Interval Computations Technology in Mathematics Research: From Help in Theoretical Breakthroughs to Practically Useful Results About Numerical Methods

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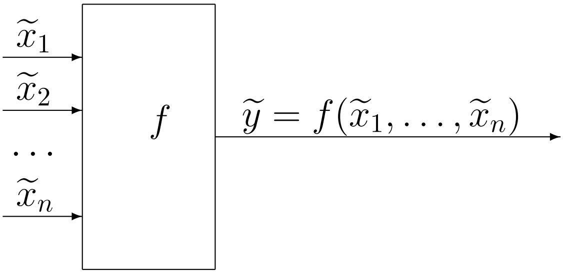
1. General Problem of Data Processing under Uncertainty

- *Indirect measurements:* way to measure y that are are difficult (or even impossible) to measure directly.
- *Idea:* $y = f(x_1, \ldots, x_n)$



- *Problem:* measurements are never 100% accurate: $\widetilde{x}_i \neq x_i$ ($\Delta x_i \neq 0$) hence

$$\widetilde{y} = f(\widetilde{x}_1, \ldots, \widetilde{x}_n) \neq y = f(x_1, \ldots, x_n).$$

What are bounds on $\Delta y \stackrel{\text{def}}{=} \widetilde{y} - y$?

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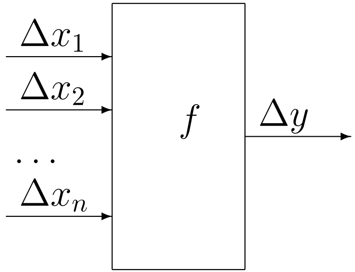
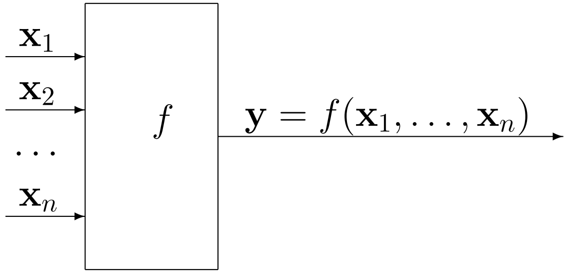
2. Probabilistic and Interval Uncertainty



- *Traditional approach:* we know probability distribution for Δx_i (usually Gaussian).
- *Where it comes from:* calibration using standard MI.
- *Problem:* calibration is not possible in:
  - fundamental science
  - manufacturing
- *Solution:* we know upper bounds Δ_i on $|\Delta x_i|$ hence

$$x_i \in [\widetilde{x}_i - \Delta_i, \widetilde{x}_i + \Delta_i].$$

3. Interval Computations: A Problem



- *Given:* an algorithm $y = f(x_1, \dots, x_n)$ and n intervals $\mathbf{x}_i = [\underline{x}_i, \overline{x}_i]$.
- *Compute:* the corresponding range of y:

$$[\underline{y}, \overline{y}] = \{f(x_1, \dots, x_n) \mid x_1 \in [\underline{x}_1, \overline{x}_1], \dots, x_n \in [\underline{x}_n, \overline{x}_n]\}.$$

- *Fact:* NP-hard even for quadratic f.
- *Challenge:* when are feasible algorithm possible?
- *Challenge:* when computing $\mathbf{y} = [\underline{y}, \overline{y}]$ is not feasible, find a good approximation $\mathbf{Y} \supseteq \mathbf{y}$.

4. Interval Computations: A Brief History

- *Origins:* Archimedes (Ancient Greece)
- *Modern pioneers:* Warmus (Poland), Sunaga (Japan), Moore (USA), 1956–59
- *First boom:* early 1960s.
- *First challenge:* taking interval uncertainty into account when planning spaceflights to the Moon.
- *Current applications* (sample):
  - design of elementary particle colliders: Berz, Kyoko (USA)
  - will a comet hit the Earth: Berz, Moore (USA)
  - robotics: Jaulin (France), Neumaier (Austria)
  - chemical engineering: Stadtherr (USA)

5. Alternative Approach: Maximum Entropy

- *Situation:* in many practical applications, it is very difficult to come up with the probabilities.
- *Traditional engineering approach:* use probabilistic techniques.
- *Problem:* many different probability distributions are consistent with the same observations.
- *Solution:* select one of these distributions – e.g., the one with the largest entropy.
- *Example – 1 variable:* if all we know is that $x \in [\underline{x}, \overline{x}]$, then MaxEnt leads to a uniform distribution on $[\underline{x}, \overline{x}]$.
- *Example – multiple variables:* different variables are independently distributed.

6. Limitations of Maximum Entropy Approach

- *Example:* simplest algorithm $y = x_1 + \ldots + x_n$.
- *Measurement errors:* $\Delta x_i \in [-\Delta, \Delta]$.
- *Analysis:* $\Delta y = \Delta x_1 + \ldots + \Delta x_n$.
- *Worst case situation:* $\Delta y = n \cdot \Delta$.
- *Maximum Entropy approach:* due to Central Limit Theorem, Δy is $\approx$ normal, with $\sigma = \Delta \cdot \dfrac{\sqrt{n}}{\sqrt{3}}$.
- *Why this may be inadequate:* we get $\Delta \sim \sqrt{n}$, but due to correlation, it is possible that $\Delta = n \cdot \Delta \sim n \gg \sqrt{n}$.
- *Conclusion:* using a single distribution can be very misleading, especially if we want guaranteed results.
- Examples: high-risk application areas such as space exploration or nuclear engineering.

7. Interval Arithmetic: Foundations of Interval Techniques

- *Problem:* compute the range
  $$[\underline{y}, \overline{y}] = \{f(x_1, \ldots, x_n) \mid x_1 \in [\underline{x}_1, \overline{x}_1], \ldots, x_n \in [\underline{x}_n, \overline{x}_n]\}.$$
- *Interval arithmetic:* for arithmetic operations $f(x_1, x_2)$ (and for elementary functions), we have explicit formulas for the range.
- *Examples:* when $x_1 \in \mathbf{x}_1 = [\underline{x}_1, \overline{x}_1]$ and $x_2 \in \mathbf{x}_2 = [\underline{x}_2, \overline{x}_2]$, then:
  - The range $\mathbf{x}_1 + \mathbf{x}_2$ for $x_1 + x_2$ is $[\underline{x}_1 + \underline{x}_2, \overline{x}_1 + \overline{x}_2]$.
  - The range $\mathbf{x}_1 - \mathbf{x}_2$ for $x_1 - x_2$ is $[\underline{x}_1 - \overline{x}_2, \overline{x}_1 - \underline{x}_2]$.
  - The range $\mathbf{x}_1 \cdot \mathbf{x}_2$ for $x_1 \cdot x_2$ is $[\underline{y}, \overline{y}]$, where
  $$\underline{y} = \min(\underline{x}_1 \cdot \underline{x}_2, \underline{x}_1 \cdot \overline{x}_2, \overline{x}_1 \cdot \underline{x}_2, \overline{x}_1 \cdot \overline{x}_2);$$
  $$\overline{y} = \max(\underline{x}_1 \cdot \underline{x}_2, \underline{x}_1 \cdot \overline{x}_2, \overline{x}_1 \cdot \underline{x}_2, \overline{x}_1 \cdot \overline{x}_2).$$
- The range $1/\mathbf{x}_1$ for $1/x_1$ is $[1/\overline{x}_1, 1/\underline{x}_1]$ (if $0 \notin \mathbf{x}_1$).

8. Straightforward Interval Computations: Example

- *Example:* $f(x) = (x-2)\cdot(x+2)$, $x \in [1,2]$.
- How will the computer compute it?
  - $r_1 := x - 2;$
  - $r_2 := x + 2;$
  - $r_3 := r_1 \cdot r_2.$
- *Main idea:* perform the same operations, but with *intervals* instead of *numbers*:
  - $\mathbf{r}_1 := [1,2] - [2,2] = [-1,0];$
  - $\mathbf{r}_2 := [1,2] + [2,2] = [3,4];$
  - $\mathbf{r}_3 := [-1,0] \cdot [3,4] = [-4,0].$
- *Actual range:* $f(\mathbf{x}) = [-3,0]$.
- *Comment:* this is just a toy example, there are more efficient ways of computing an enclosure $\mathbf{Y} \supseteq \mathbf{y}$.

9. First Idea: Use of Monotonicity

- *Reminder:* for arithmetic, we had exact ranges.
- *Reason:* $+$, $-$, $\cdot$ are monotonic in each variable.
- *How monotonicity helps:* if $f(x_1, \ldots, x_n)$ is (non-strictly) increasing ($f \uparrow$) in each x_i, then
$$f(\mathbf{x}_1, \ldots, \mathbf{x}_n) = [f(\underline{x}_1, \ldots, \underline{x}_n), f(\overline{x}_1, \ldots, \overline{x}_n)].$$
- *Similarly:* if $f \uparrow$ for some x_i and $f \downarrow$ for other x_j $(-)$.
- *Fact:* $f \uparrow$ in x_i if $\dfrac{\partial f}{\partial x_i} \geq 0$.
- *Checking monotonicity:* check that the range $[\underline{r}_i, \overline{r}_i]$ of $\dfrac{\partial f}{\partial x_i}$ on $\mathbf{x}_i$ has $\underline{r}_i \geq 0$.
- *Differentiation:* by Automatic Differentiation (AD) tools.
- *Estimating ranges of* $\dfrac{\partial f}{\partial x_i}$*:* straightforward interval comp.

10. Monotonicity: Example

- *Idea:* if the range $[\underline{r}_i, \overline{r}_i]$ of each $\dfrac{\partial f}{\partial x_i}$ on $\mathbf{x}_i$ has $\underline{r}_i \geq 0$, then

$$f(\mathbf{x}_1, \ldots, \mathbf{x}_n) = [f(\underline{x}_1, \ldots, \underline{x}_n), f(\overline{x}_1, \ldots, \overline{x}_n)].$$

- *Example:* $f(x) = (x - 2) \cdot (x + 2)$, $\mathbf{x} = [1, 2]$.
- *Case $n = 1$:* if the range $[\underline{r}, \overline{r}]$ of $\dfrac{df}{dx}$ on $\mathbf{x}$ has $\underline{r} \geq 0$, then

$$f(\mathbf{x}) = [f(\underline{x}), f(\overline{x})].$$

- *AD:* $\dfrac{df}{dx} = 1 \cdot (x + 2) + (x - 2) \cdot 1 = 2x.$
- *Checking:* $[\underline{r}, \overline{r}] = [2, 4]$, with $2 \geq 0$.
- *Result:* $f([1, 2]) = [f(1), f(2)] = [-3, 0]$.
- *Comparison:* this is the exact range.

11. Non-Monotonic Example

- *Example:* $f(x) = x \cdot (1 - x)$, $x \in [0, 1]$.
- How will the computer compute it?
  - $r_1 := 1 - x$;
  - $r_2 := x \cdot r_1$.
- *Straightforward interval computations:*
  - $\mathbf{r}_1 := [1, 1] - [0, 1] = [0, 1]$;
  - $\mathbf{r}_2 := [0, 1] \cdot [0, 1] = [0, 1]$.
- *Actual range:* min, max of f at $\underline{x}$, $\overline{x}$, or when $\dfrac{df}{dx} = 0$.
- Here, $\dfrac{df}{dx} = 1 - 2x = 0$ for $x = 0.5$, so
  - compute $f(0) = 0$, $f(0.5) = 0.25$, and $f(1) = 0$.
  - $\underline{y} = \min(0, 0.25, 0) = 0$, $\overline{y} = \max(0, 0.25, 0) = 0.25$.
- *Resulting range:* $f(\mathbf{x}) = [0, 0.25]$.

12. Second Idea: Centered Form

- *Main idea:* Intermediate Value Theorem

$$f(x_1, \ldots, x_n) = f(\widetilde{x}_1, \ldots, \widetilde{x}_n) + \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}(\chi) \cdot (x_i - \widetilde{x}_i)$$

  for some $\chi_i \in \mathbf{x}_i$.

- *Corollary:* $f(x_1, \ldots, x_n) \in \mathbf{Y}$, where

$$\mathbf{Y} = \widetilde{y} + \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}(\mathbf{x}_1, \ldots, \mathbf{x}_n) \cdot [-\Delta_i, \Delta_i].$$

- *Differentiation:* by Automatic Differentiation (AD) tools.
- *Estimating the ranges of derivatives:*
  - if appropriate, by monotonicity, or
  - by straightforward interval computations, or
  - by centered form (more time but more accurate).

13. Centered Form: Example

- *General formula:*

$$\mathbf{Y} = f(\widetilde{x}_1, \ldots, \widetilde{x}_n) + \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}(\mathbf{x}_1, \ldots, \mathbf{x}_n) \cdot [-\Delta_i, \Delta_i].$$

- *Example:* $f(x) = x \cdot (1 - x)$, $\mathbf{x} = [0, 1]$.
- Here, $\mathbf{x} = [\widetilde{x} - \Delta, \widetilde{x} + \Delta]$, with $\widetilde{x} = 0.5$ and $\Delta = 0.5$.
- *Case* $n = 1$*:* $\mathbf{Y} = f(\widetilde{x}) + \dfrac{df}{dx}(\mathbf{x}) \cdot [-\Delta, \Delta]$.
- *AD:* $\dfrac{df}{dx} = 1 \cdot (1 - x) + x \cdot (-1) = 1 - 2x$.
- *Estimation:* we have $\dfrac{df}{dx}(\mathbf{x}) = 1 - 2 \cdot [0, 1] = [-1, 1]$.
- *Result:* $\mathbf{Y} = 0.5 \cdot (1 - 0.5) + [-1, 1] \cdot [-0.5, 0.5] = 0.25 + [-0.5, 0.5] = [-0.25, 0.75]$.
- *Comparison:* actual range $[0, 0.25]$, straightforward $[0, 1]$.

14. Third Idea: Bisection

- *Known:* accuracy $O(\Delta_i^2)$ of first order formula

$$f(x_1,\ldots,x_n) = f(\widetilde{x}_1,\ldots,\widetilde{x}_n) + \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}(\chi)\cdot(x_i-\widetilde{x}_i).$$

- *Idea:* if the intervals are too wide, we:
  - split one of them in half ($\Delta_i^2 \to \Delta_i^2/4$); and
  - take the union of the resulting ranges.
- *Example:* $f(x) = x\cdot(1-x)$, where $x \in \mathbf{x} = [0,1]$.
- *Split:* take $\mathbf{x}' = [0, 0.5]$ and $\mathbf{x}'' = [0.5, 1]$.
- *1st range:* $1-2\cdot\mathbf{x} = 1-2\cdot[0,0.5] = [0,1]$, so $f\uparrow$ and $f(\mathbf{x}') = [f(0), f(0.5)] = [0, 0.25]$.
- *2nd range:* $1-2\cdot\mathbf{x} = 1-2\cdot[0.5,1] = [-1,0]$, so $f\downarrow$ and $f(\mathbf{x}'') = [f(1), f(0.5)] = [0, 0.25]$.
- *Result:* $f(\mathbf{x}')\cup f(\mathbf{x}'') = [0, 0.25]$ – exact.

15. Use of Interval Computations in Pure Mathematics: Computer-Aided Proofs

- *Main idea:* to prove (guarantee) that certain inequalities hold for all the values within given intervals.
- *Case study:* Lorenz equations – a simple model of atmospheric circulation.
- *Empirical fact:* solutions of Lorentz equations behave chaotically ("have a strange attractor").
- *Theoretical confirmation:* by Warwick Tucker using interval computations (Moore prize 2002).
- *Case study:* Kepler conjecture – that the standard layer-by-layer packing of spheres in the densest.
- *Solution:* Thomas Hales (Moore prize 2004).
- *Case study:* "double bubble" iso-perimetric problem (R. Schlafly, 1995).

16. Practical Case Study: Description

- We are interested in *indirect* measurements:
  - *we measure:* $f(\vec{x})$, resulting in $[\underline{f}(\vec{x}), \overline{f}(\vec{x})]$;
  - *we know:* that $L(u) = f$ for a known operator L;
  - *we want:* the range $[\underline{u}(\vec{x}), \overline{u}(\vec{x})]$ of possible values of $u(\vec{x})$.
- *"Monotonic" case:* if $f_1(\vec{x}) \leq f_2(\vec{x})$ for all $\vec{x}$, then $u_1(\vec{x}) \leq u_2(\vec{x})$.
- In the "monotonic" case, the range is easier to compute: $u(\vec{x}) \in [\underline{u}, \overline{u}] = [L^{-1}(\underline{f}), L^{-1}(\overline{f})]$.
- For linear operators L, "monotonic" means *non-negativity-preserving*: if $u \geq 0$, then $L(u) = f \geq 0$.
- We look for situations where L^{-1} is non-negativity-preserving.
- *Example:* find u s.t. $-u'' = f$ and $u(-1) = u(1) = 0$.

17. Finite Element Methods (FEM) and Discrete Non-Negativity Conservation Principles

- *Problem:* find u s.t. $-u'' = f$ and $u(-1) = u(1) = 0$.
- *FEM – main idea:* use (piece-wise) polynomial approximations $f_{h,p}(x)$ and $u_{h,p}(x)$ of given order p.
- *Problem:* we cannot have $z(x) \stackrel{\text{def}}{=} u''_{h,p}(x) + f_{h,p}(x) = 0$ for all x: e.g., for $p = 1$, we have $u''_{h,p} \equiv 0$.
- *In practice:* we never measure point values $z(x)$, only (regional) averages $\int z(x) \cdot w(x)\, dx$.
- *Solution:* require that $\int z(x) \cdot w_{h,p}(x)\, dx = 0$ for all polynomials $w_{h,p}$ which vanish at endpoints ($x = \pm 1$).
- *So:* $\int_{-1}^{1} u'_{h,p}(x) \cdot w'_{h,p}(x)\, dx = \int_{-1}^{1} f_{h,p}(x) \cdot w_{h,p}(x)\, dx$.
- *Question:* can we guarantee $u_{h,p}(x) \geq 0$ if $f_{h,p}(x) \geq 0$?

18. Proof of Non-Negativity Preservation: Main Ideas

- *Basis:* Lobatto shape functions $l_i(x)$ s.t. $l_i'(x)$ are orthonormal polynomials.
- *Resulting formula:* $u_{h,p}(x) = \int_{-1}^{1} f_{h,p}(z) \cdot \Phi_p(x,z)\,dz$, where $\Phi_p(x,z) \stackrel{\text{def}}{=} \sum_{i=1}^{p-1} l_{i+1}(x) \cdot l_{i+1}(z)$.
- *We want to prove:* if $f_{h,p}(x) \geq 0$, then $u_{h,p}(x) \geq 0$.
- *Idea of the proof:*
  - identify a subdomain Ω_p^+ of $(-1,1)^2$ where $\Phi_p \geq 0$;
  - find a quadrature rule of the order of accuracy $2p$ with positive weights and points lying in Ω_p^+.
- *What was known:* subdomains Ω_p^+ and quadrature rules for $p = 4, \ldots, 10$.
- *Remained to be proven:* $\Phi_p(x,z) \geq 0$ for all $(x,z) \in \Omega_p^+$.

19. Application of Interval Arithmetic, Case $p = 4$

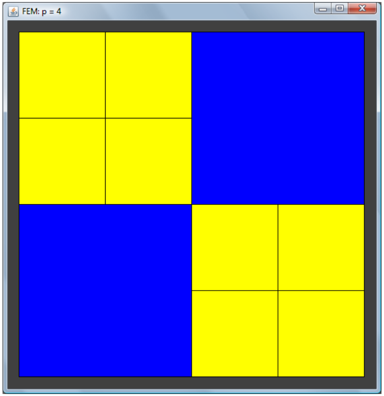
- *We need to show:* $\Phi_4(x,z) = \sum_{i=1}^{3} l_{i+1}(x) \cdot l_{i+1}(z) \geq 0.$
- $l_{i+1}(x)$ vanishes at ± 1, so $l_{i+1}(x) = (x^2 - 1) \cdot m_{i+1}(x)$.
- So, $\Phi_4(x,z) = (x^2 - 1) \cdot (z^2 - 1) \cdot \Psi_4(x,z)$, where $\Psi_4(x,z) \stackrel{\text{def}}{=} \sum_{i=1}^{3} m_{i+1}(x) \cdot m_{i+1}(z)$.
- *Consequence:* $\Phi_4(x,z) \geq 0$ for all $x, z \in (-1,1)$ if and only if $\Psi_4(x,z) \geq 0$ for all $x, z \in (-1,1)$.
- Here, $\Psi_4(x,z) = \dfrac{3}{8} + \dfrac{5}{8} \cdot x \cdot z + \dfrac{7}{128} \cdot (5x^2 - 1) \cdot (5z^2 - 1)$.
- *Idea:*
  - use interval arithmetic to compute the enclosure $[\underline{\Psi}_4, \overline{\Psi}_4]$ for the range of the function $\Psi_4(x,z)$;
  - if $\underline{\Psi}_4 \geq 0$, then $\Psi_4(x,z) \geq 0$ for all x, z.

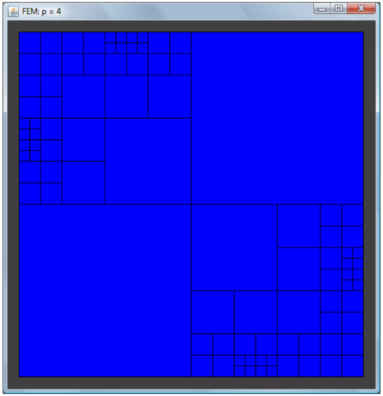
20. Application of Interval Arithmetic (cont-d)

- *Reminder:* we want to find the range of the function
$$\Psi_4(x,z)=\frac{3}{8}+\frac{5}{8}\cdot x\cdot z+\frac{7}{128}\cdot(5x^2-1)\cdot(5z^2-1).$$
- For $[-1,1]\times[-1,1]$, we get $[\underline{\Psi}_4,\overline{\Psi}_4]=\left[-\frac{25}{16},\frac{95}{32}\right]$.
- Since $\underline{\Psi}_4<0$, we subdivide the domain and evaluate the range of each sub-domain.
- For $[0,1]\times[0,1]$, we get $[\underline{\Psi}_4,\overline{\Psi}_4]=\left[\frac{5}{32},\frac{15}{8}\right]$, so $\underline{\Psi}_4\ge 0$.
- For $[-1,0]\times[-1,0]$, we similarly get $\underline{\Psi}_4=\frac{5}{32}\ge 0$.
- For $[0,1]\times[-1,0]$, we get $[\underline{\Psi}_4,\overline{\Psi}_4]=\left[-\frac{15}{32},\frac{5}{4}\right]$, so $\underline{\Psi}_4<0$.
- Thus, we need to further subdivide this sub-domain.

21. Result for the Case $p = 4$

- We subdivide the domains until (after 6 iterations) we get a partition of $[-1,1]^2$ where $[\underline{\Psi}_4, \overline{\Psi}_4] > 0$.





- *Conclusion:* $\Psi_4(x, z) \geq 0$.
- *Conclusion:* the operator $f_{h,p} \to u_{h,p}$ is non-negativity-preserving.
- Similar results are available for $p = 5, \ldots, 10$.

22. Acknowledgments

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23. Alternative Approach: Affine Arithmetic

- *So far:* we compute the range of $x \cdot (1 - x)$ by multiplying ranges of x and $1 - x$.
- *We ignore:* that both factors depend on x and are, thus, dependent.
- *Idea:* for each intermediate result a, keep an explicit dependence on $\Delta x_i = \widetilde{x}_i - x_i$ (at least its linear terms).
- *Implementation:*

$$a = a_0 + \sum_{i=1}^{n} a_i \cdot \Delta x_i + [\underline{a}, \overline{a}].$$

- *We start:* with $x_i = \widetilde{x}_i - \Delta x_i$, i.e.,

$$\widetilde{x}_i + 0 \cdot \Delta x_1 + \ldots + 0 \cdot \Delta x_{i-1} + (-1) \cdot \Delta x_i + 0 \cdot \Delta x_{i+1} + \ldots + 0 \cdot \Delta x_n + [0, 0].$$

- *Description:* $a_0 = \widetilde{x}_i$, $a_i = -1$, $a_j = 0$ for $j \neq i$, and $[\underline{a}, \overline{a}] = [0, 0]$.

24. Affine Arithmetic: Operations

- *Representation:* $a = a_0 + \sum\limits_{i=1}^{n} a_i \cdot \Delta x_i + [\underline{a}, \overline{a}]$.
- *Input:* $a = a_0 + \sum\limits_{i=1}^{n} a_i \cdot \Delta x_i + \mathbf{a}$ and $b = b_0 + \sum\limits_{i=1}^{n} b_i \cdot \Delta x_i + \mathbf{b}$.
- *Operations:* $c = a \otimes b$.
- *Addition:* $c_0 = a_0 + b_0$, $c_i = a_i + b_i$, $\mathbf{c} = \mathbf{a} + \mathbf{b}$.
- *Subtraction:* $c_0 = a_0 - b_0$, $c_i = a_i - b_i$, $\mathbf{c} = \mathbf{a} - \mathbf{b}$.
- *Multiplication:* $c_0 = a_0 \cdot b_0$, $c_i = a_0 \cdot b_i + b_0 \cdot a_i$,

$$\mathbf{c} = a_0 \cdot \mathbf{b} + b_0 \cdot \mathbf{a} + \sum_{i \neq j} a_i \cdot b_j \cdot [-\Delta_i, \Delta_i] \cdot [-\Delta_j, \Delta_j] +$$

$$\sum_i a_i \cdot b_i \cdot [-\Delta_i, \Delta_i]^2 +$$

$$\left(\sum_i a_i \cdot [-\Delta_i, \Delta_i] \right) \cdot \mathbf{b} + \left(\sum_i b_i \cdot [-\Delta_i, \Delta_i] \right) \cdot \mathbf{a} + \mathbf{a} \cdot \mathbf{b}.$$

25. Affine Arithmetic: Example

- *Example:* $f(x) = x \cdot (1 - x)$, $x \in [0, 1]$.
- Here, $n = 1$, $\widetilde{x} = 0.5$, and $\Delta = 0.5$.
- How will the computer compute it?
  - $r_1 := 1 - x$;
  - $r_2 := x \cdot r_1$.
- *Affine arithmetic:* we start with $x = 0.5 - \Delta x + [0, 0]$;
  - $\mathbf{r}_1 := 1 - (0.5 - \Delta) = 0.5 + \Delta x$;
  - $\mathbf{r}_2 := (0.5 - \Delta x) \cdot (0.5 + \Delta x)$, i.e.,

$$\mathbf{r}_2 = 0.25 + 0 \cdot \Delta x - [-\Delta, \Delta]^2 = 0.25 + [-\Delta^2, 0].$$

- *Resulting range:* $\mathbf{y} = 0.25 + [-0.25, 0] = [0, 0.25]$.
- *Comparison:* this is the exact range.

26. Affine Arithmetic: Towards More Accurate Estimates

- *In our simple example:* we got the exact range.
- *In general:* range estimation is NP-hard.
- *Meaning:* a feasible (polynomial-time) algorithm will sometimes lead to excess width: $\mathbf{Y} \supset \mathbf{y}$.
- *Conclusion:* affine arithmetic may lead to excess width.
- *Question:* how to get more accurate estimates?
- *First idea:* bisection.
- *Second idea* (Taylor arithmetic):
  - *affine arithmetic:* $a = a_0 + \sum a_i \cdot \Delta x_i + \mathbf{a}$;
  - *meaning:* we keep linear terms in Δx_i;
  - *idea:* keep, e.g., quadratic terms

$$a = a_0 + \sum a_i \cdot \Delta x_i + \sum a_{ij} \cdot \Delta x_i \cdot \Delta x_j + \mathbf{a}.$$

27. Interval Computations vs. Affine Arithmetic: Comparative Analysis

- *Objective:* we want a method that computes a reasonable estimate for the range in reasonable time.
- *Conclusion – how to compare different methods:*
  - how accurate are the estimates, and
  - how fast we can compute them.
- *Accuracy:* affine arithmetic leads to more accurate ranges.
- *Computation time:*
  - *Interval arithmetic:* for each intermediate result a, we compute two values: endpoints $\underline{a}$ and $\overline{a}$ of $[\underline{a}, \overline{a}]$.
  - *Affine arithmetic:* for each a, we compute $n + 3$ values:

$$a_0 \quad a_1, \ldots, a_n \quad \underline{a}, \overline{a}.$$

- *Conclusion:* affine arithmetic is $\sim n$ times slower.

28. Solving Systems of Equations: Extending Known Algorithms to Situations with Interval Uncertainty

- *We have:* a system of equations $g_i(y_1, \ldots, y_n) = a_i$ with unknowns y_i;
- *We know:* a_i with interval uncertainty: $a_i \in [\underline{a}_i, \overline{a}_i]$;
- *We want:* to find the corresponding ranges of y_j.
- *First case:* for exactly known a_i, we have an algorithm $y_j = f_j(a_1, \ldots, a_n)$ for solving the system.
- *Example:* system of linear equations.
- *Solution:* apply interval computations techniques to find the range $f_j([\underline{a}_1, \overline{a}_1], \ldots, [\underline{a}_n, \overline{a}_n])$.
- *Better solution:* for specific equations, we often already know which ideas work best.
- *Example:* linear equations $Ay = b$; y is monotonic in b.

29. Solving Systems of Equations When No Algorithm Is Known

- *Idea:*
  - parse each equation into elementary constraints, and
  - use interval computations to improve original ranges until we get a narrow range (= solution).
- *First example:* $x - x^2 = 0.5$, $x \in [0,1]$ (no solution).
- *Parsing:* $r_1 = x^2$, $0.5\ (= r_2)\ = x - r_1$.
- *Rules:* from $r_1 = x^2$, we extract two rules:

$$(1)\ x \to r_1 = x^2; \quad (2)\ r_1 \to x = \sqrt{r_1};$$

from $0.5 = x - r_1$, we extract two more rules:

$$(3)\ x \to r_1 = x - 0.5; \quad (4)\ r_1 \to x = r_1 + 0.5.$$

30. Solving Systems of Equations When No Algorithm Is Known: Example

- (1) $r = x^2$; (2) $x = \sqrt{r}$; (3) $r = x - 0.5$; (4) $x = r + 0.5$.
- *We start with:* $\mathbf{x} = [0, 1]$, $\mathbf{r} = (-\infty, \infty)$.

(1) $\mathbf{r} = [0, 1]^2 = [0, 1]$, so $\mathbf{r}_{\text{new}} = (-\infty, \infty) \cap [0, 1] = [0, 1]$.

(2) $\mathbf{x}_{\text{new}} = \sqrt{[0, 1]} \cap [0, 1] = [0, 1]$ – no change.

(3) $\mathbf{r}_{\text{new}} = ([0, 1] - 0.5) \cap [0, 1] = [-0.5, 0.5] \cap [0, 1] = [0, 0.5]$.

(4) $\mathbf{x}_{\text{new}} = ([0, 0.5] + 0.5) \cap [0, 1] = [0.5, 1] \cap [0, 1] = [0.5, 1]$.

(1) $\mathbf{r}_{\text{new}} = [0.5, 1]^2 \cap [0, 0.5] = [0.25, 0.5]$.

(2) $\mathbf{x}_{\text{new}} = \sqrt{[0.25, 0.5]} \cap [0.5, 1] = [0.5, 0.71]$;
round $\underline{a}$ down $\downarrow$ and $\overline{a}$ up $\uparrow$, to guarantee enclosure.

(3) $\mathbf{r}_{\text{new}} = ([0.5, 0.71] - 0.5) \cap [0.25, 5] = [0.0.21] \cap [0.25, 0.5]$,
i.e., $\mathbf{r}_{\text{new}} = \emptyset$.

- *Conclusion:* the original equation has no solutions.

31. Solving Systems of Equations: Second Example

- *Example:* $x - x^2 = 0$, $x \in [0, 1]$.
- *Parsing:* $r_1 = x^2$, $0\ (= r_2)\ = x - r_1$.
- *Rules:* (1) $r = x^2$; (2) $x = \sqrt{r}$; (3) $r = x$; (4) $x = r$.
- *We start with:* $\mathbf{x} = [0, 1]$, $\mathbf{r} = (-\infty, \infty)$.
- *Problem:* after Rule 1, we're stuck with $\mathbf{x} = \mathbf{r} = [0, 1]$.
- *Solution:* bisect $\mathbf{x} = [0, 1]$ into $[0, 0.5]$ and $[0.5, 1]$.
- *For 1st subinterval:*
  - Rule 1 leads to $\mathbf{r}_{\text{new}} = [0, 0.5]^2 \cap [0, 0.5] = [0, 0.25]$;
  - Rule 4 leads to $\mathbf{x}_{\text{new}} = [0, 0.25]$;
  - Rule 1 leads to $\mathbf{r}_{\text{new}} = [0, 0.25]^2 = [0, 0.0625]$;
  - Rule 4 leads to $\mathbf{x}_{\text{new}} = [0, 0.0625]$; etc.
  - we converge to $x = 0$.
- *For 2nd subinterval:* we converge to $x = 1$.

32. Optimization: Extending Known Algorithms to Situations with Interval Uncertainty

- *Problem:* find $y_1, \ldots, y_m$ for which

$$g(y_1, \ldots, y_m, a_1, \ldots, a_m) \to \max .$$

- *We know:* a_i with interval uncertainty: $a_i \in [\underline{a}_i, \overline{a}_i]$;
- *We want:* to find the corresponding ranges of y_j.
- *First case:* for exactly known a_i, we have an algorithm $y_j = f_j(a_1, \ldots, a_n)$ for solving the optimization problem.
- *Example:* quadratic objective function g.
- *Solution:* apply interval computations techniques to find the range $f_j([\underline{a}_1, \overline{a}_1], \ldots, [\underline{a}_n, \overline{a}_n])$.
- *Better solution:* for specific f, we often already know which ideas work best.

33. Optimization When No Algorithm Is Known

- *Idea:* divide the original box $\mathbf{x}$ into subboxes $\mathbf{b}$.
- If $\max\limits_{x\in\mathbf{b}} g(x) < g(x')$ for a known x', dismiss $\mathbf{b}$.
- *Example:* $g(x) = x \cdot (1 - x)$, $\mathbf{x} = [0, 1]$.
- Divide into 10 (?) subboxes $\mathbf{b} = [0, 0.1], [0.1, 0.2], \ldots$
- Find $g(\widetilde{b})$ for each $\mathbf{b}$; the largest is $0.45 \cdot 0.55 = 0.2475$.
- Compute $G(\mathbf{b}) = g(\widetilde{b}) + (1 - 2 \cdot \mathbf{b}) \cdot [-\Delta, \Delta]$.
- Dismiss subboxes for which $\overline{Y} < 0.2475$.
- *Example:* for $[0.2, 0.3]$, we have

$$0.25 \cdot (1 - 0.25) + (1 - 2 \cdot [0.2, 0.3]) \cdot [-0.05, 0.05].$$

- Here $\overline{Y} = 0.2175 < 0.2475$, so we dismiss $[0.2, 0.3]$.
- *Result:* keep only boxes $\subseteq [0.3, 0.7]$.
- *Further subdivision:* get us closer and closer to $x = 0.5$.