

# Dealing with Uncertainties in Computing: from Probabilistic and Interval Uncertainty to Combination of Different Approaches, with Application to Geoinformatics, Bioinformatics, and Engineering

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*Case Study: Chip Design*

*Combining Interval ...*

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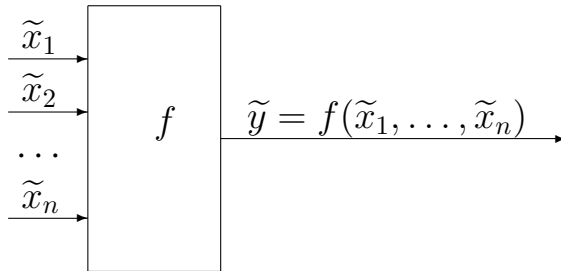
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# 1. General Problem of Data Processing under Uncertainty

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



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

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

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

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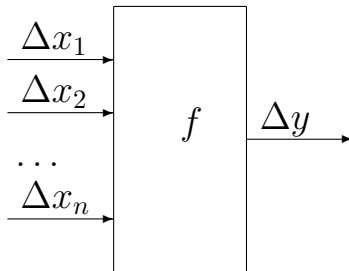
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## 2. Probabilistic and Interval Uncertainty



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

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

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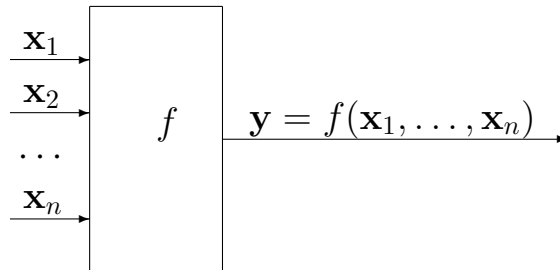
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### 3. Interval Computations: A Problem



- *Given:* an algorithm  $y = f(x_1, \dots, x_n)$  and  $n$  intervals  $\mathbf{x}_i = [\underline{x}_i, \bar{x}_i]$ .
- *Compute:* the corresponding range of  $y$ :  
$$[\underline{y}, \bar{y}] = \{f(x_1, \dots, x_n) \mid x_1 \in [\underline{x}_1, \bar{x}_1], \dots, x_n \in [\underline{x}_n, \bar{x}_n]\}.$$
- *Fact:* NP-hard even for quadratic  $f$ .
- *Challenge:* when are feasible algorithm possible?
- *Challenge:* when computing  $\mathbf{y} = [\underline{y}, \bar{y}]$  is not feasible, find a good approximation  $\mathbf{Y} \supseteq \mathbf{y}$ .

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## 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)

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## 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 – single variable*: if all we know is that  $x \in [\underline{x}, \bar{x}]$ , then MaxEnt leads to a uniform distribution on  $[\underline{x}, \bar{x}]$ .
- *Example – multiple variables*: different variables are independently distributed.

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## 6. Limitations of Maximum Entropy Approach

- *Example:* simplest algorithm  $y = x_1 + \dots + x_n$ .
- *Measurement errors:*  $\Delta x_i \in [-\Delta, \Delta]$ .
- *Analysis:*  $\Delta y = \Delta x_1 + \dots + \Delta x_n$ .
- *Worst case situation:*  $\Delta y = n \cdot \Delta$ .
- *Maximum Entropy approach:* due to Central Limit Theorem,  $\Delta y$  is  $\approx$  normal, with  $\sigma = \Delta \cdot \frac{\sqrt{n}}{\sqrt{3}}$ .
- *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.

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## 7. Interval Arithmetic: Foundations of Interval Techniques

- *Problem:* compute the range

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

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

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## 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  $\mathbf{Y} \supseteq \mathbf{y}$ .

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## 9. First Idea: Use of Monotonicity

- *Reminder:* for arithmetic, we had exact ranges.
- *Reason:*  $+$ ,  $-$ ,  $\cdot$  are monotonic in each variable.
- *How monotonicity helps:* if  $f(x_1, \dots, x_n)$  is (non-strictly) increasing ( $f \uparrow$ ) in each  $x_i$ , then

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

- *Similarly:* if  $f \uparrow$  for some  $x_i$  and  $f \downarrow$  for other  $x_j$  ( $-$ ).
- *Fact:*  $f \uparrow$  in  $x_i$  if  $\frac{\partial f}{\partial x_i} \geq 0$ .
- *Checking monotonicity:* check that the range  $[\underline{r}_i, \bar{r}_i]$  of  $\frac{\partial f}{\partial x_i}$  on  $\mathbf{x}_i$  has  $\underline{r}_i \geq 0$ .
- *Differentiation:* by Automatic Differentiation (AD) tools.
- *Estimating ranges of  $\frac{\partial f}{\partial x_i}$ :* straightforward interval comp.

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## 10. Monotonicity: Example

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

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

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

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

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

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## 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  $\underline{x}$ ,  $\bar{x}$ , or when  $\frac{df}{dx} = 0$ .
- Here,  $\frac{df}{dx} = 1 - 2x = 0$  for  $x = 0.5$ , so
  - compute  $f(0) = 0$ ,  $f(0.5) = 0.25$ , and  $f(1) = 0$ .
  - $\underline{y} = \min(0, 0.25, 0) = 0$ ,  $\bar{y} = \max(0, 0.25, 0) = 0.25$ .
- *Resulting range:*  $f(\mathbf{x}) = [0, 0.25]$ .

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## 12. Second Idea: Centered Form

- *Main idea:* Intermediate Value Theorem

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

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

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

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

- *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).

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### 13. Centered Form: Example

- *General formula:*

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

- *Example:*  $f(x) = x \cdot (1 - x)$ ,  $\mathbf{x} = [0, 1]$ .
- Here,  $\mathbf{x} = [\tilde{x} - \Delta, \tilde{x} + \Delta]$ , with  $\tilde{x} = 0.5$  and  $\Delta = 0.5$ .
- *Case  $n = 1$ :*  $\mathbf{Y} = f(\tilde{x}) + \frac{df}{dx}(\mathbf{x}) \cdot [-\Delta, \Delta]$ .
- *AD:*  $\frac{df}{dx} = 1 \cdot (1 - x) + x \cdot (-1) = 1 - 2x$ .
- *Estimation:* we have  $\frac{df}{dx}(\mathbf{x}) = 1 - 2 \cdot [0, 1] = [-1, 1]$ .
- *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  $[0, 1]$ .

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## 14. Third Idea: Bisection

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

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

- *Idea:* if the intervals are too wide, we:
  - split one of them in half ( $\Delta_i^2 \rightarrow \Delta_i^2/4$ ); 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.

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## 15. 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  $\Delta x_i = \tilde{x}_i - x_i$  (at least its linear terms).
- *Implementation:*

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

- *We start:* with  $x_i = \tilde{x}_i - \Delta x_i$ , i.e.,  
 $\tilde{x}_i + 0 \cdot \Delta x_1 + \dots + 0 \cdot \Delta x_{i-1} + (-1) \cdot \Delta x_i + 0 \cdot \Delta x_{i+1} + \dots + 0 \cdot \Delta x_n + [0, 0]$ .
- *Description:*  $a_0 = \tilde{x}_i$ ,  $a_i = -1$ ,  $a_j = 0$  for  $j \neq i$ , and  $[\underline{a}, \bar{a}] = [0, 0]$ .

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## 16. Affine Arithmetic: Operations

- *Representation:*  $a = a_0 + \sum_{i=1}^n a_i \cdot \Delta x_i + [\underline{a}, \bar{a}]$ .
- *Input:*  $a = a_0 + \sum_{i=1}^n a_i \cdot \Delta x_i + \mathbf{a}$  and  $b = b_0 + \sum_{i=1}^n b_i \cdot \Delta x_i + \mathbf{b}$ .
- *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:*  $c_0 = a_0 \cdot b_0$ ,  $c_i = a_0 \cdot b_i + b_0 \cdot a_i$ ,  
 $\mathbf{c} = a_0 \cdot \mathbf{b} + b_0 \cdot \mathbf{a} + \sum_{i \neq j} a_i \cdot b_j \cdot [-\Delta_i, \Delta_i] \cdot [-\Delta_j, \Delta_j] +$   
 $\sum_i a_i \cdot b_i \cdot [-\Delta_i, \Delta_i]^2 +$   
 $\left( \sum_i a_i \cdot [-\Delta_i, \Delta_i] \right) \cdot \mathbf{b} + \left( \sum_i b_i \cdot [-\Delta_i, \Delta_i] \right) \cdot \mathbf{a} + \mathbf{a} \cdot \mathbf{b}.$

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## 17. Affine Arithmetic: Example

- *Example:*  $f(x) = x \cdot (1 - x)$ ,  $x \in [0, 1]$ .
- Here,  $n = 1$ ,  $\tilde{x} = 0.5$ , 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.

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## 18. 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  $\Delta x_i$ ;
    - *idea:* keep, e.g., quadratic terms
- $$a = a_0 + \sum a_i \cdot \Delta x_i + \sum a_{ij} \cdot \Delta x_i \cdot \Delta x_j + \mathbf{a}.$$

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## 19. 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  $\bar{a}$  of  $[\underline{a}, \bar{a}]$ .
  - *Affine arithmetic:* for each  $a$ , we compute  $n + 3$  values:

$$a_0 \quad a_1, \dots, a_n \quad \underline{a}, \bar{a}.$$

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

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

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

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## 21. 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:

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

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

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

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## 22. 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  $\bar{a}$  up  $\uparrow$ , to guarantee enclosure.

(3)  $\mathbf{r}_{\text{new}} = ([0.5, 0.71] - 0.5) \cap [0.25, 0.5] = [0.0, 0.21] \cap [0.25, 0.5]$ ,  
i.e.,  $\mathbf{r}_{\text{new}} = \emptyset$ .

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

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## 23. 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  $x = 1$ .

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## 24. Optimization: Extending Known Algorithms to Situations with Interval Uncertainty

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

$$g(y_1, \dots, y_m, a_1, \dots, a_m) \rightarrow \max.$$

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

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## 25. Optimization When No Algorithm Is Known

- *Idea:* divide the original box  $\mathbf{x}$  into subboxes  $\mathbf{b}$ .
- If  $\max_{x \in \mathbf{b}} g(x) < g(x')$  for a known  $x'$ , dismiss  $\mathbf{b}$ .
- *Example:*  $g(x) = x \cdot (1 - x)$ ,  $\mathbf{x} = [0, 1]$ .
- Divide into 10 (?) subboxes  $\mathbf{b} = [0, 0.1], [0.1, 0.2], \dots$
- Find  $g(\tilde{\mathbf{b}})$  for each  $\mathbf{b}$ ; the largest is  $0.45 \cdot 0.55 = 0.2475$ .
- Compute  $G(\mathbf{b}) = g(\tilde{\mathbf{b}}) + (1 - 2 \cdot \mathbf{b}) \cdot [-\Delta, \Delta]$ .
- Dismiss subboxes for which  $\bar{Y} < 0.2475$ .
- *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  $\bar{Y} = 0.2175 < 0.2475$ , so we dismiss  $[0.2, 0.3]$ .
- *Result:* keep only boxes  $\subseteq [0.3, 0.7]$ .
- *Further subdivision:* get us closer and closer to  $x = 0.5$ .

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## 26. Case Study: Chip Design

- *Chip design*: one of the main objectives is to decrease the clock cycle.
- *Current approach*: uses worst-case (interval) techniques.
- *Problem*: the probability of the worst-case values is usually very small.
- *Result*: estimates are over-conservative – unnecessary over-design and under-performance of circuits.
- *Difficulty*: we only have *partial* information about the corresponding probability distributions.
- *Objective*: produce estimates valid for all distributions which are consistent with this information.
- *What we do*: provide such estimates for the clock time.

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## 27. Estimating Clock Cycle: a Practical Problem

- *Objective:* estimate the clock cycle on the design stage.
- The clock cycle of a chip is constrained by the maximum path delay over all the circuit paths

$$D \stackrel{\text{def}}{=} \max(D_1, \dots, D_N).$$

- The path delay  $D_i$  along the  $i$ -th path is the sum of the delays corresponding to the gates and wires along this path.
- Each of these delays, in turn, depends on several factors such as:
  - the variation caused by the current design practices,
  - environmental design characteristics (e.g., variations in temperature and in supply voltage), etc.

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## 28. Traditional (Interval) Approach to Estimating the Clock Cycle

- *Traditional approach:* assume that each factor takes the worst possible value.
- *Result:* time delay when all the factors are at their worst.
- *Problem:*
  - different factors are usually independent;
  - combination of worst cases is improbable.
- *Computational result:* current estimates are 30% above the observed clock time.
- *Practical result:* the clock time is set too high – chips are over-designed and under-performing.

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## 29. Robust Statistical Methods Are Needed

- *Ideal case:* we know probability distributions.
- *Solution:* Monte-Carlo simulations.
- *In practice:* we only have *partial* information about the distributions of some of the parameters; usually:
  - the mean, and
  - some characteristic of the deviation from the mean
    - e.g., the interval that is guaranteed to contain possible values of this parameter.
- *Possible approach:* Monte-Carlo with several possible distributions.
- *Problem:* no guarantee that the result is a valid bound for all possible distributions.
- *Objective:* provide *robust* bounds, i.e., bounds that work for all possible distributions.

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### 30. Towards a Mathematical Formulation of the Problem

- *General case:* each gate delay  $d$  depends on the difference  $x_1, \dots, x_n$  between the actual and the nominal values of the parameters.
- *Main assumption:* these differences are usually small.
- Each path delay  $D_i$  is the sum of gate delays.
- *Conclusion:*  $D_i$  is a linear function:  $D_i = a_i + \sum_{j=1}^n a_{ij} \cdot x_j$   
for some  $a_i$  and  $a_{ij}$ .
- The desired maximum delay  $D = \max_i D_i$  has the form

$$D = F(x_1, \dots, x_n) \stackrel{\text{def}}{=} \max_i \left( a_i + \sum_{j=1}^n a_{ij} \cdot x_j \right).$$

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## 31. Towards a Mathematical Formulation of the Problem (cont-d)

- *Known*: maxima of linear function are exactly convex functions:

$$F(\alpha \cdot x + (1 - \alpha) \cdot y) \leq \alpha \cdot F(x) + (1 - \alpha) \cdot F(y)$$

for all  $x, y$  and for all  $\alpha \in [0, 1]$ ;

- *We know*: factors  $x_i$  are independent;
  - we know distribution of some of the factors;
  - for others, we know ranges  $[x_j, \bar{x}_j]$  and means  $E_j$ .
- *Given*: a convex function  $F \geq 0$  and a number  $\varepsilon > 0$ .
- *Objective*: find the smallest  $y_0$  s.t. for all possible distributions, we have  $y \leq y_0$  with the probability  $\geq 1 - \varepsilon$ .

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## 32. Additional Property: Dependency is Non-Degenerate

- *Fact*: sometimes, we learn additional information about one of the factors  $x_j$ .
- *Example*: we learn that  $x_j$  actually belongs to a proper subinterval of the original interval  $[\underline{x}_j, \bar{x}_j]$ .
- *Consequence*: the class  $\mathcal{P}$  of possible distributions is replaced with  $\mathcal{P}' \subset \mathcal{P}$ .
- *Result*: the new value  $y'_0$  can only decrease:  $y'_0 \leq y_0$ .
- *Fact*: if  $x_j$  is irrelevant for  $y$ , then  $y'_0 = y_0$ .
- *Assumption*: irrelevant variables been weeded out.
- *Formalization*: if we narrow down one of the intervals  $[\underline{x}_j, \bar{x}_j]$ , the resulting value  $y_0$  decreases:  $y'_0 < y_0$ .

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### 33. Formulation of the Problem

GIVEN: •  $n, k \leq n, \varepsilon > 0$ ;

• a convex function  $y = F(x_1, \dots, x_n) \geq 0$ ;

•  $n - k$  cdfs  $F_j(x)$ ,  $k + 1 \leq j \leq n$ ;

• intervals  $\mathbf{x}_1, \dots, \mathbf{x}_k$ , values  $E_1, \dots, E_k$ ,

TAKE: all joint probability distributions on  $R^n$  for which:

• all  $x_i$  are independent,

•  $x_j \in \mathbf{x}_j$ ,  $E[x_j] = E_j$  for  $j \leq k$ , and

•  $x_j$  have distribution  $F_j(x)$  for  $j > k$ .

FIND: the smallest  $y_0$  s.t. for all such distributions,

$F(x_1, \dots, x_n) \leq y_0$  with probability  $\geq 1 - \varepsilon$ .

WHEN: the problem is *non-degenerate* – if we narrow down one of the intervals  $\mathbf{x}_j$ ,  $y_0$  decreases.

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## 34. Main Result and How We Can Use It

- *Result:*  $y_0$  is attained when for each  $j$  from 1 to  $k$ ,

- $x_j = \underline{x}_j$  with probability  $\underline{p}_j \stackrel{\text{def}}{=} \frac{\bar{x}_j - E_j}{\bar{x}_j - \underline{x}_j}$ , and

- $x_j = \bar{x}_j$  with probability  $\bar{p}_j \stackrel{\text{def}}{=} \frac{E_j - \underline{x}_j}{\bar{x}_j - \underline{x}_j}$ .

- *Algorithm:*

- simulate these distributions for  $x_j$ ,  $j < k$ ;
- simulate known distributions for  $j > k$ ;
- use the simulated values  $x_j^{(s)}$  to find

$$y^{(s)} = F(x_1^{(s)}, \dots, x_n^{(s)});$$

- sort  $N$  values  $y^{(s)}$ :  $y_{(1)} \leq y_{(2)} \leq \dots \leq y_{(N_i)}$ ;
- take  $y_{(N_i \cdot (1-\varepsilon))}$  as  $y_0$ .

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## 35. Comment about Monte-Carlo Techniques

- *Traditional belief*: Monte-Carlo methods are inferior to analytical:
  - they are approximate;
  - they require large computation time;
  - simulations for *several* distributions, may mis-calculate the (desired) maximum over *all* distributions.
- *We proved*: the value corresponding to the selected distributions indeed provide the desired maximum value  $y_0$ .
- *General comment*:
  - justified Monte-Carlo methods often lead to *faster* computations than analytical techniques;
  - example: multi-D integration – where Monte-Carlo methods were originally invented.

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## 36. Comment about Non-Linear Terms

- *Reminder:* in the above formula  $D_i = a_i + \sum_{j=1}^n a_{ij} \cdot x_j$ , we ignored quadratic and higher order terms in the dependence of each path time  $D_i$  on parameters  $x_j$ .
- *In reality:* we may need to take into account some quadratic terms.
- *Idea behind possible solution:* it is known that the  $\max_i D = \max_i D_i$  of convex functions  $D_i$  is convex.
- *Condition when this idea works:* when each dependence  $D_i(x_1, \dots, x_k, \dots)$  is still convex.
- *Solution:* in this case,
  - the function function  $D$  is still convex,
  - hence, our algorithm will work.

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## 37. Conclusions

- *Problem of chip design:* decrease the clock cycle.
- *How this problem is solved now:* by using worst-case (interval) techniques.
- *Limitations of this solution:* the probability of the worst-case values is usually very small.
- *Consequence:* estimates are over-conservative, hence over-design and under-performance of circuits.
- *Objective:* find the clock time as  $y_0$  s.t. for the actual delay  $y$ , we have  $\text{Prob}(y > y_0) \leq \varepsilon$  for given  $\varepsilon > 0$ .
- *Difficulty:* we only have *partial* information about the corresponding distributions.
- *What we have described:* a general technique that allows us, in particular, to compute  $y_0$ .

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## 38. Combining Interval and Probabilistic Uncertainty: General Case

- *Problem:* there are many ways to represent a probability distribution.
- *Idea:* look for an objective.
- *Objective:* make decisions  $E_x[u(x, a)] \rightarrow \max_a$ .
- *Case 1:* smooth  $u(x)$ .
- *Analysis:* we have  $u(x) = u(x_0) + (x - x_0) \cdot u'(x_0) + \dots$
- *Conclusion:* we must know moments to estimate  $E[u]$ .
- *Case of uncertainty:* interval bounds on moments.
- *Case 2:* threshold-type  $u(x)$ .
- *Conclusion:* we need cdf  $F(x) = \text{Prob}(\xi \leq x)$ .
- *Case of uncertainty:* p-box  $[\underline{F}(x), \overline{F}(x)]$ .

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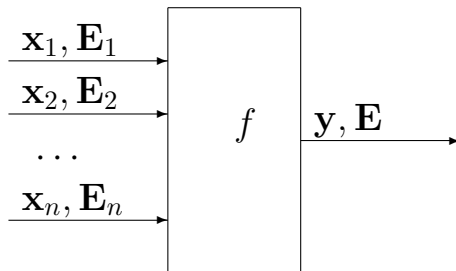
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## 39. Extension of Interval Arithmetic to Probabilistic Case: Successes

- *General solution:* parse to elementary operations  $+$ ,  $-$ ,  $\cdot$ ,  $1/x$ ,  $\max$ ,  $\min$ .
- Explicit formulas for arithmetic operations known for intervals, for p-boxes  $\mathbf{F}(x) = [\underline{F}(x), \overline{F}(x)]$ , for intervals  $+ 1\text{st moments } E_i \stackrel{\text{def}}{=} E[x_i]$ :



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## 40. Successes (cont-d)

- *Easy cases*:  $+$ ,  $-$ , product of independent  $x_i$ .
- *Example of a non-trivial case*: multiplication  $y = x_1 \cdot x_2$ , when we have no information about the correlation:

- $\underline{E} = \max(p_1 + p_2 - 1, 0) \cdot \bar{x}_1 \cdot \bar{x}_2 + \min(p_1, 1 - p_2) \cdot \bar{x}_1 \cdot \underline{x}_2 + \min(1 - p_1, p_2) \cdot \underline{x}_1 \cdot \bar{x}_2 + \max(1 - p_1 - p_2, 0) \cdot \underline{x}_1 \cdot \underline{x}_2$ ;
- $\bar{E} = \min(p_1, p_2) \cdot \bar{x}_1 \cdot \bar{x}_2 + \max(p_1 - p_2, 0) \cdot \bar{x}_1 \cdot \underline{x}_2 + \max(p_2 - p_1, 0) \cdot \underline{x}_1 \cdot \bar{x}_2 + \min(1 - p_1, 1 - p_2) \cdot \underline{x}_1 \cdot \underline{x}_2$ ,

where  $p_i \stackrel{\text{def}}{=} (E_i - \underline{x}_i) / (\bar{x}_i - \underline{x}_i)$ .

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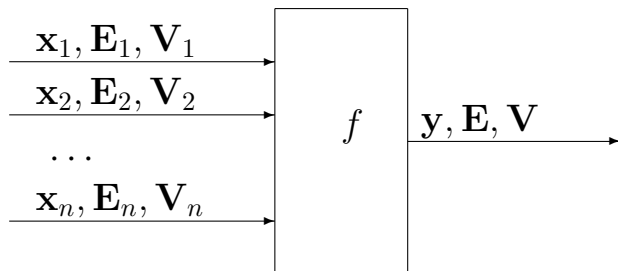
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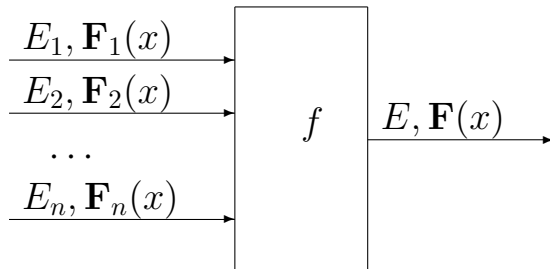
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## 41. Challenges

- intervals + 2nd moments:



- moments + p-boxes; e.g.:



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## 42. Case Study: Bioinformatics

- *Practical problem:* find genetic difference between cancer cells and healthy cells.
- *Ideal case:* we directly measure concentration  $c$  of the gene in cancer cells and  $h$  in healthy cells.
- *In reality:* difficult to separate.
- *Solution:* we measure  $y_i \approx x_i \cdot c + (1 - x_i) \cdot h$ , where  $x_i$  is the percentage of cancer cells in  $i$ -th sample.
- *Equivalent form:*  $a \cdot x_i + h \approx y_i$ , where  $a \stackrel{\text{def}}{=} c - h$ .

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### 43. Case Study: Bioinformatics (cont-d)

- If we know  $x_i$  exactly: Least Squares Method

$$\sum_{i=1}^n (a \cdot x_i + h - y_i)^2 \rightarrow \min_{a,h}, \text{ hence } a = \frac{C(x,y)}{V(x)} \text{ and}$$

$$h = E(y) - a \cdot E(x), \text{ where } E(x) = \frac{1}{n} \cdot \sum_{i=1}^n x_i,$$

$$V(x) = \frac{1}{n-1} \cdot \sum_{i=1}^n (x_i - E(x))^2,$$

$$C(x,y) = \frac{1}{n-1} \cdot \sum_{i=1}^n (x_i - E(x)) \cdot (y_i - E(y)).$$

- *Interval uncertainty:* experts manually count  $x_i$ , and only provide interval bounds  $\mathbf{x}_i$ , e.g.,  $x_i \in [0.7, 0.8]$ .
- *Problem:* find the range of  $a$  and  $h$  corresponding to all possible values  $x_i \in [\underline{x}_i, \bar{x}_i]$ .

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## 44. General Problem

- *General problem:*
  - we know intervals  $\mathbf{x}_1 = [\underline{x}_1, \overline{x}_1], \dots, \mathbf{x}_n = [\underline{x}_n, \overline{x}_n]$ ,
  - compute the range of  $E(x) = \frac{1}{n} \sum_{i=1}^n x_i$ , population variance  $V = \frac{1}{n} \sum_{i=1}^n (x_i - E(x))^2$ , etc.
- *Difficulty:* NP-hard even for variance.
- *Known:*
  - efficient algorithms for  $\underline{V}$ ,
  - efficient algorithms for  $\overline{V}$  and  $C(x, y)$  for reasonable situations.
- *Bioinformatics case:* find intervals for  $C(x, y)$  and for  $V(x)$  and divide.

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## 45. Case Study: Detecting Outliers

- In many application areas, it is important to detect *outliers*, i.e., unusual, abnormal values.
- In *medicine*, unusual values may indicate disease.
- In *geophysics*, abnormal values may indicate a mineral deposit (or an erroneous measurement result).
- In *structural integrity* testing, abnormal values may indicate faults in a structure.
- *Traditional engineering approach*: a new measurement result  $x$  is classified as an outlier if  $x \notin [L, U]$ , where

$$L \stackrel{\text{def}}{=} E - k_0 \cdot \sigma, \quad U \stackrel{\text{def}}{=} E + k_0 \cdot \sigma,$$

and  $k_0 > 1$  is pre-selected.

- *Comment*: most frequently,  $k_0 = 2, 3$ , or  $6$ .

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## 46. Outlier Detection Under Interval Uncertainty: A Problem

- In some practical situations, we only have intervals  $\mathbf{x}_i = [\underline{x}_i, \overline{x}_i]$ .
- Different  $x_i \in \mathbf{x}_i$  lead to different intervals  $[L, U]$ .
- A *possible* outlier: outside *some*  $k_0$ -sigma interval.
- *Example*: structural integrity – not to miss a fault.
- A *guaranteed* outlier: outside *all*  $k_0$ -sigma intervals.
- *Example*: before a surgery, we want to make sure that there is a micro-calcification.
- A value  $x$  is a possible outlier if  $x \notin [\overline{L}, \underline{U}]$ .
- A value  $x$  is a guaranteed outlier if  $x \notin [\underline{L}, \overline{U}]$ .
- *Conclusion*: to detect outliers, we must know the ranges of  $L = E - k_0 \cdot \sigma$  and  $U = E + k_0 \cdot \sigma$ .

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## 47. Outlier Detection Under Interval Uncertainty: A Solution

- *We need:* to detect outliers, we must compute the ranges of  $L = E - k_0 \cdot \sigma$  and  $U = E + k_0 \cdot \sigma$ .
- *We know:* how to compute the ranges  $\mathbf{E}$  and  $[\underline{\sigma}, \overline{\sigma}]$  for  $E$  and  $\sigma$ .
- *Possibility:* use interval computations to conclude that  $L \in \mathbf{E} - k_0 \cdot [\underline{\sigma}, \overline{\sigma}]$  and  $U \in \mathbf{E} + k_0 \cdot [\underline{\sigma}, \overline{\sigma}]$ .
- *Problem:* the resulting intervals for  $L$  and  $U$  are *wider* than the actual ranges.
- *Reason:*  $E$  and  $\sigma$  use the same inputs  $x_1, \dots, x_n$  and are hence not independent from each other.
- *Practical consequence:* we miss some outliers.
- *Desirable:* compute *exact* ranges for  $L$  and  $U$ .
- *Application:* detecting outliers in gravity measurements.

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## 48. Acknowledgments

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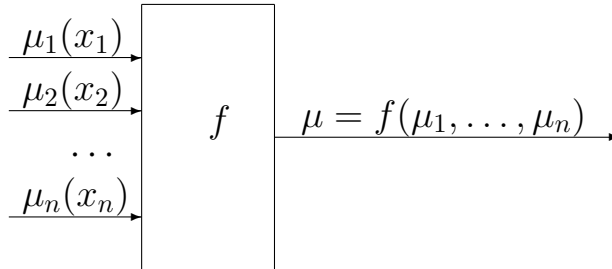
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## 49. Fuzzy Computations: A Problem



- *Given:* an algorithm  $y = f(x_1, \dots, x_n)$  and  $n$  fuzzy numbers  $\mu_i(x_i)$ .
- *Compute:*  $\mu(y) = \max_{x_1, \dots, x_n: f(x_1, \dots, x_n) = y} \min(\mu_1(x_1), \dots, \mu_n(x_n))$ .
- *Motivation:*  $y$  is a possible value of  $Y \leftrightarrow \exists x_1, \dots, x_n$  s.t. each  $x_i$  is a possible value of  $X_i$  and  $f(x_1, \dots, x_n) = y$ .
- *Details:* “and” is  $\min$ ,  $\exists$  (“or”) is  $\max$ , hence
$$\mu(y) = \max_{x_1, \dots, x_n} \min(\mu_1(x_1), \dots, \mu_n(x_n), t(f(x_1, \dots, x_n) = y)),$$
where  $t(\text{true}) = 1$  and  $t(\text{false}) = 0$ .

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## 50. Fuzzy Computations: Reduction to Interval Computations

- *Problem (reminder):*
  - *Given:* an algorithm  $y = f(x_1, \dots, x_n)$  and  $n$  fuzzy numbers  $X_i$  described by membership functions  $\mu_i(x_i)$ .
  - *Compute:*  $Y = f(X_1, \dots, X_n)$ , where  $Y$  is defined by Zadeh's extension principle:

$$\mu(y) = \max_{x_1, \dots, x_n: f(x_1, \dots, x_n) = y} \min(\mu_1(x_1), \dots, \mu_n(x_n)).$$

- *Idea:* represent each  $X_i$  by its  $\alpha$ -cuts

$$X_i(\alpha) = \{x_i : \mu_i(x_i) \geq \alpha\}.$$

- *Advantage:* for continuous  $f$ , for every  $\alpha$ , we have

$$Y(\alpha) = f(X_1(\alpha), \dots, X_n(\alpha)).$$

- *Resulting algorithm:* for  $\alpha = 0, 0.1, 0.2, \dots, 1$  apply interval computations techniques to compute  $Y(\alpha)$ .

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## 51. Proof of the Result about Chips

- Let us fix the optimal distributions for  $x_2, \dots, x_n$ ; then,

$$\text{Prob}(D \leq y_0) = \sum_{(x_1, \dots, x_n): D(x_1, \dots, x_n) \leq y_0} p_1(x_1) \cdot p_2(x_2) \cdot \dots$$

- So,  $\text{Prob}(D \leq y_0) = \sum_{i=0}^N c_i \cdot q_i$ , where  $q_i \stackrel{\text{def}}{=} p_1(v_i)$ .
- Restrictions:  $q_i \geq 0$ ,  $\sum_{i=0}^N q_i = 1$ , and  $\sum_{i=0}^N q_i \cdot v_i = E_1$ .
- Thus, the worst-case distribution for  $x_1$  is a solution to the following linear programming (LP) problem:

$$\begin{aligned} &\text{Minimize } \sum_{i=0}^N c_i \cdot q_i \text{ under the constraints } \sum_{i=0}^N q_i = 1 \text{ and} \\ &\sum_{i=0}^N q_i \cdot v_i = E_1, \quad q_i \geq 0, \quad i = 0, 1, 2, \dots, N. \end{aligned}$$

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## 52. Proof of the Result about Chips (cont-d)

- *Minimize:*  $\sum_{i=0}^N c_i \cdot q_i$  under the constraints  $\sum_{i=0}^N q_i = 1$  and  $\sum_{i=0}^N q_i \cdot v_i = E_1$ ,  $q_i \geq 0$ ,  $i = 0, 1, 2, \dots, N$ .
- *Known:* in LP with  $N + 1$  unknowns  $q_0, q_1, \dots, q_N$ ,  $\geq N + 1$  constraints are equalities.
- *In our case:* we have 2 equalities, so at least  $N - 1$  constraints  $q_i \geq 0$  are equalities.
- Hence, no more than 2 values  $q_i = p_1(v_i)$  are non-0.
- If corresponding  $v$  or  $v'$  are in  $(\underline{x}_1, \bar{x}_1)$ , then for  $[v, v'] \subset \mathbf{x}_1$  we get the same  $y_0$  – in contradiction to non-degeneracy.
- Thus, the worst-case distribution is located at  $\underline{x}_1$  and  $\bar{x}_1$ .
- The condition that the mean of  $x_1$  is  $E_1$  leads to the desired formulas for  $\underline{p}_1$  and  $\bar{p}_1$ .

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