Application-Motivated Combinations of Interval and Probability Approaches, with Application to Geoinformatics, Bioinformatics, and Engineering

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Interval computations website:
http://www.cs.utep.edu/interval-comp
1. General Problem of Data Processing under Uncertainty

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

\[
\begin{align*}
\tilde{x}_1 \\
\tilde{x}_2 \\
\vdots \\
\tilde{x}_n
\end{align*}
\rightarrow f

\[
\tilde{y} = f(\tilde{x}_1, \ldots, \tilde{x}_n)
\]

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

\[
\tilde{y} = f(\tilde{x}_1, \ldots, \tilde{x}_n) \neq y = f(x_1, \ldots, x_n).
\]

What are bounds on \( \Delta y \overset{\text{def}}{=} \tilde{y} - y \)?
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**: calibration is not possible in:
  - fundamental science
  - manufacturing
- **Solution**: we know upper bounds $\Delta_i$ on $|\Delta x_i|$ hence

$$x_i \in [\tilde{x}_i - \Delta_i, \tilde{x}_i + \Delta_i].$$
3. Interval Computations: A Problem

Given: an algorithm $y = f(x_1, \ldots, x_n)$ and $n$ intervals $x_i = [\underline{x}_i, \overline{x}_i]$.

Compute: the corresponding range of $y$:

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

Fact: NP-hard even for quadratic $f$.

Challenge: when are feasible algorithm possible?

Challenge: when computing $y = [\underline{y}, \overline{y}]$ is not feasible, find a good approximation $Y \supseteq y$. 
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 $x \in [x, \bar{x}]$, then MaxEnt leads to a uniform distribution on $[x, \bar{x}]$.
- **Example – multiple variables:** different variables are independently distributed.
5. 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, $\Delta y$ is $\approx$ normal, with $\sigma = \Delta \cdot \frac{\sqrt{n}}{\sqrt{3}}$.

- **Why this may be inadequate:** we get $\Delta \sim \sqrt{n}$, but due to correlation, it is possible that $\Delta = n \cdot \Delta \sim n \gg \sqrt{n}$.
- **Conclusion:** using a single distribution can be very misleading, especially if we want guaranteed results.
- **Examples:** high-risk application areas such as space exploration or nuclear engineering.
6. Interval Arithmetic: Foundations of Interval Techniques

- **Problem**: compute the range
  \[ [y, \overline{y}] = \{ f(x_1, \ldots, x_n) \mid x_1 \in [x_1, \overline{x}_1], \ldots, x_n \in [x_n, \overline{x}_n] \}. \]

- **Interval arithmetic**: for arithmetic operations \( f(x_1, x_2) \) (and for elementary functions), we have explicit formulas for the range.

- **Examples**: when \( x_1 \in x_1 = [x_1, \overline{x}_1] \) and \( x_2 \in x_2 = [x_2, \overline{x}_2] \), then:
  - The range \( x_1 + x_2 \) for \( x_1 + x_2 \) is \( [x_1 + x_2, \overline{x}_1 + \overline{x}_2] \).
  - The range \( x_1 - x_2 \) for \( x_1 - x_2 \) is \( [x_1 - \overline{x}_2, \overline{x}_1 - x_2] \).
  - The range \( x_1 \cdot x_2 \) for \( x_1 \cdot x_2 \) is \( [y, \overline{y}] \), where
    \[
    y = \min(x_1 \cdot x_2, \overline{x}_1 \cdot \overline{x}_2, \overline{x}_1 \cdot x_2, x_1 \cdot \overline{x}_2);
    \]
    \[
    \overline{y} = \max(x_1 \cdot x_2, \overline{x}_1 \cdot \overline{x}_2, \overline{x}_1 \cdot x_2, x_1 \cdot \overline{x}_2).
    \]
  - The range \( 1/x_1 \) for \( 1/x_1 \) is \( [1/\overline{x}_1, 1/x_1] \) (if \( 0 \not\in x_1 \)).
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:
  - $r_1 := [1, 2] - [2, 2] = [-1, 0]$;
  - $r_2 := [1, 2] + [2, 2] = [3, 4]$;
  - $r_3 := [-1, 0] \cdot [3, 4] = [-4, 0]$.

- **Actual range:** $f(x) = [-3, 0]$.

- **Comment:** this is just a toy example, there are more efficient ways of computing an enclosure $Y \supseteq y$. 
8. 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.

- **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

  \[ D \overset{\text{def}}{=} \max(D_1, \ldots, D_N). \]

- 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.
10. 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.
11. 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.
12. 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: 
  \[
  D_i = a_i + \sum_{j=1}^{n} a_{ij} \cdot x_j
  \]
  for some \( a_i \) and \( a_{ij} \).

• The desired maximum delay \( D = \max_i D_i \) has the form
  \[
  D = F(x_1, \ldots, x_n) \overset{\text{def}}{=} \max_i \left( a_i + \sum_{j=1}^{n} a_{ij} \cdot x_j \right).
  \]
13. Towards a Mathematical Formulation of the Problem (cont-d)

- **Known**: maxima of linear function are exactly convex functions:
  \[ F(\alpha \cdot x + (1 - \alpha) \cdot y) \leq \alpha \cdot F(x) + (1 - \alpha) \cdot F(y) \]
  for all \(x, y\) and for all \(\alpha \in [0, 1]\);

- **We know**: factors \(x_i\) are independent;
  - we know distribution of some of the factors;
  - for others, we know ranges \([x_j, \bar{x}_j]\) and means \(E_j\).

- **Given**: a convex function \(F \geq 0\) and a number \(\varepsilon > 0\).

- **Objective**: find the smallest \(y_0\) s.t. for all possible distributions, we have \(y \leq y_0\) with the probability \(\geq 1 - \varepsilon\).
14. 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 $[x_j, \bar{x}_j]$.
- **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 $[x_j, \bar{x}_j]$, the resulting value $y_0$ decreases: $y_0' < y_0$. 
15. Formulation of the Problem

GIVEN:  
• \( n, k \leq n, \varepsilon > 0; \)
  • a convex function \( y = F(x_1, \ldots, x_n) \geq 0; \)
  • \( n - k \) cdfs \( F_j(x), k + 1 \leq j \leq n; \)
  • intervals \( x_1, \ldots, x_k \), values \( E_1, \ldots, E_k, \)

TAKE: all joint probability distributions on \( \mathbb{R}^n \) for which:
  • all \( x_i \) are independent,
  • \( x_j \in x_j, E[x_j] = E_j \) 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, \( F(x_1, \ldots, x_n) \leq y_0 \) with probability \( \geq 1 - \varepsilon. \)

WHEN: the problem is non-degenerate – if we narrow down one of the intervals \( x_j \), \( y_0 \) decreases.
16. Main Result and How We Can Use It

- **Result:** $y_0$ is attained when for each $j$ from 1 to $k$,
  - $x_j = \bar{x}_j$ with probability $\overline{p}_j \overset{\text{def}}{=} \frac{\bar{x}_j - E_j}{\bar{x}_j - x_j}$, and
  - $x_j = \bar{x}_j$ with probability $\overline{p}_j \overset{\text{def}}{=} \frac{E_j - x_j}{\bar{x}_j - x_j}$.

- **Algorithm:**
  - simulate these distributions for $x_j$, $j < k$;
  - simulate known distributions for $j > k$;
  - use the simulated values $x_j^{(s)}$ to find
    $$y^{(s)} = F(x_1^{(s)}, \ldots, x_n^{(s)});$${} \text{\cdot}$
  - sort $N$ values $y^{(s)}$: $y(1) \leq y(2) \leq \ldots \leq y(N_i)$;
  - take $y(N_i \cdot (1 - \varepsilon))$ as $y_0$. 
17. 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.
18. 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 $y_0$. 
19. 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 $u(x) = u(x_0) + (x - x_0) \cdot u'(x_0) + \ldots$.
  - **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 $F(x) = \text{Prob}(\xi \leq x)$.
  - **Case of uncertainty**: p-box $[\underline{F}(x), \overline{F}(x)]$. 
20. Extension of Interval Arithmetic to Probabilistic Case: Successes

- **General solution:** parse to elementary operations +, −, ·, 1/x, max, min.

- Explicit formulas for arithmetic operations known for intervals, for p-boxes \( F(x) = [\underline{E}(x), \overline{F}(x)] \), for intervals + 1st moments \( E_i \overset{\text{def}}{=} E[x_i] \):

\[
\begin{align*}
  x_1, E_1 \\
  x_2, E_2 \\
  \vdots \\
  x_n, E_n \\
\end{align*}
\]

\[
\begin{align*}
  f \\
  y, E \\
\end{align*}
\]
21. Successes (cont-d)

- **Easy cases:** $+, -, \text{ product of independent } x_i$.
- **Example of a non-trivial case:** multiplication $y = x_1 \cdot x_2$, when we have no information about the correlation:
  
  - $E = \max(p_1 + p_2 - 1, 0) \cdot \bar{x}_1 \cdot \bar{x}_2 + \min(p_1, 1 - p_2) \cdot x_1 \cdot x_2 + \min(1 - p_1, p_2) \cdot x_1 \cdot \bar{x}_2 + \max(1 - p_1 - p_2, 0) \cdot x_1 \cdot x_2$;
  
  - $\bar{E} = \min(p_1, p_2) \cdot x_1 \cdot x_2 + \max(p_1 - p_2, 0) \cdot \bar{x}_1 \cdot x_2 + \max(p_2 - p_1, 0) \cdot \bar{x}_1 \cdot \bar{x}_2 + \min(1 - p_1, 1 - p_2) \cdot \bar{x}_1 \cdot \bar{x}_2$,

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


22. **Challenges**

- intervals + 2nd moments:

  \[
  x_1, E_1, V_1 \quad \xrightarrow{f} \quad y, E, V \\
  x_2, E_2, V_2 \\
  \vdots \\
  x_n, E_n, V_n
  \]

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

  \[
  E_1, F_1(x) \quad \xrightarrow{f} \quad E, F(x) \\
  E_2, F_2(x) \\
  \vdots \\
  E_n, F_n(x)
  \]
23. **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 $a \overset{\text{def}}{=} c - h$. 
24. Case Study: Bioinformatics (cont-d)

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

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

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

- Interval uncertainty: experts manually count \( x_i \), and only provide interval bounds \( x_i \), e.g., \( x_i \in [0.7, 0.8] \).

- Problem: find the range of \( a \) and \( h \) corresponding to all possible values \( x_i \in [x_i, \bar{x}_i] \).
25. General Problem

- General problem:
  - we know intervals \( x_1 = [x_1, \bar{x}_1], \ldots, x_n = [x_n, \bar{x}_n], \)
  - 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 \( V, \)
  - efficient algorithms for \( \bar{V} \) and \( C(x, y) \) for reasonable situations.

- Bioinformatics case: find intervals for \( C(x, y) \) and for \( V(x) \) and divide.
26. 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
  \[
  L \overset{\text{def}}{=} E - k_0 \cdot \sigma, \quad U \overset{\text{def}}{=} E + k_0 \cdot \sigma,
  \]
  and \( k_0 > 1 \) is pre-selected.
- Comment: most frequently, \( k_0 = 2, 3, \) or 6.
27. Outlier Detection Under Interval Uncertainty: A Problem

- In some practical situations, we only have intervals $x_i = [x_i, \bar{x}_i]$.
- Different $x_i \in x_i$ 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 $x \notin [\bar{L}, U]$.
- A value $x$ is a guaranteed outlier if $x \notin [L, \bar{U}]$.
- Conclusion: to detect outliers, we must know the ranges of $L = E - k_0 \cdot \sigma$ and $U = E + k_0 \cdot \sigma$. 
28. **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 $E$ and $[\sigma, \bar{\sigma}]$ for $E$ and $\sigma$.
- **Possibility:** use interval computations to conclude that $L \in E - k_0 \cdot [\sigma, \bar{\sigma}]$ and $L \in E + k_0 \cdot [\sigma, \bar{\sigma}]$.
- **Problem:** the resulting intervals for $L$ and $U$ are wider than the actual ranges.
- **Reason:** $E$ and $\sigma$ use the same inputs $x_1, \ldots, x_n$ 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.
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30. Proof of the Result about Chips

- Let us fix the optimal distributions for $x_2, \ldots, x_n$; then,
  \[ \text{Prob}(D \leq y_0) = \sum_{(x_1, \ldots, x_n): D(x_1, \ldots, x_n) \leq y_0} p_1(x_1) \cdot p_2(x_2) \cdots \]

- So, \( \text{Prob}(D \leq y_0) = \sum_{i=0}^{N} c_i \cdot q_i \), where \( q_i \overset{\text{def}}{=} p_1(v_i) \).

- 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:

  Minimize \( \sum_{i=0}^{N} c_i \cdot q_i \) under the constraints \( \sum_{i=0}^{N} q_i = 1 \) and

  \( \sum_{i=0}^{N} q_i \cdot v_i = E_1 \), \( q_i \geq 0 \), \( i = 0, 1, 2, \ldots, N \).
31. **Proof of the Result about Chips (cont-d)**

- **Minimize:** \( \sum_{i=0}^{N} c_i \cdot q_i \) under the constraints \( \sum_{i=0}^{N} q_i = 1 \) and \( \sum_{i=0}^{N} q_i \cdot v_i = E_1, q_i \geq 0, \; i = 0, 1, 2, \ldots, N. \)

- **Known:** in LP with \( N + 1 \) unknowns \( q_0, q_1, \ldots, q_N \geq N + 1 \) 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 \( (x_1, \bar{x}_1) \), then for \( [v, v'] \subset x_1 \) we get the same \( y_0 \) – in contradiction to non-degeneracy.

- Thus, the worst-case distribution is located at \( x_1 \) and \( \bar{x}_1 \).

- The condition that the mean of \( x_1 \) is \( E_1 \) leads to the desired formulas for \( p_1 \) and \( \bar{p}_1 \).