

# Combining Interval, Probabilistic, and Fuzzy Uncertainty: Foundations, Algorithms, Challenges – An Overview

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<http://www.cs.utep.edu/interval-comp>

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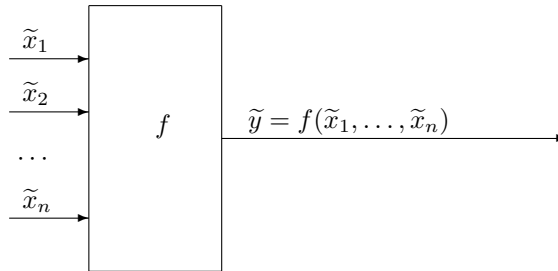
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# 1. General Problem of Data Processing under Uncertainty

- *Indirect measurements*: way to measure  $y$  that 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  $\Delta y \stackrel{\text{def}}{=} \tilde{y} - y$ ?

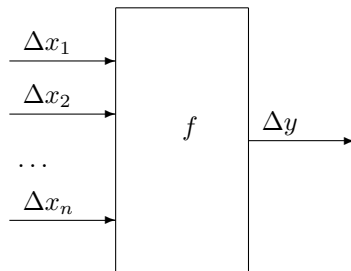
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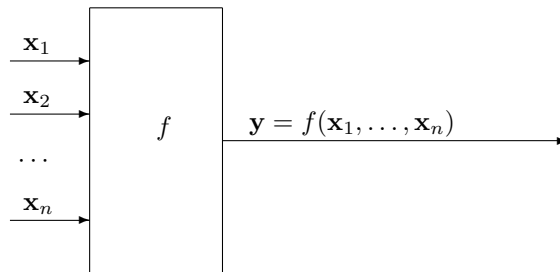
## 2. Probabilistic and Interval Uncertainty



- *Traditional approach:* we know probability distribution for  $\Delta x_i$  (usually Gaussian).
- *Where it comes from:* calibration using standard MI.
- *Problem:* sometimes we do not know the distribution because no “standard” (more accurate) MI is available. Cases:
  - fundamental science
  - manufacturing
- *Solution:* we know upper bounds  $\Delta_i$  on  $|\Delta x_i|$  hence

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

### 3. Interval Computations: A Problem



- *Given:*
  - an algorithm  $y = f(x_1, \dots, x_n)$  that transforms  $n$  real numbers  $x_i$  into a number  $y$ ;
  - $n$  intervals  $\mathbf{x}_i = [\underline{x}_i, \bar{x}_i]$ .
- *Compute:* the corresponding range of  $y$ :
$$[y, \bar{y}] = \{f(x_1, \dots, x_n) \mid x_1 \in [\underline{x}_1, \bar{x}_1], \dots, x_n \in [\underline{x}_n, \bar{x}_n]\}.$$
- *Fact:* even for quadratic  $f$ , the problem of computing the exact range  $\mathbf{y}$  is NP-hard.
- *Practical challenges:*
  - find classes of problems for which efficient algorithms are possible; and
  - for problems outside these classes, find efficient techniques for *approximating* uncertainty of  $y$ .

## 4. Why Not 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  $x \in [x, \bar{x}]$ , then MaxEnt leads to a uniform distribution on  $[x, \bar{x}]$ .
- *Example – multiple variables:* different variables are independently distributed.
- *Conclusion:* if  $\Delta y = \Delta x_1 + \dots + \Delta x_n$ , with  $\Delta x_i \in [-\Delta_i, \Delta_i]$ , then due to Central Limit Theorem,  $\Delta y$  is almost normal, with  $\sigma = \frac{1}{\sqrt{3}} \cdot \sqrt{\sum_{i=1}^n \Delta_i^2}$ .
- *Why this may be inadequate:* when  $\Delta_i = \Delta$ , we get  $\Delta \sim \sqrt{n}$ , but due to correlation, it is possible that  $\Delta = n \cdot \Delta_i \sim n \gg \sqrt{n}$ .
- *Conclusion:* using a single distribution can be very misleading, especially if we want guaranteed results – e.g., in high-risk application areas such as space exploration or nuclear engineering.

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## 5. Chip Design: Case Study When Intervals Are Not Enough

- *One of the main objectives:* decrease the chip's clock cycle  $D$ .
- *Conclusion:* it is therefore important to estimate the clock cycle on the design stage.
- *Formula – idea:*  $D$  is the maximum delay over all possible paths  $D \stackrel{\text{def}}{=} \max(D_1, \dots, D_N)$ , where  $D_i$  is the sum of the delays corresponding to the gates and wires along this path.
- *Formula – details:* each  $D_i$  depends on factors  $x_1, \dots, x_n$  – variation caused by the current design practices, environmental design characteristics (e.g., variations in temperature and in in supply voltage), etc. –

$$D_i = a_i + \sum_{j=1}^n a_{ij} \cdot x_j, \text{ so } D = \max_i \left( a_i + \sum_{j=1}^n a_{ij} \cdot x_j \right).$$

- *Traditional approach to estimating  $D$ :* worst-case (interval) analysis.
- *Result:* over-estimation up to 30% above the observed clock time, so chips are over-designed and under-performing.
- *Reason:* factors  $x_i$  are independent, so the probability that all these factors are at their worst is extremely small.
- *Challenge:* take into account the probabilistic character of the factor variations.

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## 6. General Approach: Interval-Type Step-by-Step Techniques

- *Problem:*
- *Solution:* compute an enclosure  $\mathbf{Y}$  such that  $\mathbf{y} \subseteq \mathbf{Y}$ .
- *Interval arithmetic:* for arithmetic operations  $f(x_1, x_2)$ , 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  $[y, \bar{y}]$ , 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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## 7. Interval Approach: 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:* do 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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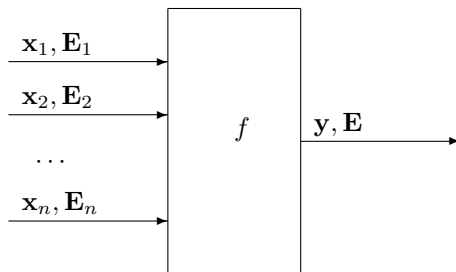


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## 8. Extension of Interval Arithmetic to Probabilistic Case: Successes

- *Objective:* make decisions  $E_x[u(x, a)] \rightarrow \max a$ .
- For smooth  $u(x)$ , we have  $u(x) = u(x_0) + (x - x_0) \cdot u'(x_0) + \dots$ , so we must know moments to estimate  $E[u]$ .
- For threshold-type  $u(x)$ , we need cdf  $F(x) = \text{Prob}(\xi \leq x)$ .
- *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  $+ 1\text{st moments } E_i \stackrel{\text{def}}{=} E[x_i]$ :



## 9. 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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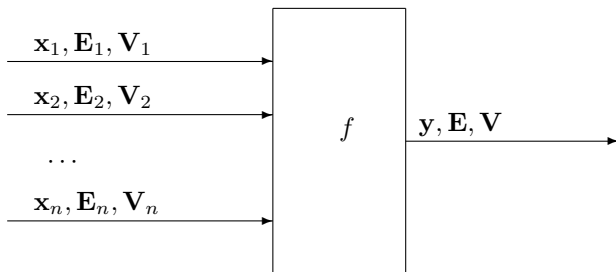
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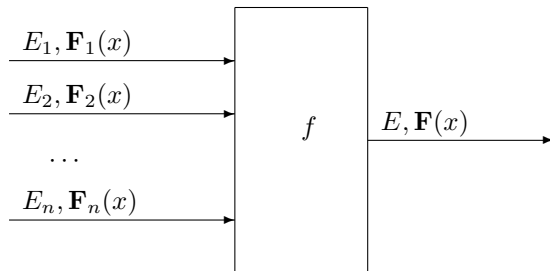
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## 10. Challenges

- intervals + 2nd moments:



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



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## 11. Problem

- *Result of interval-type approach:* over-estimation practically as bad as with interval computations.
- *Good news:* for  $D_i = a_i + \sum a_{ij} \cdot x_j$ , we use independence of  $x_i$  and get reasonable p-boxes.
- *Bad news:* the values  $D_i$  depends on same factors, so they are not independent.
- *Analogy:* this is similar to dependence-caused excess width in interval computations.
- *In interval computations:* methods beyond straightforward interval computations – centroid, affine, bisection – decrease excess width.
- *What we have done so far:* extended interval arithmetic to the probabilistic case.
- *What we need:* extend state-of-the-art interval computations techniques to the probabilistic case.

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## 12. Main Idea: Use Moments

- *What we want:* find  $D_0$  s.t.  $D \leq D_0$  with the probability  $\geq 1 - \varepsilon$  (where  $\varepsilon > 0$  is a given small probability).
- *Traditional statistical analysis:* compute moments  $M_v \stackrel{\text{def}}{=} E[D^v]$ ,  $v = 1, 2, \dots$
- *From moments to p-boxes – guaranteed:* Chebyshev inequality

$$\text{Prob}(|D - M_1| > k_0 \cdot \sigma) \leq 1/k_0^2,$$

where  $\sigma \stackrel{\text{def}}{=} \sqrt{V} = \sqrt{M_2 - M_1^2}$ .

- *Example:* for  $\varepsilon = 10^{-3}$ , we need  $D_0 = E + 30\sigma$ .
- *Problem:*  $D$  is often almost normal, so  $D_0 \approx E + 3\sigma$  – excess width.
- *Idea:* higher moments  $D_0 = M_1 + k_{2q} \cdot \sigma_{2q}$  with  $\sigma_{2q} = C_{2q}^{1/q}$  and  $k_{2q} = \varepsilon^{-1/(2q)}$ .
- *Example:* for  $\varepsilon = 10^{-3}$ ,  $k_2 \approx 30$ ,  $k_4 \approx 5.5$ ,  $k_6 \approx 3$ .
- *Central moment:*  $C_4 = E[(D - M_1)^4] = M_4 - 4 \cdot M_3 \cdot M_1 + 6 \cdot M_2 \cdot M_1^2 - 3 \cdot M_1^4$ .
- *Interval uncertainty:*  $D_0 = \overline{M}_1 + k_{2q} \cdot \overline{(C_{2q})}^{1/q}$ , where

$$\overline{C}_4 = \overline{M}_4 - 4 \cdot \underline{M}_3 \cdot \underline{M}_1 + 6 \cdot \overline{M}_2 \cdot \overline{M}_1^2 - 3 \cdot \underline{M}_1^4.$$

## 13. Formulation of the Problem: Convex Case

- GIVEN:
- natural numbers  $n, k \leq n$ , and  $v \geq 1$ ;
  - a function  $y = F(x_1, \dots, x_n)$  (algorithmically defined) such that for every combination of values  $x_{k+1}, \dots, x_n$ , the dependence of  $y$  on  $x_1, \dots, x_k$  is convex;
  - $n - k$  probability distributions  $x_{k+1}, \dots, x_n$  – e.g., given in the form of cumulative distribution function (cdf)  $F_j(x)$ ,  $k + 1 \leq j \leq n$ ;
  - $k$  intervals  $\mathbf{x}_1, \dots, \mathbf{x}_k$ , and
  - $k$  values  $E_1, \dots, E_k$ .

such that for every  $x_1 \in [\underline{x}_1, \overline{x}_1], \dots, x_k \in [\underline{x}_k, \overline{x}_k]$ , we have  $F(x_1, \dots, x_n) \geq 0$  with probability 1.

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

- all  $n$  random variables are independent;
- for each  $j$  from 1 to  $k$ ,  $x_j \in \mathbf{x}_j$  with probability 1 and the mean value of  $x_j$  is equal  $E_j$ ;
- for  $j > k$ , the variable  $x_j$  has a given distribution  $F_j(x)$ .

FIND: for the variable  $y = F(x_1, \dots, x_n)$ , find the set  $\mathbf{M}_v = [\underline{M}_v, \overline{M}_v]$  of all possible values of  $M_v \stackrel{\text{def}}{=} E[y^v]$  for all such distributions.

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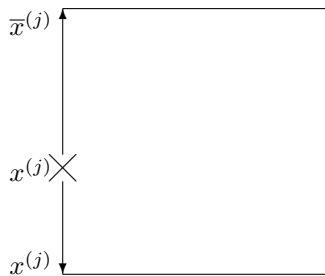
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## 14. Result

- The *smallest* possible value  $\underline{M}_v$  is attained when for each  $j$  from 1 to  $k$ , we use a 1-point distribution in which  $x_j = E_j$  with probability 1.
- The *largest* possible values  $\overline{M}_v$  is attained when for each  $j$  from 1 to  $k$ , we use a 2-point distribution for  $x_j$ , in which:
  - $x_j = \underline{x}_j$  with probability  $\underline{p}_j \stackrel{\text{def}}{=} \frac{\overline{x}_j - E_j}{\overline{x}_j - \underline{x}_j}$ .
  - $x_j = \overline{x}_j$  with probability  $\overline{p}_j \stackrel{\text{def}}{=} \frac{E_j - \underline{x}_j}{\overline{x}_j - \underline{x}_j}$ .
- *Main idea – transfer:*  $F$  is convex and  $F \geq 0$ , hence  $F^v$  is convex.



- *Algorithm:* Monte-Carlo simulations.
- *Results:* much smaller excess width.
- *Additional result:* if we also know that each distribution is unimodal.

## 15. 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, so 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  $a \stackrel{\text{def}}{=} c - h$ .

- *If we know  $x_i$  exactly:* Least Squares Method  $\sum_{i=1}^n (a \cdot x_i + h - y_i)^2 \rightarrow \min_{a,h}$ ,  
hence  $a = \frac{C(x,y)}{V(x)}$  and  $h = E(y) - a \cdot E(x)$ , where  $E(x) = \frac{1}{n} \cdot \sum_{i=1}^n x_i$ ,

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

- *Interval uncertainty:* experts manually count  $x_i$ , and only provide interval bounds  $\mathbf{x}_i$ , e.g.,  $x_i \in [0.7, 0.8]$ .
- *Fact:* different  $x_i \in \mathbf{x}_i$  lead to different  $a$  and  $h$ .
- *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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## 16. General Problem

- *General problem*: how to efficiently deduce the statistical information from, e.g., interval data.
- *Example*: we know intervals  $\mathbf{x}_1 = [\underline{x}_1, \bar{x}_1], \dots, \mathbf{x}_n = [\underline{x}_n, \bar{x}_n]$ , we want to compute the ranges of possible values of the population mean  $E(x) = \frac{1}{n} \sum_{i=1}^n x_i$ ,  
population variance  $V = \frac{1}{n} \sum_{i=1}^n (x_i - E(x))^2$ , etc.
- *Difficulty*: in general, this problem is NP-hard even for the variance.
- *Known*:
  - efficient algorithms for  $\underline{V}$ ,
  - efficient algorithms for  $\bar{V}$  for reasonable situations,
  - efficient algorithms for  $C(x, y)$  when intervals comes from a partition, etc.
- *Bioinformatics case*: we find intervals for  $C(x, y)$  and for  $V(x)$  and divide.
- *Challenges*: finding the ranges of covariance, correlation, etc., in other situations

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## 17. 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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## 18. Outlier Detection Under Interval Uncertainty: A Problem

- In some practical situations, we only have intervals  $\mathbf{x}_i = [\underline{x}_i, \overline{x}_i]$ .
- For different values  $x_i \in \mathbf{x}_i$ , we get different  $k_0$ -sigma intervals  $[L, U]$ .
- A *possible* outlier is a value outside *some*  $k_0$ -sigma interval.
- *Example*: structural integrity – not to miss a fault.
- A *guaranteed* outlier is a value 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  $x \notin [\underline{L}, \underline{U}]$ .
- 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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## 19. 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  $[\underline{\sigma}, \bar{\sigma}]$  for  $E$  and  $\sigma$ .
- *Possibility:* use interval computations to conclude that  $L \in \mathbf{E} - k_0 \cdot [\underline{\sigma}, \bar{\sigma}]$  and  $U \in \mathbf{E} + k_0 \cdot [\underline{\sigma}, \bar{\sigma}]$ .
- *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  $U$ .
- *What we do:* exactly this.
- *Application:* detecting outliers in gravity measurements.

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## 20. Fuzzy Uncertainty: In Brief

- In the fuzzy case, for each value of measurement error  $\Delta x_i$ , we describe the degree  $\mu_i(\Delta x_i)$  to which this value is possible.
- For each degree of certainty  $\alpha$ , we can determine the set of values of  $\Delta x_i$  that are possible with at least this degree of certainty – the  $\alpha$ -cut  $\{x \mid \mu(x) \geq \alpha\}$  of the original fuzzy set.
- Vice versa, if we know  $\alpha$ -cuts for every  $\alpha$ , then, for each object  $x$ , we can determine the degree of possibility that  $x$  belongs to the original fuzzy set.
- A fuzzy set can be thus viewed as a nested family of its  $\alpha$ -cuts.
- If instead of a (crisp) interval  $\mathbf{x}_i$  of possible values of the measured quantity, we have a fuzzy set  $\mu_i(x)$  of possible values, then we can view this information as a family of nested intervals  $\mathbf{x}_i(\alpha)$  –  $\alpha$ -cuts of the given fuzzy sets.
- Our objective is then to compute the fuzzy number corresponding to this the desired value  $y = f(x_1, \dots, x_n)$ .
- In this case, for each level  $\alpha$ , to compute the  $\alpha$ -cut of this fuzzy number, we can apply the interval algorithm to the  $\alpha$ -cuts  $\mathbf{x}_i(\alpha)$  of the corresponding fuzzy sets.
- The resulting nested intervals form the desired fuzzy set for  $y$ .

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## 21. Acknowledgments

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## 22. Detecting Possible Outliers: Idea

- To detect possible outliers, we need  $\bar{L}$  and  $\underline{U}$ .
- The minimum  $\underline{U}$  of a smooth function  $U$  on an interval  $[\underline{x}_i, \bar{x}_i]$  is attained:

- either inside, when  $\frac{\partial U}{\partial x_i} = 0$  – i.e., when

$$x_i = \mu \stackrel{\text{def}}{=} E - \alpha \cdot \sigma \text{ (where } \alpha \stackrel{\text{def}}{=} 1/k_0);$$

- or at  $x_i = \underline{x}_i$ , when  $\frac{\partial U}{\partial x_i} \geq 0$  – i.e., when  $\mu \leq \underline{x}_i$ ;

- or at  $x_i = \bar{x}_i$ , when  $\frac{\partial U}{\partial x_i} \leq 0$  – i.e., when  $\bar{x}_i \leq \mu$ .

- Thus, once we know how  $\mu$  is located w.r.t. all the intervals  $\mathbf{x}_i$ , we can find the optimal values of  $x_i$ .
- *Comment.* the value  $\mu$  can be obtained from the condition  $E - \alpha \cdot \sigma = \mu$ .
- Hence, to find  $\min U$ , we analyze how the endpoints  $\underline{x}_i$  and  $\bar{x}_i$  divide the real line, consider all the resulting sub-intervals, and take the smallest  $U$ .

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## 23. Computing Lower Bound for $U$ : Algorithm

- First, sort all  $2n$  values  $\underline{x}_i, \bar{x}_i$  into a sequence  $x_{(1)} \leq x_{(2)} \leq \dots \leq x_{(2n)}$ ; take  $x_{(0)} \stackrel{\text{def}}{=} -\infty, x_{(2n+1)} \stackrel{\text{def}}{=} +\infty$ .
- For each zone  $[x_{(k)}, x_{(k+1)}]$ , we compute the values

$$e_k \stackrel{\text{def}}{=} \sum_{i: \underline{x}_i \geq x_{(k+1)}} \underline{x}_i + \sum_{j: \bar{x}_j \leq x_{(k)}} \bar{x}_j,$$

$$m_k \stackrel{\text{def}}{=} \sum_{i: \underline{x}_i \geq x_{(k+1)}} (\underline{x}_i)^2 + \sum_{j: \bar{x}_j \leq x_{(k)}} (\bar{x}_j)^2,$$

and  $n_k$  = the total number of such  $i$ 's and  $j$ 's.

- Solve equation  $A - B \cdot \mu + C \cdot \mu^2 = 0$ , where

$$A \stackrel{\text{def}}{=} e_k^2 \cdot (1 + \alpha^2) - \alpha^2 \cdot m_k \cdot n,$$

$$B \stackrel{\text{def}}{=} 2e_k \cdot ((1 + \alpha^2) \cdot n_k - \alpha^2 \cdot n); \quad C \stackrel{\text{def}}{=} B \cdot \frac{n_k}{2e_k};$$

select  $\mu \in \text{zone}$  for which  $\mu \cdot n_k \leq e_k$ .

- $E_k \stackrel{\text{def}}{=} \frac{e_k}{n} + \frac{n - n_k}{n} \cdot \mu, \quad M_k \stackrel{\text{def}}{=} \frac{m_k}{n} + \frac{n - n_k}{n} \cdot \mu^2,$   
 $U_k \stackrel{\text{def}}{=} E_k + k_0 \cdot \sqrt{M_k - (E_k)^2}.$
- $\underline{U}$  is the smallest of these values  $U_k$ .

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## 24. Computing Upper Bound for $L$ : Algorithm

- First, sort all  $2n$  values  $\underline{x}_i, \bar{x}_i$  into a sequence  $x_{(1)} \leq x_{(2)} \leq \dots \leq x_{(2n)}$ ; take  $x_{(0)} \stackrel{\text{def}}{=} -\infty, x_{(2n+1)} \stackrel{\text{def}}{=} +\infty$ .
- For each zone  $[x_{(k)}, x_{(k+1)}]$ , we compute the values

$$e_k \stackrel{\text{def}}{=} \sum_{i: \underline{x}_i \geq x_{(k+1)}} \underline{x}_i + \sum_{j: \bar{x}_j \leq x_{(k)}} \bar{x}_j,$$

$$m_k \stackrel{\text{def}}{=} \sum_{i: \underline{x}_i \geq x_{(k+1)}} (\underline{x}_i)^2 + \sum_{j: \bar{x}_j \leq x_{(k)}} (\bar{x}_j)^2,$$

and  $n_k$  = the total number of such  $i$ 's and  $j$ 's.

- Solve equation  $A - B \cdot \mu + C \cdot \mu^2 = 0$ , where

$$A \stackrel{\text{def}}{=} e_k^2 \cdot (1 + \alpha^2) - \alpha^2 \cdot m_k \cdot n,$$

$$B \stackrel{\text{def}}{=} 2e_k \cdot ((1 + \alpha^2) \cdot n_k - \alpha^2 \cdot n); \quad C \stackrel{\text{def}}{=} B \cdot \frac{n_k}{2e_k};$$

select  $\mu \in \text{zone}$  for which  $\mu \cdot n_k \geq e_k$ .

- $E_k \stackrel{\text{def}}{=} \frac{e_k}{n} + \frac{n - n_k}{n} \cdot \mu, \quad M_k \stackrel{\text{def}}{=} \frac{m_k}{n} + \frac{n - n_k}{n} \cdot \mu^2,$   
 $L_k \stackrel{\text{def}}{=} E_k - k_0 \cdot \sqrt{M_k - (E_k)^2}.$
- $\bar{L}$  is the largest of these values  $L_k$ .

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## 25. Computational Complexity of Outlier Detection

- *Detecting possible outliers:* The above algorithm  $\mathcal{A}_U$  always computes  $\underline{U}$  in quadratic time.
- *Detecting possible outliers:* The above algorithm  $\overline{\mathcal{A}}_L$  always computes  $\overline{L}$  in quadratic time.
- *Detecting guaranteed outliers:* For every  $k_0 > 1$ , computing the upper endpoint  $\overline{U}$  of the interval  $[\underline{U}, \overline{U}]$  of possible values of  $U = E + k_0 \cdot \sigma$  is NP-hard.
- *Detecting guaranteed outliers:* For every  $k_0 > 1$ , computing the lower endpoint  $\underline{L}$  of the interval  $[\underline{L}, \overline{L}]$  of possible values of  $L = E - k_0 \cdot \sigma$  is NP-hard.
- *Comment.* For interval data, the NP-hardness of computing the upper bound for  $\sigma$  was known before.

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## 26. How Can We Actually Detect Guaranteed Outliers?

- *1st result:* if  $1 + (1/k_0)^2 < n$ , then  $\max U$  and  $\min L$  are attained at endpoints of  $\mathbf{x}_i$ .
- *Example:*  $k_0 > 1$  and  $n \geq 2$ .
- *Resulting algorithm:* test all  $2^n$  combinations of values  $\underline{x}_i$  and  $\bar{x}_i$ .
- *Important case:* often, measured values  $\tilde{x}_i$  are definitely different from each other, in the sense that the “narrowed” intervals

$$\left[ \tilde{x}_i - \frac{1 + \alpha^2}{n} \cdot \Delta_i, \tilde{x}_i + \frac{1 + \alpha^2}{n} \cdot \Delta_i \right]$$

do not intersect with each other.

- *Slightly more general case:* for some  $C$ , no more than  $C$  “narrowed” intervals can have a common point.

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## 27. Computing Upper Bound for $U$

- Sort all endpoints of the narrowed intervals into a sequence  $x_{(1)} \leq x_{(2)} \leq \dots \leq x_{(2n)}$ , with  $x_{(0)} \stackrel{\text{def}}{=} -\infty$ ,  $x_{(2n+1)} \stackrel{\text{def}}{=} +\infty$ .
- For each zone  $[x_{(i)}, x_{(i+1)}]$ , for each  $j$ , pick  $x_j$ :
  - if  $x_{(i+1)} < \tilde{x}_j - \frac{1 + \alpha^2}{n} \cdot \Delta_j$ , pick  $x_j = \bar{x}_j$ ;
  - if  $x_{(i+1)} > \tilde{x}_j + \frac{1 + \alpha^2}{n} \cdot \Delta_j$ , pick  $x_j = \underline{x}_j$ ;
  - for all other  $j$ , consider both  $x_j = \bar{x}_j$  and  $x_j = \underline{x}_j$ .
- We get  $\leq 2^C$  sequences of  $x_j$  for each zone.
- For each sequence  $x_j$ , check whether  $E - \alpha \cdot \sigma$  is within the zone.
- If  $E - \alpha \cdot \sigma \in \text{zone}$ , compute  $U \stackrel{\text{def}}{=} E + k_0 \cdot \sigma$ .
- Finally, we return the largest of the computed values  $U$  as  $\overline{U}$ .

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## 28. Computing Lower Bound for $L$

- Sort all endpoints of the narrowed intervals into a sequence  $x_{(1)} \leq x_{(2)} \leq \dots \leq x_{(2n)}$ , with  $x_{(0)} \stackrel{\text{def}}{=} -\infty$ ,  $x_{(2n+1)} \stackrel{\text{def}}{=} +\infty$ .
- For each zone  $[x_{(i)}, x_{(i+1)}]$ , for each  $j$ , pick  $x_j$ :
  - if  $x_{(i+1)} < \tilde{x}_j - \frac{1 + \alpha^2}{n} \cdot \Delta_j$ , pick  $x_j = \bar{x}_j$ ;
  - if  $x_{(i+1)} > \tilde{x}_j + \frac{1 + \alpha^2}{n} \cdot \Delta_j$ , pick  $x_j = \underline{x}_j$ ;
  - for all other  $j$ , consider both  $x_j = \bar{x}_j$  and  $x_j = \underline{x}_j$ .
- We get  $\leq 2^C$  sequences of  $x_j$  for each zone.
- For each sequence  $x_j$ , check whether  $E + \alpha \cdot \sigma$  is within the zone.
- If  $E + \alpha \cdot \sigma \in \text{zone}$ , compute  $L \stackrel{\text{def}}{=} E - k_0 \cdot \sigma$ .
- Finally, we return the smallest of the computed values  $L$  as  $\underline{L}$ .

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