Uncertainty in Cyberinfrastructure: Results, Algorithms, Challenges, and Request for Collaboration

Ann Gates, Vladik Kreinovich, Paulo Pinheiro da Silva, Craig Tweedie, Leonardo Salayandia, and Christian Servin

Center of Excellence for Sharing resources for the Advancement of Research and Education through Cyberinfrastructure Cyber-ShARE, University of Texas at El Paso (UTEP)
http://trust.cs.utep.edu/cybershare/
contact email vladik@utep.edu
1. Cyberinfrastructure: A Brief Overview

- Practical problem: need to combine geographically separate computational resources.
- Centralization of computational resources – traditional approach to combining computational resources.
- Limitations of centralization:
  - need to reformat all the data;
  - need to rewrite data processing programs: make compatible w/selected formats and w/each other
- Cyberinfrastructure – a more efficient approach to combining computational resources:
  - keep resources at their current locations, and
  - in their current formats.
- Technical advantages of cyberinfrastructure: a brief summary.
2. **Data Processing vs. Data Fusion**

- *Practically important situation:* difficult to measure the desired quantity $y$ with a given accuracy.

- **Data processing:**
  - measure related easier-to-measure quantities $x_1, \ldots, x_n$;
  - estimate $y$ from the results $\tilde{x}_i$ of measuring $x_i$ as $\tilde{y} = f(\tilde{x}_1, \ldots, \tilde{x}_n)$.

- **Example:** seismic inverse problem.

- **Data fusion:**
  - measure the quantity $y$ several times;
  - combine the results $\tilde{y}_1, \ldots, \tilde{y}_n$ of these measurements.

- **Specifics of cyberinfrastructure:** first looks for stored results $\tilde{x}_i$ (corr., $\tilde{y}_i$), measure only if necessary.

- **Combination of data processing and data fusion.**
3. Need for Uncertainty Propagation, and for Provenance of Uncertainty

- **Need for uncertainty propagation.**
  - main reasons for data processing and data fusion: accuracy is not high enough;
  - we must make sure that after the data processing (data fusion), we get the desired accuracy.

- **In cyberinfrastructure this is especially important:**
  - accuracy varies greatly, and
  - we do not have much control over these accuracies.

- **Need for the provenance of uncertainty:**
  - sometimes, the resulting accuracy is still too low;
  - it is desirable to find out which data points contributed most to the inaccuracy.
4. Uncertainty of the Results of Direct Measurements: Probabilistic and Interval Approaches

- Manufacturer of the measuring instrument (MI) supplies $\Delta_i$ s.t. $|\Delta x_i| \leq \Delta_i$, where $\Delta x_i \overset{\text{def}}{=} \tilde{x}_i - x_i$.

- The actual (unknown) value $x_i$ of the measured quantity is in the interval $x_i = [\tilde{x}_i - \Delta_i, \tilde{x}_i + \Delta_i]$.

- **Probabilistic uncertainty:** often, we know the probabilities of different values $\Delta x_i \in [-\Delta_i, \Delta_i]$.

- **How probabilities are determined:** by comparing our MI with a much more accurate (standard) MI.

- **Interval uncertainty:** in two cases, we do not determine the probabilities:
  - cutting-edge measurements;
  - measurements on the shop floor.

- In both cases, we only know that $x_i \in [\tilde{x}_i - \Delta_i, \tilde{x}_i + \Delta_i]$. 
5. Typical Situation: Measurement Errors are Reasonably Small

- **Typical situation:**
  - direct measurements are accurate enough;
  - the resulting approximation errors $\Delta x_i$ are small;
  - terms which are quadratic (or of higher order) in $\Delta x_i$ can be safely neglected.

- **Example:** for an error of 1%, its square is a negligible 0.01%.

- **Linearization:**
  - expand $f$ in Taylor series around the point $(\tilde{x}_1, \ldots, \tilde{x}_n);$ 
  - restrict ourselves only to linear terms:
    \[ \Delta y = c_1 \cdot \Delta x_1 + \ldots + c_n \cdot \Delta x_n, \]
    where $c_i \overset{\text{def}}{=} \frac{\partial f}{\partial x_i}.$
6. Case of Data Processing

- *Propagation (probabilistic case)*: if $\Delta x_i$ are independent with st. dev. $\sigma_i$ (and 0 mean), then $\Delta y$ has st. dev.

$$\sigma^2 = c_1^2 \cdot \sigma_1^2 + \ldots + c_n^2 \cdot \sigma_n^2.$$ 

- *Provenance*:
  - we know which component $\sigma^2$ comes from the $i$-th measurement;
  - we can predict how replacing the $i$-th measurement with a more accurate one ($\sigma_i^{\text{new}} \ll \sigma_i$) will affect $\sigma^2$.

- *Propagation of interval uncertainty*:

$$\Delta = |c_1| \cdot \Delta_1 + \ldots + |c_n| \cdot \Delta_n.$$ 

- We can predict how replacing the $i$-th measurement with a more accurate one ($\Delta_i^{\text{new}} \ll \Delta_i$) will affect $\Delta$. 
7. Beyond Probabilistic and Interval Uncertainty

- **Up to now:** we considered two extreme situations:
  - *probabilistic* uncertainty, when we know all the probabilities;
  - *interval* uncertainty, when we have no information about the probabilities.

- **Fact:** probabilistic situation is a particular case of the interval situation.

- **Conclusion:** interval bounds are wider.

- **In practice:** often, we have partial information about probabilities.

- **As a result:**
  - probabilistic bounds are too narrow,
  - interval bounds are too wide.

- **We need:** intermediate bounds.
8. Case Study: Seismic Inverse Problem in the Geosciences

- **Linearization:** \( \Delta y = \sum_{i=1}^{n} c_i \cdot \Delta x_i \), where \( c_i \overset{\text{def}}{=} \frac{\partial f}{\partial x_i} \).

- **Formulas:** \( \sigma^2 = \sum_{i=1}^{n} c_i^2 \cdot \sigma_i^2 \), \( \Delta = \sum_{i=1}^{n} |c_i| \cdot \Delta_i \).

- **Numerical differentiation:** \( n \) iterations, too long.

- **Monte-Carlo approach:** if \( \Delta x_i \) are Gaussian w/\( \sigma_i \), then \( \Delta y = \sum_{i=1}^{n} c_i \cdot \Delta x_i \) is also Gaussian, w/desired \( \sigma \).

- **Advantage:** # of iterations does not grow with \( n \).

- **Interval estimates:** if \( \Delta x_i \) are Cauchy, w/\( \rho_i(x) = \frac{\Delta_i}{\Delta_i^2 + x^2} \), then \( \Delta y = \sum_{i=1}^{n} c_i \cdot \Delta x_i \) is also Cauchy, w/desired \( \Delta \).
12. Resulting Fast (Linearized) Algorithm for Estimating Interval Uncertainty

- Apply $f$ to $\tilde{x}_i$: $\tilde{y} := f(\tilde{x}_1, \ldots, \tilde{x}_n)$;

- For $k = 1, 2, \ldots, N$, repeat the following:
  - use RNG to get $r_{i}^{(k)}$, $i = 1, \ldots, n$ from $U[0, 1]$;
  - get st. Cauchy values $c_{i}^{(k)} := \tan(\pi \cdot (r_{i}^{(k)} - 0.5))$;
  - compute $K := \max_i |c_{i}^{(k)}|$ (to stay in linearized area);
  - simulate “actual values” $x_{i}^{(k)} := \tilde{x}_i - \delta_{i}^{(k)}$, where $\delta_{i}^{(k)} := \Delta_i \cdot c_{i}^{(k)}/K$;
  - simulate error of the indirect measurement: $\delta^{(k)} := K \cdot (\tilde{y} - f(x_{1}^{(k)}, \ldots, x_{n}^{(k)}))$;

- Solve the ML equation $\sum_{k=1}^{N} \frac{1}{1 + \left(\frac{\delta^{(k)}}{\Delta}\right)^2} = \frac{N}{2}$ by bisection, and get the desired $\Delta$. 
13. A New (Heuristic) Approach

- **Problem:** guaranteed (interval) bounds are too high.
- **Gaussian case:** we only have bounds guaranteed with confidence, say, 90%.
- **How:** cut top 5% and low 5% off a normal distribution.
- **New idea:** to get similarly estimates for intervals, we “cut off” top 5% and low 5% of Cauchy distribution.
- **How:**
  - find the threshold value $x_0$ for which the probability of exceeding this value is, say, 5%;
  - replace values $x$ for which $x > x_0$ with $x_0$;
  - replace values $x$ for which $x < -x_0$ with $-x_0$;
  - use this “cut-off” Cauchy in error estimation.
- **Example:** for 95% confidence level, we need $x_0 = 12.706$. 
14. Heuristic Approach: Results with 95% Confidence Level

![Graph showing depth vs. distance and velocity]
15. Heuristic Approach: Results with 90% Confidence Level
16. Conclusions

- *In the past:* communications were much slower.
- *Conclusion:* use centralization.
- *At present:* communications are much faster.
- *Conclusion:* use cyberinfrastructure.

- *Related problems:*
  - gauge the uncertainty of the results obtained by using cyberinfrastructure;
  - which data points contributed most to uncertainty;
  - how an improved accuracy of these data points will improve the accuracy of the result.

- *We described:* algorithms for solving these problems.

- *Additional problem:* what if interval estimates are too wide and probabilistic estimates are too narrow.
17. Request for Collaboration

- Our main objective: enhance applications of CI.

- We welcome: practical problems in need of CI and uncertainty estimation.

- We expect: some problems are similar to GEON ones. For such problems,
  - in collaboration with researchers working on these problems,
  - we will be able to apply (and, if necessary adjust and modify) our CI techniques.

- We also expect: that some practical problems will lead
  - to new challenges and thus,
  - to the development of new techniques for gauging uncertainty in CI.
18. Acknowledgments

This work was supported in part by:

- by National Science Foundation grants HRD-0734825, EAR-0225670, and EIA-0080940,
- by Texas Department of Transportation contract No. 0-5453,
- by the Japan Advanced Institute of Science and Technology (JAIST) International Joint Research Grant 2006-08, and
- and by the Max Planck Institut für Mathematik.
19. Propagation of Probabilistic Uncertainty Through Data Fusion

- **Situation:** we know several results $\tilde{y}_1, \ldots, \tilde{y}_n$ of measuring the same quantity $y$ with st. dev. $\sigma_i$:

$$
\rho_i(y) = \frac{1}{\sqrt{2\pi} \cdot \sigma_i} \cdot \exp \left( -\frac{(y - \tilde{y}_i)^2}{2\sigma_i^2} \right).
$$

- **Resulting probability density:**

$$
\rho(y) = \rho_1(y) \cdot \ldots \cdot \rho_n(y) = \text{const} \cdot \exp \left( - \sum_{i=1}^{n} \frac{(y - \tilde{y}_i)^2}{2\sigma_i^2} \right).
$$

- **Maximum Likelihood Estimate:** $\rho(y) \rightarrow \text{max}$, hence

$$
\tilde{y} = \frac{1}{\sum_{i=1}^{n} \frac{1}{\sigma_i^2}} \cdot \sum_{i=1}^{n} \frac{\tilde{y}_i}{\sigma_i^2}.
$$
20. Propagation of Probabilistic Uncertainty Through Data Fusion (cont-d)

• Reminder:

\[ \tilde{y} = \frac{1}{\sum_{i=1}^{n} \frac{1}{\sigma_i^2}} \cdot \sum_{i=1}^{n} \frac{\tilde{y}_i}{\sigma_i^2}. \]

• Resulting st. dev. \( \sigma \) for \( \tilde{y} \): \( \tilde{y} \) is a linear combination of independent normal \( \tilde{y}_i \), hence its st. dev. is:

\[ \sigma^2 = \frac{1}{\left( \sum_{i=1}^{n} \frac{1}{\sigma_i^2} \right)^2} \cdot \sum_{i=1}^{n} \frac{\sigma_i^4}{\sigma_i^2} = \frac{1}{\left( \sum_{i=1}^{n} \frac{1}{\sigma_i^2} \right)^2} \cdot \sum_{i=1}^{n} \frac{1}{\sigma_i^2} = \frac{1}{\sum_{i=1}^{n} \frac{1}{\sigma_i^2}}. \]

• Simplified expression:

\[ \frac{1}{\sigma^2} = \sum_{i=1}^{n} \frac{1}{\sigma_i^2}. \]

• Provenance: we can predict how replacing \( \sigma_i \) with a “more accurate” value \( \sigma_i^{\text{new}} \ll \sigma_i \) affects \( \sigma \).
21. Propagation of Interval Uncertainty Through Data Fusion

- **Situation:** we know several results $\tilde{y}_1, \ldots, \tilde{y}_n$ of measuring the same quantity $y$ with bounds $\Delta_i$.

- **Analysis:** the unknown (actual) value $y$ belongs to $n$ intervals $y_i \overset{\text{def}}{=} [\tilde{y}_i - \Delta_i, \tilde{y}_i + \Delta_i]$.

- **Conclusion:** the range $y$ of possible values of $y$ is the intersection $y = [y, \bar{y}] = y_1 \cap \ldots \cap y_n$ of intervals $y_i$: $\left[\max(\tilde{y}_1 - \Delta_1, \ldots, \tilde{y}_n - \Delta_n), \min(\tilde{y}_1 + \Delta_1, \ldots, \tilde{y}_n + \Delta_n)\right]$.

- **Provenance – a problem:** if we replace $\Delta_i$ with the same new value $\Delta_i^{\text{new}} \ll \Delta_i$, we may get different accuracies.

- **Example:** $y_1 = [-1, 1]$, $y_2 = [-2, 2]$, and $y = [-1, 1]$. If we use $\Delta_2^{\text{new}} = 1 \ll \Delta_2 = 2$, we may get:
  - $y_2 = [-1, 1]$; then $y = [-1, 1]$ is unchanged.
  - $y_2 = [0, 2]$; then $y = [0, 1]$ is much narrower.
22. Pre-Estimating the Accuracy of Data Fusion Under Interval Uncertainty: A Problem

- **We know:** the $i$-th measurement error $\Delta y_i \in [-\Delta_i, \Delta_i]$.
- **Fact:** different values $\Delta y_i$ lead to different intersections

$$y = [\underline{y}, \bar{y}] = \bigcap_{i=1}^{n} [(y + \Delta y_i) - \Delta_i, (y + \Delta y_i) + \Delta_i].$$

- **Reasonable assumptions:**
  - $\Delta y_i$ is uniformly distributed on $[-\Delta_i, \Delta_i]$;
  - $\Delta y_i$ and $\Delta y_j$ ($i \neq j$) are independent;
  - we allow a small probability $p_0$ of mis-estimation.

- **Formulation of the problem:** find the smallest $\Delta$ s.t.:
  - the probability to have $\bar{y} \leq y + \Delta$ is at least $1 - p_0$,
  and
  - the probability to have $\underline{y} \geq y - \Delta$ is also $\geq 1 - p_0$. 
23. **Pre-Estimating the Accuracy of Data Fusion Under Interval Uncertainty: Solution**

- **Resulting formula:** when fusion is efficient \((\Delta \ll \Delta_i)\), we get \(\frac{1}{\Delta} = \text{const} \cdot \sum_{i=1}^{n} \frac{1}{\Delta_i}\), with \(\text{const} = 2|\ln(p_0)|\).

- **Example:** for \(\Delta_1 = \ldots = \Delta_n\), we get \(\Delta = \frac{\text{const}}{n} \cdot \Delta_1\).

- **Prob. case:** \(\frac{1}{\sigma^2} = \text{const} \cdot \sum_{i=1}^{n} \frac{1}{\sigma_i^2}\), w/\(\Delta_i\) instead of \(\sigma_i^2\).

- **Observation:** for prob. uncertainty, \(\sigma \sim \frac{\text{const}}{\sqrt{n}} \cdot \sigma_1\).

- **Data processing:** \(\Delta = \sum_{i=1}^{n} |c_i| \cdot \Delta_i\) vs. \(\sigma^2 = \sum_{i=1}^{n} |c_i|^2 \cdot \sigma_i^2\).

- \(\sim\): \(\parallel\) and sequential resistors \(\frac{1}{R} = \sum_{i=1}^{n} \frac{1}{R_i}\), \(R = \sum_{i=1}^{n} R_i\).
24. **Optimal Data Processing and Data Fusion**

- **Problem:** find the least expensive way to guarantee the given accuracy $\sigma$ or $\Delta$.

- **Costs:** $c_i^{\text{prob}}(\sigma_i) = \frac{C_i}{\sigma_i^{\alpha_i}}$ and $c_i^{\text{int}}(\Delta_i) = \frac{C_i}{\Delta^{\alpha_i}}$.

- **Case of data fusion:** we measure the same quantity, so $C_1 = \ldots = C_n$ and $\alpha_1 = \ldots = \alpha_n$.

- **Optimal data fusion:** minimizing cost, we get $\sigma_1 = \ldots = \sigma_n = \sqrt{n} \cdot \sigma$ and $\Delta_1 = \ldots = \Delta_n = n \cdot \Delta$.

- **Optimal data processing:** probabilistic case.
  \[
  \sigma_i = \left(\frac{\alpha_i \cdot C_i}{2\lambda \cdot c_i^2}\right)^{1/(2+\alpha_i)}, \text{ with } \sum_{i=1}^{n} c_i^2 \cdot \left(\frac{\alpha_i \cdot C_i}{2\lambda \cdot c_i^2}\right)^{2/(2+\alpha_i)} = \sigma^2.
  \]

- **Optimal data processing:** interval case.
  \[
  \Delta_i = \left(\frac{\alpha_i \cdot C_i}{\lambda \cdot |c_i|}\right)^{1/(1+\alpha_i)}, \text{ with } \sum_{i=1}^{n} |c_i| \cdot \left(\frac{\alpha_i \cdot C_i}{\lambda \cdot |c_i|}\right)^{2/(2+\alpha_i)} = \Delta.
  \]