

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

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Outline

Need for Data Processing

Measurement . . .

Interval Part: Outline

Constraint-Based Set . . .

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## 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.

## 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  $x_1, \dots, x_n$  which are related to  $y$  by a known relation  $y = f(x_1, \dots, x_n)$ ;
  - measure or estimate the values of the quantities  $x_1, \dots, x_n$ ; results are  $\tilde{x}_i \approx x_i$ ;
  - estimate  $y$  as  $\tilde{y} = f(\tilde{x}_1, \dots, \tilde{x}_n)$ .
- Computing  $\tilde{y}$  is called *data processing*.
- *Comment:* algorithm  $f$  can be complex, e.g., solving ODEs.

### 3. Measurement Uncertainty

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

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

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

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## 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.

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## 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.

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## 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  $f(\mathbf{a}, \mathbf{b})$ :

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

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

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

- *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.

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## 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  $\bar{r}$ .
- *Computation time:* increase by a factor of  $\leq 4$ .
- *Computing exact range:* NP-hard.
- *Conclusion:* excess width is inevitable.
- *More accurate techniques exist:* centered form, bisection, etc.

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## 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  $x_2 = x_1^2$ .

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## 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  $\mathbf{x}_{12} = \{(x_1, x_1^2) \mid x_1 \in [0, 1]\}$ .
- *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
$$\mathbf{x}_{ik} = \{(x_i, x_i + x_j) \mid (x_i, x_j) \in \mathbf{x}_{ij}\},$$
$$\mathbf{x}_{jk} = \{(x_j, x_i + x_j) \mid (x_i, x_j) \in \mathbf{x}_{ij}\},$$
$$\mathbf{x}_{kl} = \{(x_i + x_j, x_l) \mid (x_i, x_j) \in \mathbf{x}_{ij}, (x_i, x_l) \in \mathbf{x}_{il}, (x_j, x_l) \in \mathbf{x}_{jl}\}.$$

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## 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  $\mathbf{x}_{ij}$ .

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## 11. Implementing Arithmetic Operations

- *Example:* implementing

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

- *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

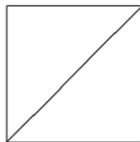
$$\{(x_i, x_i + x_j) \mid (x_i, x_j) \in \mathbf{X}_i \times \mathbf{X}_j\}$$

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  $\{0\} = [0, 0]$ .

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### 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  $\mathbf{r}_{12}$ :

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| × |   |   |   |   |

- 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.

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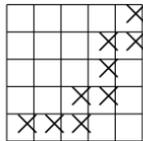
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## 14. Second Example: Computing the Range of $x - x^2$

- *Straightforwad 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  $[0, 0.25]$ .

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## 15. Limitations of This Approach

- *Fact:* to get an accuracy  $\varepsilon$ , 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%).

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## 16. Estimating Variance under Interval Uncertainty

- *We know:* intervals  $\mathbf{x}_1, \dots, \mathbf{x}_n$  of possible values of  $x_i$ .
- *We need to compute:* the range of the variance  $V = \frac{1}{n} \cdot M - \frac{1}{n^2} \cdot E^2$ , where  $M \stackrel{\text{def}}{=} \sum_{i=1}^n x_i^2$  and  $E \stackrel{\text{def}}{=} \sum_{i=1}^n x_i$ .
- *Natural idea:* compute  $M_k \stackrel{\text{def}}{=} \sum_{i=1}^k x_i^2$  and  $E_k \stackrel{\text{def}}{=} \sum_{i=1}^k x_i$ :  
 $M_0 = E_0 = 0$ ,  $(M_{k+1}, E_{k+1}) = (M_k + x_{k+1}^2, E_k + x_{k+1})$ .
- *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:*  $C_d = \frac{1}{n} \cdot \sum_{i=1}^n (x_i - \bar{x})^d$  is a linear combination of  $d$  moments  $M^{(j)} \stackrel{\text{def}}{=} \sum_{i=1}^n x_i^j$  for  $j = 1, \dots, d$ .

- *How to compute:* keep, for each  $k$ , the set of possible values of tuples  $(M_k^{(1)}, \dots, M_k^{(d)})$ , 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:*  $C = \frac{1}{n} \cdot \sum_{i=1}^n x_i \cdot y_i - \frac{1}{n^2} \cdot \sum_{i=1}^n x_i \cdot \sum_{i=1}^n y_i$ .

- *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.

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## 18. Dynamical Systems under Interval Uncertainty

- *Situation:*

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

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

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

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

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## 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  $|x_i - x_{i+1}| \leq \varepsilon$  for some  $\varepsilon > 0$  (i.e.,  $x_i$  is smooth).
- *Estimating:* a high-frequency Fourier coefficient

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

- *Usual interval computations:* enclosure  $[-2n, 2n]$ .
- *Actual range* of  $(x_1 - x_2) + (x_3 - x_4) + \dots$  is  $[-n \cdot \varepsilon, n \cdot \varepsilon]$ .
- *Set computations approach:* keep the set  $\mathbf{s}_k$  of pairs  $(f_k, x_k)$ , where  $f_k = x_1 - x_2 + \dots + (-1)^{k+1} \cdot x_k$ , then
$$\mathbf{s}_{k+1} = \{(f_k + (-1)^k \cdot x_{k+1}, x_{k+1}) \mid (f_k, x_k) \in \mathbf{s}_k \ \& \ |x_k - x_{k+1}| \leq \varepsilon\}.$$
- *Result:* almost exact bounds (modulo  $1/C$ ).

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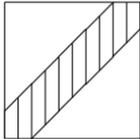
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## 20. Toy Example with Prior Dependence

- *Case study*: find the range of  $r_1 - r_2$  when  $\mathbf{r}_1 = [0, 1]$ ,  $\mathbf{r}_2 = [0, 1]$ , and  $|r_1 - r_2| \leq 0.2$ .
  - *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  $\{r_1 - r_2 \mid (r_1, r_2) \in \mathbf{r}_{12}\}$ .
- *Result*:  $[-0.2, 0.2]$ .

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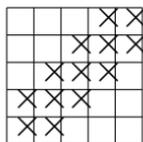
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## 21. Toy Example with Prior Dependence (cont-d)

- *Case study:* find the range of  $r_1 - r_2$  when  $\mathbf{r}_1 = [0, 1]$ ,  $\mathbf{r}_2 = [0, 1]$ , and  $|r_1 - r_2| \leq 0.1$ .
- *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

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

- 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  $F(z) \in \mathbf{F}(z)$ .

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## 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  $(x_1(t), \dots, a_1, \dots)$ .
- *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.

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## 24. Acknowledgments

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