

Statistical Data Processing under Interval Uncertainty: Algorithms and Computational Complexity

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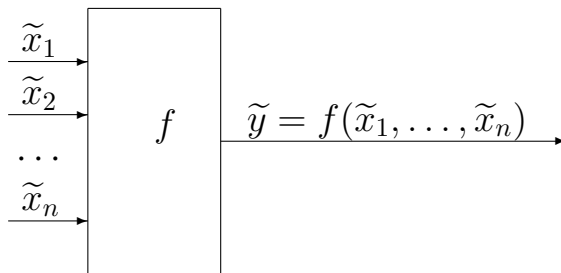
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1. General Problem of Data Processing under Uncertainty

- *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

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

- *Question:* what are bounds on $\Delta y \stackrel{\text{def}}{=} \tilde{y} - y$?

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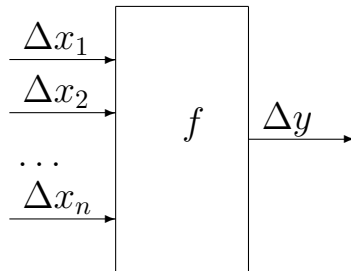
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2. Probabilistic and Interval Uncertainty



- *Traditional approach:* we know probability distribution for Δx_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 Δ_i on $|\Delta x_i|$ hence

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

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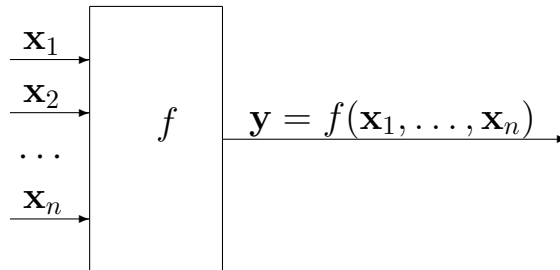
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3. Interval Computations: A Problem



- *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. 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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5. 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, Δy 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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6. 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 $0 \notin \mathbf{x}_1$).

7. 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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8. 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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9. 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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10. 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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11. 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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12. 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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13. 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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14. 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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15. 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:* $c_0 = a_0 \cdot b_0$, $c_i = a_0 \cdot b_i + b_0 \cdot a_i$,
 $\mathbf{c} = a_0 \cdot \mathbf{b} + b_0 \cdot \mathbf{a} + \sum_{i \neq j} a_i \cdot b_j \cdot [-\Delta_i, \Delta_i] \cdot [-\Delta_j, \Delta_j] +$
 $\sum_i a_i \cdot b_i \cdot [-\Delta_i, \Delta_i]^2 +$
 $\left(\sum_i a_i \cdot [-\Delta_i, \Delta_i] \right) \cdot \mathbf{b} + \left(\sum_i b_i \cdot [-\Delta_i, \Delta_i] \right) \cdot \mathbf{a} + \mathbf{a} \cdot \mathbf{b}.$

16. 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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17. 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

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

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18. 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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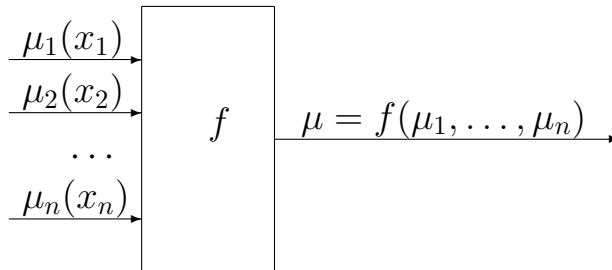
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19. Fuzzy Computations: A Problem



- *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 $t(\text{false}) = 0$.

20. 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 α -cuts

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

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

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

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

21. 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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22. 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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23. 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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24. 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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25. 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

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

26. 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 $[\underline{x}_j, \bar{x}_j]$ 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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27. 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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28. 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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29. 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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30. 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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31. 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 D is still convex,
 - hence, our algorithm will work.

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32. Case Study: 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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33. 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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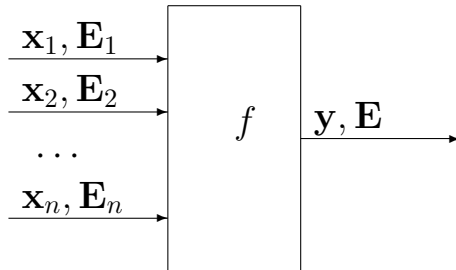
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34. Extension of Interval Arithmetic to Probabilistic Case: Successes

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



35. 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:

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

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

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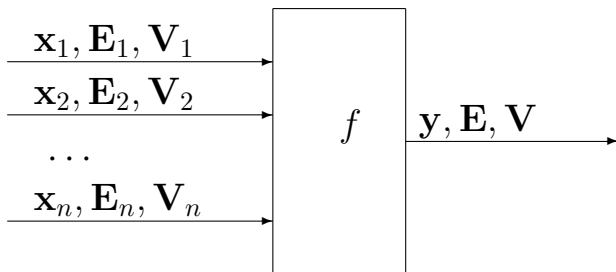
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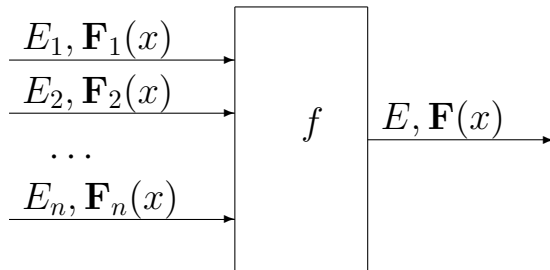
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36. Challenges

- intervals + 2nd moments:



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



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37. 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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38. 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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39. 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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40. 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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41. 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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42. 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 $U \in \mathbf{E} + k_0 \cdot [\underline{\sigma}, \overline{\sigma}]$.
- *Problem:* the resulting intervals for L and U are *wider* than the actual ranges.
- *Reason:* E and σ 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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43. Computing Amount of Information: A Problem

- *Uncertainty*: usually, there are several (n) different states which are consistent with our knowledge.
- *Question*: how much information we need to gain to determine the actual state of the world?
- *Natural measure*: average number of “yes”-“no” questions that we need to ask.
- *Probabilistic case*: sometimes, we know the probabilities p_1, \dots, p_n of different states.
- *Shannon's result*: $S = - \sum_{i=1}^n p_i \cdot \log_2(p_i)$.
- *Problem*: often, we only know intervals $\mathbf{p}_i = [\underline{p}_i, \bar{p}_i]$ of possible values of p_i .
- *Question*: find the range $\mathbf{S} = [\underline{S}, \bar{S}]$ of possible values of S .

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44. Computing Amount of Information: Results

- *Problem (reminder):*
 - *given:* intervals $\mathbf{p}_i = [\underline{p}_i, \bar{p}_i]$ of possible values of p_i .
 - *find:* the range $\mathbf{S} = [\underline{S}, \bar{S}]$ of possible values of
$$S = - \sum_{i=1}^n p_i \cdot \log_2(p_i).$$
- *Results:*
 - the problem of computing \mathbf{S} is, in general, NP-hard;
 - algorithms that efficiently compute \mathbf{S} in many practically important situations.

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45. Acknowledgments

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46. Proof of the Chip Result

- 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:

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

47. Proof of the Chip Result (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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