Enclosure Methods

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Abstract: We present an overview on existing methods for including the range of functions by interval arithmetic tools.

1. Introduction

In this paper we do not try to give a precise definition of what we mean by an enclosure method. Instead we first recall that the four basic interval operations allow to include the range of values of rational functions. Using more appropriate tools also the range of more general functions can be included. Since all enclosure methods for the solution of equations which are based on interval arithmetic tools are finally enclosure methods for the range of some function we concentrate ourselves on methods for the inclusion of the range of functions. We limit our discussion to the case of functions of one real variable. Most of the material in the present paper is well known. See [1], Chapter 3 and the books [9], [10] by Ratschek and Rokne, for example. However, there are also some new results. See Theorem 2, for example.

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2. Notation

The notation in this paper is essentially the same as in [1]. We repeat the most important ones in order that the non-specialist can also read this paper. Real intervals $[a_1;a_2]$, $[b_1;b_2]$,... are denoted by $[a]$, $[b]$,... . The four arithmetic operations for intervals are defined by

$$[a]*[b] = \{a*b \mid a \in [a] , b \in [b]\} , \quad * \in \{+,-,\times,/\} .$$

The result is an interval whose bounds can be computed from the bounds of $[a]$ and $[b]$. Similarly, vectors with intervals as components, so-called interval vectors, are denoted by $[a] = ([a]_i)$, $[b] = ([b]_i)$,... . Analogously, $[A] = ([a]_{ij})$ denotes an interval matrix. $m[a]$ is the center of $[a]$, $d[a] = a_2-a_1$ is the diameter of $[a]$, $q([a],[b]) = \max\{|a_1-b_1| , |a_2-b_2|\}$ denotes the distance of $[a]$ and $[b]$ and $q([a],0) = |[a]|$ is called the absolute value of $[a]$. These concepts are defined for interval vectors and interval matrices via the components. For additional details we refer to [1].

3. Interval arithmetic evaluation

The four basic operations for intervals are <u>inclusion monotone</u>:

If $[a] \subseteq [c]$, $[b] \subseteq [d]$ then $[a]*[b] \subseteq [c]*[d]$, $* \in \{+,-,\times,/\}$.

From this it follows that for rational functions (and more generally for all functions f which have an interval arithmetic evaluation (see [1], Chapter 3)) the range $R(f;[x])$ of f over the interval $[x]$ is contained in the interval arithmetic evaluation $f([x])$:

(1) $R(f;[x]) \subseteq f([x])$.

Example 1. Let

$$f(x) = \frac{x}{1-x} \quad , \quad x \neq 1$$

and $[x] = [2\,;\,3]$. Then

$$R(f;[x]) = [-2\,;\,-\tfrac{3}{2}] \; ,$$

$$f([x]) = \frac{[x]}{1-[x]} = \frac{[2;3]}{1-[2;3]} = [-3\,;\,-1] \; ,$$

and therefore $R(f;[x]) \subset f([x])$ holds.

For $x \neq 0$ we can rewrite $f(x)$ as

$$f(x) = \frac{x}{1-x} = \frac{1}{\frac{1}{x} - 1} \quad , \quad x \neq 0 \; .$$

For the interval arithmetic evaluation of this function over $[2;3]$ we get

$$\tilde{f}\,([x]) = \frac{1}{\frac{1}{[2;3]} - 1} = [-2\,;\,-\tfrac{3}{2}] = R(f;[x]) \; .$$

□

The preceding example shows that the overestimation of $R(f;[x])$ by $f([x])$ is strongly dependent on the arithmetic expression which is used for the interval arithmetic evaluation of the given function.

Moore [6] has shown that under reasonable assumptions the following inequality holds for the distance between $R(f;[x])$ and $f([x])$:

(2) $$q(R(f;[x]) , f([x])) \leq \gamma \, d[x] , [x] \subseteq [x]^0 , \gamma \geq 0 .$$

This means that the overestimation of $R(f;[x])$ by $f([x])$ goes linearly to zero with $d[x]$. We illustrate this using the following example.

Example 2. Let

$$f(x) = x - x^2 , \quad x \in [x]^0 = [0;1] .$$

Set $$[x] = [\tfrac{1}{2} - r ; \tfrac{1}{2} + r] , \quad 0 \leq r \leq \tfrac{1}{2} .$$

A simple discussion gives

$$R(f;[x]) = [\tfrac{1}{4} - r^2 ; \tfrac{1}{4}] .$$

For $f([x])$ we get

$$f([x]) = [\tfrac{1}{2} - r ; \tfrac{1}{2} + r] - [\tfrac{1}{2} - r ; \tfrac{1}{2} + r][\tfrac{1}{2} - r ; \tfrac{1}{2} + r]$$

$$= [\tfrac{1}{4} - 2r - r^2 ; \tfrac{1}{4} + 2r - r^2] .$$

From this we get

$$q(R(f;[x]) , f([x])) = \max \{ |\tfrac{1}{4} - 2r - r^2 - \tfrac{1}{4} + r^2| , |\tfrac{1}{4} + 2r - r^2 - \tfrac{1}{4}| \}$$

$$= \max \{2r \, , \, 2r - r^2\}$$

$$= 2r = \gamma \, d[x] \, , \, \gamma = 1 \, ,$$

as predicted by Moore's result (2). □

The second part of Example 1 rises the question whether it is possible to rearrange the variables of the given function in such a manner that the interval arithmetic evaluation gives higher than linear convergence to the range of values. The answer is "yes". Before we state the general result we consider again an example.

Example 3. The function $f(x) = x - x^2$, $x \in [0;1]$, from the preceding example can be rewritten as

$$f(x) = x - x^2 = \frac{1}{4} - (x - \frac{1}{2})(x - \frac{1}{2}) \, , \quad x \in [0;1] \; .$$

Plugging in intervals we get for the interval arithmetic evaluation

$$\tilde{f}([x]) = \frac{1}{4} - ([\frac{1}{2} - r \, ; \, \frac{1}{2} + r] - \frac{1}{2}) \, ([\frac{1}{2} - r \, ; \, \frac{1}{2} + r] - \frac{1}{2})$$

$$= \frac{1}{4} - [-r \, ; \, r] \, [-r \, ; \, r] = \frac{1}{4} + [-r^2 \, ; \, r^2]$$

$$= [\frac{1}{4} - r^2 \, ; \, \frac{1}{4} + r^2] \; .$$

Hence we get

$$q(R(f;[x]) \, , \, \tilde{f}([x])) = \max \{|\frac{1}{4} - r^2 - (\frac{1}{4} - r^2)| \, , \, |\frac{1}{4} + r^2 - \frac{1}{4}|\}$$

$$= r^2 = \frac{1}{4}(d[x])^2$$

which means that the distance goes quadratically to zero with $d[x]$.

The general result is as follows:

Theorem 1. (The centered form). Let the (rational) function $f : \mathbb{R} \to \mathbb{R}$ be represented in the form

$$(3) \qquad f(x) = f(z) + (x-z) \cdot h(x)$$

for some $z \in [x]$. If we define

$$(4) \qquad f([x]) := f(z) + ([x] - z)\, h([x])$$

then (under weak conditions on the interval arithmetic evaluation $h([x])$, see Theorem 2) it holds that

$$\text{a)} \qquad R(f;[x]) \subseteq f([x])$$

and

$$(5) \quad \text{b)} \qquad q(R(f;[x]) \, , \, f([x])) \leq \gamma \, (d[x])^2 \; . \qquad \square$$

Inequality (5) is called "Quadratic approximation property" of the centered form. (3) was introduced by Moore in [6], where he conjectured that (5) holds. (5) was first proved by E. Hansen [5].

How can one find the centered form?

Consider first the case that $f(x)$ is a polynomial

$$f(x) = a_o + a_1 x + \dots + a_n x^n \ .$$

Using the Taylorpolynomial (which can be computed by applying the complete Horner-scheme) we get

$$f(x) = f(z) + \frac{f'(z)}{1!} (x-z) + \dots + \frac{f^{(n)}(z)}{n!} (x-z)^n$$

$$= f(z) + (x-z)\, h(x)$$

where

$$h(x) = f'(z) + \frac{x-z}{2!} f''(z) + \dots + \frac{f^{(n)}(z)}{n!} (x-z)^{n-1} \ .$$

If $f(x)$ is a general rational function then (see Ratschek [7], [8]) for $s(x) \neq 0$ we can write

$$f(x) = \frac{r(x)}{s(x)} = f(z) + \frac{r(x) - f(z)\, s(x)}{s(x)}$$

$$= f(z) + (x-z) \frac{r(x) - f(z)\, s(x)}{(x-z)\, s(x)}$$

$$= f(z) + (x-z)\, h(x)$$

where

$$h(x) = \frac{r(x) - f(z)\, s(x)}{(x-z)\, s(x)} \quad .$$

Since $r(z) - f(z)\, s(z) = 0$ and $s(z) \neq 0$ the term $x-z$ appears both in the nominator and in the denominator of $h(x)$ and therefore can be cancelled out.

Example 4. Let

$$f(x) = \frac{r(x)}{s(x)} = \frac{x-x^2}{x-3} \,, \quad x \neq 3 \;.$$

For $z = \frac{1}{2}$ we have $f(z) = -\frac{1}{10}$ and therefore

$$f(x) = -\frac{1}{10} + (x - \tfrac{1}{2}) \frac{r(x) - (-\frac{1}{10})\, s(x)}{(x - \frac{1}{2})\, s(x)}$$

$$= -\frac{1}{10} + (x - \tfrac{1}{2}) \frac{\frac{1}{4} - (x - \frac{1}{2})\,(x - \frac{1}{2}) - (-\frac{1}{10})\,((x - \frac{1}{2}) - \frac{5}{2})}{(x - \frac{1}{2})\,((x - \frac{1}{2}) - \frac{5}{2})}$$

$$= -\frac{1}{10} + (x - \tfrac{1}{2}) \frac{\frac{1}{10} - (x - \frac{1}{2})}{-\frac{5}{2} + (x - \frac{1}{2})}$$

$$= -\frac{1}{10} + (x - \tfrac{1}{2})\, h(x)$$

where

$$h(x) = \frac{\frac{1}{10} - (x - \frac{1}{2})}{-\frac{5}{2} + (x - \frac{1}{2})} \quad . \qquad \square$$

The question whether there exists a representation of f such that for the interval arithmetic evaluation of this representation it holds that

$$q(R(f;[x]), f([x])) \leq \gamma \, (d[x])^m$$

where $m \geq 3$ is an open question. However, in special cases this can be achieved.

Theorem 2. (Generalized centered forms). Let the (rational) function $f : \mathbb{R} \to \mathbb{R}$ be represented in the form

(6) $$f(x) = \varphi_0 + \ell(x) \cdot h(x) \quad , \quad x \in [x] \, ,$$

where $\varphi_0 \in \mathbb{R}$. Assume that there exist intervals $\ell([x])$ and $h([x])$ such that

(7) $$\ell(x) \in \ell([x]) \, , \quad x \in ([x]) \, ,$$

(8) $$h(x) \in h([x]) \, , \quad x \in [x] \, ,$$

(9) $$|\ell([x])| \leq \tau (d[x])^n \, ,$$

(10) $$d(h([x])) \leq \sigma \, d[x] \, .$$

If we define

(11) $f([x]) := \varphi_0 + R(\ell;[x]) \cdot h([x])$

then

(12) $R(f;[x]) \subseteq f([x])$,

(13) $q(R(f;[x]) , f([x])) \leq \kappa(d[x])^{n+1}$. □

A proof of Theorem 2 has been performed in [1].

Example 5. a) Assume that

(14) $\ell(x) = (x-c)^n , \quad c \in [x]$.

Then

$$|\ell([x])| = |([x] - c)^n| \leq (d[x])^n$$

and therefore (9) holds.

For $n = 1$ in (14) we have the classical centered form (see Theorem 1). For $n > 1$ in (14) the result of Theorem 2 was already proved in [2].

b) Assume that

(15) $\ell(x) = (x-x_1) \cdot \ldots \cdot (x-x_n) , \quad x_i \in [x] , \quad i = 1(1)n$.

Then again

$$|\ell([x])| \leq (d[x])^n$$

and therefore (9) holds.

Whereas $R(\ell;[x])$ is easy to compute in case a) this is in general not true in case b). On the other hand it might be much easier to find a representation of $f(x)$ of the form (6) with $\ell(x)$ defined by (15) compared with finding such a representation using (14). □

We illustrate the preceding Theorem 2 by a simple example.

Example 6. Consider the real polynomial

$$f(x) = x^3 - 6x^2 + (12 - \epsilon^2)x - (8 - 2\epsilon^2) , \quad \epsilon \geq 0 ,$$

which has the zeroes

$$x_1 = 2 - \epsilon , \quad x_2 = 2 , \quad x_3 = 2 + \epsilon .$$

For $[x] = [2-\delta ; 2+\delta]$, $\epsilon \leq \delta \leq 2$, the zeroes are contained in $[x]$.

a) If $\delta^3 - \epsilon^2\delta \geq \frac{2}{9}\sqrt{3}\,\epsilon^3$ then

$$R(f;[x]) = [- \delta^3 + \epsilon^2\delta ; \delta^3 - \epsilon^2\delta] .$$

b) If $\delta^3 - \epsilon^2\delta < \frac{2}{9}\sqrt{3}\,\epsilon^3$ then

$$R(f;[x]) = \frac{2}{9}\sqrt{3}\,\epsilon^3\,[-1\,;\,1]\,.$$

We consider three different cases for the inclusion of $R(f;[x])$ by the evaluation of interval expressions.

A) $f([x]) = f([2-\delta\,;\,2+\delta])$

$$=[-\delta^3 + \delta\epsilon^2 - 48\delta\,;\,\delta^3 - \epsilon^2\delta + 48\delta]$$

from which it follows that

$$q(R(f;[x])\,,\,f([x])) \le \gamma\, d[x]\,.$$

This agrees with Moore's result (2).

B) $f(x)$ can be written as

$$f(x) = \varphi_o + \ell(x)\cdot h(x)$$

where $\varphi_o = 0\,,\;\ell(x) = x-2\,,\;h(x) = x^2 - 4x + 4 - \epsilon^2\,.$

From this we get

$$f([x]) := \varphi_o + R(\ell;[x])\cdot h([x])$$

$$= [-\delta\ ;\ \delta]\ ([2-\delta\ ;\ 2+\delta][2-\delta\ ;\ 2+\delta] - 4[2-\delta\ ;\ 2+\delta] + 4 - \epsilon^2)$$

$$= [-\delta^3 + \delta\epsilon^2 - 8\delta^2\ ;\ \delta^3 - \delta\epsilon^2 + 8\delta^2]$$

and therefore

$$q(R(f;[x])\ ,\ f([x])) \leq \gamma\ (d[x])^2$$

which agrees with the statement (5) of Theorem 1.

C) If we write f(x) as

$$f(x) = \varphi_0 + \ell(x) \cdot h(x)$$

where

$$\varphi_0 = 0\ ,\ \ \ell(x) = (x-2)\ (x - (2+\epsilon))\ ,\ h(x) = x - (2-\epsilon)$$

then

(16) $$f([x]) = \varphi_0 + R(\ell;[x]) \cdot h([x])$$

$$= [\min\ \{-\frac{\epsilon^2}{4}(\delta + \epsilon)\ ,\ \ -(\delta - \epsilon)(\delta^2 + \epsilon\delta)\}\ ;$$

$$\max\ \{\frac{\epsilon^2}{4}(\delta - \epsilon)\ ,\ \ (\delta^2 + \epsilon\delta)(\delta + \epsilon)\}]$$

and therefore

(17) $q(R(f;[x]) , f([x])) \leq \gamma \, (d[x])^3$

which agrees with the statement (13) for $n = 2$ of Theorem 2. See Example 5, case a). It is important to note that (17) is no longer true if we replace $R(\ell;[x])$ by $\ell([x])$ (the interval arithmetic evaluation) in (16). □

Cornelius and Lohner [4] had the idea to consider so-called remainder forms of f for including the range of f by higher order methods.

Theorem 3. (Remainder form). Let $f : D \subseteq \mathbb{R} \to \mathbb{R}$ have a representation of the form

$$f(x) = g(x) + s(x) \quad , \quad x \in D \ .$$

Assume that

$$R(s;[x]) \subseteq s([x]) \quad , \quad [x] \subseteq D \ .$$

Define

(18) $f([x]) := R(g;[x]) + s([x])$.

Then

a) $R(f;[x]) \subseteq f([x])$

b) $$q(R(f;[x]), f([x])) \leq d(s([x])) \leq 2|s([x])| . \quad \square$$

How can one find a remainder form of f ?

Suppose that f has derivatives of sufficiently high order. Let $p_\sigma(x)$ be the unique polynomial of degree $\sigma \geq 0$ solving the Hermite interpolation problem:

(19) $$p_\sigma^{(j)}(x_i) = f^{(j)}(x_i) \; ; \quad j = 0(1)m_i - 1 , \; m_i \in \mathbb{N} , \quad i = 0(1)n , \; n \geq 0 ,$$

where $x_o, x_1, \dots , x_n \in [x]$ are pairwise distinct and

$$\sigma + 1 = \sum_{i=o}^{n} m_i .$$

Then it is well known that

(20) $$f(x) = p_\sigma(x) + \frac{f^{(\sigma+1)}(\xi(x))}{(\sigma+1)!} \prod_{i=o}^{n} (x-x_i)^{m_i}$$

$$= g(x) + s(x) , \quad x \in [x]$$

where we have set $g(x) = p_\sigma(x)$ and $s(x)$ is the remainder term. Assume now that the derivative $f^{(\sigma+1)}$ has an interval arithmetic evaluation over $[x]$. Then, since $\xi(x) \in [x]$, we can set

$$s([x]) = \frac{f^{(\sigma+1)}([x])}{(\sigma+1)!} \prod_{i=o}^{n} ([x]-x_i)^{m_i} .$$

Using this $s([x])$ in (18) Lohner and Cornelius [4] have proved that

$$(21) \qquad q(R(f;[x]) , f([x])) \le \gamma(d[x])^{\sigma+1} .$$

Of course it must be stressed that practically only small values of σ are possible for finding $R(g;[x])$ in (18).

Example 7. Take

$$n = 0 , \quad m_o = 3 , \quad \sigma = 2 .$$

Then we have given

$$p_2^{(j)}(x_o) = f^{(j)}(x_o) , \quad j = 0(1)2 , \quad x_o \in [x] ,$$

and (20) reads

$$f(x) = f(x_o) + \frac{f'(x_o)}{1!}(x-x_o) + \frac{f''(x_o)}{2!}(x-x_o)^2 + \frac{1}{3!} f'''(\xi(x))(x-x_o)^3$$

$$= g(x) + s(x)$$

where

$$g(x) = f(x_o) + \frac{f'(x_o)}{1!}(x-x_o) + \frac{f''(x_o)}{2!}(x-x_o)^2 ,$$

$$s(x) = \frac{1}{3!} f'''(\xi(x))(x-x_o)^3 .$$

$R(g;[x])$ is easy to compute in this case since $g(x)$ is a quadratic polynomial. For

$$f([x]) := R(g;[x]) + \frac{1}{3!} f'''([x])([x]-x_0)^3$$

we have by (21)

$$q(R(f;[x]) , f([x])) \le \gamma(d[x])^3 . \qquad \square$$

4. Outlook

The discussion in the preceding chapter shows that although it is easy to include the range of functions using interval arithmetic tools it is in general not obvious how to find very good inclusions with a reasonable amount of work. Therefore this problem needs very careful further investigations.

We have not considered functions of several variables. From a practical point of view including the range of such a function is even of much greater importance. See [10], for example, where optimization algorithms, based on interval arithmetic tools, are discussed. In principle all results of the present paper hold for the multidimensional case. However, getting good inclusions is in general much more laborious than for the one dimensional case.

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