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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.

Key words. slope tuple, interval analysis, automatic slope computation, range enclosure

AMS subject classifications. 65G20, 65G99

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 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

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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 $[x] = [\underline{x}, \overline{x}] = \{x = (x_i) \in \mathbb{R}^n, \underline{x_i} \le x_i \le \overline{x_i}\}$ 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.

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

Furthermore, by

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

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 $p(x) = \sum_{i=0}^{n} a_i x^i$ be the Hermitian interpolation polynomial for f with respect to the nodes $x_0, \dots, x_n \in D$. Here, exactly $k+1$ elements of $x_0, \dots, x_n$ are equal to x_i, if $f(x_i), \dots, f^{(k)}(x_i)$ 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 $x_0, \dots, x_n$. *Notation:*

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

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 $\delta_n f(x_0, \dots, x_n)$ be the slope of $n-$th order of f with respect to $x_0, \dots, x_n$. Then, the following statements hold:*

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

b) For $x_i \ne x_j$ 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

$$f(x) = \sum_{i=0}^{n-1} \delta_i f(x_0, \dots, x_i) \cdot \omega_i(x) + \delta_n f(x_0, \dots, x_{n-1}, x) \cdot \omega_n(x), \quad n \ge 1. \tag{2.1}$$

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

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

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is continuous.

e) For the nodes $x_0 \le x_1 \le \ldots \le x_n$ 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*

$$f\,(x) = f\,(x_0) + \delta f(x; x_0) \cdot (x - x_0)\,, \quad x \in D, \tag{2.2}$$

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 $x = x_0$, (2.2) is fulfilled for an arbitrary $\delta f(x_0; x_0) \in \mathbb{R}$. If f is differentiable at x_0, then we always set $\delta f(x_0; x_0) := f^{'}(x_0)$. Often, the midpoint 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 (2.2), we have

$$f\,(x) \;\in\; f\,(x_0) + \delta f([x]\,; x_0) \cdot ([x] - x_0) \tag{2.3}$$

for all $x \in [x]$.

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

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

Therefore, (2.3) 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.,

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

with $x_0 = 0$, $[x] = [-1, 1]$. If f is continuous on $[x]$ and differentiable at $x_0 \in [x]$, 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 $\delta f_{\lim}\,([x_0]) \in \mathbb{IR}$ *is*

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

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

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

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

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

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

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

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

$$\delta f_{\lim}\left([x_0]\right)\ \subseteq\ \partial f\left(x_0\right), \tag{2.4}$$

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

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

holds and also a sufficient condition for equality in (2.4).

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

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

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

$$f\left(x\right)\in f\left(x_0\right)+f^{'}\left(x_0\right)\cdot\left(x-x_0\right)+\delta_2 f([x]\,;x_0,x_0)\cdot\left(x-x_0\right)^2,\quad x\in[x]\,, \tag{2.5}$$

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 at x_0, then we set $\delta_2 f(x;x_0) := \frac{1}{2}f^{''}(x_0)$.

REMARK 2.11. Assume that (2.5) holds. Then, we have the enclosure

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

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*

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

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*

$$u(x) \in U_x, \tag{3.1}$$

$$u(x_0) \in U_{x_0}, \tag{3.2}$$

$$\delta u_{\lim}([x_0]) \subseteq \delta U_{x_0}, \tag{3.3}$$

$$u(x) - u(x_0) \in \delta U \cdot (x - x_0), \tag{3.4}$$

$$u(x) - u(x_0) \in \delta U_{x_0} \cdot (x - x_0) + \delta_2 U \cdot (x - x_0)^2, \tag{3.5}$$

for all $x \in [x]$.

REMARK 3.3. Property (3.5) does not imply that $\delta_2 U$ is a second-order slope enclosure in the sense of (2.5) 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 (3.1)-(3.5) we get the enclosures

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

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 (3.4) and (3.5) 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

$$\left\{ \delta\varphi\left(\widetilde{u_{x_0}}; u_{x_0}\right) \mid \widetilde{u_{x_0}} \in U_{x_0}, u_{x_0} \in U_{x_0} \right\}, \tag{3.6}$$

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

$$\left\{ \delta\varphi(u_x; u_{x_0}) \mid u_x \in U_x, u_{x_0} \in U_{x_0} \right\}, \tag{3.7}$$

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

$$\left\{ \delta_2\varphi(u_x; u_{x_0}) \mid u_x \in U_x, u_{x_0} \in U_{x_0} \right\}. \tag{3.8}$$

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 (3.1)-(3.5).*

Proof. The proof of (3.1), (3.2), and (3.4) for $\mathcal{W}$ are analogous to those in [14, 16]. So, we only need to prove (3.3) and (3.5). 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

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

and thus obtain

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

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which is (3.3) 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

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

which proves (3.5).

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 (3.3) for $\mathcal{W} = \varphi(\mathcal{U})$. Because of

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

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 (3.5). □

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 (3.1)-(3.5). 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 $\delta\varphi\left(U_{x_0}; U_{x_0}\right)$, $\delta\varphi\left(U_x; U_{x_0}\right)$, $\delta_2\varphi\left(U_x; U_{x_0}\right) \in \mathbb{IR}$ of (3.6)-(3.8), where φ is twice continuously differentiable. Note that such enclosures exist because the sets (3.6)-(3.8) 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

$$\delta\varphi\left(U_{x_0}; U_{x_0}\right) = \varphi^{'}\left(U_{x_0}\right), \tag{3.9}$$

$$\delta\varphi\left(U_x; U_{x_0}\right) = \varphi^{'}\left(U_x\right), \tag{3.10}$$

and

$$\delta_2\varphi\left(U_x; U_{x_0}\right) = \frac{1}{2}\,\varphi^{''}\left(U_x\right) \tag{3.11}$$

of (3.6)-(3.8). However, for some functions, such as $\varphi\left(x\right) = x^2$ and $\varphi\left(x\right) = \sqrt{x}$, sharper enclosures for (3.7) and (3.8) can be found. By explicit computation of $\delta\varphi\left(u_x; u_{x_0}\right)$ and $\delta_2\varphi\left(u_x; u_{x_0}\right)$ 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 $\varphi : \mathbb{R} \to \mathbb{R}$, $\varphi\left(x\right) = x^2$. Then, we have the enclosures*

$$\delta\varphi\left(u_x; u_{x_0}\right) \;\in\; U_x + U_{x_0},$$

$$\delta_2\varphi\left(u_x; u_{x_0}\right) \;\in\; [1, 1]$$

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* $\inf\left(U_x\right) \geq 0$ *and* $\inf\left(U_{x_0}\right) > 0$. *Furthermore, let $\varphi : \mathbb{R}_{\geq 0} \to \mathbb{R}$, $\varphi\left(x\right) = \sqrt{x}$. Then, for all $u_x \in U_x$ and all $u_{x_0} \in U_{x_0}$ we have*

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

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

Furthermore, by exploiting convexity or concavity of φ and $\varphi^{'}$ we can get sharper enclosures for (3.7) and (3.8) than by (3.10) and (3.11). The formulas and the proofs can be found in [9] and [16]. Moreover, exploiting a unique point of inflection of φ or $\varphi^{'}$ may also give sharper enclosures for (3.7) or (3.8) than (3.10) or (3.11). This applies to functions such as $\varphi\left(x\right) = \sinh x$, $\varphi\left(x\right) = \cosh x$, etc. We omit the details of these formulas and refer to [20].

REMARK 3.12. Let f be twice continuously differentiable and

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

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 (3.5). Hence, by (2.5), $\delta_2 F$ 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.

3.1. 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

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

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

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

where

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

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

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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. $w(x) = \max\{u(x), v(x)\}$:
We define the evaluation of the max-function for two intervals $[a]$ and $[b]$ by

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

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

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

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

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

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 $\mathcal{W} = \varphi(\mathcal{U}) = abs(\mathcal{U})$ 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 (3.1), (3.2), and (3.4) for $\mathcal{W}$ can be found in [14]. Therefore, we only need to check (3.3) and (3.5).

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1. $w(x) = \varphi(u(x)) = |u(x)|$:
We prove (3.3). 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

$$\delta w_{\,\mathrm{lim}}\,([x_0]) \subseteq \delta W_{x_0}.$$

Next, we prove (3.5).
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

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

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

$$0 \;\leq\; \frac{2\,u(x)}{\big(u(x) - u(x_0)\big)^2} \;\leq\; \frac{2\,u(x)}{\big(u(x) - \overline{u_{x_0}}\big)^2}. \tag{3.12}$$

By computing the maximum of the right expression in (3.12) 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

$$\frac{2\,u(x)}{\big(u(x) - u(x_0)\big)^2} \;\in\; \left[0,\; -\frac{1}{2\,\overline{u_{x_0}}}\right]. \tag{3.13}$$

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

$$
\begin{aligned}
w(x) - w(x_0) \quad &\in \quad -\delta U_{x_0} \cdot (x - x_0) + \Big(\delta\varphi\,(U_x; U_{x_0}) \cdot \delta_2 U \\
&\qquad + \left[0,\ -\frac{1}{2\,\overline{u_{x_0}}}\right] \cdot \delta U_{x_0} \cdot \delta U\Big) \cdot (x - x_0)^2
\end{aligned}
\tag{3.14}
$$

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, (3.14) 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 (3.13), we get

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

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

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

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 (3.3) and (3.5) 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 (3.3). Next, we prove (3.5).

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

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

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and therefore,

$$w(x) - w(x_0) \in (\delta U_{x_0} \,\underline{\cup}\, \delta V_{x_0}) \cdot (x - x_0) + (\delta_2 U \,\underline{\cup}\, \delta_2 V) \cdot (x - x_0)^2 \tag{3.15}$$

holds. Clearly, (3.15) also holds, if

$$\max\{u(x), v(x)\} = u(x) \quad \text{and} \quad \max\{u(x_0), v(x_0)\} = u(x_0).$$

Analogously, (3.15) is fulfilled, if u and v are interchanged. Therefore, we get (3.5). □

3.2. 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 ite : $\mathbb{R}^3 \longrightarrow \mathbb{R}$ ("if-then-else").

DEFINITION 3.14. *ite* : $\mathbb{R}^3 \longrightarrow \mathbb{R}$ *is the function*

$$ite(z, u, v) := \begin{cases} u & \text{if } z < 0 \\ v & \text{otherwise.} \end{cases} \tag{3.16}$$

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

$$w(x) = \mathrm{ite}\big(z(x), u(x), v(x)\big). \tag{3.17}$$

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*

$$ite\big([z], [u], [v]\big) := \begin{cases} [u] & \text{if } \overline{z} < 0 \\ [v] & \text{if } \underline{z} \geq 0 \\ [u] \,\underline{\cup}\, [v] & \text{otherwise.} \end{cases} \tag{3.18}$$

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* $w(x) = ite\big(z(x), u(x), v(x)\big)$ *be continuous on* $[x]$. *We define the 5-tuple* $\mathcal{W} = ite(\mathcal{Z}, \mathcal{U}, \mathcal{V})$

by

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

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

Proof. See [22] and [23]. □

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

$$S_1 := F_{x_0} + \delta F \cdot ([x] - x_0) \tag{4.1}$$

and

$$S_2 := F_{x_0} + \delta F_{x_0} \cdot ([x] - x_0) + \delta_2 F \cdot ([x] - x_0)^2 \tag{4.2}$$

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

$$D_1 := f(x_0) + f^{'}([x]) \cdot ([x] - x_0) \tag{4.3}$$

and

$$D_2 := f(x_0) + f^{'}(x_0) \cdot ([x] - x_0) + \frac{1}{2} f^{''}([x]) \cdot ([x] - x_0)^2 . \tag{4.4}$$

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 (3.1)-(3.5) are preserved. Hence, by applying machine interval arithmetic, we obtain verified range enclosures.

We consider the following examples:

1. $f(x) = (x + \sin x) \cdot \exp(-x^2)$
2. $f(x) = x^4 - 10x^3 + 35x^2 - 50x + 24$
3. $f(x) = \left(\ln(x + 1.25) - 0.84x\right)^2$
4. $f(x) = \frac{2}{100}x^2 - \frac{3}{100}\exp\left(-\left(20(x - 0.875)\right)^2\right)$
5. $f(x) = \exp(x^2)$
6. $f(x) = x^4 - 12x^3 + 47x^2 - 60x - 20\exp(-x)$
7. $f(x) = x^6 - 15x^4 + 27x^2 + 250$
8. $f(x) = \left(\arctan(|x - 1|)\right)^2 / \left(x^6 - 2x^4 + 20\right)$
9. $f(x) = \max\left\{\exp(-x), \sin\left(|x - 1|\right)\right\}$
10. $f(x) = \mathrm{ite}\left(x - 1,\ x^4 - 1 + \sin(x - 1),\ \left|x^2 - \frac{5}{2}x + \frac{3}{2}\right|\right)$
11. $f(x) = \left|(x - 1)\left(x^2 + x + 5\right)\right| \cdot \exp\left((x - 2)^2\right)$
12. $f(x) = \max\left\{x^5 - x^2 + x,\ \exp(x) \cdot (x - 1) + 1\right\}$
13. $f(x) = \mathrm{ite}\Big(x - 1,\ (x - 1) \cdot \arctan x \cdot \exp(x + \sin x),$ $\left|\left(x^2 - \frac{5}{2}x + \frac{3}{2}\right) \cdot \sin x\right|\Big)$

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 results in Table 4.1. 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.

TABLE 4.1
Range enclosure for examples 1-13

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]

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*

$$u(x) \in U_x, \tag{5.1}$$

$$u(x_0) \in U_{x_0}, \tag{5.2}$$

$$\delta u_{\lim}([x_0]) \subseteq \delta U_{x_0}, \tag{5.3}$$

$$u(x) - u(x_0) \in \delta U^T \cdot (x-x_0), \tag{5.4}$$

$$u(x) - u(x_0) \in \delta U_{x_0}^T \cdot (x-x_0) + (x-x_0)^T \cdot \delta_2 U \cdot (x-x_0) \tag{5.5}$$

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) $\mathcal{X} = \left([x]_i, (x_0)_i, e^i, e^i, 0\right)$ *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.*

REMARK 5.6. 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].

5.1. 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 5.7. *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*

$$\mathcal{G}_i := \left\{ \begin{array}{l} g : [x]_i \subseteq \mathbb{R} \to \mathbb{R}, \quad g(t) := u(x_1,\ldots,x_{i-1},t,x_{i+1},\ldots,x_n) \\ \text{with } x_j \in [x]_j \text{ fixed for } j \in \{1,\ldots,n\},\ j \neq i. \end{array} \right\} \tag{5.6}$$

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 5.8. *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 (5.6).*

REMARK 5.9. 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

$$u\,(x) \;\in\; U_{x_0} + \delta U \cdot \Big(\,[x]_i - (x_0)_i\Big) \tag{5.7}$$

and

$$u\,(x) \;\in\; U_{x_0} + \delta U_{x_0} \cdot \Big(\,[x]_i - (x_0)_i\Big) + \delta_2 U \cdot \Big(\,[x]_i - (x_0)_i\Big)^2. \tag{5.8}$$

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 5.10. *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*

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

REMARK 5.11. Using a technique similar to [6, 7], we obtain range enclosures that are sharper than (5.7) and (5.8). For a fixed $x_0 \in [x] \subseteq D$ we have

$$\begin{aligned} & f\big(x_1, \ldots, x_n\big) - f\big(\,(x_0)_1\,, \ldots, (x_0)_n\,\big) \\ &\quad = \; f\big(x_1, \ldots, x_n\big) - f\big(\,(x_0)_1\,, x_2, \ldots, x_n\big) \\ &\qquad + f\big(\,(x_0)_1\,, x_2, \ldots, x_n\big) - f\big(\,(x_0)_1\,, (x_0)_2\,, x_3, \ldots, x_n\big) \\ &\qquad + f\big(\,(x_0)_1\,, (x_0)_2\,, x_3, \ldots, x_n\big) - + \cdots \\ &\qquad + f\big(\,(x_0)_1\,, \ldots, (x_0)_{n-1}\,, x_n\big) - f\big(\,(x_0)_1\,, \ldots, (x_0)_n\,\big). \end{aligned} \tag{5.9}$$

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

$$f_i : \big(\,(x_0)_1\,, \ldots, (x_0)_{i-1}\,, [x]_i\,, [x]_{i+1}\,, \ldots, [x]_n\,\big) \to \mathbb{R},$$

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

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 (5.9) we have

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

for all $x \in [x]$.

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

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

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 Remark 5.6, 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 $[x]$, as introduced in Definition 5.4. Then, by (5.1)-(5.5) 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 $\delta_2 F \in \mathbb{IR}^{n\times n}$.

In Table 5.1, we compare the range enclosures $S_{m;1}$ and $S_{m;2}$ with $S_{c;1}$ and $S_{c;2}$ obtained via Remark 5.11. 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.

TABLE 5.1
Comparison of range enclosures $S_{m;1}$ and $S_{m;2}$ with $S_{c;1}$ and $S_{c;2}$.

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

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 [21, 22].

REFERENCES

[1] G. ALEFELD AND J. HERZBERGER, *Introduction to Interval Computations*, Academic Press, New York, 1983.
[2] F. H. CLARKE, *Optimization and Nonsmooth Analysis*, John Wiley & Sons, New York, 1983.
[3] P. DEUFLHARD AND A. HOHMANN, *Numerical Analysis*, de Gruyter, Berlin, 1995.
[4] A. FROMMER, B. LANG, AND M. SCHNURR, *A comparison of the Moore and Miranda existence tests*, Computing, 72 (2004), pp. 349–354.
[5] A. GOLDSZTEJN, *Comparison of the Hansen-Sengupta and the Frommer-Lang-Schnurr existence tests*, Computing, 79 (2007), pp. 53–60.
[6] E. R. HANSEN, *Interval forms of Newton's method*, Computing, 20 (1978), pp. 153–163.
[7] E. R. HANSEN AND G. W. WALSTER, *Global Optimization Using Interval Analysis*, Second Ed., Revised and Expanded, Marcel Dekker, New York, 2004.
[8] R. B. KEARFOTT, *Rigorous Global Search: Continuous Problems*, Kluwer Academic Publishers, Dordrecht, 1996.
[9] L. KOLEV, *Use of interval slopes for the irrational part of factorable functions*, Reliab. Comput., 3 (1997), pp. 83–93.
[10] R. KRAWCZYK AND A. NEUMAIER, *Interval slopes for rational functions and associated centered forms*, SIAM J. Numer. Anal., 22 (1985), pp. 604–616.
[11] R. E. MOORE, *A test for existence of solutions to nonlinear systems*, SIAM J. Numer. Anal., 14 (1977), pp. 611–615.
[12] H. MUÑOZ AND R. B. KEARFOTT, *Slope intervals, generalized gradients, semigradients, slant derivatives, and csets*, Reliab. Comput., 10 (2004), pp. 163–193.
[13] L. B. RALL, *Automatic Differentiation: Techniques and Applications*, Lecture Notes in Comput. Sci., Vol. 120, Springer, Berlin, 1981.
[14] D. RATZ, *Automatic Slope Computation and its Application in Nonsmooth Global Optimization*, Shaker Verlag, Aachen, 1998.

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[15] ———, *A nonsmooth global optimization technique using slopes – the one-dimensional case*, J. Global Optim., 14 (1999), pp. 365–393.

[16] S. M. RUMP, *Expansion and estimation of the range of nonlinear functions*, Math. Comp., 65 (1996), pp. 1503–1512.

[17] U. SCHÄFER AND M. SCHNURR, *A comparison of simple tests for accuracy of approximate solutions to nonlinear systems with uncertain data*, J. Ind. Manag. Optim., 2 (2006), pp. 425–434.

[18] M. SCHNURR, *Webpage for software download*. http://iamlasun8.mathematik.uni-karlsruhe.de/~ae26/software/.

[19] ———, *On the proofs of some statements concerning the theorems of Kantorovich, Moore, and Miranda*, Reliab. Comput., 11 (2005), pp. 77–85.

[20] ———, *Computing slope enclosures by exploiting a unique point of inflection*, to appear in Appl. Math. Comput.

[21] ———, *A second-order pruning step for verified global optimization*, to appear in J. Global Optim.

[22] ———, *Steigungen höherer Ordnung zur verifizierten globalen Optimierung*, PhD thesis, Department of Mathematics, Universität Karlsruhe, 2007. http://digbib.ubka.uni-karlsruhe.de/volltexte/1000007229.

[23] M. SCHNURR AND D. RATZ, *Slope enclosures for functions given by two or more branches*, submitted for publication.

[24] Z. SHEN AND M. A. WOLFE, *On interval enclosures using slope arithmetic*, Appl. Math. Comput., 39 (1990), pp. 89–105.

[25] XSC WEBSITE, *Website on programming languages for scientific computing with validation*. http://www.xsc.de [December 2007].