x \odot y \mid x \in \boldsymbol{x} \text{ and } y \in \boldsymbol{y}\}.$$

- This definition can be made operational; for example, for $\boldsymbol{x} = [\underline{x}, \overline{x}]$ and $\boldsymbol{y} = [\underline{y}, \overline{y}]$, $\boldsymbol{x} + \boldsymbol{y} = [\underline{x} + \underline{y}, \overline{x} + \overline{y}]$; similarly, ranges of functions such as sin, exp can be computed.
- Evaluation of an expression with this interval arithmetic gives *bounds* on the range of the expression.
- With *directed rounding* (e.g. using IEEE standard arithmetic), the computer can give mathematically rigorous bounds on ranges.

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Interval Operations
Advantages

- Computing sharp bounds on ranges is an NP-hard problem.
- Computing range bounds with interval computations is quick and simple.
- The range bounds get sharper asymptotically as the widths of the domain intervals tend to zero, and, with *second-order extensions*, will do so rapidly.

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Interval Operations

Pitfalls

- The interval values contain the actual ranges, but are possibly significantly larger. For example, if $f(x) = (x+1)(x-1)$, then

$$\begin{aligned} \boldsymbol{f}([-2,2]) &= \big([-2,2]+1\big)\big([-2,2]-1\big) \\ &= [-1,3][-3,1] = [-9,3], \end{aligned}$$

  whereas the exact range is $[-1,3]$.

- However, if we write f equivalently as $f(x) = x^2 - 1$, and we suppose we compute the range of x^2 exactly, we obtain

$$\boldsymbol{f}([-2,2]) = [-2,2]^2 - 1 = [0,4] - 1 = [-1,3],$$

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Dependency and Overestimation

Consequences

- This range overestimation above is caused by the arithmetic not taking account of the fact that, when $x = 2$ in $(x + 1)$, x must also equal 2 in $(x - 1)$.
- This phenomenon is at the root of many failures of interval arithmetic.
- For this reason, interval arithmetic should be used with skill, only in appropriate places.
- Naively converting a floating point code to interval computation by simply changing the data types is far more likely to fail than succeed.
- However, there are some notable successes.

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Fast Bounds on Ranges

A *Filter* in Branch and Bound Methods

- In branch and bound methods for global optimization, methods are needed for rejecting regions $\boldsymbol{x}$ that cannot contain global optimizing points.
- $\boldsymbol{x}$ can contain a global optimizing point only if
  - It contains points x that satisfy constraints $c_i(x) = 0$ and $g_j(x) \le 0$.
  - It contains points x such that the quantity φ to be optimized obeys $\varphi(x) \le \overline{\varphi}$, where $\overline{\varphi}$ is a previously computed upper bound on the global optimum value.
- Regions $\boldsymbol{x}$ can sometimes be quickly eliminated by evaluating φ, the c_i, and the g_j and checking violation of the conditions. For example, if the lower bound on one of the $g_j(\boldsymbol{x})$ is greater than 0, then $\boldsymbol{x}$ may be eliminated from further consideration.
- This technique is widely acknowledged in the general literature and used in leading commercial software.

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Use in Branch and Bound Methods

Constraint Propagation

- This is based on a simple idea: Solve a relation in many variables for one of the variables, then plug in bounds on the other constraints to compute new bounds on the original constraint.
- The technique is the foundation of an entire field, with expertise at UTEP (Martine Ceberio).
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Constraint Propagation

A Simple Illustrative Example

Consider

$$\begin{aligned} \text{minimize } & \varphi(x) = x_1^2 - x_2^2 \\ \text{subject to } & x_1^2 + x_2^2 = 1, \\ & x_1 + x_2 \le 0. \end{aligned}$$

- Suppose we have already found the feasible point $\hat{x} = (0, -1)$ with $\varphi(\hat{x}) = -1$, so -1 is an upper bound on the optimum.
- Suppose we are searching in the box $([-1, 1], [-1, 1])$.
- Using the upper bound $\overline{\varphi}$ gives

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- Solving this for x_1 gives $\cdots$

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Constraint Propagation
(Simple Example, Continued)

- (solving for x_1 in the objective condition)

$$x_1 \le \sqrt{[-1,1]^2 - 1} = \sqrt{[0,1] - 1} = \sqrt{[-1,0]}$$

and

$$x_1 \ge \sqrt{[-1,1]^2 - 1} = \sqrt{[0,1] - 1} = \sqrt{[-1,0]}.$$

- Here, it is appropriate to interpret $\sqrt{[-1,0]} = 0$, so we obtain $x_1 = 0$.
- We now solve for x_2 in $x_1^2 + x_2^2 = 1$ and plug in $x_1 = 0$ to get

$$x_2 = 1 \quad \text{or} \quad x_2 = -1,$$

- Plugging $x_1 = 0$, $x_2 = 1$ into $x_1 + x_2 \le 0$ gives a contradiction, leading to the unique point $x = (0, -1)$ in $([-1,1],[-1,1])$ that can be a global optimizer.

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Verified Paths

COSY Infinity and Taylor Arithmetic

- Martin Berz and Kyoko Makino have included these methods in the *COSY Infinity* software for modeling beams in particle accelerators. This software is used by thousands of beam theorists worldwide.
- The techniques have been used to predict
  - Bounds on orbits of near-Earth objects (proving they will not hit the Earth),
  - Bounds on paths of particles in actual and planned particle accelerators (proving feasibility before expensive accelerators are built).
- Berz and Makino are recipients of this year's Moore Prize (presentation to be given 1:15–2:00 today).

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Other Verified ODE Solutions

Chemical Engineering and Biological Models

- Mark Stadtherr and his students (originally Youdong Lin) have produced success in using interval techniques (with Taylor models) to find the range of responses to systems, subject to initial conditions that vary.
- Enszer and Stadtherr will be giving a talk related to this in a “Biomedical Applications” session at 5:30PM on Tuesday.

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Computer-Aided Proofs

Proofs of Some Famous Mathematical Conjectures

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Proof of the Kepler Conjecture Exhibit the way to arrange spheres in space to maximize the ratio of filled to unfilled space, and prove it is optimal. This was done by Thomas Hales, who received the 2004 Moore prize for his success.

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Use in Diverse Applications

(with the INTLAB toolbox)

- Siegfried Rump has maintained a high-quality MATLAB toolbox INTLAB for interval computations.
- The widespread availability of this toolbox has stimulated its use in diverse applications, both within and outside the area of interval computations research.
- Siegfried has compiled a list of about 200 salient references that use INTLAB to obtain results, with many science and engineering fields represented. See `http://www.ti3.tu-harburg.de/rump/intlab/INTLABref.pdf`
- Siegfried is scheduled to be at SCAN 2008.

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- Siegfried has compiled a list of about 200 salient references that use INTLAB to obtain results, with many science and engineering fields represented. See `http://www.ti3.tu-harburg.de/rump/intlab/INTLABref.pdf`
- Siegfried is scheduled to be at SCAN 2008.

Outline

Molecular Properties

Minimum-energy spatial conformations

- Mark Stadtherr and his students have used interval arithmetic with global optimization techniques to obtain minimum-energy atomic configurations and prove that they are correct.
- The work has resulted in significant revision of tables of molecular properties.
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- Rafi Muhanna and Robert Mullen have put forward very promising methods for structural analysis that uses interval methods to take account of measurement uncertainties and tolerances in components.
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- Related papers, will be presented at an "Applications to Civil Engineering" session.
- Various others have also contributed to this area.

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Various PDE Problems

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Finance and Decision Making

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What Have I Forgotten

- Is there some important application I have failed to mention?
- Are some of the things I have listed as "promising" actually *faites accomplis*?

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