From Interval Computations to Constraint-Related Set Computations: Towards Faster Estimation of Statistics and ODEs under Interval and p-Box Uncertainty

Martine Ceberio, Vladik Kreinovich,
and Andrzej Pownuk
University of Texas, El Paso, Texas 79968, USA
emails mceberio@cs.utep.edu, vladik@utep.edu

1. Outline

- *Interval computations:* at each intermediate stage of the computation, we have intervals of possible values.
- In our previous papers, we proposed an extension of this technique to *set computations*.
- *Set computations:* on each stage,
  - in addition to *intervals* of possible values of the quantities,
  - we also keep *sets* of possible values of pairs (triples, etc.).
- In this paper, we consider several practical problems:
  - estimating statistics (variance, correlation, etc.),
  - solving ordinary differential equations (ODEs).
- For these problems, the new formalism enables us to find estimates in feasible (polynomial) time.

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2. Need for Data Processing

- *Situation:* We are interested in the value of a physical quantity y.
- *Problem:* often, y that is difficult or impossible to measure directly.
- *Examples:* distance to a star, amount of oil in a well.
- *Solution:*
  - find easier-to-measure quantities $x_1, \ldots, x_n$ which are related to y by a known relation $y = f(x_1, \ldots, x_n)$;
  - measure or estimate the values of the quantities $x_1, \ldots, x_n$; results are $\widetilde{x}_i \approx x_i$;
  - estimate y as $\widetilde{y} = f(\widetilde{x}_1, \ldots, \widetilde{x}_n)$.
- Computing $\widetilde{y}$ is called *data processing.*
- *Comment:* algorithm f can be complex, e.g., solving ODEs.

3. Measurement Uncertainty

- *Measurement errors:* measurement are never 100% accurate, so $\Delta x_i \stackrel{\text{def}}{=} \widetilde{x}_i - x_i \neq 0$.
- *Result:* the estimate $\widetilde{y} = f(\widetilde{x}_1, \ldots, \widetilde{x}_n)$ is, in general, different from the actual value $y = f(x_1, \ldots, x_n)$.
- *Problem:* based on the information about Δx_i, estimate the error $\Delta y \stackrel{\text{def}}{=} \widetilde{y} - y$.
- *What do we know about Δx_i:* the manufacturer of the measuring instrument (MI) supplies an upper bound Δ_i:

$$|\Delta x_i| \leq \Delta_i.$$

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

4. Measurement Uncertainty: from Probabilities to Intervals

- *Reminder:* we know that $\Delta x_i \in [-\Delta_i, \Delta_i]$.
- *Probabilistic uncertainty:* often, we also know the probability of different values $\Delta x_i \in [\Delta_i, \Delta_i]$.
- We can determine these probabilities by using standard measuring instruments.
- Two cases when this is not done:
  - cutting edge measurements (e.g., Hubble telescope);
  - manufacturing.
- In these cases, we have a purely interval uncertainty.

5. Interval Part: Outline

- We start by recalling the basic techniques of interval computations and their drawbacks.
- Then we will describe the new set computation techniques.
- We describe a class of problems for which these techniques are efficient.
- Finally, we talk about how we can extend these techniques to other types of uncertainty.
- Example of other types of uncertainty: classes of probability distributions.

6. Straightforward Interval Computations: Main Idea

- *Parsing:* inside the computer, every algorithm consists of elementary operations ($+$, $-$, $\cdot$, min, max, etc.).
- *Interval arithmetic:* for each elementary operation $f(a,b)$,
  – if we know the intervals $\mathbf{a}$ and $\mathbf{b}$,
  – we can compute the exact range $f(\mathbf{a},\mathbf{b})$:

$$[\underline{a},\overline{a}]+[\underline{b},\overline{b}]=[\underline{a}+\underline{b},\overline{a}+\overline{b}];\quad [\underline{a},\overline{a}]-[\underline{b},\overline{b}]=[\underline{a}-\overline{b},\overline{a}-\underline{b}];$$

$$[\underline{a},\overline{a}]\cdot[\underline{b},\overline{b}]=[\min(\underline{a}\cdot\underline{b},\underline{a}\cdot\overline{b},\overline{a}\cdot\underline{b},\overline{a}\cdot\overline{b}),\max(\underline{a}\cdot\underline{b},\underline{a}\cdot\overline{b},\overline{a}\cdot\underline{b},\overline{a}\cdot\overline{b})];$$

$$\frac{1}{[\underline{a},\overline{a}]}=\left[\frac{1}{\overline{a}},\frac{1}{\underline{a}}\right]\text{ if }0\notin[\underline{a},\overline{a}];\quad \frac{[\underline{a},\overline{a}]}{[\underline{b},\overline{b}]}=[\underline{a},\overline{a}]\cdot\frac{1}{[\underline{b},\overline{b}]}.$$

- *Main idea:* replace each elementary operation in f by the corresponding operation of interval arithmetic.
- *Known:* we get an enclosure $\mathbf{Y}\supseteq\mathbf{y}$ for the desired range.

7. Discussion

- *Fact:* not every real number can be exactly implemented in a computer, so:
  - after implementing an operation of interval arithmetic,
  - we must enclose the result $[r^-, r^+]$ in a computer-representable interval:
    * round-off r^- to a smaller computer-representable value $\underline{r}$, and
    * round-off r^+ to a larger computer-representable value $\overline{r}$.
- *Computation time:* increase by a factor of ≤ 4.
- *Computing exact range:* NP-hard.
- *Conclusion:* excess width is inevitable.
- *More accurate techniques exist:* centered form, bisection, etc.

8. Reason for Excess Width

- *Main reason:*
  - intermediate results are dependent on each other;
  - straightforward interval computations ignore this.
- *Example:* the range of $f(x_1) = x_1 - x_1^2$ over $\mathbf{x}_1 = [0, 1]$ is $\mathbf{y} = [0, 0.25]$.
- *Parsing:*
  - we first compute $x_2 := x_1^2$,
  - then subtract x_2 from x_1.
- *Straightforward interval computations:*
  - compute $\mathbf{r} = [0, 1]^2 = [0, 1]$,
  - then $\mathbf{x}_1 - \mathbf{x}_2 = [0, 1] - [0, 1] = [-1, 1]$.
- *Illustration:* the values of x_1 and x_2 are not independent: x_2 is uniquely determined by x_1, as $x_2 = x_1^2$.

9. Constraint-Based Set Computations

- *Main idea* (Shary): at every computation stage, we also keep *sets*:
  - sets $\mathbf{x}_{ij}$ of possible values of pairs (x_i, x_j);
  - if needed, sets $\mathbf{x}_{ijk}$ of possible values of triples (x_i, x_j, x_k).
- *Example:*
  - in addition to intervals $\mathbf{x}_1 = \mathbf{x}_2 = [0, 1]$,
  - we also generate the set $\mathbf{x}_{12} = \{(x_1, x_1^2) \,|\, x_1 \in [0, 1]\}$.
- *Result:* Then, the desired range is computed as the range of $x_1 - x_2$ over this set – which is exactly $[0, 0.25]$.
- *Set arithmetic:* e.g., if $x_k := x_i + x_j$, we set

$$\mathbf{x}_{ik} = \{(x_i, x_i + x_j) \,|\, (x_i, x_j) \in \mathbf{x}_{ij}\},$$

$$\mathbf{x}_{jk} = \{(x_j, x_i + x_j) \,|\, (x_i, x_j) \in \mathbf{x}_{ij}\},$$

$$\mathbf{x}_{kl} = \{(x_i + x_j, x_l) \,|\, (x_i, x_j) \in \mathbf{x}_{ij}, (x_i, x_l) \in \mathbf{x}_{il}, (x_j, x_l) \in \mathbf{x}_{jl}\}.$$

10. From Main Idea to Actual Computer Implementation

- We fix the number C of granules (e.g., $C = 10$).
- We divide each interval $\mathbf{x}_i$ into C equal parts $\mathbf{X}_i$.
- Thus each box $\mathbf{x}_i \times \mathbf{x}_j$ is divided into C^2 subboxes $\mathbf{X}_i \times \mathbf{X}_j$.
- We then describe each set $\mathbf{x}_{ij}$ by listing all subboxes $\mathbf{X}_i \times \mathbf{X}_j$ which have common elements with $\mathbf{x}_{ij}$.
- The union of such subboxes is an enclosure for the desired set $\mathbf{x}_{ij}$.

11. Implementing Arithmetic Operations

- *Example:* implementing

$$\mathbf{x}_{ik} = \{(x_i, x_i + x_j) \,|\, (x_i, x_j) \in \mathbf{x}_{ij}\}.$$

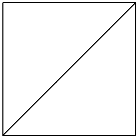
- *Step 1:* we take all the subboxes $\mathbf{X}_i \times \mathbf{X}_j$ that form the set $\mathbf{x}_{ij}$.
- *Step 2:* for each of these subboxes, we enclosure the corresponding set of pairs

$$\{(x_i, x_i + x_j) \,|\, (x_i, x_j) \in \mathbf{X}_i \times \mathbf{X}_j\}$$

  into a set $\mathbf{X}_i \times (\mathbf{X}_i + \mathbf{X}_j)$.
- *Step 3:* we add all subboxes $\mathbf{X}_i \times \mathbf{X}_k$ intersecting with this set to the enclosure for $\mathbf{x}_{ik}$.
- *Enclosure property:* we always have enclosure.
- *Relative accuracy:* $1/C$.

12. First Example: Computing the Range of $x - x$

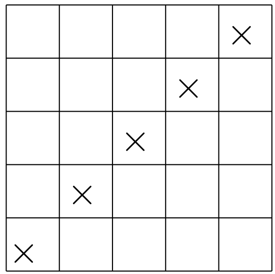
- For $f(x) = x - x$ on $[0, 1]$, the actual range is $[0, 0]$;
- *Problem:* straightforward interval computations lead to an enclosure $[0, 1] - [0, 1] = [-1, 1]$.
- In straightforward interval computations:
  - we have $r_1 = x$ with interval $\mathbf{r}_1 = [0, 1]$;
  - we have $r_2 = x$ with interval $\mathbf{x}_2 = [0, 1]$;
  - the variables r_1 and r_2 are dependent, but we ignore this dependence.
- *New approach:* $\mathbf{r}_1 = \mathbf{r}_2 = [0, 1]$, and $\mathbf{r}_{12}$:



- The resulting set is the exact range $\{0\} = [0, 0]$.

13. First Example (cont-d)

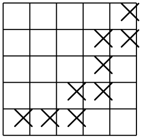
- *Problem:* compute the range of $f(x) = x - x$ on $[0, 1]$.
- In the new approach: we have $\mathbf{r}_1 = \mathbf{r}_2 = [0, 1]$, and we also have $\mathbf{r}_{12}$:



- For each small box, we have $[-0.2, 0.2]$, so the union is $[-0.2, 0.2]$.
- If we divide into more pieces, we get close to 0.

14. Second Example: Computing the Range of $x - x^2$

- *Straightforwrad approach:* $r_1 = x$ with $\mathbf{r}_1 = [0, 1]$, $r_2 = x^2$ with $\mathbf{r}_2 = [0, 1]$, $[0, 1] - [0, 1] = [-1, 1] \supset [0, 0.25]$.
- *New approach:* for $\mathbf{R}_1 = [0.2, 0.4]$, we have $\mathbf{R}_1^2 = [0.04, 0.16] \subseteq [0, 0.2]$.
- For $\mathbf{R}_1 = [0.4, 0.6]$, $\mathbf{R}_1^2 = [0.16, 0.25] \subseteq [0, 0.2] \cup [0.2, 0.4]$, etc.



- For each pair $\mathbf{R}_1 \times \mathbf{R}_2$, we have $\mathbf{R}_1 - \mathbf{R}_2 = [-0.2, 0.2]$, $[0, 0.4]$ and $[0.2, 0.6]$.
- So, the union of sets $\mathbf{R}_1 - \mathbf{R}_2$ is $\mathbf{r}_3 = [-0.2, 0.6]$.
- If we divide into more pieces, we get closer to $[0, 0.25]$.

15. Limitations of This Approach

- *Fact:* to get an accuracy ε, we must use $\sim 1/\varepsilon$ granules.
- *Reasonable situation:* we want to compute the result with k digits of accuracy, i.e., with accuracy $\varepsilon = 10^{-k}$.
- *Problem:* we must consider exponentially many boxes ($\sim 10^k$).
- *Conclusion:* this method is only applicable
  - when we want to know the desired quantity
  - with a given accuracy (e.g., 10%).

16. Estimating Variance under Interval Uncertainty

- *We know:* intervals $\mathbf{x}_1, \ldots, \mathbf{x}_n$ of possible values of x_i.
- *We need to compute:* the range of the variance $V = \dfrac{1}{n} \cdot M - \dfrac{1}{n^2} \cdot E^2$, where $M \stackrel{\text{def}}{=} \sum\limits_{i=1}^{n} x_i^2$ and $E \stackrel{\text{def}}{=} \sum\limits_{i=1}^{n} x_i$.
- *Natural idea:* compute $M_k \stackrel{\text{def}}{=} \sum\limits_{i=1}^{k} x_i^2$ and $E_k \stackrel{\text{def}}{=} \sum\limits_{i=1}^{k} x_i$: $M_0 = E_0 = 0$, $(M_{k+1}, E_{k+1}) = (M_k + x_{k+1}^2, E_k + x_{k+1})$.
- *Set computations:* $\mathbf{p}_0 = \{(M_0, E_0)\} = \{(0,0)\}$,

$$\mathbf{p}_{k+1} = \{(M_k + x^2, E_k + x) \mid (M_k, E_k) \in \mathbf{p}_k, x \in \mathbf{x}_{k+1}\},$$

$$\mathbf{V} = \left\{ \frac{1}{n} \cdot M - \frac{1}{n^2} \cdot E^2 \mid (E, M) \in \mathbf{p}_n \right\}.$$

- *Accuracy:* after n steps, we add the inaccuracy of n/C. Thus, to get $n/C \approx \varepsilon$, we must choose $C = n/\varepsilon$.
- *Computation time:* C^3 subboxes on n steps – $O(n^4)$.

17. Other Statistical Characteristics

- *Central moment:* $C_d = \dfrac{1}{n} \cdot \displaystyle\sum_{i=1}^{n} (x_i - \overline{x})^d$ is a linear combination of d moments $M^{(j)} \stackrel{\text{def}}{=} \sum_{i=1}^{n} x_i^j$ for $j = 1, \ldots, d$.
- *How to compute:* keep, for each k, the set of possible values of tuples $(M_k^{(1)}, \ldots, M_k^{(d)})$, where $M_k^{(j)} \stackrel{\text{def}}{=} \sum_{i=1}^{k} x_i^j$.
- *Computation time:* $n \cdot C^{d+1} \sim n^{d+2}$ steps.
- *Covariance:* $C = \dfrac{1}{n} \cdot \displaystyle\sum_{i=1}^{n} x_i \cdot y_i - \dfrac{1}{n^2} \cdot \sum_{i=1}^{n} x_i \cdot \sum_{i=1}^{n} y_i$.
- *How to compute:* keep the values of the triples (C_k, X_k, Y_k), where $C_k \stackrel{\text{def}}{=} \sum_{i=1}^{k} x_i \cdot y_i$, $X_k \stackrel{\text{def}}{=} \sum_{i=1}^{k} x_i$, and $Y_k \stackrel{\text{def}}{=} \sum_{i=1}^{k} y_i$.
- *Correlation* $\rho = C/\sqrt{V_x \cdot V_y}$: similar.

18. Dynamical Systems under Interval Uncertainty

- *Situation:*

  $$x_i(t+1) = f_i(x_1(t), \ldots, x_m(t), t, a_1, \ldots, a_k, b_1(t), \ldots, b_l(t)),$$

  where:

  – the dependence f_i is known,

  – we know the intervals $\mathbf{a}_j$ of possible values of the global parameters a_i, and

  – we know the intervals $\mathbf{b}_j(t)$ of possible values of the noise-like parameters $b_j(t)$.

- *Set computations solution:*

  – keep the set of all possible values of a tuple

  $$(x_1(t), \ldots, x_m(t), a_1, \ldots, a_k),$$

  – use the dynamic equations to get the exact set of possible values of this tuple at the moment $t+1$.

19. Possibility to Take Constraints into Account

- *Traditional formulation:* all combinations of $x_i \in \mathbf{x}_i$ are possible.
- *In practice:* we may have additional constraints on x_i.
- *Example:* $\mathbf{x}_i = [-1, 1]$ and $|x_i - x_{i+1}| \le \varepsilon$ for some $\varepsilon > 0$ (i.e., x_i is smooth).
- *Estimating:* a high-frequency Fourier coefficient

$$f = x_1 - x_2 + x_3 - x_4 + \ldots + x_{2n-1} - x_{2n}.$$

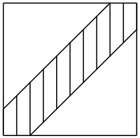
- *Usual interval computations:* enclosure $[-2n, 2n]$.
- *Actual range* of $(x_1 - x_2) + (x_3 - x_4) + \ldots$ is $[-n \cdot \varepsilon, n \cdot \varepsilon]$.
- *Set computations approach:* keep the set $\mathbf{s}_k$ of pairs (f_k, x_k), where $f_k = x_1 - x_2 + \ldots + (-1)^{k+1} \cdot x_k$, then

$$\mathbf{s}_{k+1} = \{(f_k + (-1)^k \cdot x_{k+1}, x_{k+1}) \,|\, (f_k, x_k) \in \mathbf{s}_k \,\&\, |x_k - x_{k+1}| \le \varepsilon\}.$$

- *Result:* almost exact bounds (modulo $1/C$).

20. Toy Example with Prior Dependence

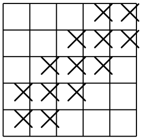
- *Case study:* find the range of $r_1 - r_2$ when $\mathbf{r}_1 = [0,1]$, $\mathbf{r}_2 = [0,1]$, and $|r_1 - r_2| \le 0.2$.
- *Actual range:* $[-0.2, 0.2]$.
- *Straightforward interval computations:* $[0,1] - [0,1] = [-1,1]$.
- *New approach:*
  - First, we describe the set $\mathbf{r}_{12}$:



  - Next, we compute $\{r_1 - r_2 \,|\, (r_1, r_2) \in \mathbf{r}_{12}\}$.
- *Result:* $[-0.2, 0.2]$.

21. Toy Example with Prior Dependence (cont-d)

- *Case study:* find the range of $r_1 - r_2$ when $\mathbf{r}_1 = [0, 1]$, $\mathbf{r}_2 = [0, 1]$, and $|r_1 - r_2| \le 0.1$.
- *Actual range:* $[-0.2, 0.2]$.
- *Straightforward approach:* $[0, 1] - [0, 1] = [-1, 1]$.
- *New approach:* first, we describe the constraint in terms of subboxes:



- Next, we compute $\mathbf{R}_1 - \mathbf{R}_2$ for all possible pairs and take the union.
- *Result:* $[-0.6, 0.6]$.
- If we divide into more pieces, we get the enclosure closer to $[-0.2, 0.2]$.

22. p-Boxes and Classes of Probability Distributions

- *Situation:*
  - in addition to $\mathbf{x}_i$,
  - we may also have *partial* information about the probabilities of different values $x_i \in \mathbf{x}_i$.
- An *exact* probability distribution can be described, e.g., by its cumulative distribution function

$$F_i(z) = \text{Prob}(x_i \le z).$$

- A *partial* information means that instead of a single cdf, we have a *class* $\mathcal{F}$ of possible cdfs.
- *p-box:*
  - for every z, we know an interval $\mathbf{F}(z) = [\underline{F}(z), \overline{F}(z)]$;
  - we consider all possible distributions for which, for all z, we have $F(z) \in \mathbf{F}(z)$.

23. Set Computations for p-Boxes and Classes of Probability Distributions

- *Idea:* keep and update, for all t, the set of possible joint *distributions* for the tuple $(x_1(t), \ldots, a_1, \ldots)$.
- *Implementation:*
  - divide both the x-range and the probability (p-) range into C granules, and
  - describe, for each x-granule, which p-granules are covered.
- *Remaining challenge:*
  - to describe a p-subbox, we need to attach one of C probability granules to each of C x-granules;
  - these are $\sim C^C$ such attachments, so we need $\sim C^C$ subboxes;
  - for $C = 10$, we already get an unrealistic 10^{10} increase in computation time.

24. Acknowledgments

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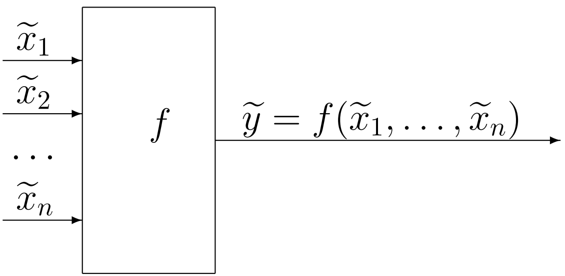
25. General Problem of Data Processing under Uncertainty

- *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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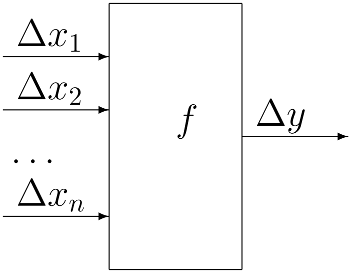
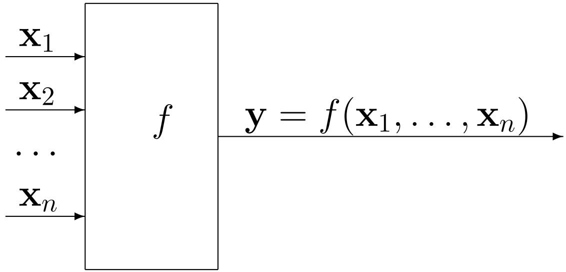
26. Probabilistic and Interval Uncertainty



- *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

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

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

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28. 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)

29. 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 $x \in [\underline{x}, \overline{x}]$, then MaxEnt leads to a uniform distribution on $[\underline{x}, \overline{x}]$.
- *Example – multiple variables:* different variables are independently distributed.

30. 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.

31. 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 $0 \notin \mathbf{x}_1$).

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

33. 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.

34. 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.

35. 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:* $f(\mathbf{x}) = [0, 0.25]$.

36. 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).

37. 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 $[0, 1]$.

38. 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.

39. 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 $[\underline{a}, \overline{a}] = [0, 0]$.

40. 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:* $c_0 = a_0 \cdot b_0$, $c_i = a_0 \cdot b_i + b_0 \cdot a_i$,

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

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

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

41. 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.

42. 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

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

43. 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.

44. 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.

45. 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:

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

46. 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.

47. 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 $x = 1$.

48. 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.

49. 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 $x = 0.5$.

50. 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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51. 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

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

- 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.

52. 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.

53. 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.

54. Towards a Mathematical Formulation of the Problem

- *General case:* each gate delay d depends on the difference $x_1, \ldots, x_n$ 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: $D_i = a_i + \sum\limits_{j=1}^{n} a_{ij} \cdot x_j$ for some a_i and a_{ij}.
- The desired maximum delay $D = \max\limits_i D_i$ has the form

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

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

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

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

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 $[\underline{x}_j, \overline{x}_j]$ and means E_j.
- *Given:* a convex function $F \ge 0$ and a number $\varepsilon > 0$.
- *Objective:* find the smallest y_0 s.t. for all possible distributions, we have $y \le y_0$ with the probability $\ge 1-\varepsilon$.

56. 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 $[\underline{x}_j, \overline{x}_j]$.
- *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: $y_0' \le y_0$.
- *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 $[\underline{x}_j, \overline{x}_j]$, the resulting value y_0 decreases: $y_0' < y_0$.

57. Formulation of the Problem

GIVEN:
- n, $k \le n$, $\varepsilon > 0$;
- a convex function $y = F(x_1, \ldots, x_n) \ge 0$;
- $n - k$ cdfs $F_j(x)$, $k + 1 \le j \le n$;
- intervals $\mathbf{x}_1, \ldots, \mathbf{x}_k$, values $E_1, \ldots, E_k$,

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 $j \le k$, and
- x_j have distribution $F_j(x)$ for $j > k$.

FIND: the smallest y_0 s.t. for all such distributions, $F(x_1, \ldots, x_n) \le y_0$ with probability $\ge 1 - \varepsilon$.

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

58. 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 $\underline{p}_j \stackrel{\text{def}}{=} \dfrac{\overline{x}_j - E_j}{\overline{x}_j - \underline{x}_j}$, and
  - $x_j = \overline{x}_j$ with probability $\overline{p}_j \stackrel{\text{def}}{=} \dfrac{E_j - \underline{x}_j}{\overline{x}_j - \underline{x}_j}$.
- *Algorithm:*
  - simulate these distributions for x_j, $j < k$;
  - simulate known distributions for $j > k$;
  - use the simulated values $x_j^{(s)}$ to find

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

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

59. 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.

60. Comment about Non-Linear Terms

- *Reminder:* in the above formula $D_i = a_i + \sum\limits_{j=1}^{n} a_{ij} \cdot x_j$, 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 $D = \max\limits_i D_i$ of convex functions D_i is convex.
- *Condition when this idea works:* when each dependence $D_i(x_1, \ldots, x_k, \ldots)$ is still convex.
- *Solution:* in this case,
  - the function function D is still convex,
  - hence, our algorithm will work.

61. Conclusions

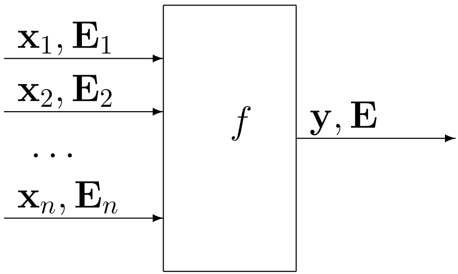
- *Problem of chip design:* decrease the clock cycle.
- *How this problem is solved now:* by using worst-case (interval) techniques.
- *Limitations of this solution:* the probability of the worst-case values is usually very small.
- *Consequence:* estimates are over-conservative, hence over-design and under-performance of circuits.
- *Objective:* find the clock time as y_0 s.t. for the actual delay y, we have $\text{Prob}(y > y_0) \le \varepsilon$ 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.

62. 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 $E_x[u(x,a)] \to \max\limits_a$.
- *Case 1:* smooth $u(x)$.
- *Analysis:* we have $u(x) = u(x_0) + (x - x_0) \cdot u'(x_0) + \ldots$
- *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 $F(x) = \text{Prob}(\xi \le x)$.
- *Case of uncertainty:* p-box $[\underline{F}(x), \overline{F}(x)]$.

63. 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 + 1st moments $E_i \stackrel{\text{def}}{=} E[x_i]$:



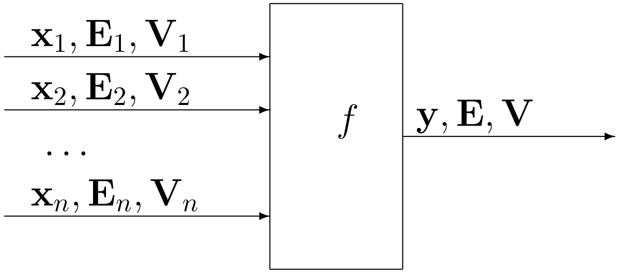
64. Successes (cont-d)

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

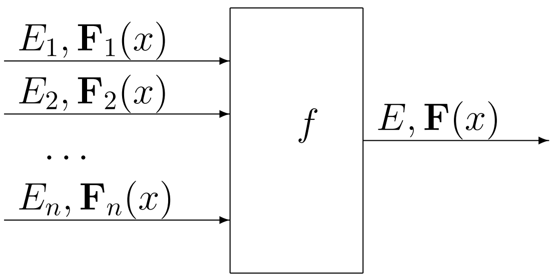
  where $p_i \stackrel{\text{def}}{=} (E_i - \underline{x}_i)/(\overline{x}_i - \underline{x}_i)$.

65. Challenges

- intervals + 2nd moments:



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



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66. 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 $a \stackrel{\text{def}}{=} c - h$.

67. Case Study: Bioinformatics (cont-d)

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

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

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

- *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 $x_i\in[\underline{x}_i,\overline{x}_i]$.

68. General Problem

- *General problem:*
  - we know intervals $\mathbf{x}_1 = [\underline{x}_1, \overline{x}_1]$, ..., $\mathbf{x}_n = [\underline{x}_n, \overline{x}_n]$,
  - compute the range of $E(x) = \dfrac{1}{n}\sum\limits_{i=1}^{n} x_i$, population variance $V = \dfrac{1}{n}\sum\limits_{i=1}^{n}(x_i - E(x))^2$, 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.

69. 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.

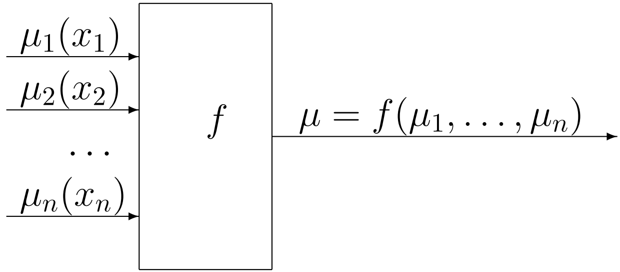
70. Outlier Detection Under Interval Uncertainty: A Problem

- 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 $U = E + k_0 \cdot \sigma$.

71. 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 σ.
- *Possibility:* use interval computations to conclude that $L \in \mathbf{E} - k_0 \cdot [\underline{\sigma}, \overline{\sigma}]$ and $L \in \mathbf{E} + k_0 \cdot [\underline{\sigma}, \overline{\sigma}]$.
- *Problem:* the resulting intervals for L and U are *wider* than the actual ranges.
- *Reason:* E and σ use the same inputs $x_1, \ldots, x_n$ 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.

72. Fuzzy Computations: A Problem



- *Given:* an algorithm $y = f(x_1, \dots, x_n)$ and n fuzzy numbers $\mu_i(x_i)$.
- *Compute:* $\mu(y) = \max\limits_{x_1,\dots,x_n : f(x_1,\dots,x_n)=y} \min(\mu_1(x_1), \dots, \mu_n(x_n))$.
- *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 $t(\text{false}) = 0$.

73. Fuzzy Computations: Reduction to Interval Computations

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

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

- *Idea:* represent each X_i by its α-cuts

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

- *Advantage:* for continuous f, for every α, we have

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

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

74. Proof of the Result about Chips

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

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

- So, $\text{Prob}(D \le y_0) = \sum\limits_{i=0}^{N} c_i \cdot q_i$, where $q_i \stackrel{\text{def}}{=} p_1(v_i)$.

- Restrictions: $q_i \ge 0$, $\sum\limits_{i=0}^{N} q_i = 1$, and $\sum\limits_{i=0}^{N} q_i \cdot v_i = E_1$.

- Thus, the worst-case distribution for x_1 is a solution to the following linear programming (LP) problem:

Minimize $\sum\limits_{i=0}^{N} c_i \cdot q_i$ under the constraints $\sum\limits_{i=0}^{N} q_i = 1$ and

$$\sum_{i=0}^{N} q_i \cdot v_i = E_1,\ q_i \ge 0, \quad i = 0, 1, 2, \ldots, N.$$

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

- *Minimize:* $\sum\limits_{i=0}^{N} c_i \cdot q_i$ under the constraints $\sum\limits_{i=0}^{N} q_i = 1$ and $\sum\limits_{i=0}^{N} q_i \cdot v_i = E_1$, $q_i \ge 0$, $i = 0, 1, 2, \ldots, N$.
- *Known:* in LP with $N+1$ unknowns $q_0, q_1, \ldots, q_N$, $\ge N+1$ constraints are equalities.
- *In our case:* we have 2 equalities, so at least $N-1$ constraints $q_i \ge 0$ are equalities.
- Hence, no more than 2 values $q_i = p_1(v_i)$ are non-0.
- If corresponding v or v' are in $(\underline{x}_1, \overline{x}_1)$, 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 $\overline{x}_1$.
- The condition that the mean of x_1 is E_1 leads to the desired formulas for $\underline{p}_1$ and $\overline{p}_1$.