Use of Grothendieck's Inequality in Interval Computations: Quadratic Terms are Estimated Accurately (Modulo a Constant Factor)

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1. Interval Computations (IC): Brief Reminder

- One of the main problem of interval computations:
  - *Given:* a function $f(x_1, \ldots, x_n)$ and intervals
  $$\boldsymbol{x}_i = [\underline{x}_i, \overline{x}_i] = [\widetilde{x}_i - \Delta_i, \widetilde{x}_i + \Delta_i],$$
  - *Compute:* the range
  $$\boldsymbol{y} = f(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n) = \{f(x_1, \ldots, x_n) : x_i \in \boldsymbol{x}_i\}.$$
- Computing the exact range is known to be NP-hard, even for quadratic $f(x_1, \ldots, x_n)$.
- So, instead, we compute an enclosure $\boldsymbol{Y} \supseteq \boldsymbol{y}$, with excess width $\text{wid}(\boldsymbol{Y}) - \text{wid}(\boldsymbol{y}) > 0$.
- One of the most widely used methods of efficiently computing $\boldsymbol{Y}$ is the Mean Value (MV) method:
$$\boldsymbol{Y} = f(\widetilde{x}_1, \ldots, \widetilde{x}_n) + \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}(\boldsymbol{x}_1 \times \ldots \times \boldsymbol{x}_n) \cdot [-\Delta_i, \Delta_i].$$

2. Interval Computations: Reminder (cont-d)

- Mean Value (MV) method (reminder):

$$\boldsymbol{Y} = f(\widetilde{x}_1, \ldots, \widetilde{x}_n) + \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}(\boldsymbol{x}_1 \times \ldots \times \boldsymbol{x}_n) \cdot [-\Delta_i, \Delta_i].$$

- The ranges of the derivatives $f_{,i} \stackrel{\text{def}}{=} \dfrac{\partial f}{\partial x_i}$ can be estimated, e.g., by using straightforward IC:
  - *parse* the expression $f_{,i}$, i.e., represent it as a sequence of elementary arithmetic operations, and
  - replace each operation with numbers by the corresponding operation of interval arithmetic.
- The Mean Value method has excess width $O(\Delta^2)$, where

$$\Delta \stackrel{\text{def}}{=} \max \Delta_i.$$

3. Can We Get Better Enclosures?

- The Mean Value method has excess width $O(\Delta^2)$
- Can we come up with more accurate enclosures?
- We cannot get too drastic an improvement:
  - even for quadratic functions $f(x_1 \ldots, x_n)$, computing the interval range is NP-hard
  - and therefore (unless P=NP), a feasible algorithm with excess width $O(\Delta^{2+\varepsilon})$ is impossible.
- What we can do is try to decrease the overestimation of the quadratic term.
- It turns out that such a possibility follows from an inequality proven by A. Grothendieck in 1953.

4. Main Idea

- The MV method is based on the 1st order Mean Value Theorem (MVT):

$$f(\widetilde{x}+\Delta x) = f(\widetilde{x})+\sum f_{,i}(\widetilde{x}+\eta)\cdot\Delta x_i \text{ for some } \eta_i \in [-\Delta_i, \Delta_i].$$

- Instead, we propose to use 3rd order MVT:

$$f(\widetilde{x}+\Delta x) = f(\widetilde{x})+\sum f_{,i}(\widetilde{x})\cdot\Delta x_i+\frac{1}{2}\cdot\sum f_{,ij}(\widetilde{x})\cdot\Delta x_i\cdot\Delta x_j+$$
$$\frac{1}{6}\cdot\sum f_{,ijk}(\widetilde{x}+\eta)\cdot\Delta x_i\cdot\Delta x_j\cdot\Delta x_k.$$

- Specifically, we propose to add estimates for ranges of linear, quadratic, and cubic terms.
- The range of the cubic term is estimated via straightforward interval comp.; the estimate is $O(\Delta^3)$.
- The range of the linear term $f(\widetilde{x})+\sum f_{,i}(\widetilde{x})\cdot\Delta x_i$ can be explicitly described as $[\widetilde{y}-\Delta, \widetilde{y}+\Delta]$, where

$$\widetilde{y} \stackrel{\text{def}}{=} f(\widetilde{x}) \text{ and } \Delta = \sum |f_{,i}(\widetilde{x})|\cdot\Delta_i.$$

5. Main Idea (cont-d)

- Reminder: we use the 3rd order MVT:

$$f(\widetilde{x}+\Delta x) = f(\widetilde{x})+\sum f_{,i}(\widetilde{x})\cdot\Delta x_i+\frac{1}{2}\cdot\sum f_{,ij}(\widetilde{x})\cdot\Delta x_i\cdot\Delta x_j+$$

$$\frac{1}{6}\cdot\sum f_{,ijk}(\widetilde{x}+\eta)\cdot\Delta x_i\cdot\Delta x_j\cdot\Delta x_k.$$

- Specifically, we propose to add estimates for ranges of linear, quadratic, and cubic terms.
- The range of the linear term can be computed exactly.
- The range of the cubic term is $O(\Delta^3) \ll O(\Delta^2)$.
- What remains is to estimate the range $[-Q, Q]$ of the quadr. term $\sum\limits_{i,j=1}^{n} a_{ij}\cdot\Delta x_i\cdot\Delta x_j$ $\left(a_{ij} \stackrel{\text{def}}{=} \frac{1}{2}\cdot f_{,ij}(\widetilde{x})\right)$ on

$$[-\Delta_1,\Delta_1]\times\ldots\times[-\Delta_n,\Delta_n].$$

6. Relation to Grothendieck Inequality

- *Problem:* estimating the range $[-Q, Q]$ of
$$\sum_{i,j=1}^{n} a_{ij} \cdot \Delta x_i \cdot \Delta x_j \text{ on } [-\Delta_1, \Delta_1] \times \ldots \times [-\Delta_n, \Delta_n].$$
- *Re-scaling:* for $z_i \stackrel{\text{def}}{=} \Delta x_i / \Delta_i$, we have $z_i \in [-1, 1]$, $\Delta x_i = \Delta_i \cdot z_i$, and the quadratic form becomes:
$$\sum_{i,j=1}^{n} b_{ij} \cdot z_i \cdot z_j, \text{ with } b_{ij} \stackrel{\text{def}}{=} a_{ij} \cdot \Delta_i \cdot \Delta_j.$$
- *Thus:* $Q = \max \left\{ \sum_{i,j=1}^{n} b_{ij} \cdot z_i \cdot z_j : z_i \in [-1, 1] \right\}$.
- *Grothendieck's inequality* enables us to estimate the maximum Q' of a related bilinear function
$$b(z, t) \stackrel{\text{def}}{=} \sum_{i,j=1}^{n} b_{ij} \cdot z_i \cdot t_j, \quad z_i, t_j \in \{-1, 1\}.$$

7. Grothendieck Inequality (cont-d)

- *Auxiliary problem:* estimating

$$Q' = \max\left\{\sum_{i,j=1}^{n} b_{ij}\cdot z_i\cdot t_j : z_i, t_j \in \{-1,1\}\right\}.$$

- This problem is known to be NP-hard.
- *General fact:* discrete optimization problems are more complex than continuous ones.
- *Observation:* the discrete set $\{-1,1\}$ is a unit sphere in 1-D Euclidean space.
- *Interesting:* for larger dimensions, a unit sphere is connected (hence not discrete).
- *Grothendieck's idea:* consider z_i and t_j from the unit sphere in a Hilbert space (= ∞-dim. Euclidean space).

8. Grothendieck's Result and Related Algorithm

- *We want to compute:*

$$Q' = \max \left\{ \sum_{i,j=1}^{n} b_{ij} \cdot z_i \cdot t_j : z_i, t_j \in \{-1, 1\} \right\}.$$

- *We estimate instead:*

$$Q'' \stackrel{\text{def}}{=} \max \left\{ \sum_{i,j=1}^{n} b_{ij} \cdot \langle z_i, t_j \rangle : z_i, t_j \in S \right\}.$$

- *Grothendieck's inequality:* for some universal constant $K_G \in [1, 1.782]$, we have $\frac{1}{K_G} \cdot Q'' \le Q' \le Q''$.

- *Comment:* the part $Q' \le Q''$ is trivial, since we can have all z_i and t_j equal to $\pm e$ for some unit vector e.

- *Computational result:* an ellipsoid method – similar to linear programming one – can feasibly compute Q''.

9. How to Use This Algorithm to Estimate the Range $[-Q, Q]$ of the Quadratic Part

- *We want to estimate:* $Q = \max\{B(z) : z_i \in [-1, 1]\}$, where $B(z) \stackrel{\text{def}}{=} b(z, z)$ and $b(z, t) = \sum\limits_{i,j=1}^{n} b_{ij} \cdot z_i \cdot t_j$.
- *We know:* $Q' = \max\{b(z, t) : z_i \in \{-1, 1\}, t_j \in \{-1, 1\}\}$.
- *Fact:* a bilinear f-n $b(z, t)$ attains its max at endpoints.
- *Hence:* $Q' = \max\{b(z, t) : z_i \in [-1, 1], t_j \in [-1, 1]\}$.
- *Since* $b(z, t) = B((z + t)/2) - B((z - t)/2)$, we have $Q' \le 2Q$. Clearly, $Q \le Q'$, hence $Q'/2 \le Q \le Q'$.
- *From* $K_G^{-1} \cdot Q'' \le Q' \le Q''$, we can now conclude that
$$\frac{Q''}{2K_G} \le Q \le Q''.$$
- *Hence:* by computing Q'', we can feasibly estimate Q accurately modulo a small constant factor $2K_G \le 3.6$.

10. Resulting Algorithm

- According to the 3rd order Mean Value Theorem, for $\Delta x_i \in [-\Delta_i, \Delta_i]$, we have:

$$f(\widetilde{x} + \Delta x) = T_1 + T_2 + T_3, \text{ where:}$$

$$T_1 \stackrel{\text{def}}{=} f(\widetilde{x}) + \sum f_{,i}(\widetilde{x}) \cdot \Delta x_i;$$

$$T_2 \stackrel{\text{def}}{=} \sum a_{ij} \cdot \Delta x_i \cdot \Delta x_j, \text{ where } a_{ij} = \frac{1}{2} \cdot f_{,ij}(\widetilde{x}); \text{ and}$$

$$T_3 \stackrel{\text{def}}{=} \frac{1}{6} \cdot \sum f_{,ijk}(\widetilde{x} + \eta) \cdot \Delta x_i \cdot \Delta x_j \cdot \Delta x_k.$$

- As an enclosure for the range of f, we take the sum of enclosures for T_1, T_2, and T_3.
- For T_1, we compute the exact range in linear time $O(n)$.
- For T_3, we use straightforward interval computations and get an enclosure of width

$$O(\Delta^3) \ll O(\Delta^2).$$

11. Resulting Algorithm (cont-d)

- To estimate the range $[-Q, Q]$ of the quadratic term $T_2 = \sum a_{ij} \cdot \Delta x_i \cdot \Delta x_j$, we do the following:
  - compute an auxiliary matrix $b_{ij} = a_{ij} \cdot \Delta_i \cdot \Delta_j$, and
  - use the ellipsoid method to compute

$$Q'' \stackrel{\text{def}}{=} \max \left\{ \sum_{i,j=1}^{n} b_{ij} \cdot \langle z_i, t_j \rangle : z_i, t_j \in S \right\}.$$

- Then, $\dfrac{Q''}{2K_G} \le Q \le Q''$, with $2 \le 2K_G \le 3.6$.
- *Why this is better* that the Mean Value method:
  - we still get excess width $O(\Delta^2)$, but
  - this time, we overestimate the quadratic terms by no more than a known constant factor.

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