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Computing Slope Enclosures by Exploiting a Unique Point of Inflection*

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Abstract

Using slope enclosures may provide sharper bounds for the range of a function than using enclosures of the derivative. Hence, slope enclosures may be useful in verifying the assumptions for existence tests or in algorithms for global optimization. Previous papers by Kolev and Ratz show how to compute slope enclosures for convex and concave functions. In this paper, we generalize these formulas and show how to obtain slope enclosures for a function that has exactly one point of inflection or whose derivative has exactly one point of inflection.

1 Introduction

Many algorithms require an enclosure for the range of a function $f : D \subset \mathbb{R}^n \to \mathbb{R}$ on an interval $[x]$. For this purpose, the mean value form [9] using an interval enclosure of the derivative f' is a well-known tool. Sharper enclosures of the range of f can be obtained by using slope enclosures. Slopes and slope enclosures have various applications, for example in existence tests [3, 4, 10, 14, 15] or in global optimization [5, 6, 12, 13, 16, 17].

Using interval analysis [1, 9], slope enclosures for factorable functions can be computed by a technique analogous to automatic differentiation [11]. This technique is due to Krawczyk and Neumaier [8], and it was extended to second-order slopes by Shen and Wolfe [18]. These approaches require slope enclosures for elementary functions $\varphi : D \subseteq \mathbb{R} \to \mathbb{R}$. First-order slope enclosures for some elementary functions are given by Ratz [12]. Kolev [7] shows how to compute first-order slope enclosures if φ is convex or concave, and how to compute second-order slope enclosures if φ' is convex or concave. For other elementary functions, however, enclosures of the derivatives are used as slope enclosures.

In this paper, we show how first-order slope enclosures can be computed for some elementary functions that have exactly one point of inflection, and how second-order slope enclosures can be computed for some elementary functions φ whose derivative has exactly one point of inflection. The formulas of the present paper provide sharper bounds

*This paper contains and extends some results from the author's dissertation [17].

than enclosures of the respective derivatives. Therefore, they improve the enclosures used in [7, 12, 18]. The slope enclosures given in this paper can be used both for automatic computation of slope enclosures and for theoretical aspects.

Throughout this paper, $[x] \in \mathbb{IR}$ denotes a compact interval, $\mathbb{IR}$ being the set of all compact intervals $[x] \subset \mathbb{R}$.

2 Slopes and Slope Enclosures

Definition 2.1 Let $\varphi : D \subseteq \mathbb{R} \to \mathbb{R}$, $\varphi \in C^n(D)$. Furthermore, let $p(x) = \sum_{i=0}^{n} a_i x^i$ be the Hermitian interpolation polynomial for φ 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 $\varphi(x_i), \ldots, \varphi^{(k)}(x_i)$ are given for some node x_i. The leading coefficient a_n of p is called the *slope of n-th order of φ with respect to* $x_0, \ldots, x_n$. Notation:

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

For details, see [2].

Some properties of slopes are given in the following theorem. The statements d) and e) in Theorem 2.2 are easy consequences of the Hermite-Genocchi Theorem (see, e.g., [2]).

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

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

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

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

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

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

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

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

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

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

Definition 2.3 Let $\varphi : D \subseteq \mathbb{R} \to \mathbb{R}$, $\varphi \in C^1(D)$, and let $x_0 \in D$ be fixed. A function $\delta\varphi : D \to \mathbb{R}$ satisfying

$$\varphi(x) = \varphi(x_0) + \delta\varphi(x; x_0) \cdot (x - x_0), \quad x \in D, \tag{1}$$

is called a *first-order slope function of* φ *with respect to* x_0. We set $\delta\varphi(x_0;x_0) := \varphi^{'}(x_0)$.

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

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

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

Remark 2.4 Let $\delta\varphi([x]\,;x_0) \in \mathbb{IR}$ be a first-order slope enclosure of φ on $[x]$. Then, the range of φ on $[x]$ is enclosed by

$$\varphi(x) \in \varphi(x_0) + \delta\varphi([x]\,;x_0) \cdot ([x] - x_0)\,, \quad x \in [x]\,.$$

Definition 2.5 Let $\varphi : D \subseteq \mathbb{R} \to \mathbb{R}$, $\varphi \in C^2(D)$, and let $x_0, x_1 \in D$ fixed. A function $\delta_2\varphi : D \to \mathbb{R}$ satisfying

$$\varphi(x) = \varphi(x_0) + \delta\varphi(x_1, x_0) \cdot (x - x_0) + \delta_2\varphi(x; x_1, x_0) \cdot (x - x_0) \cdot (x - x_1)\,, \ \ x \in D,$$

is called a *second-order slope function of* φ *with respect to* x_0 *and* x_1. As in [7] and [18], we only consider the case $x_1 = x_0$ in this paper, and as an abbreviation we set $\delta_2\varphi(x;x_0) = \delta_2\varphi(x;x_0,x_0)$. Furthermore, we set $\delta_2\varphi(x_0;x_0) := \frac{1}{2}\,\varphi^{''}(x_0)$.

An interval $\delta_2\varphi([x]\,;x_0) \in \mathbb{IR}$ satisfying

$$\delta_2\varphi([x]\,;x_0) \supseteq \{\delta_2\varphi(x;x_0) \mid x \in [x]\}$$

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

Remark 2.6 Let $\delta_2\varphi([x]\,;x_0) \in \mathbb{IR}$ be a second-order slope enclosure of φ on $[x]$. Then, the range of φ on $[x]$ is enclosed by

$$\varphi(x) \in \varphi(x_0) + \varphi^{'}(x_0) \cdot ([x] - x_0) + \delta\varphi([x]\,;x_0) \cdot ([x] - x_0)^2\,, \quad x \in [x]\,.$$

Let $\varphi : D \subseteq \mathbb{R} \to \mathbb{R}$ be a twice continuously differentiable elementary function, and let $[x_0] \subseteq [x] \subseteq D$. Furthermore, let $f : \mathbb{R}^n \to \mathbb{R}$ be a function given by a function expression containing φ. In order to perform automatic computation of a slope enclosure of f on a floating-point computer using interval arithmetic (cf. [12]) we need enclosures of

$$\left\{\delta\varphi(x;x_0) \mid x \in [x]\,, x_0 \in [x_0]\,\right\} \tag{2}$$

and

$$\left\{\delta_2\varphi(x;x_0) \mid x \in [x]\,, x_0 \in [x_0]\,\right\}. \tag{3}$$

Obviously, we have

$$\Big\{\delta\varphi(x;x_0) \mid x \in [x]\,, x_0 \in [x_0]\,\Big\} \subseteq \Big\{\varphi^{'}(x) \mid x \in [x]\Big\}$$

and

$$\Big\{\delta_2\varphi(x;x_0) \mid x \in [x]\,, x_0 \in [x_0]\,\Big\} \subseteq \left\{\frac{1}{2}\,\varphi^{''}(x) \mid x \in [x]\right\}.$$

Hence, (2) and (3) can be enclosed by using enclosures of the first and second derivative, respectively. However, often sharper enclosures of (2) and (3) can be found, see [7] and [12]. Kolev [7] shows how enclosures of (2) and (3) can be computed by using convexity or concavity of φ and φ', respectively. In the next section, we restate these theorems. Theorem 3.2 is a slight generalization of [7] because we include the case $x_0 \neq x_1$ and we allow intervals $[x_0]$ and $[x_1]$ instead of real values x_0 and x_1. In section 4, we show how slope enclosures can be computed by exploiting a unique point of inflection. The formulas of section 4 provide sharper bounds for (2) and (3) than using the first and second derivative, respectively. Some examples in section 5 illustrate this.

3 Computing Slope Enclosures by Exploiting Convexity and Concavity

In this section, we show how slope enclosures can be computed by exploiting convexity or concavity of φ and φ', respectively.

Theorem 3.1 Let $\varphi : D \subseteq \mathbb{R} \to \mathbb{R}$ be twice continuously differentiable on the interval $[x] = [\,\underline{x}, \overline{x}\,] \subseteq D$ and let $[x_0] = \left[\,\underline{x_0}, \overline{x_0}\,\right] \subseteq [x]$.

If $\varphi''(x) \geq 0$, $x \in [x]$, i.e. if φ is convex on $[x]$, then

$$\delta\varphi\left(\underline{x}; \underline{x_0}\right) \leq \delta\varphi\left(x; x_0\right) \leq \delta\varphi\left(\overline{x}; \overline{x_0}\right) \tag{4}$$

holds for all $x \in [x]$, $x_0 \in [x_0]$.

If $\varphi''(x) \leq 0$, $x \in [x]$, i.e. if φ is concave on $[x]$, then

$$\delta\varphi\left(\underline{x}; \underline{x_0}\right) \geq \delta\varphi\left(x; x_0\right) \geq \delta\varphi\left(\overline{x}; \overline{x_0}\right) \tag{5}$$

holds for all $x \in [x]$, $x_0 \in [x_0]$.

Proof: See [7, 12]. □

The following theorem is an easy generalization of a theorem of Kolev [7], which treats the case $x_1 = x_0$.

Theorem 3.2 Let $\varphi : D \subseteq \mathbb{R} \to \mathbb{R}$ be three times continuously differentiable and let $[x_0] = \left[\,\underline{x_0}, \overline{x_0}\,\right] \subseteq [x]$ and $[x_1] = \left[\,\underline{x_1}, \overline{x_1}\,\right] \subseteq [x]$.

If $\varphi'''(x) \geq 0$, $x \in [x]$, i.e. if φ' is convex on $[x]$, then

$$\delta_2\varphi\left(\underline{x}; \underline{x_1}, \underline{x_0}\right) \leq \delta_2\varphi\left(x; x_1, x_0\right) \leq \delta_2\varphi\left(\overline{x}; \overline{x_1}, \overline{x_0}\right) \tag{6}$$

holds for all $x \in [x]$, $x_1 \in [x_1]$ and $x_0 \in [x_0]$.

If $\varphi'''(x) \leq 0$, $x \in [x]$, i.e. if φ' is concave on $[x]$, then

$$\delta_2\varphi\left(\underline{x}; \underline{x_1}, \underline{x_0}\right) \geq \delta_2\varphi\left(x; x_1, x_0\right) \geq \delta_2\varphi\left(\overline{x}; \overline{x_1}, \overline{x_0}\right) \tag{7}$$

holds for all $x \in [x]$, $x_1 \in [x_1]$ and $x_0 \in [x_0]$.

Proof: We prove (6). Consider $g : [x] \times [x_1] \times [x_0] \to \mathbb{R}$ defined by

$$g\left(x, x_1, x_0\right) \quad := \quad \delta_2\varphi\left(x; x_1, x_0\right).$$

By Theorem 2.2, we have

$$\begin{aligned}
\frac{\partial g\left(x, x_1, x_0\right)}{\partial x} &= \lim_{\tilde{x} \to x} \frac{\delta_2\varphi\left(\tilde{x}; x_1, x_0\right) - \delta_2\varphi\left(x; x_1, x_0\right)}{\tilde{x} - x} \\
&= \lim_{\tilde{x} \to x} \delta_3\varphi\left(x; \tilde{x}, x_1, x_0\right) \\
&= \delta_3\varphi\left(x; x, x_1, x_0\right).
\end{aligned}$$

Because of

$$\delta_3\varphi\,(x;x,x_1,x_0) \;=\; \frac{1}{6}\,\varphi'''(\xi) \;\geq\; 0, \qquad \xi \in [x]\,,$$

$g\,(x,x_1,x_0)$ increases monotonically with respect to x.

By Theorem 2.2 a), $g\,(x,x_1,x_0)$ increases monotonically with respect to x_1, if x and x_0 are fixed, and $g\,(x,x_1,x_0)$ increases monotonically with respect to x_0, if x and x_1 are fixed. Hence, we obtain (6).

The proof of (7) is analogous. □

As a corollary we obtain the theorem from Kolev [7]:

Theorem 3.3 Let $\varphi : D \subseteq \mathbb{R} \to \mathbb{R}$ be three times continuously differentiable on $[x] \subseteq D$ and let $[x_0] = \left[\,\underline{x_0}, \overline{x_0}\,\right] \subseteq [x]$.

If $\varphi'''(x) \geq 0$, $x \in [x]$, i.e. if φ' is convex on $[x]$, then we have

$$\delta_2\varphi\left(\underline{x};\underline{x_0}\right) \leq \delta_2\varphi\,(x;x_0) \leq \delta_2\varphi\,(\overline{x};\overline{x_0}) \tag{8}$$

for all $x \in [x]$, $x_0 \in [x_0]$.

If $\varphi'''(x) \leq 0$, $x \in [x]$, i.e. if φ' is concave on $[x]$, then we have

$$\delta_2\varphi\left(\underline{x};\underline{x_0}\right) \geq \delta_2\varphi\,(x;x_0) \geq \delta_2\varphi\,(\overline{x};\overline{x_0}) \tag{9}$$

for all $x \in [x]$, $x_0 \in [x_0]$.

Proof: The claim follows directly from Theorem 3.2, because

$$g : [x] \times [x_1] \times [x_0] \to \mathbb{R}, \qquad g\,(x,x_1,x_0) := \delta_2\varphi\,(x;x_1,x_0)\,,$$

is continuous by Theorem 2.2. □

4 Computing Slope Enclosures by Exploiting a Unique Point of Inflection

In this section, we set

$$\begin{aligned}
m_1 \;&:=\; \min\left\{\delta\varphi\left(\underline{x};\underline{x_0}\right), \delta\varphi\,(\overline{x};\overline{x_0})\right\}, \\
M_1 \;&:=\; \max\left\{\delta\varphi\left(\underline{x};\underline{x_0}\right), \delta\varphi\,(\overline{x};\overline{x_0})\right\}, \\
m_2 \;&:=\; \min\left\{\delta_2\varphi\left(\underline{x};\underline{x_0}\right), \delta_2\varphi\,(\overline{x};\overline{x_0})\right\}, \\
M_2 \;&:=\; \max\left\{\delta_2\varphi\left(\underline{x};\underline{x_0}\right), \delta_2\varphi\,(\overline{x};\overline{x_0})\right\}.
\end{aligned}$$

Ratz [12] gives a formula that provides a first-order slope enclosure for $\varphi\,(x) = x^n$, $n \in \mathbb{N}$ odd. The following theorem generalizes this by exploiting a unique point of inflection of φ. It also applies, e.g., to $\varphi\,(x) = \sinh x$.

Theorem 4.1 Let $\varphi : D \subseteq \mathbb{R} \to \mathbb{R}$ be twice continuously differentiable on $[x] \subseteq D$ and let $[x_0] = \left[\underline{x_0}, \overline{x_0}\right] \subseteq [x]$. Furthermore, let $\varphi^{'}(x) \geq 0$ on $[x]$, $\varphi^{''}(x) \leq 0$ on $\{x \in [x] \mid x \leq 0\}$, and $\varphi^{''}(x) \geq 0$ on $\{x \in [x] \mid x \geq 0\}$. Set

$$\delta\varphi\left([x]\,;[x_0]\right) = \begin{cases} \left[\delta\varphi\left(\underline{x};\underline{x_0}\right), \delta\varphi\left(\overline{x};\overline{x_0}\right)\right] & \text{if } \underline{x} \geq 0, \\ \left[\delta\varphi\left(\overline{x};\overline{x_0}\right), \delta\varphi\left(\underline{x};\underline{x_0}\right)\right] & \text{if } \overline{x} \leq 0, \\ \left[\max\left\{\dfrac{\varphi(0) - \varphi\left(\overline{x_0}\right)}{\overline{x} - \overline{x_0}}, \varphi^{'}(0)\right\},\ M_1\right] & \text{if } \underline{x} \leq \overline{x_0} < 0 < \overline{x}, \\ \left[\max\left\{\dfrac{\varphi(0) - \varphi\left(\underline{x_0}\right)}{\underline{x} - \underline{x_0}}, \varphi^{'}(0)\right\},\ M_1\right] & \text{if } \underline{x} < 0 < \underline{x_0} \leq \overline{x}, \\ \left[\varphi^{'}(0),\ M_1\right] & \text{if } 0 \in [x] \ \wedge\ 0 \in [x_0]\,. \end{cases}$$

Then, we have the enclosure

$$\delta\varphi\left([x]\,;[x_0]\right) \ \supseteq\ \left\{\delta\varphi\left(x;x_0\right) \mid x \in [x]\,, x_0 \in [x_0]\ \right\}. \tag{10}$$

Proof. Let $x \in [x]$ and $x_0 \in [x_0]$.

If $\underline{x} \geq 0$, then φ is convex on $[x]$. Therefore, we can apply Theorem 3.1 and obtain (10). If $\overline{x} \leq 0$, then φ is concave on $[x]$, and by Theorem 3.1 we have (10).

Next, we prove the enclosure (10) for the remaining three cases. We begin by proving $\delta\varphi\left(x;x_0\right) \leq M_1$ in three steps:

i) Suppose $x \leq 0$ and $x_0 \leq 0$. By Theorem 3.1 we have $\delta\varphi\left(x;x_0\right) \leq \delta\varphi\left(\underline{x};\underline{x_0}\right)$, because φ is concave on $\{x \in [x] \mid x \leq 0\}$. Analogously, $\delta\varphi\left(x;x_0\right) \leq \delta\varphi\left(\overline{x};\overline{x_0}\right)$ holds for all $x \geq 0$, $x_0 \geq 0$.

ii) Suppose $\underline{x_0} < 0$. We prove that $\delta\varphi\left(x;x_0\right) \leq M_1$ holds for all $x \geq 0$, $x_0 \leq 0$.

First, for all $x_0 \leq 0$ and all $x \in [x]$ with $\varphi^{'}(x) \leq \varphi^{'}\left(\underline{x_0}\right)$ we have

$$\begin{aligned} \delta\varphi\left(x;x_0\right) &= \varphi^{'}(\xi)\,, \qquad \xi \text{ between } x_0 \text{ and } x, \\ &\leq \varphi^{'}\left(\underline{x_0}\right) \\ &= \delta\varphi\left(\underline{x_0};\underline{x_0}\right) \end{aligned} \tag{11}$$

by Theorem 2.2. Hence, by i) we obtain

$$\delta\varphi\left(x;x_0\right) \leq \delta\varphi\left(\underline{x};\underline{x_0}\right) \tag{12}$$

for all $x_0 \leq 0$ and all $x \in [x]$ with $\varphi^{'}(x) \leq \varphi^{'}\left(\underline{x_0}\right)$.

Now, we consider an arbitrary $\tilde{x}_0 \leq 0$, $\tilde{x}_0 \in [x_0]$, and an arbitrary $\tilde{x} > 0$, $\tilde{x} \in [x]$, with $\varphi^{'}(\tilde{x}) > \varphi^{'}\left(\underline{x_0}\right)$. By (11) and by $\varphi^{''}(x) \geq 0$ on $\{x \in [x] \mid x \geq 0\}$, we get $\varphi^{'}(x) \geq \varphi^{'}(\xi)$ for all $x \geq \tilde{x}$ and all $\xi \in [\tilde{x}_0, x]$. Hence, we obtain

$$\frac{\partial\left(\delta\varphi\left(x;\tilde{x}_0\right)\right)}{\partial x} = \frac{\varphi^{'}(x) - \dfrac{\varphi(x) - \varphi\left(\tilde{x}_0\right)}{x - \tilde{x}_0}}{x - \tilde{x}_0} \ \geq\ 0$$

for all $x \geq \tilde{x}$. Therefore, $\delta\varphi(x; \tilde{x}_0)$ increases monotonically for $x \geq \tilde{x}$ with respect to x. Thus, we have

$$\delta\varphi(\tilde{x}; \tilde{x}_0) \leq \delta\varphi(\overline{x}; \tilde{x}_0). \tag{13}$$

On the one hand, if $\delta\varphi(\overline{x}; \tilde{x}_0) \leq \varphi^{'}(\tilde{x}_0)$, then by (i) we get

$$\delta\varphi(\tilde{x}; \tilde{x}_0) \; \leq \; \varphi^{'}(\tilde{x}_0) \; \leq \; \delta\varphi\left(\underline{x}; \underline{x_0}\right).$$

On the other hand, if $\delta\varphi(\overline{x}; \tilde{x}_0) > \varphi^{'}(\tilde{x}_0)$, then for the function $g : [\tilde{x}_0, 0] \to \mathbb{R}$, $g(t) = \delta\varphi(\overline{x}; t)$ we have

$$\begin{aligned} g^{'}(t) = \frac{\partial\left(\delta\varphi(\overline{x}; t)\right)}{\partial t} &= \frac{-\varphi^{'}(t) + \delta\varphi(\overline{x}; t)}{\overline{x} - t} \\ &\geq \frac{-\varphi^{'}(\tilde{x}_0) + g(t)}{\overline{x} - t} \end{aligned}$$

and

$$g^{'}(\tilde{x}_0) \; > \; 0.$$

Thus, g increases monotonically on $[\tilde{x}_0, 0]$, and we obtain

$$\delta\varphi(\overline{x}; \tilde{x}_0) \leq \begin{cases} \delta\varphi(\overline{x}; \overline{x_0}), & \text{if } \overline{x_0} \leq 0, \\ \delta\varphi(\overline{x}; 0), & \text{if } \overline{x_0} > 0. \end{cases}$$

Using (13) and i), we get

$$\delta\varphi(\tilde{x}; \tilde{x}_0) \quad \leq \quad \delta\varphi(\overline{x}; \overline{x_0}) \tag{14}$$

for all $\tilde{x}_0 \leq 0$, $\tilde{x}_0 \in [x_0]$, and all $\tilde{x} > 0$, $\tilde{x} \in [x]$, with $\varphi^{'}(\tilde{x}) > \varphi^{'}\left(\underline{x_0}\right)$. Hence, by (12) and (14) we have $\delta\varphi(x; x_0) \leq M_1$ for all $x \geq 0$ and all $x_0 \leq 0$.

iii) The proof for the case $\overline{x_0} > 0$ is analogous to ii), and we obtain that $\delta\varphi(x; x_0) \leq M_1$ holds for all $x \leq 0$, $x_0 \geq 0$.

By i)-iii) we have shown that

$$\delta\varphi(x; x_0) \quad \leq \quad \max\left\{\delta\varphi\left(\underline{x}; \underline{x_0}\right), \delta\varphi(\overline{x}; \overline{x_0})\right\} \; = \; M_1$$

holds for all $x \in [x]$ and all $x_0 \in [x_0]$.

Finally, we complete the proof by showing that the lower bounds for (10) given in the theorem hold for the remaining three cases:

- First, we have

  $$\delta\varphi(x; x_0) = \varphi^{'}(\xi) \geq \varphi^{'}(0). \tag{15}$$

  If $0 \in [x_0]$, then the lower bound of $\left\{\delta\varphi(x; x_0) \mid x \in [x], x_0 \in [x_0]\right\}$ is $\varphi^{'}(0)$ because of $\delta\varphi(0; 0) = \varphi^{'}(0)$.

- Suppose $\overline{x_0} < 0$. By (5) we get

  $$\delta\varphi(x; x_0) \; \geq \; \delta\varphi(0; \overline{x_0}) \; \geq \; \frac{\varphi(0) - \varphi(\overline{x_0})}{\overline{x} - \overline{x_0}} \tag{16}$$

  for all $x \leq 0$ and all $x_0 \in [x_0]$. For all $x \geq 0$ we have $\varphi(x) \geq \varphi(0)$, and therefore, we obtain

  $$\delta\varphi(x; x_0) \; = \; \frac{\varphi(x) - \varphi(x_0)}{x - x_0} \; \geq \; \frac{\varphi(0) - \varphi(x_0)}{x - x_0}$$

for all $x \geq 0$, $x_0 \in [x_0]$. The function $h(x, x_0) := \dfrac{\varphi(0) - \varphi(x_0)}{x - x_0}$, $x \geq 0$, $x_0 \in [x_0]$, decreases monotonically with respect to both x and x_0 because of

$$\frac{\partial(h(x, x_0))}{\partial x} = \frac{\varphi(x_0) - \varphi(0)}{(x - x_0)^2} \leq 0$$

and

$$\begin{aligned}
\frac{\partial(h(x, x_0))}{\partial x_0} &= \frac{-\varphi'(x_0) + \dfrac{\varphi(0) - \varphi(x_0)}{x - x_0}}{x - x_0} \\
&\leq \frac{-\varphi'(x_0) + \dfrac{\varphi(0) - \varphi(x_0)}{0 - x_0}}{x - x_0} \\
&= \frac{-\varphi'(x_0) + \varphi'(\xi)}{x - x_0}, \qquad \xi \in [x_0, 0], \\
&\leq 0.
\end{aligned}$$

Hence, for all $x \geq 0$ and all $x_0 \in [x_0]$ we have

$$\delta\varphi(x; x_0) \geq \frac{\varphi(0) - \varphi(x_0)}{x - x_0} \geq \frac{\varphi(0) - \varphi(\overline{x_0})}{\overline{x} - \overline{x_0}}. \tag{17}$$

Therefore, by (15), (16), and (17) we obtain

$$\delta\varphi(x; x_0) \geq \max\left\{\frac{\varphi(0) - \varphi(\overline{x_0})}{\overline{x} - \overline{x_0}}, \varphi'(0)\right\}$$

for all $x \in [x]$ and all $x_0 \in [x_0]$.

- The proof for $\underline{x_0} > 0$ is analogous to the case of $\overline{x_0} < 0$.

$\square$

Theorem 4.2 Let $\varphi : D \subseteq \mathbb{R} \to \mathbb{R}$ be twice continuously differentiable on $[x] \subseteq D$ and let $[x_0] = \left[\underline{x_0}, \overline{x_0}\right] \subseteq [x]$. Furthermore, let $\varphi'(x) \geq 0$ on $[x]$, $\varphi''(x) \geq 0$ on $\{x \in [x] \mid x \leq 0\}$, and $\varphi''(x) \leq 0$ on $\{x \in [x] \mid x \geq 0\}$. Set

$$\delta\varphi([x]; [x_0]) = \begin{cases}
\left[\delta\varphi(\overline{x}; \overline{x_0}), \delta\varphi\left(\underline{x}; \underline{x_0}\right)\right] & \text{if } \underline{x} \geq 0, \\
\left[\delta\varphi\left(\underline{x}; \underline{x_0}\right), \delta\varphi(\overline{x}; \overline{x_0})\right] & \text{if } \overline{x} \leq 0, \\
\left[m_1,\ \min\left\{\dfrac{\varphi(\overline{x}) - \varphi(\overline{x_0})}{-\overline{x_0}}, \varphi'(0)\right\}\right] & \text{if } \underline{x} \leq \overline{x_0} < 0 < \overline{x}, \\
\left[m_1,\ \min\left\{\dfrac{\varphi(\underline{x}) - \varphi\left(\underline{x_0}\right)}{-\underline{x_0}}, \varphi'(0)\right\}\right] & \text{if } \underline{x} < 0 < \underline{x_0} \leq \overline{x}, \\
\left[m_1,\ \varphi'(0)\right] & \text{if } 0 \in [x] \wedge 0 \in [x_0].
\end{cases}$$

Then, we have the enclosure

$$\delta\varphi([x]; [x_0]) \supseteq \left\{\delta\varphi(x; x_0) \mid x \in [x], x_0 \in [x_0]\right\}. \tag{18}$$

Proof: The proof is analogous to Theorem 4.1. $\square$

Similarly, we get the following theorems for $\delta_2\varphi(x;x_0)$ by exploiting a unique point of inflection of φ'.

Theorem 4.3 Let $\varphi : D \subseteq \mathbb{R} \to \mathbb{R}$ be three times continuously differentiable on $[x] \subseteq D$ and let $[x_0] = \left[\underline{x_0}, \overline{x_0}\right] \subseteq [x]$. Furthermore, let $\varphi'(x) = -\varphi'(-x)$ on $\{x \in [x] \mid -x \in [x]\}$, $\varphi''(x) \geq 0$ on $[x]$, $\varphi'''(x) \leq 0$ on $\{x \in [x] \mid x \leq 0\}$, and $\varphi'''(x) \geq 0$ on $\{x \in [x] \mid x \geq 0\}$. Set

$$\delta_2\varphi([x];[x_0]) = \begin{cases} \left[\delta_2\varphi\left(\underline{x};\underline{x_0}\right), \delta_2\varphi\left(\overline{x};\overline{x_0}\right)\right] & \text{if } \underline{x} \geq 0, \\[1ex] \left[\delta_2\varphi\left(\overline{x};\overline{x_0}\right), \delta_2\varphi\left(\underline{x};\underline{x_0}\right)\right] & \text{if } \overline{x} \leq 0, \\[1ex] \left[\max\left\{\dfrac{\varphi(0) - \varphi(\overline{x_0}) - \varphi'(\overline{x_0})\cdot(0-\overline{x_0})}{(\overline{x}-\overline{x_0})^2}, \tfrac{1}{2}\varphi''(0)\right\}, M_2\right] \\ \text{if } \underline{x} \leq \overline{x_0} < 0 < \overline{x}, \\[1ex] \left[\max\left\{\dfrac{\varphi(0) - \varphi\left(\underline{x_0}\right) - \varphi'\left(\underline{x_0}\right)\cdot\left(0-\underline{x_0}\right)}{\left(\underline{x}-\underline{x_0}\right)^2}, \tfrac{1}{2}\varphi''(0)\right\}, M_2\right] \\ \text{if } \underline{x} < 0 < \underline{x_0} \leq \overline{x}, \\[1ex] \left[\tfrac{1}{2}\varphi''(0), M_2\right] & \text{if } 0 \in [x] \wedge 0 \in [x_0]. \end{cases}$$

Then, we get the enclosure

$$\delta_2\varphi([x];[x_0]) \supseteq \left\{\delta_2\varphi(x;x_0) \mid x \in [x], x_0 \in [x_0]\right\}.$$

Proof: The proof is similar to the proof of Theorem 4.1. For details see [17]. $\square$

Theorem 4.4 Let $\varphi : D \subseteq \mathbb{R} \to \mathbb{R}$ be three times continuously differentiable on $[x] \subseteq D$ and let $[x_0] = \left[\underline{x_0}, \overline{x_0}\right] \subseteq [x]$. Furthermore, let $\varphi'(x) = -\varphi'(-x)$ on $\{x \in [x] \mid -x \in [x]\}$, $\varphi''(x) \geq 0$ on $[x]$, $\varphi'''(x) \geq 0$ on $\{x \in [x] \mid x \leq 0\}$, and $\varphi'''(x) \leq 0$ on $\{x \in [x] \mid x \geq 0\}$. Set

$$\delta_2\varphi([x];[x_0]) = \begin{cases} \left[\delta_2\varphi\left(\overline{x};\overline{x_0}\right), \delta_2\varphi\left(\underline{x};\underline{x_0}\right)\right] & \text{if } \underline{x} \geq 0, \\[1ex] \left[\delta_2\varphi\left(\underline{x};\underline{x_0}\right), \delta_2\varphi\left(\overline{x};\overline{x_0}\right)\right] & \text{if } \overline{x} \leq 0, \\[1ex] \left[m_2, \max\left\{\dfrac{\varphi(\overline{x}) - \varphi(\overline{x_0}) - \varphi'(\overline{x_0})\cdot(\overline{x}-\overline{x_0})}{\overline{x_0}^2}, \tfrac{1}{2}\varphi''(0)\right\}\right] \\ \text{if } \underline{x} \leq \overline{x_0} < 0 < \overline{x}, \\[1ex] \left[m_2, \max\left\{\dfrac{\varphi\left(\underline{x}\right) - \varphi\left(\underline{x_0}\right) - \varphi'\left(\underline{x_0}\right)\cdot\left(\underline{x}-\underline{x_0}\right)}{\underline{x_0}^2}, \tfrac{1}{2}\varphi''(0)\right\}\right] \\ \text{if } \underline{x} < 0 < \underline{x_0} \leq \overline{x}, \\[1ex] \left[m_2, \tfrac{1}{2}\varphi''(0)\right] & \text{if } 0 \in [x] \wedge 0 \in [x_0]. \end{cases}$$

Then, we get the enclosure

$$\delta_2\varphi\left([x]\,;[x_0]\right) \quad \supseteq \quad \left\{\delta_2\varphi\left(x;x_0\right) \mid x\in[x]\,, x_0\in[x_0]\ \right\}.$$

Proof: The proof is similar to the proof of Theorem 4.3. □

5 Examples

Theorems 3.1-4.4 apply to some elementary functions such as $\exp x$, $\ln x$, x^n, $\sinh x$, $\cosh x$, $\tan x$ or $\arctan x$. Next, we consider some examples.

Example 5.1 $\varphi\left(x\right)=\sinh x,\ [x]=[-5,1],\ x_0=[-2,-2].$

By Theorem 4.1 we get

$$\begin{aligned}\delta\varphi\left([x]\,;[x_0]\right) &= \left[\max\left\{\frac{-\sinh\left(-2\right)}{3},1\right\},\max\left\{\delta\varphi\left(\underline{x};\underline{x_0}\right),\delta\varphi\left(\overline{x};\overline{x_0}\right)\right\}\right]\\ &\subseteq [1.208,\ 23.526]\,,\end{aligned}$$

whereas

$$\varphi^{'}\left([x]\right)=\left[\cosh\left(0\right),\,\cosh\left(-5\right)\right]\subseteq[1,\ 74.21]\,.$$

Furthermore, by (8) we obtain

$$\delta_2\varphi\left([x]\,;[x_0]\right)\subseteq[-6.588,\ -0.7205]\,,$$

whereas

$$\frac{1}{2}\,\varphi^{''}([x])=\frac{1}{2}\,\left[\sinh\left(-5\right),\,\sinh\left(1\right)\right]\subseteq[-37.102,\ 0.588]\,.$$

Example 5.2 $\varphi\left(x\right)=\sinh x,\ [x]=[-6,2],\ x_0=[-2,-2].$

By Theorem 4.1 we get

$$\begin{aligned}\delta\varphi\left([x]\,;[x_0]\right) &= \left[\max\left\{\frac{-\sinh\left(-2\right)}{4},1\right\},\max\left\{\delta\varphi\left(\underline{x};\underline{x_0}\right),\delta\varphi\left(\overline{x};\overline{x_0}\right)\right\}\right]\\ &\subseteq [1,\ 49.522]\,,\end{aligned}$$

whereas

$$\varphi^{'}\left([x]\right)=\left[\cosh\left(0\right),\,\cosh\left(-6\right)\right]\subseteq[1,\ 201.716]\,.$$

Furthermore, by (8) we obtain

$$\delta_2\varphi\left([x]\,;[x_0]\right)\subseteq[-11.44,\ -0.487]\,,$$

whereas

$$\frac{1}{2}\,\varphi^{''}([x])=\frac{1}{2}\,\left[\sinh\left(-6\right),\,\sinh\left(2\right)\right]\subseteq[-100.857,\ 1.814]\,.$$

Example 5.3 $\varphi(x) = \cosh x$, $[x] = [-4, 1]$, $x_0 = [-2, -1.5]$.

By (4) we get

$$\delta\varphi([x]\,;[x_0]) \subseteq [-11.774,\ -0.323]\,,$$

whereas

$$\varphi'([x]) = [\sinh(-4)\,,\ \sinh(1)] \subseteq [-27.29,\ 1.176]\,.$$

Furthermore, by Theorem 4.3 we obtain

$$\delta_2\varphi([x]\,;[x_0]) \subseteq [0.5,\ 4.074]\,,$$

whereas

$$\frac{1}{2}\,\varphi''([x]) = \frac{1}{2}\ [\cosh(0)\,,\ \cosh(-4)] \subseteq [0.5,\ 13.655]\,.$$

Example 5.4 $\varphi(x) = x^4$, $[x] = [-3, 1]$, $x_0 = [-1, -0.9]$.

By (4) we get

$$\delta\varphi([x]\,;[x_0]) \subseteq [-40,\ 0.181]\,,$$

whereas

$$\varphi'([x]) = [-108,\ 4]\,.$$

Furthermore, by Theorem 4.3 we obtain

$$\delta_2\varphi([x]\,;[x_0]) \subseteq [0.545,\ 18]\,,$$

whereas

$$\frac{1}{2}\,\varphi''([x]) = [0,\ 54]\,.$$

Example 5.5 $\varphi(x) = \arctan x$, $[x] = [-3, 1]$, $x_0 = [-2, -2]$.

By $\varphi'(x) = \dfrac{1}{1+x^2}$ and $\varphi''(x) = \dfrac{-2x}{(1+x^2)^2}$ we can apply Theorem 4.2. We get

$$\delta\varphi([x]\,;[x_0]) \subseteq [0.141,\ 0.947]\,,$$

whereas

$$\varphi'([x]) = [0.1,\ 1]\,.$$

Because $\varphi'''(x) = \dfrac{-2+6x^2}{(1+x^2)^3}$, we can not apply the theorems of this paper. Therefore, we have to use the enclosure

$$\left\{\delta_2\varphi(x; x_0) \mid x \in [x]\,, x_0 \in [x_0]\ \right\} \subseteq \frac{1}{2}\,\varphi''([x]) = \left[-\frac{3\sqrt{3}}{16},\ \frac{3\sqrt{3}}{16}\right].$$

6 Conclusion

Using slope enclosures may provide sharper bounds of the function range than using enclosures of the derivative. Automatic compuatation of slope enclosures, which can be applied to global optimization [5, 6, 12, 13, 16, 17], requires first-order and second-order slope enclosures for elementary functions φ. This may be obtained by using enclosures of φ' or φ''. Sharper enclosures can be computed by using the convexity or concavity of φ or φ' (see [7] and section 3).

In this paper, we have computed first-order and second-order slope enclosures by exploiting a unique point of inflection of φ or φ'. The formulas given in this paper apply to functions such as $\exp x$, $\ln x$, x^n, $\sinh x$, $\cosh x$, $\tan x$ or $\arctan x$. They provide sharper bounds than enclosures using derivatives. Some examples in section 5 illustrate this. The enclosures given in this paper can be used both for automatic computation of slope enclosures and for theoretical aspects.

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