Use of Grothendieck Inequality in Interval Computations: Quadratic Terms are Estimated Accurately Modulo a Constant Factor*

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Abstract

One of the main problems of interval computations is, given a function f and intervals, to compute the range of this function over the intervals. For a linear function, we can feasibly estimate its range, but for quadratic (and for more complex) functions, the problem of computing the exact range is NP-hard. So, if we limit ourselves to feasible algorithms, we have to compute *enclosures* instead of the actual ranges. It is known that asymptotically the smallest possible excess width of these enclosures is $O(\Delta^2)$, where Δ is the largest radius (half-width) of the input intervals. This asymptotics is attained for the Mean Value methods, which are among most widely used methods for estimating the range.

The excess width is caused by quadratic (and higher order) terms in the function f. It is therefore desirable to come up with an estimation method for which the excess width decreases when the maximum of this quadratic term decreases. In this paper, we show that, by using Grothendieck inequality, we can create a modification of the Mean Value methods in which the quadratic term is estimated accurately modulo a small multiplicative constant – i.e., in which the excess width is guaranteed to be bounded by 3.6 times the size of the quadratic term.

Keywords: interval computations, Grothendieck inequality, Mean Value form
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1 Formulation of the Problem

Interval computations: brief reminder. One of the main problems of interval computations (see, e.g., [11]) is:

- *given:* a function $f(x_1, \ldots, x_n)$ and intervals $\mathbf{x}_i = [\underline{x}_i, \overline{x}_i] = [\widetilde{x}_i - \Delta_i, \widetilde{x}_i + \Delta_i]$, $1 \le i \le n$,

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- *compute:* the range $\mathbf{y} = f(\mathbf{x}_1, \ldots, \mathbf{x}_n) = \{f(x_1, \ldots, x_n) : x_i \in \mathbf{x}_i \text{ for all } i\}$.

Computing the exact range is known to be NP-hard, even for quadratic $f(x_1, \ldots, x_n)$; see, e.g., [3, 4, 10]. This means, crudely speaking, that (unless P = NP), we cannot hope to have a feasible (i.e., polynomial-time) algorithm that always computes the exact range of a given function.

Since we cannot feasibly compute the exact range $\mathbf{y}$, instead, we compute an enclosure $\mathbf{Y} \supseteq \mathbf{y}$, with excess width $\mathrm{wid}(\mathbf{Y}) - \mathrm{wid}(\mathbf{y}) > 0$, and we try to make this excess width as small as possible.

Moreover, if we fix some accuracy $\varepsilon > 0$ and want to compute the endpoints $\underline{y}$ and $\overline{y}$ of the desired range $\mathbf{y} = [\underline{y}, \overline{y}]$ with this accuracy – i.e., to compute values $\underline{Y}$ and $\overline{Y}$ for which $\left|\underline{y} - \underline{Y}\right| \le \varepsilon$ and $\left|\overline{y} - \overline{Y}\right| \le \varepsilon$ – this problem remains NP-hard [3, 4, 10]. The only way to make the problem feasible is to have different approximation accuracies for different problems.

Mean Value methods. Among the most widely used methods of efficiently computing $\mathbf{Y}$ are the Mean Value methods:

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

In these methods, the ranges of the derivatives $f_{,i} \stackrel{\text{def}}{=} \dfrac{\partial f}{\partial x_i}$ can be estimated, e.g., by using the following technique known as *natural interval extension* or *straightforward interval computations* (see, e.g., [11]):

- we *parse* the expression $f_{,i}$, i.e., represent it as a sequence of elementary arithmetic operations, and
- we *replace* each operation with numbers by the corresponding operation of interval arithmetic [11].

The Mean Value methods have excess width $O(\Delta^2)$, where $\Delta \stackrel{\text{def}}{=} \max \Delta_i$.

Can we get better enclosures? Can we come up with more accurate enclosures? It is known that we cannot get too drastic an improvement: for any $\varepsilon > 0$, even for quadratic functions $f(x) \stackrel{\text{def}}{=} f(x_1 \ldots, x_n)$, computing the interval range is NP-hard and therefore (unless P=NP), a feasible algorithm with excess width $O(\Delta^{2+\varepsilon})$ is impossible; see, e.g., [9].

What we can do is try to decrease the overestimation of the quadratic term.

What we do in this paper. We show that it is possible to decrease the overestimation of the quadratic term if we use an inequality proven by A. Grothendieck in 1953 [5, 13].

2 Main Idea

Mean Value methods: reminder. The Mean Value methods are based on the following *first* order Mean Value Theorem:

$$f(\widetilde{x} + \Delta x) = f(\widetilde{x}) + \sum_{i=1}^{n} f_{,i}(\widetilde{x} + \eta) \cdot \Delta x_i \text{ for some } \eta_i \in [-\Delta_i, \Delta_i].$$

To get an enclosure, we estimate each term in this expression one by one, and then use interval arithmetic to combine these estimates.

Specifically, since $\eta_i \in [-\Delta_i, \Delta_i]$, we conclude that $\widetilde{x}_i + \eta_i \in [\widetilde{x}_i - \Delta_i, \widetilde{x}_i - \Delta_i] = \mathbf{x}_i$. Thus, $f_{,i}(\widetilde{x} + \eta) \in f_{,i}(\mathbf{x}_1, \ldots, \mathbf{x}_n)$. From this inclusion and from $\Delta x_i \in [-\Delta_i, \Delta_i]$, we conclude that

$$f_{,i}(\widetilde{x} + \eta) \cdot \Delta x_i \in f_{,i}(\mathbf{x}_1, \ldots, \mathbf{x}_n) \cdot [-\Delta_i, \Delta_i].$$

By adding the value $f(\widetilde{x})$ and n interval bounds on $f_{,i}(\widetilde{x} + \eta) \cdot \Delta x_i$, we conclude that

$$f(\widetilde{x} + \Delta x) \in f(\widetilde{x}_1, \ldots, \widetilde{x}_n) + \sum_{i=1}^{n} f_{,i}(\mathbf{x}_1, \ldots, \mathbf{x}_n) \cdot [-\Delta_i, \Delta_i].$$

How to get a more accurate estimate: natural idea. The first order Mean Value Theorem uses first order terms in the Taylor expansion. It is known that the more terms in the Taylor expansion we use, the more accurately we approximate the original function. Let us use this idea and utilize the following *third* order Mean Value Theorem (see, e.g., [8]):

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

$$\frac{1}{6} \cdot \sum_{i,k,k=1}^{n} f_{,ijk}(\widetilde{x} + \eta) \cdot \Delta x_i \cdot \Delta x_j \cdot \Delta x_k.$$

(for completeness, the derivation of this formula is given in the Appendix).

Then, we can estimate the ranges of linear, quadratic, and cubic terms in this formula, and add up the enclosures for these ranges.

The range of the linear part $f(\widetilde{x}) + \sum\limits_{i=1}^{n} f_{,i}(\widetilde{x}) \cdot \Delta x_i$ can be explicitly described as $[\widetilde{y} - \Delta, \widetilde{y} + \Delta]$, where $\widetilde{y} \stackrel{\text{def}}{=} f(\widetilde{x})$ and $\Delta = \sum\limits_{i=1}^{n} |f_{,i}(\widetilde{x})| \cdot \Delta_i$.

The range of the cubic part $\dfrac{1}{6} \cdot \sum\limits_{i,j,k=1}^{n} f_{,ijk}(\widetilde{x} + \eta) \cdot \Delta x_i \cdot \Delta x_j \cdot \Delta x_k$ can be estimated via straightforward interval computations; the estimate is $O(\Delta^3) \ll O(\Delta^2)$.

The only non-trivial task is estimating the range $[-Q, Q]$ of the quadratic part $\sum\limits_{i,j=1}^{n} a_{ij} \cdot \Delta x_i \cdot \Delta x_j$, where $a_{ij} \stackrel{\text{def}}{=} \dfrac{1}{2} \cdot f_{,ij}(\widetilde{x})$, on the box $[-\Delta_1, \Delta_1] \times \ldots \times [-\Delta_n, \Delta_n]$. We will show that the Grothendieck inequality will help in estimating the range of this quadratic expression. To explain how it can help, let us first recall what is Grothendieck inequality.

Grothendieck inequality: reminder. To introduce Grothendieck inequality, we will follow [13] and consider the following auxiliary computational problem: estimate the value

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

This problem is known to be NP-hard; see, e.g., [10, 12]. This means that we cannot always feasibly compute the value Q'. Instead, we compute approximations to Q'.

One way to get such approximations is to take into account that, in general, discrete optimization problems are more complex than similar continuous ones; see, e.g., [10, 12]. One can easily observe that in the problem of estimating Q', the discrete set $\{-1, 1\}$ is a unit sphere in 1-D Euclidean space, and that in larger dimensions, a unit sphere is connected (hence not discrete). So, Grothendieck's idea was to consider z_i and t_j from the unit sphere S in a Hilbert space (i.e., in effect, in an infinite-dimensional Euclidean space), i.e., to compute the value

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

where $\langle a, b\rangle$ denotes the scalar product: for two elements $a = (a_1, \ldots, a_n, \ldots)$ and $b = (b_1, \ldots, b_n, \ldots)$ in the Hilbert space, $\langle a, b\rangle \stackrel{\text{def}}{=} \sum\limits_{i=1}^{\infty} a_i \cdot b_i$.

Since we can have all z_i and t_j equal to $\pm e$ for some unit vector e, the maximum in Q'' is always larger than or equal to the maximum in Q': $Q' \le Q''$.

Grothendieck showed that for some universal constant $K_G \in [1, 1.782]$, we have $\dfrac{1}{K_G} \cdot Q'' \le Q'$. Thus, we have $\dfrac{1}{K_G} \cdot Q'' \le Q' \le Q''$.

It turns out that a feasible ellipsoid-based method – similar to feasible ellipsoid methods used in linear programming – can compute Q'' [1, 13]. Thus, by using Grothendieck inequality, we can feasibly estimate the value Q' modulo a small multiplicative constant.

How to use this result to estimate Q. We want to estimate the range $[-Q, Q]$ of the expression $\sum\limits_{i,j=1}^{n} a_{ij} \cdot \Delta x_i \cdot \Delta x_j$ on $[-\Delta_1, \Delta_1] \times \ldots \times [-\Delta_n, \Delta_n]$. We can make this problem closer to the Grothendieck's problem if we introduce new variables $z_i \stackrel{\text{def}}{=} \Delta x_i/\Delta_i$. For these variables, we have $z_i \in [-1, 1]$, $\Delta x_i = \Delta_i \cdot z_i$, and the above quadratic form takes the following form:

$$\sum_{i,j=1}^{n} b_{ij} \cdot z_i \cdot z_j, \text{ with } b_{ij} \stackrel{\text{def}}{=} a_{ij} \cdot \Delta_i \cdot \Delta_j.$$

Thus, we can conclude that $Q = \max\{B(z) : z_i \in [-1, 1]\}$, where $B(z) \stackrel{\text{def}}{=} b(z, z)$ and $b(z, t) \stackrel{\text{def}}{=} \sum\limits_{i,j=1}^{n} b_{ij} \cdot z_i \cdot t_j$. Grothendieck's inequality enables us to estimate the maximum Q' of the bilinear function $b(z, t)$: $Q' = \max\{b(z, t) : z_i \in \{-1, 1\}, t_j \in \{-1, 1\}\}$ on the values ± 1.

There are two differences between Q and Q':

- in Q, we maximize $b(z, z)$ as opposed to $b(z, t)$ in Q', and
- in Q, we maximize over the whole interval $[-1, 1]$ as opposed to over the two-valued set $\{-1, 1\}$ in Q'.

The second difference is not important, since a bilinear function $b(z, t)$ is linear in each of its variables and thus, attains its maximum at endpoints. Hence,

$$Q' = \max\{b(z, t) : z_i \in [-1, 1], t_j \in [-1, 1]\}.$$

Now, the only remaining difference is between maximizing $B(z) = b(z, z)$ and $b(z, t)$.

Clearly, since maximizing over all possible pairs (z,t) includes maximizing over pairs (z,z), we have $Q \le Q'$. Vice versa, to bound Q' (maximum of $b(z,t)$) in terms of Q (maximum of $B(z)$), it is reasonable to use a known expression of a bilinear form $b(z,t)$ in terms of its diagonal terms $B(z)=b(z,z)$: $b(z,t)=B((z+t)/2)-B((z-t)/2)$. Because of this expression, the maximum Q' of the absolute value of $b(z,t)$ cannot exceed twice the maximum Q of the expression $B(z)$: $Q' \le 2Q$. Since $Q \le Q'$, we get $Q'/2 \le Q \le Q'$.

Now, from the Grothendieck inequality $K_G^{-1} \cdot Q'' \le Q' \le Q''$, we can conclude that

$$\frac{Q''}{2K_G} \le Q \le Q''.$$

In other words, by feasibly computing the value Q'', we can feasibly estimate the quadratic-expression bound Q accurately – modulo a small constant factor $2K_G \le 3.6$.

Thus, we arrive at the following algorithm.

3 Resulting Algorithm

Preamble. According to the third order Mean Value Theorem, for $\Delta x_i \in [-\Delta_i, \Delta_i]$, we have: $f(\widetilde{x}+\Delta x)=T_1+T_2+T_3$, where:

$$T_1 \stackrel{\text{def}}{=} f(\widetilde{x}) + \sum_{i=1}^{n} f_{,i}(\widetilde{x}) \cdot \Delta x_i;$$

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

$$T_3 \stackrel{\text{def}}{=} \frac{1}{6} \cdot \sum_{i,j,k=1}^{n} f_{,ijk}(\widetilde{x}+\eta) \cdot \Delta x_i \cdot \Delta x_j \cdot \Delta x_k.$$

Algorithm. 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 $O(\Delta^3) \ll O(\Delta^2)$.
- To estimate the range $[-Q,Q]$ of the quadratic term $T_2 = \sum\limits_{i,j=1}^{n} a_{ij} \cdot \Delta x_i \cdot \Delta x_j$, we do the following:
  - we compute an auxiliary matrix $b_{ij} = a_{ij} \cdot \Delta_i \cdot \Delta_j$, and
  - we use the ellipsoid method described in [1] to compute the value

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

Then, $\dfrac{Q''}{2K_G} \le Q \le Q''$, with $2 \le 2K_G \le 3.6$.

Discussion: why this is better than the Mean Value methods. We still get excess width $O(\Delta^2)$, but this time, we overestimate the quadratic terms by no more than a known constant factor.

Remaining open problem. In interval computing, it is often beneficial to use slopes instead of derivatives; see, e.g., [6]. It would be great to extend Grothendieck-based techniques to slope-based methods.

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A Third Order Mean Value Theorem: Derivation

According to the Lagrange form of the Taylor's theorem (see, e.g., [2, 7]), for each three times differentiable function $F(x)$ of one variable, and for all $a \neq b$, there exists a point η between a and b for which

$$F(b) = F(a) + F'(a) \cdot (b-a) + \frac{1}{2} \cdot F''(a) \cdot (b-a)^2 + \frac{1}{6} \cdot F'''(\varkappa) \cdot (b-a)^3.$$

By applying this formula to an auxiliary function

$$F(x) = f(\widetilde{x}_1 + x \cdot (x_1 - \widetilde{x}_1), \ldots, \widetilde{x}_n + x \cdot (x_n - \widetilde{x}_n))$$

and the values $a = 0$ and $b = 1$, and taking into account that $F(0) = f(\widetilde{x}_1, \ldots, \widetilde{x}_n)$ and $F(1) = f(x_1, \ldots, x_n)$, we get the desired expression for the third order Mean Value Theorem, with $\eta_i = \varkappa \cdot (x_i - \widetilde{x}_i)$. Since $\varkappa \in (0,1)$ and $|x_i - \widetilde{x}_i| \leq \Delta_i$, we have $\eta_i \in [-\Delta_i, \Delta_i]$.