BIT manuscript No.
(will be inserted by the editor)

On a quality measure for interval inclusions

Siegfried M. Rump and Takeshi Ogita

Received: date / Accepted: date

Abstract Verification methods compute intervals which contain the solution of a given problem with mathematical rigor. In order to compare the quality of intervals some measure is desirable. We identify some anticipated properties and propose a method avoiding drawbacks of previous definitions.

Keywords Verification methods, interval, relative error, INTLAB

Mathematics Subject Classification (2000) 65G40

1 Main result

Verification methods produce mathematically rigorous error bounds for the solution of a numerical problem including the proof that the problem is solvable. For an overview of verification methods cf. [4,7] and [in Japanese] [5].

When developing a new verification method, it is desirable to have some measure for the quality of an inclusion. We consider an inclusion interval X as error bounds for an unknown real quantity $\hat{x}$, i.e., $\hat{x} \in X$. Depending on the situation, we use synonymous notations for an inclusion interval, namely

$$\begin{aligned} X = [\underline{x}, \overline{x}] &:= \{x \in \mathbb{R} : \underline{x} \leqslant x \leqslant \underline{x}\} = \\ \langle m, r\rangle &:= \{x \in \mathbb{R} : m - r \leqslant x \leqslant m + r\} \ . \end{aligned}$$

A colloquial notation is $\langle m, r\rangle = m \pm r$. Consider

$$X_1 := [-1, 2], \quad X_2 := [-1, 1], \quad \text{and} \quad X_3 := [1, 2] \ .$$

S. M. Rump
Institute for Reliable Computing, Hamburg University of Technology, Am Schwarzenberg-Campus 3, Hamburg 21073, Germany, and Visiting Professor at Waseda University, Faculty of Science and Engineering, 3–4–1 Okubo, Shinjuku-ku, Tokyo 169–8555, Japan E-mail: rump@tuhh.de

Takeshi Ogita
Faculty of Science and Engineering, Waseda University, 3-4-1 Okubo, Shinjuku-ku, Tokyo 169-8555, Japan (`t.ogita@waseda.jp`).

All three intervals may be considered as not giving much information, only X_3 proves at least that $\hat{x}$ is positive. Now let A be a symmetric matrix with $\|A\| = 10^{10}$ and let the X_ν be inclusions of an eigenvalue. Then all three inclusions X_ν reveal that the condition number of A is at least $5 \cdot 10^9$.

It follows that the quality of an interval inclusion depends on the context. Having said that, it may nevertheless be desirable to define a measure for the quality of an interval, knowing the pros and cons of such an attempt. There is some folklore about such measures, however, to that end we found only one paper in the literature, see below.

Let $\varrho : \mathbb{R} \times \mathbb{R}_{\geqslant 0} \to \mathbb{R}_{\geqslant 0}$ be such a function for the quality $\varrho(m,r)$ of $\langle m, r \rangle$. The letter ϱ may remind of "relative error", however, we prefer the wording "quality" because mathematically ϱ may be interpreted as relative error, but only in a certain sense (seee below). Note that $\varrho(m,r) = 0$ means best quality. We first list some desirable properties of such a function:

I)	non-negativity	$\varrho(m,r) \geqslant 0$
II)	zero value	$\varrho(m,r) = 0 \;\Leftrightarrow\; r = 0$
III)	scaling invariance	$\varrho(X) = \varrho(\alpha X)$ for $0 \neq \alpha \in \mathbb{R}$
IV)	monotonicity for fixed m	$r' > r \;\Rightarrow\; \varrho(m,r') > \varrho(m,r)$
V)	monotonicity for fixed r	$\lvert m'\rvert > \lvert m\rvert \;\Rightarrow\; \varrho(m',r) < \varrho(m,r)$

The rationale is as follows. Properties I) and II) are clear. As for III), the quality of an inclusion interval X may well depend on the scaling for different settings, see the above example. However, without knowing any setting, invariance with respect to scaling seems the only option. For the monotonicity, an interval with constant midpoint but increasing radius gives less information, and with constant radius but increasing absolute value of the midpoint[1] the interval contains, in some sense, more information.

Moreover, we may demand ϱ to be continuous in m and r exept for $m = r = 0$ because for $r > 0$ it follows $\varrho(0,0) < \varrho(0,r) = \varrho(0,1)$. As for differentiability note that $\varrho(m,r) = \varrho(-m,r)$ would imply $\frac{d\varrho}{dm}(0,r) = 0$ for all $r > 0$, but then V) and I) lead to a contradiction. Therefore

VI)	continuity	$\varrho(m,r)$ is everywhere continuous except for $m = r = 0$
VII)	differentiability	$\varrho(m,r)$ is everywhere differentiable except for $m = 0$

Having listed the desired properties, we look for possible candidates. An obvious choice is to use the midpoint m of $X = \langle m, r \rangle$ as an approximation and define $\varrho(X)$ to be the largest relative error of $x \in X$ with respect to m:

$$\varrho_1(m,r) := \max_{x \in X} \left| \frac{x-m}{m} \right| \quad \text{implying} \quad \varrho_1(X) = \left| \frac{\overline{x} - \underline{x}}{\underline{x} + \overline{x}} \right| . \tag{1.1}$$

All properties I) to VII) are satisfied, however, there is an obvious problem for zero midpoints. If our unknown real quantity $\hat{x}$ is equal to zero, then $\varrho_1(0,r)$ is infinite no matter how small the radius r is.

[1] Note that III) implies $\varrho(m,r) = \varrho(-m,r)$.

A remedy is to use the maximum over the minimal relative error against some $\tilde{x} \in X$, i.e.,

$$\varrho_2(X) := \min_{\tilde{x}\in X} \max_{x\in X} \left| \frac{\tilde{x} - x}{\tilde{x}} \right| . \tag{1.2}$$

That is the definition in [3], the only reference we found. It is shown that

$$\varrho_2(m,r) = \begin{cases} \dfrac{r}{|m|} & \text{if } |m| - r \geqslant 0 \\ \dfrac{2r}{\max(|m-r|, m+r)} & \text{otherwise} \end{cases} .$$

The properties I) to VI) are satisfied for ϱ_2, however, differentiability VII) is not met:

$$\varrho_2(1, 1+e) = \begin{cases} 1+e & \text{if } e \leqslant 0 \\ \dfrac{1+e}{1+e/2} & \text{if } e \geqslant 0 . \end{cases}$$

As has been mentioned there is some folklore about quality measures, in particular

$$\varrho_3(X) := \frac{\overline{x} - \underline{x}}{|\underline{x}| + |\overline{x}|} \tag{1.3}$$

with $0/0 := 0$. That avoids the zero midpoint problem, but for all intervals X containing zero $\underline{x} \leqslant 0 \leqslant \overline{x}$ implies

$$0 \in X : \quad \varrho_3(X) = \frac{\overline{x} + |\underline{x}|}{|\underline{x}| + \overline{x}} = 1 .$$

The properties I) to VI are satisfied, but ϱ_3 is not differentiable for one endpoint zero:

$$\varrho_3([0,e]) = \begin{cases} 1 & \text{if } e > 0 \\ \dfrac{e}{|e|} & \text{if } e < 0 . \end{cases}$$

In order to find a function ϱ sharing all properties I) to VII) but avoiding the problems for zero midpoint we use, in view of $\varrho(m,r) = \varrho(-m,r)$, the ansatz

$$\varrho(m,r) = \frac{\alpha|m| + \beta r}{\gamma|m| + \delta r}$$

for constants $\alpha, \beta, \gamma, \delta$ to be determined. Property II) implies $\alpha = 0$ and $\gamma \neq 0$, so that using III) and some scaling we can restrict our attention to

$$\varrho(m,r) = \psi \, \frac{r}{\varphi|m| + r}$$

with a scaling factor ψ defining the maximum of ϱ. Rewriting $\varrho(m,r) = \psi \left(\varphi \frac{|m|}{r} + 1 \right)^{-1}$ it is easy to verify that this definition satisfies all properties I) to VII) for any $\varphi > 0$. In order to find a suitable choice for φ we look at intervals with fixed left endpoint $\underline{x} = -1$ and right endpoints $-1 \leqslant \overline{x} \leqslant 1$, that is $X_r := \langle -1+r, r\rangle$ for $0 \leqslant r \leqslant 1$. Then

$$\varrho(X_r) = \frac{\psi r}{\varphi(1-r)+r}.$$

A good choice may be $\varphi = 1$ in which case $\varrho(X_r)$ grows linearly. Hence,

$$\varrho(m,r) := \frac{\psi r}{|m|+r}\ .$$

Now it is a matter of taste to fix ψ. We may feel that $\varrho([0,1]) = 1$ should hold. That implies $\psi = 2$, so that we define

$$\varrho_4(m,r) := \frac{2r}{|m|+r} \tag{1.4}$$

implying $\varrho_4(m,r) \leqslant 2$ for all m, r. For $X = [\underline{x}, \overline{x}]$ it follows

$$\varrho_4(X) = \min\left(\left|\frac{\overline{x}-\underline{x}}{\underline{x}}\right|, \left|\frac{\overline{x}-\underline{x}}{\overline{x}}\right|\right),$$

the minimal relative error of the midpoints against each other. In verification methods $\mathrm{mag}(X) := \max\{|x| : x \in X\}$ is called the magnitude of an interval. Hence $\varrho_4(X) = \mathrm{diam}(X)/\mathrm{mag}(X)$. An advantage over ϱ_3 is that no case distinction is necessary in the computation. An almost identical formulation

$$\varrho_4'(X) = \frac{\overline{x}-\underline{x}}{\max(|\underline{x}|, |\overline{x}|, \eta)}$$

was suggested by Demmel [1]. It is equal to ϱ_4 except that it is tailored to IEEE754 [2] arithmetic standard by using the underflow unit $\eta = 2^{-1074}$.

In Figure 1.1 the four definitions ϱ_ν are compared for fixed midpoint $m = 1$ and for fixed left endpoint $\underline{x} = -1$.

The first function ϱ_1 [relative error against midpoint, red] shows a linear behavior for fixed midpoint and growing radius, and tends to infinity if the midpoint approaches zero. As discussed the second function ϱ_2 [Kreinovich's definition, black with circles] it is not differentiable at $m = r$. The "folklore" function ϱ_3 [green] is not differentiable for zero endpoint and flat equal to the maximal value 1 for intervals containing zero, no discrimination in terms of small or large radius. Finally, the new definition ϱ_4 [blue] is, as ϱ_1, linear for fixed midpoint and growing radius, and everywhere differentiable except for $m = 0$.

The first three definitions coincide in the left picture for $X = \langle 1, r\rangle$ with $r \in [0,1]$, and in the right picture for $X = [-1, -1+d]$ with $d \in [0,1]$. In both pictures Kreinovich's definition ϱ_3 and the proposed ϱ_4 coincide for $r \geqslant 1$ and $d \geqslant 1$, respectively. So the proposed measure ϱ_4 differs from the other definitions for $r \in [0,1]$ and $d \in [0,1]$ in the left and right picture, respectively. This ensures differentiability everywhere except zero midpoint.

The definition $\varrho_4(X) = \frac{\mathrm{diam}(X)}{\mathrm{mag}(X)}$ with the interpretation $\frac{0}{0} = 0$ can be used for complex intervals as well. It will replace the function `relerr` in INTLAB [6], the Matlab/Octave toolbox for reliable computing.

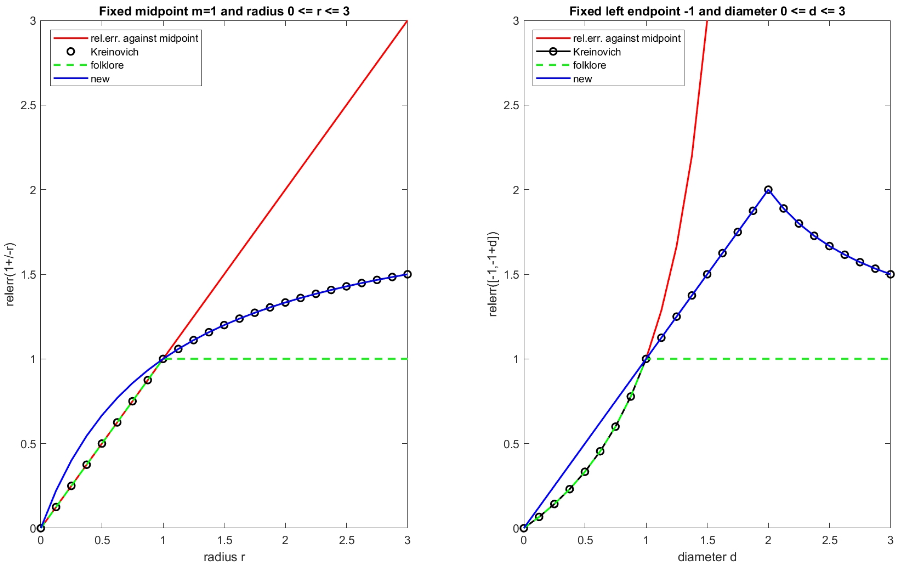

Fig. 1.1: The functions ϱ_ν for fixed midpoint $m = 1$ (left) and fixed left endpoint -1 (right)

2 Conflict of interest

Not applicable.

References

1. J.B. Demmel. private communication, 2012.
2. IEEE standard for floating-point arithmetic. *IEEE Std 754-2019 (Revision of IEEE 754-2008)*, pages 1–84, 2019.
3. Vladik Kreinovich. How to define relative approximation error of an interval estimate: a proposal. *Applied Mathematical Sciences*, 7(5):211–216, 2013.
4. Arnold Neumaier. *Interval methods for systems of equations*. Encyclopedia of Mathematics and its Applications. Cambridge University Press, 1990.
5. Shin'ichi Oishi, Kazuhiro Ichihara, Masahide Kashiwagi, Takuma Kimura, Xuefeng Liu, Hidetoshi Masai, Yusuke Morikura, Takeshi Ogita, Katsuhisa Ozaki, Siegfried M. Rump, Kouta Sekine, Akitoshi Takayasu, and Naoya Yamanaka. *Principle of Verified Numerical Computations*. Corona publisher, Tokyo, Japan, 2018. [in Japanese].
6. Siegfried M. Rump. INTLAB – INTerval LABoratory. In Tibor Csendes, editor, *Developments in Reliable Computing*, pages 77–104. Springer Netherlands, Dordrecht, 1999.
7. Siegfried M. Rump. Verification methods: Rigorous results using floating-point arithmetic. *Acta Numer.*, 19:287–449, 2010.