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The Automatic Computation of Second-Order Slope Tuples for Some Nonsmooth Functions*

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Abstract

In this paper, we show how the automatic computation of second-order slope tuples can be performed. The algorithm allows for nonsmooth functions, such as $\varphi(x) = |u(x)|$ and $\varphi(x) = \max\{u(x), v(x)\}$, to occur in the function expression of the underlying function. Furthermore, we allow the function expression to contain functions given by two or more branches. By using interval arithmetic, second-order slope tuples provide verified enclosures of the range of the underlying function. We give some examples comparing range enclosures given by a second-order slope tuple with enclosures from previous papers.

1 Introduction

Automatic differentiation [13] is a tool for evaluating functions and derivatives simultaneously without using an explicit formula for the derivative. Combining this technique with interval analysis [1], enclosures of the function range and the derivative range on an interval $[x]$ may be computed simultaneously.

By using an arithmetic analogous to automatic differentiation, the automatic computation of first-order slope tuples is possible. For this purpose, the operations $+, -, \cdot, /$ and the evaluation of elementary functions need to be defined for first-order slope tuples. This approach goes back to Krawczyk and Neumaier [10] and was extended by Rump [16] and Ratz [14]. First-order slope tuples provide enclosures of the function range that may be sharper than enclosures obtained by the well-known mean value form. Moreover, slope tuples can be used in existence tests [4, 5, 11, 17, 19] or for verified global optimization [7, 8, 14, 15, 21].

In this paper, we extend this technique by defining a second-order slope tuple and by describing how the automatic computation of such tuples can be carried out. Shen and Wolfe [24] introduced an arithmetic for the automatic computation of second-order slope enclosures, and Kolev [9] improved this by providing optimal enclosures for convex and

*This paper contains some results from the author's dissertation [22].

concave elementary functions. However, both papers require the underlying function $f : D \subseteq \mathbb{R} \to \mathbb{R}$ to be twice continuously differentiable. In this paper, we present similar results that allow for nonsmooth functions $\varphi : D \subseteq \mathbb{R} \to \mathbb{R}$ occuring in the function expression of f, such as $\varphi(x) = |u(x)|$ and $\varphi(x) = \max\{u(x), v(x)\}$. Furthermore, the function expression of f may contain functions given by two or more branches. Moreover, intermediate results are enclosed by intervals. Hence, these algorithms can be used for verified computations on a floating-point computer.

The paper is organized as follows. Section 2 recalls slope functions and slope enclosures. In section 3, we define second-order slope tuples for univariate functions and explain how the automatic computation can be performed. In Section 4, we compare range enclosures obtained by second-order slope tuples with range enclosures given by other methods. Section 5 extends the technique from section 3 to multivariate functions. Furthermore, we explain an alternative approach called componentwise computation of slope tuples and give examples for both methods.

The numerical results were computed using Pascal-XSC programs on a floating-point computer under the operating system Suse Linux 9.3. The source code of the programs is freely available [18]. A current Pascal-XSC compiler is provided by the working group "Scientific Computing / Software Engineering" of the University of Wuppertal [25].

Throughout this paper, we let $[x] = [\underline{x}, \overline{x}] = \left\{x = (x_i) \in \mathbb{R}^n,\ \underline{x_i} \le x_i \le \overline{x_i}\right\}$ with $\underline{x}, \overline{x} \in \mathbb{R}^n$ denote an interval vector. The set of all interval vectors $[x] \subset \mathbb{R}^n$ is denoted by $\mathbb{IR}^n$. For two interval vectors $[x], [y] \in \mathbb{IR}^n$, the *interval hull* $[x] \,\underline{\cup}\, [y]$ is the smallest interval vector in $\mathbb{IR}^n$ containing $[x]$ and $[y]$, i.e.

$$([x] \,\underline{\cup}\, [y])_i := \left[\min\left\{\underline{x_i}, \underline{y_i}\right\}, \max\left\{\overline{x_i}, \overline{y_i}\right\}\right].$$

Furthermore, by

$$\operatorname{mid}[x] := \frac{\overline{x} + \underline{x}}{2}$$

we define the midpoint of $[x]$. Analogously, $\mathbb{IR}^{n \times n}$ denotes the set of interval matrices $[A] = \left([a]_{ij}\right) = \left\{A \in \mathbb{R}^{n \times n},\ \underline{a_{ij}} \le A_{ij} \le \overline{a_{ij}}\right\}$.

In the following sections, we assume that a function f is given by a function expression consisting of a finite number of operations $+, -, \cdot, /$, and elementary functions (cf. [1]). Furthermore, we suppose that an interval arithmetic evaluation $f([x])$ on a given interval $[x]$ exists.

2 Slope Tuples

In this section, we consider functions $f : D \subseteq \mathbb{R} \to \mathbb{R}$.

Definition 2.1 (cf. [3]) Let $f \in C^n(D)$. Furthermore, let $p(x) = \sum\limits_{i=0}^{n} a_i x^i$ be the Hermitian interpolation polynomial for f with respect to the nodes $x_0, \ldots, x_n \in D$. Here, exactly $k+1$ elements of $x_0, \ldots, x_n$ are equal to x_i, if $f(x_i), \ldots, f^{(k)}(x_i)$ are given for some node x_i. The leading coefficient a_n of p is called the *slope of $n-$th order of f with respect to* $x_0, \ldots, x_n$. Notation:

$$\delta_n f(x_0, \ldots, x_n) := a_n.$$

In the following theorem, we give some basic properties of slopes. The statements d) and e) in Theorem 2.2 are easy consequences of the Hermite-Genocchi Theorem (see [3]).

Theorem 2.2 Let $f \in C^n(D)$ and let $\delta_n f(x_0, \ldots, x_n)$ be the slope of $n-$th order of f with respect to $x_0, \ldots, x_n$. Then, the following statements hold:

a) $\delta_n f(x_0, \ldots, x_n)$ is symmetric with respect to its arguments x_i.

b) For $x_i \neq x_j$ we have the recursion formula

$$\delta_n f(x_0, ..., x_n) = \frac{\delta_{n-1} f(x_0, ..., x_{i-1}, x_{i+1}, ..., x_n) - \delta_{n-1} f(x_0, ..., x_{j-1}, x_{j+1}, ..., x_n)}{x_j - x_i}.$$

c) Setting $\omega_k(x) := \prod_{j=0}^{k-1} (x - x_j)$, we have

$$f(x) = \sum_{i=0}^{n-1} \delta_i f(x_0, \ldots, x_i) \cdot \omega_i(x) + \delta_n f(x_0, \ldots, x_{n-1}, x) \cdot \omega_n(x), \quad n \geq 1. \tag{1}$$

d) The function $g : D \subseteq \mathbb{R}^{n+1} \to \mathbb{R}$ defined by

$$g(x_0, \ldots, x_n) := \delta_n f(x_0, \ldots, x_n)$$

is continuous.

e) For the nodes $x_0 \leq x_1 \leq \ldots \leq x_n$ there exists a $\xi \in [x_0, x_n]$ such that

$$\delta_n f(x_0, \ldots, x_n) = \frac{f^{(n)}(\xi)}{n!}.$$

Definition 2.3 Let f be continuous and $x_0 \in D$ be fixed. A function $\delta f : D \to \mathbb{R}$ satisfying

$$f(x) = f(x_0) + \delta f(x; x_0) \cdot (x - x_0), \quad x \in D, \tag{2}$$

is called a *first-order slope function of f with respect to x_0.*

An interval $\delta f([x]; x_0) \in \mathbb{IR}$ that encloses the range of $\delta f(x; x_0)$ on the interval $[x] \subseteq D$, i.e.

$$\delta f([x]; x_0) \supseteq \{\delta f(x; x_0) \mid x \in [x]\},$$

is called a *(first-order) slope enclosure of f on $[x]$ with respect to x_0.*

In $x = x_0$, (2) is fulfilled for an arbitrary $\delta f(x_0; x_0) \in \mathbb{R}$. If f is differentiable in x_0, then we always set $\delta f(x_0; x_0) := f'(x_0)$. Often, the midpoint $\operatorname{mid}[x]$ of the interval $[x]$ is used for x_0.

Remark 2.4 a) Let $\delta f([x]; x_0) = \left[\underline{\delta f}, \overline{\delta f}\right]$ be a first-order slope enclosure of f on $[x]$. Then, by (2), we have

$$f(x) \in f(x_0) + \delta f([x]; x_0) \cdot ([x] - x_0) \tag{3}$$

for all $x \in [x]$.

b) Let f be differentiable on $[x]$ and $x_0 \in [x]$. Then, we have

$$\{\delta f(x; x_0) \mid x \in [x], x \neq x_0\} \subseteq \left\{f'(x) \mid x \in [x]\right\}.$$

Therefore, (3) may provide sharper enclosures of the range of f on $[x]$ than the well-known mean value form.

For some continuous functions f and some $x_0 \in [x] \subseteq D$, a slope enclosure $\delta f([x]\,;x_0) \in \mathbb{IR}$ does not exist, e.g.

$$f(x) = \begin{cases} \sqrt{x} & \text{for } x \geq 0, \\ 0 & \text{for } x < 0, \end{cases}$$

with $x_0 = 0$, $[x] = [-1, 1]$. If f is continuous on $[x]$ and differentiable in $x_0 \in [x]$, then a slope enclosure $\delta f([x]\,;x_0) \in \mathbb{IR}$ exists. For a sufficient, more general existence criterion, we define the *limiting slope interval* [12].

Definition 2.5 Let f be continuous on $[x]$ and $x_0 \in [x]$. Suppose that both

$$\liminf_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0}$$

and

$$\limsup_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0}$$

exist. Then, the *limiting slope interval* $\delta f_{\text{lim}}([x_0]) \in \mathbb{IR}$ is

$$\delta f_{\text{lim}}([x_0]) := \left[\liminf_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0},\ \limsup_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0}\right].$$

Remark 2.6 If f is Lipschitz continuous in some neighbourhood of x_0, then the limiting slope interval $\delta f_{\text{lim}}([x_0])$ exists.

Example 2.7 For $f(x) = |x|$, $x_0 = 0$ we have $\delta f_{\text{lim}}([x_0]) = [-1, 1]$.

Lemma 2.8 Let f be continuous on $[x]$ and $x_0 \in [x]$. If $\delta f_{\text{lim}}([x_0]) \in \mathbb{IR}$ exists, then

$$\delta f([x]\,;x_0) = \left[\inf_{\substack{x \in [x] \\ x \neq x_0}} \frac{f(x) - f(x_0)}{x - x_0},\ \sup_{\substack{x \in [x] \\ x \neq x_0}} \frac{f(x) - f(x_0)}{x - x_0}\right]$$

is a slope enclosure of f on $[x]$ with respect to x_0.

Proof: $g : [x] \setminus \{x_0\} \to \mathbb{R}$, $g(x) := \dfrac{f(x) - f(x_0)}{x - x_0}$, is bounded. □

Remark 2.9 Let f be Lipschitz continuous in some neighbourhood of x_0. Then, Muñoz und Kearfott [12] show the inclusion

$$\delta f_{\text{lim}}([x_0]) \subseteq \partial f(x_0), \tag{4}$$

where $\partial f(x_0)$ is the generalized gradient (see [2]). Furthermore, they give an example where

$$\delta f_{\text{lim}}([x_0]) \subset \partial f(x_0)$$

holds and also a sufficient condition for equality in (4).

Definition 2.10 Let f be continuous, $[x] \subseteq D$ and $x_0 \in [x]$. Assume that $f^{'}(x_0)$ exists. A function $\delta_2 f : D \to \mathbb{R}$ satisfying

$$f(x) = f(x_0) + f^{'}(x_0) \cdot (x - x_0) + \delta_2 f(x; x_0, x_0) \cdot (x - x_0)^2, \quad x \in D,$$

is called a *second-order slope function of f with respect to x_0*. An interval $\delta_2 f([x]; x_0, x_0) \in \mathbb{IR}$ with

$$f(x) \in f(x_0) + f^{'}(x_0) \cdot (x - x_0) + \delta_2 f([x]; x_0, x_0) \cdot (x - x_0)^2, \quad x \in [x], \tag{5}$$

is called a *second-order slope enclosure of f on $[x]$ with respect to x_0*.

As an abbreviation we set $\delta_2 f(x; x_0) := \delta_2 f(x; x_0, x_0)$ and $\delta_2 f([x]; x_0) := \delta_2 f([x]; x_0, x_0)$. Furthermore, if f is twice differentiable in x_0, then we always set $\delta_2 f(x; x_0) := \frac{1}{2} f^{''}(x_0)$.

Remark 2.11 Assume that (5) holds. Then, we have the enclosure

$$f(x) \in f(x_0) + f^{'}(x_0) \cdot ([x] - x_0) + \delta_2 f([x]; x_0) \cdot ([x] - x_0)^2$$

for all $x \in [x]$.

3 The automatic computation of second-order slope tuples for univariate functions

In this section, we consider univariate functions $u, v, w, z : D \subseteq \mathbb{R} \to \mathbb{R}$.

First, we recall the definition of a first-order slope tuple [14, 16]. Afterwards, we give a definition of second-order slope tuples that also permits nonsmooth functions.

Definition 3.1 Let u be continuous, $[x] \subseteq D$ and $x_0 \in [x]$. A triple $\mathcal{U} = (U_x, U_{x_0}, \delta U)$ with $U_x, U_{x_0}, \delta U \in \mathbb{IR}$ satisfying

$$\begin{aligned} u(x) &\in U_x, \\ u(x_0) &\in U_{x_0}, \\ u(x) - u(x_0) &\in \delta U \cdot (x - x_0), \end{aligned}$$

for all $x \in [x]$ is called a *first-order slope tuple for u on $[x]$ with respect to x_0*.

Definition 3.2 Let u be continuous, $[x] \subseteq D$ and $x_0 \in [x]$. A *second-order slope tuple for u on $[x]$ with respect to x_0* is a 5-tuple $\mathcal{U} = (U_x, U_{x_0}, \delta U_{x_0}, \delta U, \delta_2 U)$ with $U_x, U_{x_0}, \delta U_{x_0}, \delta U, \delta_2 U \in \mathbb{IR}$, $U_{x_0} \subseteq U_x$, satisfying

$$u(x) \in U_x, \tag{6}$$

$$u(x_0) \in U_{x_0}, \tag{7}$$

$$\delta u_{\lim}([x_0]) \subseteq \delta U_{x_0}, \tag{8}$$

$$u(x) - u(x_0) \in \delta U \cdot (x - x_0), \tag{9}$$

$$u(x) - u(x_0) \in \delta U_{x_0} \cdot (x - x_0) + \delta_2 U \cdot (x - x_0)^2, \tag{10}$$

for all $x \in [x]$.

Remark 3.3 (10) does not imply that $\delta_2 U$ is a second-order slope enclosure in the sense of (5) because δU_{x_0} is a superset of $\delta u_{\lim}([x_0])$. However, Remark 3.12 will explain why the term *slope tuple* is justified.

Remark 3.4 By (6)-(10) we get the enclosures

$$\begin{array}{rcl} u(x) & \in & U_x, \\ u(x) & \in & U_{x_0} + \delta U \cdot ([x] - x_0), \\ u(x) & \in & U_{x_0} + \delta U_{x_0} \cdot ([x] - x_0) + \delta_2 U \cdot ([x] - x_0)^2, \end{array}$$

for the range of u on $[x]$, where

$$([x] - x_0)^2 = \left[\min_{x \in [x]} (x - x_0)^2, \max_{x \in [x]} (x - x_0)^2 \right].$$

Remark 3.5 If $x = x_0$, then (9) and (10) are fulfilled for arbitrary δU, δU_{x_0} and $\delta_2 U$. So in checking these relations, we can restrict ourselves to $x \neq x_0$.

Lemma 3.6 $\mathcal{K} = (k, k, 0, 0, 0)$ is a second-order slope tuple for the constant function $u(x) \equiv k \in \mathbb{R}$ and $\mathcal{X} = ([x], x_0, 1, 1, 0)$ is a second-order slope tuple for the identity function $u(x) = x$ (both on $[x]$ with respect to $x_0 \in [x]$).

Definition 3.7 Let $\mathcal{U}$ and $\mathcal{V}$ be second-order slope tuples for the continuous functions u and v, respectively, on $[x] \subseteq D$ with respect to $x_0 \in [x]$.

a) For the addition or subtraction of $\mathcal{U}$ and $\mathcal{V}$ we define the 5-tuple $\mathcal{W} := \mathcal{U} \pm \mathcal{V}$ by

$$\begin{array}{lcl} W_x & := & U_x \pm V_x, \\ W_{x_0} & := & U_{x_0} \pm V_{x_0}, \\ \delta W_{x_0} & := & \delta U_{x_0} \pm \delta V_{x_0}, \\ \delta W & := & \delta U \pm \delta V, \\ \delta_2 W & := & \delta_2 U \pm \delta_2 V. \end{array}$$

b) The multiplication $\mathcal{W} := \mathcal{U} \cdot \mathcal{V}$ is defined by

$$\begin{array}{lcl} W_x & := & U_x \cdot V_x, \\ W_{x_0} & := & U_{x_0} \cdot V_{x_0}, \\ \delta W_{x_0} & := & \delta U_{x_0} \cdot V_{x_0} + U_{x_0} \cdot \delta V_{x_0}, \\ \delta W & := & \delta U \cdot V_{x_0} + U_x \cdot \delta V, \\ \delta_2 W & := & \delta_2 U \cdot V_{x_0} + U_x \cdot \delta_2 V + \delta U \cdot \delta V_{x_0}. \end{array}$$

c) If $0 \notin V_x$, then the division $\mathcal{W} := \mathcal{U} / \mathcal{V}$ is defined by

$$\begin{array}{lcl} W_x & := & U_x / V_x, \\ W_{x_0} & := & U_{x_0} / V_{x_0}, \\ \delta W_{x_0} & := & (\delta U_{x_0} - W_{x_0} \cdot \delta V_{x_0}) / V_{x_0}, \\ \delta W & := & (\delta U - W_{x_0} \cdot \delta V) / V_x, \\ \delta_2 W & := & (\delta_2 U - W_{x_0} \cdot \delta_2 V - \delta W \cdot \delta V) / V_{x_0}. \end{array}$$

d) If φ is twice continuously differentiable, we define $\mathcal{W} := \varphi(\mathcal{U})$ by

$$\begin{array}{lcl} W_x & := & \varphi(U_x)\,, \\ W_{x_0} & := & \varphi(U_{x_0})\,, \\ \delta W_{x_0} & := & \delta\varphi(U_{x_0}; U_{x_0}) \cdot \delta U_{x_0}, \\ \delta W & := & \delta\varphi(U_x; U_{x_0}) \cdot \delta U, \\ \delta_2 W & := & \delta\varphi(U_x; U_{x_0}) \cdot \delta_2 U + \delta_2\varphi(U_x; U_{x_0}) \cdot \delta U_{x_0} \cdot \delta U. \end{array}$$

Here, we require $\varphi(U_x) \in \mathbb{IR}$ and $\varphi(U_{x_0}) \in \mathbb{IR}$ to enclose the range of φ on U_x and U_{x_0}, respectively, and $\delta\varphi(U_{x_0}; U_{x_0}) \in \mathbb{IR}$ to enclose

$$\{\delta\varphi(\widetilde{u_{x_0}}; u_{x_0}) \mid \widetilde{u_{x_0}} \in U_{x_0}, u_{x_0} \in U_{x_0}\}, \tag{11}$$

$\delta\varphi(U_x; U_{x_0}) \in \mathbb{IR}$ to enclose

$$\{\delta\varphi(u_x; u_{x_0}) \mid u_x \in U_x, u_{x_0} \in U_{x_0}\}, \tag{12}$$

and $\delta_2\varphi(U_x; U_{x_0}) \in \mathbb{IR}$ to enclose

$$\{\delta_2\varphi(u_x; u_{x_0}) \mid u_x \in U_x, u_{x_0} \in U_{x_0}\}. \tag{13}$$

Theorem 3.8 The 5-tuples $\mathcal{W} = (W_x, W_{x_0}, \delta W_{x_0}, \delta W, \delta_2 W)$ in Definition 3.7 are second-order slope tuples for the functions $w = u \circ v$, $\circ \in \{+, -, \cdot, /\}$ and $w(x) = \varphi(u(x))$ on $[x]$ with respect to x_0, i.e. they satisfy (6)-(10).

Proof: The proof of (6), (7), and (9) for $\mathcal{W}$ are analogous to those in [14, 16]. So, we only need to prove (8) and (10). We will show this for $\mathcal{W} := \mathcal{U} \cdot \mathcal{V}$ and $\mathcal{W} := \varphi(\mathcal{U})$. The proofs for addition, subtraction, and division are similar. Details can be found in [22].

For $w(x) = u(x) \cdot v(x)$ and $x \in [x]$ we have

$$\begin{array}{rcl} w(x) - w(x_0) & = & u(x)\,v(x) - u(x)\,v(x_0) + u(x)\,v(x_0) - u(x_0)\,v(x_0) \\ & = & \Big(u(x) \cdot \delta v(x; x_0) + \delta u(x; x_0) \cdot v(x_0)\Big) \cdot (x - x_0) \end{array}$$

and thus obtain

$$\begin{array}{rcl} \delta w_{\lim}([x_0]) & \subseteq & u(x_0) \cdot \delta v_{\lim}([x_0]) + \delta u_{\lim}([x_0]) \cdot v(x_0) \\ & \subseteq & U_{x_0} \cdot \delta V_{x_0} + \delta U_{x_0} \cdot V_{x_0}, \end{array}$$

which is (8) for $\mathcal{W} = \mathcal{U} \cdot \mathcal{V}$.

Furthermore, by using interval analysis and the slope tuple properties of $\mathcal{U}$ and $\mathcal{V}$ we have

$$\begin{array}{rcl} w(x) - w(x_0) & = & u(x)\big(v(x) - v(x_0)\big) + v(x_0)\big(u(x) - u(x_0)\big) \\ & \in & u(x)\Big(\delta V_{x_0} \cdot (x - x_0) + \delta_2 V \cdot (x - x_0)^2\Big) \\ & & + v(x_0)\Big(\delta U_{x_0} \cdot (x - x_0) + \delta_2 U \cdot (x - x_0)^2\Big) \\ & = & \Big(u(x) \cdot \delta V_{x_0} + v(x_0) \cdot \delta U_{x_0}\Big) \cdot (x - x_0) \\ & & + \Big(u(x) \cdot \delta_2 V + v(x_0) \cdot \delta_2 U\Big) \cdot (x - x_0)^2 \\ & \subseteq & \Big(\Big(u(x_0) + \delta U \cdot (x - x_0)\Big) \cdot \delta V_{x_0} + v(x_0) \cdot \delta U_{x_0}\Big) \cdot (x - x_0) \\ & & + \Big(u(x) \cdot \delta_2 V + v(x_0) \cdot \delta_2 U\Big) \cdot (x - x_0)^2 \\ & \subseteq & \delta W_{x_0} \cdot (x - x_0) + \delta_2 W \cdot (x - x_0)^2\,, \end{array}$$

which proves (10).

Next, we consider $w(x) = \varphi(u(x))$ and $x \in [x]$. By

$$w(x) - w(x_0) \;=\; \delta\varphi\big(u(x)\,;u(x_0)\big)\cdot\big(u(x) - u(x_0)\big)$$

we get

$$\delta w_{\lim}([x_0]) \;\subseteq\; \varphi'(u(x_0))\cdot\delta U_{x_0} \;\subseteq\; \delta\varphi(U_{x_0};U_{x_0})\cdot\delta U_{x_0},$$

which is (8) for $\mathcal{W} = \varphi(\mathcal{U})$. Because of

$$\begin{aligned}\varphi(u(x)) \;&=\; \varphi(u(x_0)) + \varphi'(u(x_0))\cdot\big(u(x) - u(x_0)\big)\\ &\quad + \delta_2\varphi\big(u(x)\,;u(x_0)\big)\cdot\big(u(x) - u(x_0)\big)^2\end{aligned}$$

we obtain

$$\delta\varphi\big(u(x)\,;u(x_0)\big) \;=\; \varphi'(u(x_0)) + \delta_2\varphi\big(u(x)\,;u(x_0)\big)\cdot\big(u(x) - u(x_0)\big).$$

Hence, we have

$$\begin{aligned} w(x) - w(x_0) \;&=\; \delta\varphi\big(u(x)\,;u(x_0)\big)\cdot\big(u(x) - u(x_0)\big)\\ &\in\; \delta\varphi\big(u(x)\,;u(x_0)\big)\cdot\Big(\delta U_{x_0}\cdot(x - x_0) + \delta_2 U\cdot(x - x_0)^2\Big)\\ &=\; \varphi'(u(x_0))\cdot\delta U_{x_0}\cdot(x - x_0)\\ &\quad +\delta_2\varphi\big(u(x)\,;u(x_0)\big)\cdot\delta U_{x_0}\cdot\big(u(x) - u(x_0)\big)\cdot(x - x_0)\\ &\quad + \delta\varphi\big(u(x)\,;u(x_0)\big)\cdot\delta_2 U\cdot(x - x_0)^2\\ &\subseteq\; \delta\varphi\big(U_{x_0};U_{x_0}\big)\cdot\delta U_{x_0}\cdot(x - x_0)\\ &\quad + \Big(\delta_2\varphi\big(U_x;U_{x_0}\big)\cdot\delta U_{x_0}\cdot\delta U + \delta\varphi\big(U_x;U_{x_0}\big)\cdot\delta_2 U\Big)\cdot(x - x_0)^2\\ &\subseteq\; \delta W_{x_0}\cdot(x - x_0) + \delta_2 W\cdot(x - x_0)^2, \end{aligned}$$

which is (10). □

Remark 3.9 It is possible to define δW and $\delta_2 W$ differently in Definition 3.7 b)-d), such that they still satisfy (6)-(10). For example, an alternative definition of δW for the multiplication $\mathcal{W} = \mathcal{U}\cdot\mathcal{V}$ would be $\delta W := \delta U\cdot V_x + U_{x_0}\cdot\delta V$. Furthermore, the intersection of this alternative δW with the δW from Definition 3.7 b) may be used (cf. [16]).

Next, we compute enclosures $\delta\varphi(U_{x_0};U_{x_0})$, $\delta\varphi(U_x;U_{x_0})$, $\delta_2\varphi(U_x;U_{x_0}) \in \mathbb{IR}$ of (11)-(13), where φ is twice continuously differentiable. Note that such enclosures exist because the sets (11)-(13) are bounded as a consequence of the assumptions on φ and $\mathcal{U}$.

By the Mean Value Theorem and Taylor's Theorem we have the enclosures

$$\delta\varphi(U_{x_0};U_{x_0}) = \varphi'(U_{x_0}), \tag{14}$$

$$\delta\varphi(U_x;U_{x_0}) = \varphi'(U_x), \tag{15}$$

and

$$\delta_2\varphi(U_x;U_{x_0}) = \frac{1}{2}\varphi''(U_x) \tag{16}$$

of (11)-(13). However, for some functions, such as $\varphi(x) = x^2$ and $\varphi(x) = \sqrt{x}$, sharper enclosures for (12) and (13) can be found. By explicit computation of $\delta\varphi(u_x;u_{x_0})$ and $\delta_2\varphi(u_x;u_{x_0})$ we get the following two lemmas.

Lemma 3.10 Let $\mathcal{U}$ be a second-order slope tuple for u on $[x]$ with respect to $x_0 \in [x]$, and let $\varphi : \mathbb{R} \to \mathbb{R}$, $\varphi(x) = x^2$. Then, we have the enclosures

$$\delta\varphi(u_x; u_{x_0}) \in U_x + U_{x_0},$$
$$\delta_2\varphi(u_x; u_{x_0}) \in [1, 1]$$

for all $u_x \in U_x$ and all $u_{x_0} \in U_{x_0}$.

Lemma 3.11 Let $\mathcal{U}$ be a second-order slope tuple for u on $[x]$ with respect to $x_0 \in [x]$ such that $\inf(U_x) \geq 0$ and $\inf(U_{x_0}) > 0$. Furthermore, let $\varphi : \mathbb{R}_{\geq 0} \to \mathbb{R}$, $\varphi(x) = \sqrt{x}$. Then, for all $u_x \in U_x$ and all $u_{x_0} \in U_{x_0}$ we have

$$\delta\varphi(u_x; u_{x_0}) \in \frac{1}{\sqrt{U_x} + \sqrt{U_{x_0}}},$$
$$\delta_2\varphi(u_x; u_{x_0}) \in -\frac{1}{2\sqrt{U_{x_0}}\left(\sqrt{U_x} + \sqrt{U_{x_0}}\right)^2}.$$

Furthermore, by exploiting convexity or concavity of φ and φ' we can get sharper enclosures for (12) and (13) than by (15) and (16). The formulas and the proofs can be found in [9] and [16]. Moreover, exploiting a unique point of inflection of φ or φ' may also give sharper enclosures for (12) or (13) than (15) or (16). This applies to functions such as $\varphi(x) = \sinh x$, $\varphi(x) = \cosh x$, etc. We omit the details of these formulas and refer to [20].

Remark 3.12 Let f be twice continuously differentiable and $\mathcal{F} = (F_x, F_{x_0}, \delta F_{x_0}, \delta F, \delta_2 F)$ be a second-order slope tuple for f on $[x]$ obtained by using Lemma 3.6 and Definition 3.7. Then, we get

$$f(x) - f(x_0) \in f'(x_0) \cdot (x - x_0) + \delta_2 F \cdot (x - x_0)^2, \quad x \in [x],$$

analogously to the proof of Theorem 3.8. This is stronger than (10). Hence, by (5), $\delta_2 F$ is a second-order slope enclosure of f on $[x]$ with respect to x_0. This justifies the term *second-order slope tuple* in Definition 3.2.

Nonsmooth elementary functions

Let $\mathcal{U}$ and $\mathcal{V}$ be second-order slope tuples for u and v on $[x] \subseteq D$ with respect to $x_0 \in [x]$. We compute a second-order slope tuple $\mathcal{W}$ for $w(x) = |u(x)|$, $w(x) = \max\{u(x), v(x)\}$ and $w(x) = \min\{u(x), v(x)\}$, so that the automatic computation of second-order slope tuples can be extended to some nonsmooth functions.

1. $w(x) = \varphi(u(x)) = |u(x)|$:

We define the evaluation of $\varphi(x) = |x|$ on an interval $[x] \in \mathbb{IR}$ by

$$|[x]| = \operatorname{abs}([x]) := \{|x| \mid x \in [x]\} = \left[\min_{x \in [x]} |x|, \max_{x \in [x]} |x|\right].$$

Furthermore, we compute $\mathcal{W} = \varphi(\mathcal{U}) = \operatorname{abs}(\mathcal{U})$ by

$$\begin{array}{rcl} W_x & = & \operatorname{abs}(U_x), \\ W_{x_0} & = & \operatorname{abs}(U_{x_0}), \\ \delta W_{x_0} & = & \delta\varphi(U_{x_0}; U_{x_0}) \cdot \delta U_{x_0}, \\ \delta W & = & \delta\varphi(U_x; U_{x_0}) \cdot \delta U, \\ \delta_2 W & = & [r], \end{array}$$

where

$$\delta\varphi\left(U_{x_0};U_{x_0}\right)=\begin{cases}[-1,-1] & \text{if } \overline{u_x}\leq 0\\ [1,1] & \text{if } \underline{u_x}\geq 0\\ [-1,-1] & \text{if } 0\in U_x\ \wedge\ \overline{u_{x_0}}<0\\ [1,1] & \text{if } 0\in U_x\ \wedge\ \underline{u_{x_0}}>0\\ [-1,1] & \text{otherwise,}\end{cases}$$

$$\delta\varphi\left(U_x;U_{x_0}\right)\ =\ \begin{cases}[-1,-1] & \text{if } \overline{u_x}\leq 0\\ [1,1] & \text{if } \underline{u_x}\geq 0\\ \left[\frac{\left|\underline{u_x}\right|-\left|\underline{u_{x_0}}\right|}{\underline{u_x}-\underline{u_{x_0}}},\ \frac{\left|\overline{u_x}\right|-\left|\overline{u_{x_0}}\right|}{\overline{u_x}-\overline{u_{x_0}}}\right] & \text{if } 0\in U_x\wedge\underline{u_x}\neq\underline{u_{x_0}}\wedge\overline{u_x}\neq\overline{u_{x_0}}\\ \left[-1,\ \frac{\left|\overline{u_x}\right|-\left|\overline{u_{x_0}}\right|}{\overline{u_x}-\overline{u_{x_0}}}\right] & \text{if } 0\in U_x\wedge\underline{u_x}=\underline{u_{x_0}}\wedge\overline{u_x}\neq\overline{u_{x_0}}\\ \left[\frac{\left|\underline{u_x}\right|-\left|\underline{u_{x_0}}\right|}{\underline{u_x}-\underline{u_{x_0}}},\ 1\right] & \text{if } 0\in U_x\wedge\underline{u_x}\neq\underline{u_{x_0}}\wedge\overline{u_x}=\overline{u_{x_0}}\\ [-1,1] & \text{otherwise,}\end{cases}$$

and

$$[r]\ =\ \begin{cases}-1\cdot\delta_2 U & \text{if } \overline{u_x}\leq 0\\ \delta_2 U & \text{if } \underline{u_x}\geq 0\\ \delta\varphi\left(U_x;U_{x_0}\right)\cdot\delta_2 U+\left[0,\ -\frac{1}{2\cdot\overline{u_{x_0}}}\right]\cdot\delta U_{x_0}\cdot\delta U & \text{if } 0\in U_x\wedge\overline{u_{x_0}}<0\wedge-\overline{u_{x_0}}\in U_x\\ \delta\varphi\left(U_x;U_{x_0}\right)\cdot\delta_2 U+\left[0,\ \frac{2\cdot\overline{u_x}}{\left(\overline{u_x}-\overline{u_{x_0}}\right)^2}\right]\cdot\delta U_{x_0}\cdot\delta U & \text{if } 0\in U_x\wedge\overline{u_{x_0}}<0\wedge-\overline{u_{x_0}}\notin U_x\\ \delta\varphi\left(U_x;U_{x_0}\right)\cdot\delta_2 U+\left[0,\ \frac{1}{2\cdot\underline{u_{x_0}}}\right]\cdot\delta U_{x_0}\cdot\delta U & \text{if } 0\in U_x\wedge\underline{u_{x_0}}>0\wedge-\underline{u_{x_0}}\in U_x\\ \delta\varphi\left(U_x;U_{x_0}\right)\cdot\delta_2 U+\left[0,-\frac{2\cdot\underline{u_x}}{\left(\underline{u_x}-\underline{u_{x_0}}\right)^2}\right]\cdot\delta U_{x_0}\cdot\delta U & \text{if } 0\in U_x\wedge\underline{u_{x_0}}>0\wedge-\underline{u_{x_0}}\notin U_x\\ [-1,1]\cdot\delta_2 U & \text{otherwise.}\end{cases}$$

2. $w\left(x\right)=\max\left\{u\left(x\right),v\left(x\right)\right\}$:

We define the evaluation of the max-function for two intervals $[a]$ and $[b]$ by

$$\max\left\{[a],[b]\right\}\ :=\ \left[\max\left\{\underline{a},\underline{b}\right\},\max\left\{\overline{a},\overline{b}\right\}\right].$$

Furthermore, we compute $\mathcal{W} = \max\{\mathcal{U}, \mathcal{V}\}$ by

$$\begin{aligned}
W_x &= \max\{U_x, V_x\}, \\
W_{x_0} &= \max\{U_{x_0}, V_{x_0}\}, \\
\delta W_{x_0} &= \begin{cases} \delta U_{x_0} & \text{if } \underline{u_x} \geq \overline{v_x} \\ \delta V_{x_0} & \text{if } \underline{v_x} \geq \overline{u_x} \\ \delta U_{x_0} \mathbin{\underline{\cup}} \delta V_{x_0} & \text{otherwise,} \end{cases} \\
\delta W &= \begin{cases} \delta U & \text{if } \underline{u_x} \geq \overline{v_x} \\ \delta V & \text{if } \underline{v_x} \geq \overline{u_x} \\ \delta U \mathbin{\underline{\cup}} \delta V & \text{otherwise,} \end{cases} \\
\delta_2 W &= \begin{cases} \delta_2 U & \text{if } \underline{u_x} \geq \overline{v_x} \\ \delta_2 V & \text{if } \underline{v_x} \geq \overline{u_x} \\ \delta_2 U \mathbin{\underline{\cup}} \delta_2 V & \text{otherwise.} \end{cases}
\end{aligned}$$

We compute $\mathcal{W}$ for $w(x) = \min\{u(x), v(x)\}$ analogously to $w(x) = \max\{u(x), v(x)\}$.

Theorem 3.13 Let $\mathcal{U}$ and $\mathcal{V}$ be second-order slope tuples for u and v, respectively, on $[x] \subseteq D$ with respect to $x_0 \in [x]$. Then, the tuples $\mathcal{W} = \varphi(\mathcal{U}) = \mathrm{abs}(\mathcal{U})$ and $\mathcal{W} = \max\{\mathcal{U}, \mathcal{V}\}$ defined above are second-order slope tuples for the functions $w(x) = \varphi(u(x)) = |u(x)|$ and $w(x) = \max\{u(x), v(x)\}$, respectively.

Proof: The proof of (6), (7), and (9) for $\mathcal{W}$ can be found in [14]. Therefore, we only need to check (8) and (10).

1. $w(x) = \varphi(u(x)) = |u(x)|$:

We prove (8). For each $x \in [x]$ with $u(x) = u(x_0)$ we have

$$w(x) - w(x_0) \;=\; [a] \cdot \big(u(x) - u(x_0)\big)$$

with an arbitrary $[a] \in \mathbb{IR}$. If $u(x) \neq u(x_0)$, then

$$\frac{w(x) - w(x_0)}{x - x_0} \;=\; \frac{|u(x)| - |u(x_0)|}{u(x) - u(x_0)} \cdot \frac{u(x) - u(x_0)}{x - x_0}$$

holds. By considering the various cases in the definition of δW_{x_0} we obtain $\delta w_{\lim}([x_0]) \subseteq \delta W_{x_0}$.

Next, we prove (10).

Case 1: $\overline{u_x} \leq 0$.

We have

$$\begin{aligned}
w(x) - w(x_0) = &\; -1 \cdot \big(u(x) - u(x_0)\big) \\
&\in -1 \cdot \delta U_{x_0} \cdot (x - x_0) - 1 \cdot \delta_2 U \cdot (x - x_0)^2 .
\end{aligned}$$

Case 2: $\underline{u_x} \geq 0$. This case is analogous to the previous case.

Case 3: $0 \in U_x \,\wedge\, \overline{u_{x_0}} < 0 \,\wedge\, -\overline{u_{x_0}} \in U_x$.

For all $x \in [x]$ with $u(x) \geq 0$ we get

$$\begin{aligned}
w(x) - w(x_0) &\in \frac{|u(x)| - |u(x_0)|}{u(x) - u(x_0)} \cdot \Big(\delta U_{x_0} \cdot (x - x_0) + \delta_2 U \cdot (x - x_0)^2\Big) \\
&= \Big(-1 + \frac{2\, u(x)}{u(x) - u(x_0)}\Big) \cdot \delta U_{x_0} \cdot (x - x_0) \\
&\quad + \frac{|u(x)| - |u(x_0)|}{u(x) - u(x_0)} \cdot \delta_2 U \cdot (x - x_0)^2 \\
&= -\delta U_{x_0} \cdot (x - x_0) + \Bigg(\frac{|u(x)| - |u(x_0)|}{u(x) - u(x_0)} \cdot \delta_2 U \\
&\quad + \frac{2\, u(x)}{\big(u(x) - u(x_0)\big)^2} \cdot \frac{u(x) - u(x_0)}{x - x_0} \cdot \delta U_{x_0}\Bigg) \cdot (x - x_0)^2 .
\end{aligned}$$

Because of $u(x) \geq 0$ we have

$$0 \leq \frac{2\, u(x)}{\big(u(x) - u(x_0)\big)^2} \leq \frac{2\, u(x)}{\big(u(x) - \overline{u_{x_0}}\big)^2}. \tag{17}$$

By computing the maximum of the right expression in (17) and by using $u(x) \geq 0$ and $-\overline{u_{x_0}} \in U_x$, we obtain

$$\frac{2\, u(x)}{\big(u(x) - \overline{u_{x_0}}\big)^2} \leq \frac{2\,(-\overline{u_{x_0}})}{\big(-\overline{u_{x_0}} - \overline{u_{x_0}}\big)^2}.$$

Thus, we have

$$\frac{2\, u(x)}{\big(u(x) - u(x_0)\big)^2} \in \left[0,\ -\frac{1}{2\,\overline{u_{x_0}}}\right]. \tag{18}$$

Therefore, for all $x \in [x]$ with $u(x) \geq 0$ we have shown that

$$\begin{aligned}
w(x) - w(x_0) \in\ & -\delta U_{x_0} \cdot (x - x_0) + \Big(\delta\varphi(U_x; U_{x_0}) \cdot \delta_2 U \\
& + \left[0,\ -\frac{1}{2\,\overline{u_{x_0}}}\right] \cdot \delta U_{x_0} \cdot \delta U\Big) \cdot (x - x_0)^2
\end{aligned} \tag{19}$$

holds. For all $x \in [x]$ with $u(x) < 0$ we get

$$\begin{aligned}
w(x) - w(x_0) &= \big(u(x) - u(x_0)\big) \\
&\in -\delta U_{x_0} \cdot (x - x_0) - \delta_2 U \cdot (x - x_0)^2 .
\end{aligned}$$

Because of $-1 \in \delta\varphi(U_x; U_{x_0})$ and $0 \in \left[0,\ -\frac{1}{2\,\overline{u_{x_0}}}\right]$ we have

$$\begin{aligned}
& -1 \cdot \delta_2 U \cdot (x - x_0)^2 \\
\subseteq\ & \Big(\delta\varphi(U_x; U_{x_0}) \cdot \delta_2 U + \left[0,\ -\frac{1}{2\,\overline{u_{x_0}}}\right] \cdot \delta U_{x_0} \cdot \delta U\Big) \cdot (x - x_0)^2 .
\end{aligned}$$

Hence, (19) also holds for all $x \in [x]$ with $u(x) < 0$. Thus, we have

$$w(x) - w(x_0) \subseteq \delta W_{x_0} \cdot (x - x_0) + \delta_2 W \cdot (x - x_0)^2$$

for all $x \in [x]$.

Case 4: $0 \in U_x \;\wedge\; \overline{u_{x_0}} < 0 \;\wedge\; -\overline{u_{x_0}} \notin U_x$.

The proof is analogous to case 3. Instead of (18), we get

$$\frac{2 \cdot u(x)}{\big(u(x) - u(x_0)\big)^2} \quad \in \quad \left[0,\, \frac{2 \cdot \overline{u_x}}{\left(\overline{u_x} - \overline{u_{x_0}}\right)^2}\right].$$

Case 5: $0 \in U_x \wedge \underline{u_{x_0}} > 0 \wedge -\underline{u_{x_0}} \in U_x$. This case is analogous to case 3.

Case 6: $0 \in U_x \wedge \underline{u_{x_0}} > 0 \wedge -\underline{u_{x_0}} \notin U_x$. This case is analogous to case 4.

Case 7: We have

$$\begin{aligned} |u(x)| - |u(x_0)| \quad &\in \quad [-1,1] \cdot \Big(u(x) - u(x_0)\Big) \\ &\subseteq \quad [-1,1] \cdot \delta U_{x_0} \cdot (x - x_0) + [-1,1] \cdot \delta_2 U \cdot (x - x_0)^2, \end{aligned}$$

which completes the proof.

2. $w(x) = \max\{u(x), v(x)\}$:

Case 1: $\underline{u_x} \geq \overline{v_x}$.

We have $\max\{u(x), v(x)\} = u(x)$ and $\max\{u(x_0), v(x_0)\} = u(x_0)$. Therefore, the proof of (8) and (10) is obvious.

Case 2: $\underline{v_x} \geq \overline{u_x}$. This case can be proven analogously to case 1.

Case 3: In the remaining case we have

$$\delta w_{\lim}([x_0]) \;\subseteq\; \delta U_{x_0} \,\underline{\cup}\, \delta V_{x_0}.$$

Therefore, we get (8). Next, we prove (10).

If $\max\{u(x), v(x)\} = u(x)$ and $\max\{u(x_0), v(x_0)\} = v(x_0)$, then we have

$$v(x) - v(x_0) \quad \leq \quad u(x) - v(x_0) \quad \leq \quad u(x) - u(x_0)\;,$$

and therefore,

$$w(x) - w(x_0) \;\in\; (\delta U_{x_0} \,\underline{\cup}\, \delta V_{x_0}) \cdot (x - x_0) + (\delta_2 U \,\underline{\cup}\, \delta_2 V) \cdot (x - x_0)^2 \tag{20}$$

holds. Clearly, (20) also holds, if $\max\{u(x), v(x)\} = u(x)$ and $\max\{u(x_0), v(x_0)\} = u(x_0)$. Analogously, (20) is fulfilled, if u and v are interchanged. Therefore, we get (10).

□

Continuous functions given by two or more branches

In order to automatically compute second-order slope tuples for continuous functions given by two or more branches, we first define the function $\mathrm{ite} : \mathbb{R}^3 \longrightarrow \mathbb{R}$ ("if-then-else").

Definition 3.14 $\mathrm{ite} : \mathbb{R}^3 \longrightarrow \mathbb{R}$ is the function

$$\mathrm{ite}(z, u, v) \quad := \quad \begin{cases} u & \text{if } z < 0 \\ v & \text{otherwise.} \end{cases} \tag{21}$$

Let $u, v, z : D \subseteq \mathbb{R} \longrightarrow \mathbb{R}$ be continuous, $[x] \subseteq D$ and define $w : D \subseteq \mathbb{R} \longrightarrow \mathbb{R}$ by

$$w(x) = \operatorname{ite}\big(z(x), u(x), v(x)\big). \tag{22}$$

w is now a function given by two branches u and v, with the function z determining which branch is chosen. For details see [23].

Definition 3.15 We define the evaluation of the ite-function for intervals $[z] = [\underline{z}, \overline{z}]$, $[u] = [\underline{u}, \overline{u}]$ and $[v] = [\underline{v}, \overline{v}]$ by

$$\operatorname{ite}\big([z], [u], [v]\big) := \begin{cases} [u] & \text{if } \overline{z} < 0 \\ [v] & \text{if } \underline{z} \geq 0 \\ [u] \mathbin{\underline{\cup}} [v] & \text{otherwise.} \end{cases} \tag{23}$$

Theorem 3.16 Let $\mathcal{U}$, $\mathcal{V}$ and $\mathcal{Z}$ be second-order slope tuples for the continuous functions u, v and z on some interval $[x] \subseteq D$ with respect to $x_0 \in [x]$. Furthermore, let $w(x) = \operatorname{ite}\big(z(x), u(x), v(x)\big)$ be continuous on $[x]$. We define the 5-tuple $\mathcal{W} = \operatorname{ite}(\mathcal{Z}, \mathcal{U}, \mathcal{V})$ by

$$\begin{aligned}
W_x &= \operatorname{ite}(Z_x, U_x, V_x), \\
W_{x_0} &= \operatorname{ite}(Z_{x_0}, U_{x_0}, V_{x_0}), \\
\delta W_{x_0} &= \begin{cases} \delta U_{x_0} & \text{if } \overline{z_x} < 0 \\ \delta V_{x_0} & \text{if } \underline{z_x} \geq 0 \\ \delta U_{x_0} \mathbin{\underline{\cup}} \big(\delta V_{x_0} + (\delta U_{x_0} - \delta V_{x_0}) \cdot [0,1]\big) & \text{if } 0 \in Z_x \wedge \overline{z_{x_0}} < 0 \\ \delta V_{x_0} \mathbin{\underline{\cup}} \big(\delta U_{x_0} + (\delta V_{x_0} - \delta U_{x_0}) \cdot [0,1]\big) & \text{if } 0 \in Z_x \wedge \underline{z_{x_0}} \geq 0 \\ \Big(\delta U_{x_0} \mathbin{\underline{\cup}} \big(\delta V_{x_0} + (\delta U_{x_0} - \delta V_{x_0}) \cdot [0,1]\big)\Big) & \\ \mathbin{\underline{\cup}} \Big(\delta V_{x_0} \mathbin{\underline{\cup}} \big(\delta U_{x_0} + (\delta V_{x_0} - \delta U_{x_0}) \cdot [0,1]\big)\Big) & \text{otherwise,} \end{cases} \\
\delta W &= \begin{cases} \delta U & \text{if } \overline{z_x} < 0 \\ \delta V & \text{if } \underline{z_x} \geq 0 \\ \delta U \mathbin{\underline{\cup}} \big(\delta V + (\delta U - \delta V) \cdot [0,1]\big) & \text{if } 0 \in Z_x \wedge \overline{z_{x_0}} < 0 \\ \delta V \mathbin{\underline{\cup}} \big(\delta U + (\delta V - \delta U) \cdot [0,1]\big) & \text{if } 0 \in Z_x \wedge \underline{z_{x_0}} \geq 0 \\ \Big(\delta U \mathbin{\underline{\cup}} \big(\delta V + (\delta U - \delta V) \cdot [0,1]\big)\Big) & \\ \mathbin{\underline{\cup}} \Big(\delta V \mathbin{\underline{\cup}} \big(\delta U + (\delta V - \delta U) \cdot [0,1]\big)\Big) & \text{otherwise,} \end{cases} \\
\delta_2 W &= \begin{cases} \delta U & \text{if } \overline{z_x} < 0 \\ \delta V & \text{if } \underline{z_x} \geq 0 \\ \delta_2 U \mathbin{\underline{\cup}} \big(\delta_2 V + (\delta_2 U - \delta_2 V) \cdot [0,1]\big) & \text{if } 0 \in Z_x \wedge \overline{z_{x_0}} < 0 \\ \delta_2 V \mathbin{\underline{\cup}} \big(\delta_2 U + (\delta_2 V - \delta_2 U) \cdot [0,1]\big) & \text{if } 0 \in Z_x \wedge \underline{z_{x_0}} \geq 0 \\ \Big(\delta_2 U \mathbin{\underline{\cup}} \big(\delta_2 V + (\delta_2 U - \delta_2 V) \cdot [0,1]\big)\Big) & \\ \mathbin{\underline{\cup}} \Big(\delta_2 V \mathbin{\underline{\cup}} \big(\delta_2 U + (\delta_2 V - \delta_2 U) \cdot [0,1]\big)\Big) & \text{otherwise.} \end{cases}
\end{aligned}$$

Then, $\mathcal{W} = \operatorname{ite}(\mathcal{Z}, \mathcal{U}, \mathcal{V})$ is a second-order slope tuple for w on $[x]$ with respect to x_0.

Proof: See [22] and [23]. $\square$

Remark 3.17 In some papers, the formula

$$\delta W = \begin{cases} \delta U & \text{if } \overline{z} < 0 \\ \delta V & \text{if } \underline{z} \geq 0 \\ \delta U \,\underline{\cup}\, \delta V & \text{otherwise} \end{cases}$$

is used for computation of a first-order slope tuple for $w(x) = \mathrm{ite}\big(z(x), u(x), v(x)\big)$ on $[x]$. However, this formula is not correct because it does not provide a slope enclosure of w on $[x]$ for all possible choices of z, u, v. For details see [22] and [23].

4 Numerical results

We use the technique from the previous section to automatically compute a second-order slope tuple

$$\mathcal{F} = (F_x, F_{x_0}, \delta F_{x_0}, \delta F, \delta_2 F)$$

for f on $[x]$ with respect to $x_0 \in [x]$. In this way, we obtain the range enclosures

$$S_1 := F_{x_0} + \delta F \cdot ([x] - x_0) \tag{24}$$

and

$$S_2 := F_{x_0} + \delta F_{x_0} \cdot ([x] - x_0) + \delta_2 F \cdot ([x] - x_0)^2 \tag{25}$$

of f on $[x]$ (see Remark 3.4). S_1 was already considered in [14]. If f is twice continuously differentiable, we can also compare these results with the centered forms

$$D_1 := f(x_0) + f^{'}([x]) \cdot ([x] - x_0) \tag{26}$$

and

$$D_2 := f(x_0) + f^{'}(x_0) \cdot ([x] - x_0) + \frac{1}{2} f^{''}([x]) \cdot ([x] - x_0)^2 . \tag{27}$$

Here, $f^{'}([x])$ and $f^{''}([x])$ are enclosures of the range of $f^{'}$ and $f^{''}$ on $[x]$. They are computed via automatic differentiation.

Remark 4.1 By using machine interval arithmetic on a floating-point computer for the operations from section 3, the slope tuple properties (6)-(10) are preserved. Hence, by applying machine interval arithmetic, we obtain verified range enclosures.

We consider the following examples:

1. $f(x) = (x + \sin x) \cdot \exp\left(-x^2\right)$
2. $f(x) = x^4 - 10x^3 + 35x^2 - 50x + 24$
3. $f(x) = \big(\ln(x + 1.25) - 0.84x\big)^2$
4. $f(x) = \dfrac{2}{100}x^2 - \dfrac{3}{100}\exp\Big(-\big(20(x - 0.875)\big)^2\Big)$
5. $f(x) = \exp\left(x^2\right)$
6. $f(x) = x^4 - 12x^3 + 47x^2 - 60x - 20\exp(-x)$
7. $f(x) = x^6 - 15x^4 + 27x^2 + 250$

$$8. \quad f(x) = \big(\arctan(|x-1|)\big)^2 / \left(x^6 - 2x^4 + 20\right)$$

$$9. \quad f(x) = \max\Big\{\exp(-x),\ \sin\big(|x-1|\big)\Big\}$$

$$10. \quad f(x) = \mathrm{ite}\left(x-1,\ x^4 - 1 + \sin(x-1),\ \left|x^2 - \frac{5}{2}x + \frac{3}{2}\right|\right)$$

$$11. \quad f(x) = \left|(x-1)\left(x^2+x+5\right)\right| \cdot \exp\left((x-2)^2\right)$$

$$12. \quad f(x) = \max\left\{x^5 - x^2 + x,\ \exp(x)\cdot(x-1)+1\right\}$$

$$13. \quad f(x) = \mathrm{ite}\Big(x-1,\ (x-1)\cdot\arctan x \cdot \exp\left(x + \sin x\right),\ \Big|\left(x^2 - \frac{5}{2}x + \frac{3}{2}\right)\cdot \sin x\Big|\Big)$$

In each case, we consider $[x] = [0.75, 1.75]$ and set $x_0 := \mathrm{mid}\,[x]$. Examples 1-7 have also been considered in [14].

We obtained the following results:

No.	D_1	D_2	S_1	S_2
1	[-2.262, 3.184]	[-0.910, 2.889]	[-0.939, 1.861]	[-0.247, 1.476]
2	[-44.75, 42.95]	[-5.215, 7.598]	[-22.84, 21.04]	[-1.778, 3.536]
3	[-0.376, 0.412]	[-0.042, 0.190]	[-0.199, 0.235]	[-0.041, 0.151]
4	[-10.51, 10.57]	[-1835, 3.062]	[-0.133, 0.195]	[-0.345, 0.115]
5	[-32.65, 42.19]	[-1.193, 48.82]	[-11.84, 21.39]	[-1.193, 21.39]
6	[-85.86, 29.28]	[-40.03, -11.73]	[-61.07, 4.492]	[-35.76, -16.47]
7	[119.5, 399.3]	[182.7, 304.4]	[185.9, 332.9]	[210.4, 275.1]
8	-	-	[-0.333, 0.339]	[-0.386, 0.233]
9	-	-	[-0.214, 0.787]	[-0.284, 1.271]
10	-	-	[-7.375, 7.500]	[-5.945, 7.516]
11	-	-	[-19.85, 26.70]	[-8.953, 34.22]
12	-	-	[-10.13, 15.61]	[-2.615, 15.11]
13	-	-	[-15.00, 15.12]	[-12.64, 13.27]

For the examples 1-7, S_1 and S_2 provide sharper enclosures than D_1 and D_2, respectively. Furthermore, S_2 is a subset of S_1 for the examples 1-7 except for example 4.

For nonsmooth functions φ, it is possible that a very large interval $\delta_2 W$ is computed for $\mathcal{W} = \varphi(\mathcal{U})$. Hence, S_2 is not always contained in S_1 in our examples. However, except for example 9, one or both bounds of S_2 provide sharper bounds for the range of f than S_1.

5 The automatic computation of second-order slope tuples for multivariate functions

In this section, let $f : D \subseteq \mathbb{R}^n \to \mathbb{R}$. We define slope enclosures and the limiting slope interval analogously to section 2.

Definition 5.1 Let f be continuous and $x_0 \in D$ be fixed. A function $\delta f : D \to \mathbb{R}^{1\times n}$ satisfying

$$f(x) = f(x_0) + \delta f(x; x_0)\cdot(x - x_0), \quad x \in D,$$

is called a *first-order slope function of f with respect to x_0.*

An interval matrix $\delta f([x]\,;x_0) \in \mathbb{IR}^{1\times n}$ with

$$\delta f([x]\,;x_0) \supseteq \{\delta f(x;x_0) \mid x \in [x]\}$$

is called a *(first-order) slope enclosure of f on $[x]$ with respect to x_0.*

A slope function of $f : \mathbb{R}^n \to \mathbb{R}$ is not unique, and there are various ways for computing one, see for example [6, 7].

Definition 5.2 Let f be continuous on $[x] \in \mathbb{IR}^n$, $[x] \subseteq D$. Furthermore, let $x_0 \in [x]$ and $f_i\,(t) := f\big((x_0)_1\,, \ldots, (x_0)_{i-1}\,, t, (x_0)_{i+1}\,, \ldots, (x_0)_n\big)$. If

$$\liminf_{t\to (x_0)_i} \frac{f_i\,(t) - f_i\big((x_0)_i\big)}{t-(x_0)_i}$$

and

$$\limsup_{t\to (x_0)_i} \frac{f_i\,(t) - f_i\big((x_0)_i\big)}{t-(x_0)_i}$$

exist for all $i \in \{1,\ldots,n\}$, then we define the *limiting slope interval $\delta f_{\lim}\,([x_0]) \in \mathbb{IR}^n$* by

$$\Big(\delta f_{\lim}\,([x_0])\Big)_i \;:=\; \left[\liminf_{t\to (x_0)_i} \frac{f_i\,(t) - f_i\big((x_0)_i\big)}{t-(x_0)_i},\; \limsup_{t\to (x_0)_i} \frac{f_i\,(t) - f_i\big((x_0)_i\big)}{t-(x_0)_i}\right].$$

Definition 5.3 Let f be continuous, $[x] \subseteq D$, $x_0 \in [x]$, and assume that $f^{'}(x_0)$ exists. A function $\delta_2 f : D \to \mathbb{R}^{n\times n}$ satisfying

$$f\,(x) \;=\; f\,(x_0) + f^{'}(x_0)\cdot(x-x_0) + (x-x_0)^T\cdot \delta_2 f(x;x_0,x_0)\cdot(x-x_0)\,,\quad x\in D,$$

is called a *second-order slope function of f with respect to x_0.*

An interval matrix $\delta_2 f([x]\,;x_0,x_0) \in \mathbb{IR}^{n\times n}$ with

$$f\,(x) \;\in\; f\,(x_0) + f^{'}(x_0)\cdot(x-x_0) + (x-x_0)^T\cdot \delta_2 f([x]\,;x_0,x_0)\cdot(x-x_0)\,,\quad x\in [x]\,,$$

is called a *second-order slope enclosure of f on $[x]$ with respect to x_0.*

Definition 5.4 Let $u : D \subseteq \mathbb{R}^n \to \mathbb{R}$ be continuous, $[x] \in \mathbb{IR}^n$ with $[x] \subseteq D$, and $x_0 \in [x]$. A *second-order slope tuple for u on $[x]$ with respect to x_0* is a 5-tuple $\mathcal{U} = (U_x, U_{x_0}, \delta U_{x_0}, \delta U, \delta_2 U)$ with $U_x, U_{x_0} \in \mathbb{IR}$, $\delta U_{x_0}, \delta U \in \mathbb{IR}^n$, $\delta_2 U \in \mathbb{IR}^{n\times n}$, $U_{x_0} \subseteq U_x$, satisfying

$$\begin{aligned}
u\,(x) &\;\in\; U_x, && (28)\\
u\,(x_0) &\;\in\; U_{x_0}, && (29)\\
\delta u_{\lim}\,([x_0]) &\;\subseteq\; \delta U_{x_0}, && (30)\\
u\,(x) - u\,(x_0) &\;\in\; \delta U^T\cdot(x-x_0)\,, && (31)\\
u\,(x) - u\,(x_0) &\;\in\; \delta U_{x_0}^T\cdot(x-x_0) + (x-x_0)^T\cdot\delta_2 U\cdot(x-x_0) && (32)
\end{aligned}$$

for all $x \in [x]$.

Lemma 5.5 Let $[x] \in \mathbb{IR}^n$, $x_0 \in [x]$, $i \in \{1, \ldots, n\}$, and let $e^i \in \mathbb{R}^n$ be the i-th unit vector.

a) $\mathcal{K} = (k, k, 0, 0, 0)$ is a second-order slope tuple for the constant function $u : \mathbb{R}^n \to \mathbb{R}$, $u(x) \equiv k \in \mathbb{R}$, on $[x]$ with respect to x_0. Here, the first and the second 0 symbolize the zero vector, and the last 0 stands for the zero matrix.

b) $\mathcal{X} = \big([x]_i, (x_0)_i, e^i, e^i, 0\big)$ is a second-order slope tuple for $u : \mathbb{R}^n \to \mathbb{R}$, $u(x) = x_i$, on $[x]$ with respect to x_0. Here, 0 stands for the zero matrix.

For the automatic computation of second-order slope tuples, the definitions and theorems are completely analogous to section 3. We only have to take into account that $\delta U_{x_0}, \delta U, \delta V_{x_0}, \delta V \in \mathbb{IR}^n$ and $\delta_2 U, \delta_2 V \in \mathbb{IR}^{n \times n}$. Therefore, we get $\delta U_{x_0} \cdot \delta U^T$ instead of $\delta U_{x_0} \cdot \delta U$ and $(x - x_0)^T \cdot \delta_2 U \cdot (x - x_0)$ instead of $\delta_2 U \cdot (x - x_0)^2$. For details, see [22].

The componentwise computation of second-order slope tuples

The automatic computation of slope tuples for multivariate functions can be reduced to the one-dimensional case by the *componentwise computation of slope tuples.* For first-order slope tuples, Ratz [14] uses this technique for verified global optimization. Hence, we also consider the componentwise computation of second-order slope tuples in this paper.

Definition 5.6 Let $u : \mathbb{R}^n \to \mathbb{R}$ be continuous on $[x]$ and let $i \in \{1, \ldots, n\}$ be fixed. We define the family of functions

$$\mathcal{G}_i \;:=\; \left\{ \begin{array}{l} g : [x]_i \subseteq \mathbb{R} \to \mathbb{R}, \quad g(t) := u(x_1, \ldots, x_{i-1}, t, x_{i+1}, \ldots, x_n) \\ \text{with } x_j \in [x]_j \text{ fixed for } j \in \{1, \ldots, n\},\ j \neq i. \end{array} \right\} \tag{33}$$

Each $g \in \mathcal{G}_i$ is a continuous function of one variable t. Hence, for each $g \in \mathcal{G}_i$ the automatic computation of a second-order slope tuple on $[x]_i$ with respect to a fixed $(x_0)_i \in [x]_i$, $(x_0)_i \in \mathbb{R}$, is defined as in section 3.

For the componentwise computation we have to modify the definition of a second-order slope tuple as follows:

Definition 5.7 Let $u : D \subseteq \mathbb{R}^n \to \mathbb{R}$ be continuous and $[x] \in \mathbb{IR}^n$, $[x] \subseteq D$. Furthermore, let $i \in \{1, \ldots, n\}$ and $(x_0)_i \in [x]_i \subseteq \mathbb{R}$ be fixed. A *second-order slope tuple for u on $[x]$ with respect to the i-th component* is a 5-tuple $\mathcal{U} = (U_x, U_{x_0}, \delta U_{x_0}, \delta U, \delta_2 U)$ with $U_x, U_{x_0}, \delta U_{x_0}, \delta U, \delta_2 U \in \mathbb{IR}$, $U_{x_0} \subseteq U_x$, satisfying

$$\begin{array}{rcl} g(x_i) & \in & U_x, \\ g\big((x_0)_i\big) & \in & U_{x_0}, \\ \delta g_{\lim}\big([x_0]_i\big) & \subseteq & \delta U_{x_0}, \\ g(x_i) - g\big((x_0)_i\big) & \in & \delta U \cdot \big(x_i - (x_0)_i\big), \\ g(x_i) - g\big((x_0)_i\big) & \in & \delta U_{x_0} \cdot \big(x_i - (x_0)_i\big) + \delta_2 U \cdot \big(x_i - (x_0)_i\big)^2 \end{array}$$

for all $x_i \in [x]_i$ and all $g \in \mathcal{G}_i$, where $\mathcal{G}_i$ is defined by (33).

Remark 5.8 Let $\mathcal{U}$ be a second-order slope tuple for u on $[x]$ with respect to the i-th component. Then, for all $x \in [x]$ we have

$$u(x) \;\in\; U_{x_0} + \delta U \cdot \Big([x]_i - (x_0)_i\Big), \tag{34}$$

$$u(x) \in U_{x_0} + \delta U_{x_0} \cdot \Big([x]_i - (x_0)_i \Big) + \delta_2 U \cdot \Big([x]_i - (x_0)_i \Big)^2. \tag{35}$$

Hence, we have reduced the automatic computation of second-order slope tuples to the one-dimensional case from section 3. Therefore, the same formulas can be used except for Lemma 3.6. We need to modify Lemma 3.6 as follows:

Lemma 5.9 Let $[x] \in \mathbb{IR}^n$, $x_0 \in [x]$, and $i \in \{1, \ldots, n\}$.

a) For each $i \in \{1, \ldots, n\}$, the tuple $\mathcal{K} = (k, k, 0, 0, 0)$ is a second-order slope tuple for the constant function $u : \mathbb{R}^n \to \mathbb{R}$, $u(x) \equiv k \in \mathbb{R}$, on $[x]$ with respect to the i-th component.

b) For $u : \mathbb{R}^n \to \mathbb{R}$, $u(x) = x_k$, a second-order slope tuple on $[x]$ with respect to the i-th component is given by

$$\mathcal{X} = \begin{cases} \big([x]_k, [x]_k, 0, 0, 0 \big), & \text{if } k \neq i, \\ \big([x]_i, (x_0)_i, 1, 1, 0 \big), & \text{if } k = i. \end{cases}$$

Remark 5.10 Using a technique similar to [6, 7], we obtain range enclosures that are sharper than (34) and (35). For a fixed $x_0 \in [x] \subseteq D$ we have

$$\begin{aligned} f\big(x_1, \ldots, x_n\big) - f\big((x_0)_1, \ldots, (x_0)_n \big) \\ = \; & f\big(x_1, \ldots, x_n\big) - f\big((x_0)_1, x_2, \ldots, x_n\big) \\ & + f\big((x_0)_1, x_2, \ldots, x_n\big) - f\big((x_0)_1, (x_0)_2, x_3, \ldots, x_n\big) \\ & + f\big((x_0)_1, (x_0)_2, x_3, \ldots, x_n\big) - + \cdots \\ & + f\big((x_0)_1, \ldots, (x_0)_{n-1}, x_n\big) - f\big((x_0)_1, \ldots, (x_0)_n \big). \end{aligned} \tag{36}$$

for all $x \in [x]$. For each $i \in \{1, \ldots, n\}$, we now compute a second-order slope tuple

$$\mathcal{F}_i := (F_{x;i}, F_{x_0;i}, \delta F_{x_0;i}, \delta F_i, \delta_2 F_i)$$

for the function

$$\begin{aligned} f_i : \big((x_0)_1, \ldots, (x_0)_{i-1}, [x]_i, [x]_{i+1}, \ldots, [x]_n \big) \to \mathbb{R}, \\ f_i(x) := u\big((x_0)_1, \ldots, (x_0)_{i-1}, x_i, x_{i+1}, \ldots, x_n\big) \\ \text{for } x \in \big((x_0)_1, \ldots, (x_0)_{i-1}, [x]_i, [x]_{i+1}, \ldots, [x]_n \big), \end{aligned}$$

on $\big((x_0)_1, \ldots, (x_0)_{i-1}, [x]_i, [x]_{i+1}, \ldots, [x]_n \big)$ with respect to the i-th component.

Then, by (36) we have

$$f(x) \in F_{x;1}, \tag{37}$$

$$f(x) \in F_{x_0;n} + \sum_{j=1}^{n} \delta F_j \cdot \Big([x]_j - (x_0)_j \Big) =: S_{c;1}, \tag{38}$$

$$f(x) \in F_{x_0;n} + \sum_{j=1}^{n} \delta F_{x_0;j} \cdot \Big([x]_j - (x_0)_j \Big) + \sum_{j=1}^{n} \delta_2 F_j \cdot \Big([x]_j - (x_0)_j \Big)^2 =: S_{c;2} \tag{39}$$

for all $x \in [x]$.

Examples

We consider the following examples $f : \mathbb{R}^n \to \mathbb{R}$. Most of them have been considered in [14]:

$$
\begin{aligned}
1.\quad f(x) = {} & \Big(\big(\tfrac{5}{\pi}x_4 - \tfrac{5.1}{4\pi^2}x_4^2 + x_2 - 6\big)^2 + 10\big(1 - \tfrac{1}{8\pi}\big)\cos x_4 + 10 \Big) \cdot x_3^2 \\
& - x_1^5 + x_2 \frac{\sinh(x_5)}{x_6^2 + 1} x_6 - \exp(x_3) \cdot x_5 \\
2.\quad f(x) = {} & 4x_1^2 - 2.1x_1^4 + \frac{1}{3}x_1^6 + x_1x_2 - 4x_2^2 + 4x_2^4 \\
3.\quad f(x) = {} & 100\left(x_2 - x_1^2\right)^2 + (x_1 - 1)^2 \\
4.\quad f(x) = {} & 12x_1^2 - 6.3x_1^4 + x_1^6 + 6x_2(x_2 - x_1) \\
5.\quad f(x) = {} & \sin x_1 + \sin\big(\tfrac{10}{3}x_1\big) + \ln x_1 - 0.84x_1 + 1000x_1x_2^2\exp\left(-x_3^2\right) \\
6.\quad f(x) = {} & (x_1 + \sin x_1)\exp\left(-x_1^2\right) + \ln(x_3)\frac{x_2^2}{x_1}
\end{aligned}
$$

In each example, we take

$$[x] = \big([x]_1, \ldots, [x]_n\big) = \big([4, 4.25], \ldots, [4, 4.25]\big)$$

and $x_0 = \operatorname{mid}[x]$.

Using the technique from section 5, we compute a second-order slope tuple

$$\mathcal{F} = (F_x, F_{x_0}, \delta F_{x_0}, \delta F, \delta_2 F)$$

for f on $[x]$. Then, by (28)-(32) we have

$$f(x) \in F_{x_0} + \delta F^T \cdot ([x] - x_0) =: S_{m;1}$$

and

$$f(x) \in F_{x_0} + \delta F_{x_0}^T \cdot ([x] - x_0) + ([x] - x_0)^T \cdot \delta_2 F \cdot ([x] - x_0) =: S_{m;2}$$

with $F_{x_0} \in \mathbb{IR}$, $\delta F_{x_0}, \delta F \in \mathbb{IR}^n$ and $\delta_2 F \in \mathbb{IR}^{n \times n}$.

We compare the range enclosures $S_{m;1}$ and $S_{m;2}$ with $S_{c;1}$ and $S_{c;2}$ obtained via Remark 5.10.

We obtained the following results:

No.	$S_{m;1}$	$S_{m;2}$	$S_{c;1}$	$S_{c;2}$
1	[-1497.1, -973.01]	[-1494.0, -976.12]	[-1497.9, -972.20]	[-1495.2, -986.94]
2	[1809.5, 2609.1]	[1816.2, 2602.5]	[1809.5, 2609.1]	[1843.0, 2602.5]
3	[13 467, 19 786]	[13 467, 19 786]	[13 467, 19 786]	[13 619, 19 786]
4	[2538.7, 4074.7]	[2558.4, 4055.0]	[2538.7E, 4074.7]	[2619.5, 4055.0]
5	[-2.1275, -1.7755]	[-2.0521, -1.8508]	[-2.1275, -1.7755]	[-2.0499, -1.9322]
6	[5.1531, 6.5377]	[5.1529, 6.5379]	[5.1532, 6.5376]	[5.1647, 6.5357]

Except for the first example, we have $S_{c;1} \subseteq S_{m;1}$ and $S_{c;2} \subseteq S_{m;2}$. Furthermore, for each of the examples $S_{c;2} \subseteq S_{c;1}$ holds.

6 Conclusion

In this paper, we have shown how the automatic computation of second-order slope tuples can be performed. Here, the function expression of the underlying function may contain nonsmooth functions such as $\varphi(x) = |u(x)|$ and $\varphi(x) = \max\{u(x), v(x)\}$. Furthermore, we allow for functions given by two or more branches. Some examples illustrated that second-order slope tuples may provide sharper enclosures of the function range than first-order slope enclosures. Machine interval arithmetic yields verified range enclosures on a floating-point computer. Hence, the automatic computation of second-order slope tuples can also be applied to verified global optimization [22].

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