

EXPANSION AND ESTIMATION OF THE RANGE OF NONLINEAR FUNCTIONS

S. M. RUMP

ABSTRACT. Many verification algorithms use an expansion $f(x) \in f(\tilde{x}) + S \cdot (x - \tilde{x})$, $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ for $x \in X$, where the set of matrices S is usually computed as a gradient or by means of slopes. In the following, an expansion scheme is described which frequently yields sharper inclusions for S . This allows also to compute sharper inclusions for the range of f over a domain. Roughly speaking, f has to be given by means of a computer program. The process of expanding f can then be fully automatized. The function f need not be differentiable. For locally convex or concave functions special improvements are described. Moreover, in contrast to other methods, $\tilde{x} \cap X$ may be empty without implying large overestimations for S . This may be advantageous in practical applications.

0. NOTATION

We denote by \mathbb{IR} the set of real intervals

$$X \in \mathbb{IR} \Rightarrow X = [\inf(X), \sup(X)] = \{x \in \mathbb{R} \mid \inf(X) \leq x \leq \sup(X)\}.$$

By \mathbb{PT} we denote the power set over a given set T , and we use the canonical embedding $\mathbb{IR} \subseteq \mathbb{PR}$. The set of n -dimensional interval vectors is denoted by \mathbb{IR}^n , i.e.,

$$X \in \mathbb{IR}^n \Rightarrow X = \{(x_i) \in \mathbb{R}^n \mid x_i \in X_i\} \quad \text{with } X_i \in \mathbb{IR}, 1 \leq i \leq n.$$

Interval vectors are compact. Interval operations and power set operations are defined in the usual way. Details can be found in standard books on interval analysis, among others [10, 2, 11]. If not explicitly noted otherwise, all operations are power set operations.

1. EXPANSION OF NONLINEAR FUNCTIONS

A differentiable function $f : D \subseteq \mathbb{R}^n \rightarrow \mathbb{R}$ can be locally expanded by its gradient. For $\tilde{x} \in D$, $X \subseteq D$, and $[g] \in \mathbb{IR}^n$ with $\nabla f(\tilde{x} \sqcup X) \subseteq [g]$ there holds

$$(1.0) \quad \forall x \in X \exists g \in [g] : f(x) - f(\tilde{x}) = g^T \cdot (x - \tilde{x}).$$

Here, \sqcup denotes the convex hull, and $\nabla f(\tilde{x} \sqcup X)$ denotes the range of ∇f over $\tilde{x} \sqcup X$. The gradient, for real and for interval arguments, can be computed using automatic differentiation [4, 12]. This process is fully automatized. This approach has three disadvantages:

- (1) f needs to be differentiable,

Received by the editor January 11, 1995 and, in revised form, November 2, 1995.
1991 *Mathematics Subject Classification*. Primary 65G10; Secondary 65D15.

- (2) $[g]$ expands f with respect to every $x \in \tilde{x} \sqcup X$ rather than with respect to some specific $\tilde{x} \in D$,
- (3) $\tilde{x} \sqcup X$ has to be used, enlarging $[g]$ if $\tilde{x} \notin X$.

Item (2) means that (1.0) still holds if \tilde{x} in (1.0) is replaced by any $y \in \tilde{x} \sqcup X$. Item (3) expresses that, according to the n -dimensional Mean Value Theorem, for all $x \in X$ some $\zeta \in \tilde{x} \sqcup x$ exists with $f(x) - f(\tilde{x}) = \nabla f(\zeta) \cdot (x - \tilde{x})$. Using $[g] \supseteq \nabla f(\tilde{x} \sqcup X)$ assures (1.0).

The three problems can be solved by means of so-called slopes. They have been introduced and described in [13, 5, 9, 11]. For another, very interesting application of slopes in the computation of inclusions for Peano functionals, see the paper by Heindl [7]. In the following, we give some generalization and improvement for slopes.

We start with a 1-dimensional function, and we will see that the approach easily extends to the n -dimensional case. The first steps very much follow the treatment in [11].

Definition 1. Let $f : D \subseteq \mathbb{R} \rightarrow \mathbb{R}$ and $\tilde{X}, X \subseteq D$ be given. The triple $(f_c, f_r, f_s) \in \mathbb{P}\mathbb{R} \times \mathbb{P}\mathbb{R} \times \mathbb{P}\mathbb{R}$ expands f in X with respect to \tilde{X} if

$$\begin{aligned} \forall \tilde{x} \in \tilde{X} : \quad & f(\tilde{x}) \in f_c, \\ \forall x \in X : \quad & f(x) \in f_r, \\ \forall \tilde{x} \in X \quad \forall x \in X \quad \exists \tilde{f}_s \in f_s : \quad & f(x) - f(\tilde{x}) = \tilde{f}_s \cdot (x - \tilde{x}). \end{aligned}$$

Furthermore, the slope of f in X with respect to \tilde{X} is defined by

$$\text{sl}(f) := \text{sl}(f, \tilde{X}, X) := \left\{ \frac{f(x) - f(\tilde{x})}{x - \tilde{x}} \mid \tilde{x} \in \tilde{X}, x \in X, x \neq \tilde{x} \right\}.$$

For Theorem 3 we also need the following definition. If $\tilde{X}, X \subseteq D$ both consist of a single point $\tilde{x}, x \in D$, respectively, then $\text{sl}(f) = (f(x) - f(\tilde{x})) / (x - \tilde{x})$ provided $\tilde{x} \neq x$. We define for $\tilde{x} \neq x$,

$$\underline{\text{sl}}^+(f, \tilde{x}, x) = \underline{\text{sl}}^-(f, \tilde{x}, x) = \overline{\text{sl}}^+(f, \tilde{x}, x) = \overline{\text{sl}}^-(f, \tilde{x}, x) := \text{sl}(f, \tilde{x}, x),$$

and for $\tilde{x} = x$,

$$\begin{aligned} \underline{\text{sl}}^+(f, \tilde{x}, x) &:= \underline{\lim}_{\varepsilon \rightarrow 0^+} \frac{f(\tilde{x} + \varepsilon) - f(\tilde{x})}{\varepsilon}, & \underline{\text{sl}}^-(f, \tilde{x}, x) &:= \underline{\lim}_{\varepsilon \rightarrow 0^-} \frac{f(\tilde{x} + \varepsilon) - f(\tilde{x})}{\varepsilon}, \\ \overline{\text{sl}}^+(f, \tilde{x}, x) &:= \overline{\lim}_{\varepsilon \rightarrow 0^+} \frac{f(\tilde{x} + \varepsilon) - f(\tilde{x})}{\varepsilon}, & \overline{\text{sl}}^-(f, \tilde{x}, x) &:= \overline{\lim}_{\varepsilon \rightarrow 0^-} \frac{f(\tilde{x} + \varepsilon) - f(\tilde{x})}{\varepsilon}. \end{aligned}$$

This definition is only needed for convex or concave f . The values for $\underline{\text{sl}}, \overline{\text{sl}}$ are allowed in $[-\infty, +\infty]$.

Instead of (f_c, f_r, f_s) we sometimes write $(f_c(\tilde{X}, X), f_r(\tilde{X}, X), f_s(\tilde{X}, X))$ in order to emphasize the dependence on \tilde{X} and X . Clearly, if (f_c, f_r, f_s) expands f in X with respect to \tilde{X} , then

$$f(\tilde{X}) \subseteq f_c, \quad f(X) \subseteq f_r, \quad \text{sl}(f, \tilde{X}, X) \subseteq f_s,$$

and $(f(\tilde{X}), f(X), \text{sl}(f, \tilde{X}, X))$ expands f in X with respect to \tilde{X} .

The following theorem can essentially be found in [11]. Note that intersection for multiplication and division is possible because we are in the 1-dimensional case. This is no longer possible in n dimensions because the slope is no longer unique.

Theorem 2. A constant $c \in \mathbb{R}$ and $f(x) \equiv x$ is expanded in $X \subseteq \mathbb{R}$ with respect to $\tilde{X} \subseteq \mathbb{R}$ by $(c, c, 0)$ and $(\tilde{X}, X, 1)$, respectively. Let $f, g : D \subseteq \mathbb{R} \rightarrow \mathbb{R}$ and $\tilde{X}, X \subseteq D$ be given. If $(f_c, f_r, f_s), (g_c, g_r, g_s)$ expand f, g in X with respect to \tilde{X} , respectively, then (h_c, h_r, h_s) expands $f \circ g$ for $\circ \in \{+, -, \cdot, /\}$ in X with respect to \tilde{X} , where

$$\begin{aligned} h_c &:= f_c \circ g_c, & h_r &:= f_r \circ g_r & \text{for } \circ \in \{+, -, \cdot, /\}, \\ h_s &:= f_s \circ g_s & & & \text{for } \circ \in \{+, -\}, \\ h_s &:= (f_s \cdot g_r + f_c \cdot g_s) \cap (f_r \cdot g_s + f_s \cdot g_c) & \text{for } \circ = \cdot, \\ h_s &:= (f_s - h_c \cdot g_s)/g_r \cap (f_s - h_r \cdot g_s)/g_c & \text{for } \circ = /, \end{aligned}$$

provided no division by zero occurs. If $g(f_c \cup f_r) \subseteq D$, the same holds for $h = g(f)$ with

$$\begin{aligned} h_c &:= g(f_c), & h_r &:= g(f_r) & \text{and} \\ h_s &:= \text{sl}(g, f_c, f_r) \cdot f_s. \end{aligned}$$

These statements remain valid if h_r is replaced by

$$h_r := h_r \cap \{h_c + h_s \cdot (X - \tilde{X})\}.$$

The proof is given for $f \cdot g, f/g$, and $g(f)$. The other cases follow similarly. Computation of h_c and h_r is obvious. For $h = f \cdot g$ we have

$$\text{sl}(f \cdot g) = \left\{ \frac{f(x) \cdot g(x) - f(\tilde{x}) \cdot g(\tilde{x})}{x - \tilde{x}} \mid \tilde{x} \in \tilde{X}, x \in X, x \neq \tilde{x} \right\}.$$

For fixed but arbitrary $\tilde{x} \in X, x \in X$ there exist $\tilde{f}_s \in f_s, \tilde{g}_s \in g_s$ with

$$\begin{aligned} f(x) \cdot g(x) - f(\tilde{x}) \cdot g(\tilde{x}) &= [f(\tilde{x}) + \tilde{f}_s \cdot (x - \tilde{x})] \cdot [g(\tilde{x}) + \tilde{g}_s \cdot (x - \tilde{x})] - f(\tilde{x}) \cdot g(\tilde{x}) \\ &= [\tilde{f}_s \cdot g(x) + f(\tilde{x}) \cdot \tilde{g}_s] \cdot (x - \tilde{x}). \end{aligned}$$

Hence $\text{sl}(f \cdot g) \subseteq f_s \cdot g_r + f_c \cdot g_s$ and therefore $\text{sl}(f \cdot g) = \text{sl}(g \cdot f) \subseteq f_r \cdot g_s + f_s \cdot g_c$. For fixed but arbitrary $\tilde{x} \in \tilde{X}, x \in X$ there exist $\tilde{f}_s \in f_s, \tilde{g}_s \in g_s$ with

$$\begin{aligned} \frac{f(x)}{g(x)} - \frac{f(\tilde{x})}{g(\tilde{x})} &= \frac{[f(\tilde{x}) + \tilde{f}_s \cdot (x - \tilde{x})] \cdot g(\tilde{x}) - f(\tilde{x}) \cdot [g(\tilde{x}) + \tilde{g}_s \cdot (x - \tilde{x})]}{g(x) \cdot g(\tilde{x})} \\ &= \frac{\tilde{f}_s \cdot (g(x) - \tilde{g}_s \cdot (x - \tilde{x})) - (f(x) - \tilde{f}_s \cdot (x - \tilde{x})) \cdot \tilde{g}_s}{g(x) \cdot g(\tilde{x})} \cdot (x - \tilde{x}) \\ &= \left\{ \frac{\tilde{f}_s}{g(\tilde{x})} - \frac{f(x) \cdot \tilde{g}_s}{g(x) \cdot g(\tilde{x})} \right\} \cdot (x - \tilde{x}), \end{aligned}$$

proving the second part of the formula for h_s for division. The first part can be derived similarly, cf. also [11]. For $h = g(f)$ we have

$$\text{sl}(h) = \left\{ \frac{g(f(x)) - g(f(\tilde{x}))}{x - \tilde{x}} \mid \tilde{x} \in \tilde{X}, x \in X, x \neq \tilde{x} \right\}.$$

For $f(x) \neq f(\tilde{x})$ we have

$$\frac{g(f(x)) - g(f(\tilde{x}))}{x - \tilde{x}} = \frac{g(f(x)) - g(f(\tilde{x}))}{f(x) - f(\tilde{x})} \cdot \frac{f(x) - f(\tilde{x})}{x - \tilde{x}} \in \text{sl}(g, f_c, f_r) \cdot f_s.$$

If $f(x) = f(\tilde{x})$ for $x \neq \tilde{x}$, then $0 \in f_s$, and this yields $\text{sl}(g(f)) \subseteq \text{sl}(g, f_c, f_r) \cdot f_s$. \square

The intersection for h_r in Theorem 2 combines naive interval evaluation with centered forms. For example, $(\tilde{X}, X, 1)$ expands the function $f(x) \equiv x$ in X with respect to \tilde{X} . Defining $g(x) := x - x$, we obtain $g(X) \subseteq X - X = [-\text{diam}(X), +\text{diam}(X)]$ by naive interval calculation. The intersection $g_r := g_r \cap (g_c + g_s \cdot (X - \tilde{X}))$ yields $g_r = g_r \cap (g_c + 0 \cdot (X - \tilde{X})) = g_c = 0$.

It has already been observed in [11] that $\text{sl}(g, f_c, f_r)$ can be replaced by $g'(f_c \sqcup f_r)$ when g is differentiable. The disadvantage is that this set may be large. It covers $\text{sl}(g, f_c \sqcup f_r, f_c \sqcup f_r)$, thus expanding g in $f_c \sqcup f_r$ with respect to each $\tilde{x} \in f_c \sqcup f_r$. In special cases, $\text{sl}(g, f_c, f_r)$ can be computed explicitly. For example, let $g(x) = x^2$. Then for every $\tilde{y} \in f_c, y \in f_r, y \neq \tilde{y}$ there holds

$$(1.1) \quad \frac{g(y) - g(\tilde{y})}{y - \tilde{y}} = \frac{y^2 - \tilde{y}^2}{y - \tilde{y}} = y + \tilde{y} \Rightarrow \text{sl}(g, f_c, f_r) \subseteq f_c + f_r.$$

For $g(x) = \sqrt{x}$ we have

$$(1.2) \quad \frac{g(y) - g(\tilde{y})}{y - \tilde{y}} = \frac{\sqrt{y} - \sqrt{\tilde{y}}}{y - \tilde{y}} = (\sqrt{y} + \sqrt{\tilde{y}})^{-1} \Rightarrow \text{sl}(g, f_c, f_r) \subseteq (g_c + g_r)^{-1}.$$

A similar principle can be extended to locally convex or concave functions. This may sharpen the inclusion interval for slopes significantly.

Theorem 3. *Let $f : D \subseteq \mathbb{R} \rightarrow \mathbb{R}, \tilde{X}, X \subseteq D$ be given and $(f_c, f_r, f_s) \in \mathbb{P}\mathbb{R} \times \mathbb{P}\mathbb{R} \times \mathbb{P}\mathbb{R}$, expanding f in X with respect to \tilde{X} . Let $g : D' \subseteq \mathbb{R} \rightarrow \mathbb{R}, f_c \sqcup f_r \subseteq D'$ be given and define $h_c := g(f_c), h_r := g(f_r)$. If g is convex on $f_c \sqcup f_r$, then (h_c, h_r, h_s) expands $g(f)$ on X with respect to \tilde{X} provided*

$$(1.3) \quad h_s \supseteq \left[\underline{\text{sl}}^+(g, \inf(f_c), \inf(f_r)), \overline{\text{sl}}^-(g, \sup(f_c), \sup(f_r)) \right] \cdot f_s.$$

If g is concave on $f_c \sqcup f_r$, then the same holds provided

$$(1.4) \quad h_s \supseteq \left[\overline{\text{sl}}^+(g, \sup(f_c), \sup(f_r)), \underline{\text{sl}}^-(g, \inf(f_c), \inf(f_r)) \right] \cdot f_s.$$

Proof. Let g be convex on $f_c \sqcup f_r$. We prove that $\text{sl}(g, y_1, y_2)$ increases when y_1 or y_2 increase. Let $y_1 < y < y_2$ with $y = \alpha y_1 + (1 - \alpha)y_2, 0 < \alpha < 1, y_1, y, y_2 \in f_c \sqcup f_r$. Then, owing to convexity, $g(\alpha y_1 + (1 - \alpha)y_2) \leq \alpha g(y_1) + (1 - \alpha)g(y_2)$ and

$$\frac{g(y_2) - g(y_1)}{y_2 - y_1} = \alpha \cdot \frac{g(y_2) - g(y_1)}{y_2 - y} \leq \frac{\alpha g(y_2) - g(y) + (1 - \alpha)g(y_2)}{y_2 - y} = \frac{g(y_2) - g(y)}{y_2 - y}.$$

We proceed similarly for $y_1 \leq y_2 < y$. Thus, $\text{sl}(g, f_c, f_r)$ achieves its extreme values at the extremes of f_c and f_r , and this proves (1.3). Concavity is treated similarly. □

Note that in the calculation of (1.3) and (1.4) only slopes of g for points, not for intervals, are necessary. Theorem 3 yields sharper slopes for many functions. Moreover, it extends the expansion principle to nondifferentiable functions.

As an example, consider e^{x^2} for $\tilde{X} = \{1\}$ and $X = [0.5, 1.5]$. In the following table we compare a standard gradient evaluation $\nabla f(\tilde{x} \sqcup X)$, the slope using $\text{sl}(g, f_c, f_r) \subseteq g'(f_c \sqcup f_r)$, and the slope computed by Theorem 3. Results are rounded to 4 figures.

TABLE 1. Expansions for $\tilde{X} = \{1\}$, $X = [0.5, 1.5]$

| | $\nabla f(\tilde{X} \sqcup X)$ | standard slope | new slope (Theorem 3) |
|-----------|--------------------------------|----------------|-----------------------|
| x^2 | [1, 3] | [1.5, 2.5] | [1.5, 2.5] |
| e^{x^2} | [1.284, 28.46] | [1.926, 23.72] | [2.869, 13.54] |

Here we set $\tilde{X} = \{\text{mid}(X)\}$. In practical applications, one cannot always ensure $\tilde{X} \subseteq X$ unless extra function evaluations are necessary. If we take the same $X = [0.5, 1.5]$, but $\tilde{X} = \{2\}$, then Table 1 looks as follows.

TABLE 2. Expansions for $\tilde{X} = \{2\}$, $X = [0.5, 1.5]$

| | $\nabla f(\tilde{X} \sqcup X)$ | standard slope | new slope (Theorem 3) |
|-----------|--------------------------------|----------------|-----------------------|
| x^2 | [1, 4] | [2.5, 3.5] | [2.5, 3.5] |
| e^{x^2} | [1.284, 218.4] | [3.21, 191.1] | [35.54, 90.22] |

In order to apply Theorems 2 and 3 to the n -dimensional case, we first generalize Definition 1 in the following way.

Definition 4. Let $F : \mathbb{R} \rightarrow \mathbb{P}\mathbb{R}$ and $\tilde{X}, X \subseteq D$ be given. The triple $(F_c, F_r, F_s) \in \mathbb{P}\mathbb{R}^3$ expands F in X with respect to \tilde{X} if

$$\begin{aligned} \forall \tilde{x} \in \tilde{X} : & F(\tilde{x}) \subseteq F_c, \\ \forall x \in X : & F(x) \subseteq F_r, \\ \forall \tilde{x} \in \tilde{X} \quad \forall x \in X \quad \forall \tilde{y} \in F(\tilde{x}) \quad \forall y \in F(x) \quad \exists \tilde{F}_s \in F_s : & y - \tilde{y} = \tilde{F}_s \cdot (x - \tilde{x}). \end{aligned}$$

Furthermore, the slope of F with respect to X and \tilde{X} is defined by

$$\text{sl}(F) := \text{sl}(F, \tilde{X}, X) := \left\{ \frac{y - \tilde{y}}{x - \tilde{x}} \mid y \in F(X), \tilde{y} \in F(\tilde{X}), x \in X, \tilde{x} \in \tilde{X}, x \neq \tilde{x} \right\}.$$

For simplicity of notation and formulation, we assume F to be defined on \mathbb{R} rather than on a subset $D \subseteq \mathbb{R}$. A generalization of the following to functions being defined only on a subset of \mathbb{R} is straightforward.

As before, we have $F(\tilde{X}) \subseteq F_c$, $F(X) \subseteq F_r$ and $\text{sl}(F, \tilde{X}, X) \subseteq F_s$ and $(F(\tilde{X}), F(X), \text{sl}(F, \tilde{X}, X))$ expands F in X with respect to \tilde{X} .

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ and let $\tilde{X}, X \in \mathbb{I}\mathbb{R}^n$ be given. We need Definition 4 to apply it to the following ‘‘component functions’’ $F^k : \mathbb{R} \rightarrow \mathbb{P}\mathbb{R}$ defined by

$$F^k(y) := f(X_1, \dots, X_{k-1}, y, \tilde{X}_{k+1}, \dots, \tilde{X}_n) \quad \text{for } 1 \leq k \leq n.$$

Then $(F^k(\tilde{X}_k), F^k(X_k), \text{sl}(F^k, \tilde{X}_k, X_k))$ expands F^k in X_k with respect to \tilde{X}_k , and by induction it follows for $x \in X$, $\tilde{x} \in \tilde{X}$ and $0 \leq k \leq n$ that

$$f(x_1, \dots, x_k, \tilde{x}_{k+1}, \dots, \tilde{x}_n) \subseteq f(\tilde{x}) + \sum_{\nu=1}^k \text{sl}(F^\nu, \tilde{X}_\nu, X_\nu) \cdot (X_\nu - \tilde{X}_\nu).$$

Of course, Definition 4 could replace 1 at the beginning; we separated them for didactical reasons. Theorems 2 and 3 can be adapted to Definition 4 and applied to

every component function F^k in a straightforward way. In the practical application, the vector $V = (V_0, \dots, V_n) \in \mathbb{I}\mathbb{R}^n$ with

$$(1.5) \quad f(X_1, \dots, X_k, \tilde{X}_{k+1}, \dots, \tilde{X}_n) \subseteq V_k \quad \text{for } 0 \leq k \leq n$$

is stored and

$$F^k(\tilde{X}_k) \subseteq V_{k-1} \quad \text{and} \quad F^k(X_k) \subseteq V_k$$

is used. The difference to Neumaier's approach [11] is that he stores $(f_c, f_r, f_s) \in \mathbb{I}\mathbb{R} \times \mathbb{I}\mathbb{R} \times \mathbb{I}\mathbb{R}^n$ with $f(\tilde{X}) \subseteq f_c$, $f(X) \subseteq f_r$ and corresponding slope. In the approach described above, more information is stored. This is very much in the spirit of Hansen [6], where the concept of componentwise application of the n -dimensional Mean Value Theorem is used to improve gradients; see also [1].

2. IMPLEMENTATION AND EXAMPLES

In the following we give some remarks regarding implementation and computational results. We use a Pascal-like notation together with an operator concept. In fact, it is the notation of TPX (Turbo Pascal eXtended, [8], a precompiler for Turbo Pascal offering these and other features). We use the data structure

```
expansion = record
    r : array[0..n] of interval;
    s : array[1..n] of interval;
end;
```

The constants $\tilde{X}, X \in \mathbb{I}\mathbb{R}$ are fixed and globally available. \tilde{X} is denoted by Xs . Then $f.r$ represents the range vector V as in (1.5), and for all $\tilde{x} \in \tilde{X}$, $x \in X$ we have

$$f(x_1, \dots, x_k, \tilde{x}_{k+1}, \dots, \tilde{x}_n) \in f.r[k] \quad \text{for } 0 \leq k \leq n,$$

$$f(x) \in f(\tilde{x}) + \sum_{i=1}^n f.s[i] \cdot (x_i - \tilde{x}_i).$$

As an example, we display the algorithm for the multiplication operator.

ALGORITHM 2.1. Multiplication for expansions

```
function mul(f, g : expansion): expansion implements * ;
var i : integer; R : interval;
begin
    R := f.r[0] * g.r[0]; mul.r[0] := R;
    for i := 1 to n do begin
        mul.s[i] := intersection(f.r[i] * g.s[i] + g.r[i-1] * f.s[i],
                               g.r[i] * f.s[i] + f.r[i-1] * g.s[i]);
        R := R + mul.s[i] * (X[i] - Xs[i]);
        mul.r[i] := intersection(f.r[i] * g.r[i], R);
    end;
end {mul};
```

The procedure gives enough detail for an implementation of basic operators for the computation of slope expansions. Note that all operations are interval operations. The main point is that replacing the data type *double* in some function by *expansion* creates automatically the slope expansion. This process is fully automatized.

We close the implementation remarks by giving a procedure for the absolute value, a convex but not everywhere differentiable function. It implements Theorem 3. We assume the function abs to be given for interval arguments, that is $abs(X) := \{ |x| \mid x \in X \}$.

ALGORITHM 2.2. Slope expansion of absolute value

```

function  $abs$  ( $f$ : expansion) : expansion;
var  $i$  : integer;  $R$  : interval;  $Sl, Su$  : double;
begin
   $R := abs(f.r[0]); abs.r[0] := R$ ;
  for  $i := 1$  to  $n$  do begin
    if  $f.r[i].inf = f.r[i-1].inf$  then
      if  $f.r[i].inf >= 0.0$  then  $Sl := 1.0$  else  $Sl := -1.0$ 
    else
       $Sl := (abs(f.r[i].inf) - abs(f.r[i-1].inf)) / (f.r[i].inf - f.r[i-1].inf)$ ;
    if  $f.r[i].sup = f.r[i-1].sup$  then
      if  $f.r[i].sup <= 0.0$  then  $Su := -1.0$  else  $Su := 1.0$ 
    else
       $Su := (abs(f.r[i].sup) - abs(f.r[i-1].sup)) /$ 
         $(f.r[i].sup - f.r[i-1].sup)$ ;
     $abs.s[i] := hull(Sl, Su) * f.s[i]$ ;
     $R := R + abs.s[i] * (X[i] - Xs[i])$ ;
     $abs.r[i] := intersection(abs(f.r[i]), R)$ ;
  end;
end { $abs$ };

```

For the implementation of nonglobally convex or concave functions, case distinctions for local convexity and/or local concavity can be used.

As an example which cannot be treated by gradients, consider $g(x) := \sqrt{|x|}$ for $X := [-1, 1]$ and $\tilde{x} := 2$. The computation of the slope according to Theorem 3 is fully automatized. Algorithm 2.2 yields

$$f(x) = |x| \Rightarrow (2, [0, 1], [\frac{1}{3}, 1]) \text{ expands } f \text{ in } X \text{ with respect to } \tilde{x}.$$

Applying Theorem 3 then gives

$$sl(g, f_c, f_r) \subseteq \left[\frac{\sqrt{2} - \sqrt{1}}{2 - 1}, \frac{\sqrt{2} - \sqrt{0}}{2 - 0} \right] = [\sqrt{2} - 1, \frac{1}{2}\sqrt{2}],$$

and (1.4) yields

$$g(x) = \sqrt{|x|} \Rightarrow (\sqrt{2}, [0, 1], [\frac{1}{3}(\sqrt{2} - 1), \frac{1}{2}\sqrt{2}]) \text{ expands } g \text{ in } X \text{ with respect to } \tilde{x}.$$

In this example, the computed slope is even sharp. A graph of the function g together with the slopes is displayed below (Figure 1).

Next we compare the following three methods for expanding a function:

- Method 1: Gradients ∇f
- Method 2: Slopes according to [11]
- Method 3: Slopes as described above

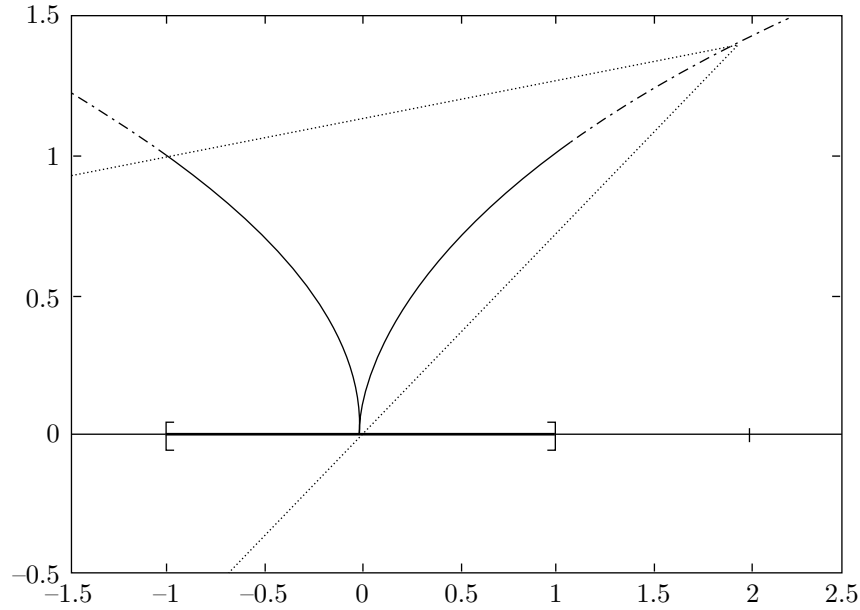


FIGURE 1. $g(x) := \sqrt{|x|}$ with slopes for $X := [-1, 1]$ and $\tilde{x} := 2$

As an example for comparing these methods, we use $f : \mathbb{R}^2 \rightarrow \mathbb{R}$ with

$$(2.1) \quad f(x, y) := e^{xy} - x \quad \text{for } X = [-1, 1], Y = [0, 2], \tilde{X} = 0, \tilde{Y} = 1.$$

Method 1 with automatic differentiation yields

TABLE 2.1. Method 1 for (2.1)

| | $z_i(X, Y)$ | $\nabla z_i(X, Y)$ | |
|-----------------------|-------------------|--------------------|-------------------|
| $z_1 = X$ | $[-1, 1]$ | 1 | 0 |
| $z_2 = Y$ | $[0, 2]$ | 0 | 1 |
| $z_3 = z_1 \cdot z_2$ | $[-2, 2]$ | $[0, 2]$ | $[-1, 1]$ |
| $z_4 = e^{z_3}$ | $[0.135, 7.390]$ | $[0, 14.779]$ | $[-7.390, 7.390]$ |
| $z_5 = z_4 - z_1$ | $[-0.865, 8.390]$ | $[-1, 13.779]$ | $[-7.390, 7.390]$ |

The final value z_5 gives an interval containing the range of f on $X \times Y$. Slopes according to [11] compute as follows:

TABLE 2.2. Method 2 (slopes) for (2.1)

| | $(z_i)_c$ | $(z_i)_r$ | $(z_i)_s$ | |
|-----------------------|-----------|-------------------|-------------------|-------------------|
| $z_1 = X$ | 0 | $[-1, 1]$ | 1 | 0 |
| $z_2 = Y$ | 1 | $[0, 2]$ | 0 | 1 |
| $z_3 = z_1 \cdot z_2$ | 0 | $[-2, 2]$ | 1 | $[-1, 1]$ |
| $z_4 = e^{z_3}$ | 1 | $[0.135, 7.390]$ | $[0.135, 7.390]$ | $[-7.390, 7.390]$ |
| $z_5 = z_4 - z_1$ | 1 | $[-0.865, 8.390]$ | $[-0.865, 6.390]$ | $[-7.390, 7.390]$ |

The results of Table 2.2 are exactly the same for the componentwise definition of gradients according to Hansen [6]. The estimation for the range $f(X, Y)$ is the same as for Method 1. It cannot be improved by using

$$f(X, Y) \subseteq \{f_c + f_s \cdot (X - \tilde{X}, Y - \tilde{Y})^T\} \cap f_r.$$

Finally, we give the results for the new Method 3, using Theorems 2 and 3.

TABLE 2.3. Method 3 for (2.1)

| | $(R_{z_i})_0$ | $(R_{z_i})_1$ | $(R_{z_i})_2$ | $(S_{z_i})_1$ | $(S_{z_i})_2$ |
|-----------------------|---------------|------------------|-------------------|-------------------|-------------------|
| $z_1 = X$ | 0 | $[-1, 1]$ | $[-1, 1]$ | 1 | 0 |
| $z_2 = Y$ | 1 | 1 | $[0, 2]$ | 0 | 1 |
| $z_3 = z_1 \cdot z_2$ | 0 | $[-1, 1]$ | $[-2, 2]$ | 1 | $[-1, 1]$ |
| $z_4 = e^{z_3}$ | 1 | $[0.367, 2.719]$ | $[0.135, 7.390]$ | $[0.633, 1.719]$ | $[-4.671, 4.671]$ |
| $z_5 = z_4 - z_1$ | 1 | $[0.281, 1.719]$ | $[-0.865, 6.390]$ | $[-0.367, 0.719]$ | $[-4.671, 4.671]$ |

Method 3 stores more information and computes better inclusions. The last line of Table 2.3 shows a sharper inclusion $[-0.865, 6.390]$ for the range $f(X, Y)$ and sharper slopes. The true range is $[0, 6.390]$, thus the upper bound is already sharp.

Slope expansions for noncontinuous functions like $\text{signum}(x)$ or $[x] := \max\{k \in \mathbb{Z} \mid k \leq x\}$ according to Theorems 2 and 3 can easily be implemented along the lines of Algorithms 2.1 and 2.2.

The following example is taken from Broyden's function [3]:

$$f(x_1, x_2) := (1 - 1/(4\pi)) \cdot (e^{2x_1} - e) + x_2 \cdot e/\pi - 2ex_1.$$

Setting $\tilde{X} = (0.5, \pi)$ and $X := \tilde{X} \cdot [1 - 0.3, 1 + 0.3]$, we obtain the following ranges computed by Methods 1, 2, and 3, the latter without and with using Theorem 3.

| method | range $f(X)$ |
|----------------------------|--------------------|
| Method 1 | $[-3.019, +3.947]$ |
| Method 2 | $[-3.019, +3.947]$ |
| Method 3 without Theorem 3 | $[-1.364, +1.364]$ |
| Method 3 with Theorem 3 | $[-0.761, +0.762]$ |

We summarize the main properties of our expansion scheme:

- The method is applicable to rather general, nondifferentiable and even noncontinuous functions and can be used in an automatized way similar to automatic differentiation.
- The quality of the inclusions is improved through various intersections and special treatment of locally convex or concave functions.
- In practical applications, expansions may be necessary with respect to some $\tilde{x} \in \mathbb{R}^n$ not exactly representable on the computer; therefore, $\tilde{X} \in \mathbb{IR}^n$ can be used instead of \tilde{x} .
- We neither require $\tilde{X} \subseteq X$ nor use $\tilde{X} \sqcup X$.
- The computational effort and storage as compared to standard slopes increase by about a factor of 2.

ACKNOWLEDGEMENT

The author would like to thank Professor Heindl from Wuppertal for many helpful remarks.

REFERENCES

1. G. Alefeld, *Intervallanalytische Methoden bei nichtlinearen Gleichungen*, In S.D. Chatterji et al., editors, Jahrbuch Überblicke Mathematik 1979, pp. 63–78. Bibliographisches Institut, Mannheim, 1979. MR **81a**:65049
2. G. Alefeld and J. Herzberger, *Introduction to interval computations*, Academic Press, New York, 1983. MR **85d**:65001
3. C.G. Broyden, *A new method of solving nonlinear simultaneous equations*, Comput. J. **12** (1969), 94–99. MR **39**:6509
4. A. Griewank, *On automatic differentiation*, Mathematical Programming 88, Kluwer Academic Publishers, Boston, 1989. MR **92k**:65002
5. E. Hansen, *A generalized interval arithmetic*, Interval Mathematics (K. Nickel, editor), vol. 29, Springer, Berlin, 1975, pp. 7–18.
6. E. R. Hansen, *On solving systems of equations using interval arithmetic*, Math. Comput. **22** (1968), 374–384. MR **37**:4985
7. G. Heindl, *Zur numerischen Einschließung der Werte von Peanofunktionalen*, Z. Angew. Math. Mech. **75** (1995), S637–S638.
8. D. Husung, *Precompiler for scientific computation (TPX)*, Technical Report 91.1, Inst. for Computer Science III, TU Hamburg-Harburg, 1989.
9. R. Krawczyk and A. Neumaier, *Interval slopes for rational functions and associated centered forms*, SIAM J. Numer. Anal. **22** (1985), 604–616. MR **86h**:65064
10. R.E. Moore, *Interval analysis*. Prentice-Hall, Englewood Cliffs, N.J., 1966. MR **37**:7069
11. A. Neumaier, *Interval methods for systems of equations*, Encyclopedia of Mathematics and its Applications, vol. 37, Cambridge University Press, 1990. MR **92b**:65004
12. L.B. Rall, *Automatic differentiation: techniques and applications*, Lecture Notes in Comput. Sci., vol. 120, Springer Verlag, Berlin–Heidelberg–New York, 1981.
13. J.W. Schmidt, *Die Regula Falsi für Operationen in Banachräumen*, Z. Angew. Math. Mech. **41** (1961), T61–T63.

ARBEITSBEREICH INFORMATIK III, TECHNISCHE UNIVERSITÄT HAMBURG-HARBURG, D-21071 HAMBURG, GERMANY

E-mail address: `rump@tu-harburg.d400.de`