POWER AND BEAUTY OF INTERVAL METHODS

Marek W. Gutowski

Institute of Physics, Polish Academy of Sciences
02–668 Warszawa, Al. Lotników 32/46, Poland
e-mail: gutow@ifpan.edu.pl

Abstract

Interval calculus is a relatively new branch of mathematics. Initially understood as a set of tools to assess the quality of numerical calculations (rigorous control of rounding errors), it became a discipline in its own rights today. Interval methods are useful whenever we have to deal with uncertainties, which can be rigorously bounded. Fuzzy sets, rough sets and probability calculus can perform similar tasks, yet only the interval methods are able to (dis)prove, with mathematical rigor, the (non)existence of desired solution(s). Known are several problems, not presented here, which cannot be effectively solved by any other means.

This paper presents basic notions and main ideas of interval calculus and two examples of useful algorithms.

Keywords

reliable computations; guaranteed results; global optimization; algebraic systems; automatic result verification; constraint satisfaction

I. WHAT IS AN INTERVAL ANYWAY?

Definition: The interval is a bounded subset of real numbers. Formally:

\( (X = [a, b]) \) is an interval \( \iff (X = \{x \in \mathbb{R} | a \leq x \leq b\}) \),

where \( a, b \in \mathbb{R} \) (set of all real numbers); in particular \( a, b \), or even both of them may be infinite.

Geometrically, interval is just a section of a real line, uniquely determined by its own endpoints. The set of all intervals is commonly denoted as \( \mathbb{IR} \). Lower and upper endpoint of interval \( X \) is usually referred to as \( X \) and \( \overline{X} \), respectively. Intervals with property \( X = \overline{X} \) are called thin (or degenerate), any of them contains exactly one real number and can be thus formally identified with this very number. Two basic real-valued functions defined on intervals (i.e. of type \( \mathbb{IR} \mapsto \mathbb{R} \)) are: width: \( w(X) = |X| \equiv |\overline{X} - X| \), and center: \( \text{mid}(X) \equiv \frac{1}{2}|X + \overline{X}| \).

Algebraic operations on intervals are defined in such a way that their results always contain every possible outcome of the corresponding algebraic operation on real numbers. More specifically: the result of \( X \odot Y \) is again an interval, \( Z \), with property

\( X \odot Y = Z = \{z = x \odot y \mid x \in X, y \in Y\} \),

where \( \odot \) belongs to the set \( \{+,-,\times,\div\} \). One can easily prove that arithmetic operations on intervals can be expressed in terms of ordinary arithmetics on their endpoints:

\[
X + Y = [X + Y, \overline{X} + \overline{Y}] \quad X - Y = [X - \overline{Y}, \overline{X} - Y]
\]

\[
X \cdot Y = [\min(X \cdot Y, X \cdot \overline{Y}, \overline{X} \cdot Y, \overline{X} \cdot \overline{Y}), \max(X \cdot Y, X \cdot \overline{Y}, \overline{X} \cdot Y, \overline{X} \cdot \overline{Y})]
\]

\[
X/Y = [\min(X/Y, X/\overline{Y}, \overline{X}/Y, \overline{X}/\overline{Y}), \max(X/Y, X/\overline{Y}, \overline{X}/Y, \overline{X}/\overline{Y})]
\]
with an extra condition for division: \( 0 \notin Y \).

In computer realization we have to take care of proper rounding of every intermediate result in order to preserve the property that the final results are guaranteed. The appropriate rounding is called *outward* or *directed rounding*, i.e. \( \underline{X} \) must be always rounded down (‘towards \( -\infty \)’) and \( \overline{Y} \) has to be rounded up (‘towards \( +\infty \)’). This is achieved either in hardware, by proper switching back and forth the processor’s rounding mode (still rare), or in software as *simulated rounding* (majority of existing software packages).

**Intervals as sets.** Since intervals are sets, it is possible to carry typical set operations on them. For example we can consider the intersections of intervals, like \( Y = X_1 \cap X_2 \).

However, the intersection of two disjoint intervals is an empty set! This shows the necessity of considering the **empty interval** as a legitimate member of the set \( \mathbb{R} \). It is usually denoted as \( \emptyset \) and in machine representation should be, for many reasons, expressed as \([INF, -INF]\), where \( INF \) is the largest machine-representable positive number.

Unfortunately, the **union** of two intervals is not always an interval. Instead, we can define the **interval hull** of two arbitrary intervals (or of any other subset of \( \mathbb{R} \) as well) as the smallest interval containing them both:

\[
\text{hull}(X, Y) = \left[ \min(X, Y), \max(X, Y) \right]
\]

There is no problem with checking whether \( X \subset Y \) (or \( X \subseteq Y \)).

It is worth to mention that addition and multiplication of intervals are both commutative: \( X \odot Y = Y \odot X \), and associative: \( X \odot Y \odot Z = (X \odot Y) \odot Z = X \odot (Y \odot Z) \). However, it is surprising that in general the following holds:

\[
X \cdot (X + Z) \subseteq X \cdot Z + X \cdot Y
\]

(and not just equality!) i.e. the multiplication is only *subdistributive* with respect to addition. We can also see, that using the same variable more than once (here: \( X \)), in rational expression, leads inadvertently to the overestimation of the final result. This phenomenon is known under the name of **dependency problem**. This property, together with the lack of good order in \( \mathbb{IR} \) (\( \mathbb{IR} \) is only partially ordered set (poset)) makes conversion of ordinary computer programs into their interval equivalents not a straightforward task. In particular, every computer instruction of the type

```java
if x < y
    then . . .
else . . .
end if
```

has to be carefully redesigned.

**Example:**

Before shopping I had exactly 100.00 monetary units in my pocket and my wife had something between 42.00 and 45.00 units. So we had together \([142, 145]\) units. We have already spent 127.99 units, so we still have \([14.01, 17.01]\) units. Can we afford to call a taxi with estimated cost \([13, 15]\) units? **Possibly** . . .

But, without any credit, we **certainly** can buy two bottles of milk at the cost \(2 \times [1.19, 3.59] = [2.38, 7.18]\) units. Guaranteed.

**Interval vectors and matrices.** Any \( n \)-dimensional vector with at least one interval component may be called interval vector or **box**. Any matrix with at least one interval entry will be called an interval matrix. Ordinary linear algebra can be done on those
objects, if only every elementary arithmetic operation is substituted by its suitable interval counterpart, as defined earlier. The most often used norms for interval vectors are: \( \| \cdot \|_1 \), equal to the sum of widths of all its components, and \( \| \cdot \|_\infty \) being the width of the widest component.

II. INTERVAL FUNCTIONS

An obvious requirement for the good interval substitute \( F \) of the real-valued function \( f \) is following

\[
F(X) = \bigcap_{x \in X} f(x) = \left[ \inf_{x \in X} f(x), \sup_{x \in X} f(x) \right]
\]

We would call such an \( F(X) \) a range function for \( f \). The explicit construction of range function may be difficult, so we often work with the so called inclusion or inclusive functions. These are not unique, but any such function satisfies

\[
F(X) \supseteq f(x) \quad \forall x \in X
\]

\( F \) is also called an interval extension for \( f \). Note, that:

- \( F \) may be ‘broader’ than the range function, i.e. it usually overestimates the range of function \( f \), and
- there is no explicit specification how large (or small) this overestimation can be.

The most desirable are the so called monotonic inclusion functions, i.e. such inclusion functions, which additionally satisfy the implication

\[
\left( X \to x \right) \Rightarrow \left( F(X) \to f(x) \right) \quad \forall x \in X
\]

more properly formulated as

\[
\left( X_1 \subset X_2 \right) \Rightarrow \left( F(X_1) \subset F(X_2) \right)
\]

This is only possible for functions, which are everywhere continuous. Shortly one can say that range functions and monotonically inclusive functions produce thin intervals for thin arguments, while functions, which are only inclusive generally return ‘true’ (i.e. non-degenerate) intervals — even if their arguments are thin.

Example:

Let \( f(x) = \text{sign} \ x = \begin{cases} +1 & \text{when } x > 0 \\ 0 & \text{when } x = 0 \\ -1 & \text{when } x < 0 \end{cases} \)

The range function corresponding to sign is:

\[
\text{SIGN}(X) = \begin{cases} +1 & \text{when } \ X > 0 \\ 0, +1 & \text{when } \ X = 0 \\ -1, +1 & \text{when } \ X < 0 \\ -1, 0 & \text{when } \ X = 0 \\ -1 & \text{when } \ X < 0 \\ 0 & \text{when } \ X = [0, 0] \end{cases}
\]

and one of its many inclusion functions may be given as

\[
F(X) = [-1.5, 2.5]
\]

while no monotonically inclusive function exists for this case, since the original function is discontinuous.

Important remark. The value of the range function for argument \( X \) should be calculated only for \( x \in X \cap D(f) \), where \( D(f) \) is domain of \( f \). Empty set should be returned whenever \( X \cap D(f) = \emptyset \). Therefore \( \sqrt{[-4, +4]} = [0, 2] \) and \( \sqrt{[-20, -10]} = \emptyset \).
III. INTERVAL-ORIENTED ALGORITHMS

As George Corliss pointed out, usual (i.e. non-interval) algorithms only rarely are a good starting point for interval oriented ones. The vast majority of work done so far was concentrated on optimization problems and on solving systems of algebraic equations in many variables. There are remarkable results achieved in this field with interval version of Newton method being the most honored.

The typical example of interval methods is the algorithm due to Ramon E. Moore and Stieg Skelboe, which belongs to the class of ‘divide and bound’ algorithms. Suppose our task is to find the global minimum of a real-valued function $f$ of $n$ variables over the box $V_0 = X_1 \times X_2 \times \cdots \times X_n$. The initial step is to construct an interval extension $F$ for the function $f$. The algorithm operates on the list of $n$-dimensional boxes, $L$, which initially contains the only element, a pair: the box $V_0$ and the interval $F(V_0)$. We will also need a real number, $f_{\text{test}}$, initially equal to $\uparrow f$ (any $x \in V_0$) or just $F(V_0)$. The outline of the rest of algorithm, in pseudo code, follows:

```plaintext
do while diameter of the first box on the list $L$ exceeds some predefined value
pick the first element $V$ and its bounds $F(V)$ from list $L$
remove $V$ from $L$
if $F(V) \leq f_{\text{test}}$ then
  bisect $V$ perpendicularly to its longest edge obtaining $V_1 \cup V_2 = V$
calculate intervals $F_1 = F(V_1)$ and $F_2 = F(V_2)$
  for $i = 1, 2$ do
    if $F_i > f_{\text{test}}$
      then discard box $V_i$
    else put pair $(V_i, F_i(V_i))$ at the end of $L$
  end if
  $f_{\text{test}} \leftarrow \min \left(f_{\text{test}}, \overline{F_i}, \uparrow f(\text{center of } V_i)\right)$
end if
end for
end if
end do
```

The operation ‘$\uparrow$’ means round the next number up. The algorithm continuously ‘grinds’ boxes on the list $L$, making them smaller and smaller. Some of them disappear forever. At exit we can say that the global minimizer(s) $x^*$, such that $f(x^*) = \min_{x \in V_0} f(x)$, is (are) contained with certainty in the union of all the boxes still present on $L$. Numerous variants of the above algorithm do exist for less general cases, for example, when $f$ is differentiable almost everywhere in $V_0$. It is absolutely essential, from the performance point of view, to get rid of ‘bad’ (sub)boxes as early as possible. And the reason is clear: to test all subboxes, which are twice smaller than $V_0$ (in each direction), it is necessary to consider up to $2^n$ of them. The properties of $f$ and its interval extension $F$ as well, can influence the speed of convergence, which may be arbitrarily slow.

Due to space limitations, we have to stop here with this introductory course. More, and most likely better, materials can be found in the web [1]. The excellent starting point, with pointers to other valuable sites, is also [2]. Those, who prefer classical forms are encouraged to see the book [3].
IV. WHERE ARE WE TODAY?

Interval analysis started as a part of numerical analysis, devoted mainly to automatic verification of computer-generated results. The four basic arithmetic operations were everything what was needed for this purpose. There were two goals in front of researchers and users of interval calculus:

- to obtain guaranteed bounds for results in every case, and
- to make every possible effort to have those bounds as tight as possible.

They are still important, therefore better and better methods for construction of inclusion functions are discussed. Besides naive (natural) expressions we have at our disposal mean value theorem, Lipschitz forms, centered forms, and — recently — Taylor centered forms. After (re)discovering various old theorems, and proving new ones, it became clear, that interval methods, mostly those based on fixed point theorems, have enormous power to prove or disprove, with mathematical rigor, the existence of solutions to nonlinear systems of equations. As a complete surprise we learned that some problems, thought hopeless, can be successfully attacked with interval methods, while no other method apply.

Two kinds of research activity is visible today:

- introduction of interval methods into other branches of ‘hard’ science, like physics, astronomy or chemistry, as well as into engineering and business everyday practice
- establishing connections with other branches of pure and applied mathematics like, for example, fuzzy set theory, mathematical statistics and others.

The first area is ‘easy’. Just learn, implement and use. Continuously increasing computing power makes interval calculations feasible and acceptable, regardless that they are usually 8–20 times slower than their regular floating-point counterparts. This is no longer a serious problem. Commercial and free software is also easily available.

The second kind of activity goes much deeper. New ideas are emerging, interval methods inspire specialists from other fields. One can clearly notice gradual shift of interest into, generally speaking, imprecise probability theory. Practical consequences are important in environmental protection, risk analysis, robotics, fuzzy sets theory and applications, experimental data processing, quality control, electric power distribution, constraint propagation, logic programming, differential equations — to name a few.

V. NEW PARADIGMS IN EXPERIMENTAL SCIENCES

Parameter identification in engineering and data fitting in experimental sciences are code words for nearly the same thing. The task of reconstruction of values of unknown parameters, given experimental observations, lies at the heart of the so called inverse problems. The problem is usually formulated as follows:

**given:**

- $N$ observations $y_1, y_2, \ldots, y_N$,
- taken for the corresponding values $x_1, x_2, \ldots, x_N$ of the control variable $x$,
- depending additionally on $p$ unknown parameters $a_1, a_2, \ldots, a_p$, $p < N$,
- and the mathematical model, $f(x, y, a) = 0$, relating $y$’s with $x$’s and with the constant vector $a$

**find** the numerical values of all parameters $a_1, a_2, \ldots, a_p$.

There is a bunch of, more or less standard, approaches to this problem, especially, when the relation $f(x, y, a) = 0$ is simply a function $y = f(x, a)$. The most popular are: least squares method (LSQ), least absolute deviations (LAD) and maximum entropy methods (MEM). All they are based on finding the absolute (global) minimum of the appropriately
chosen functional. We would like to find the most appropriate set of unknown parameters, which is also the minimizer of such a functional. It is obvious, that the final result may vary, depending on which functional shall be used.

Let us now present the interval-type approach to this very problem. We will replace minimization procedure by solution of suitable constraint satisfaction problem. Both the $x$’s and $y$’s, due to unavoidable experimental uncertainties, should be treated as intervals containing the (unknown) true value. We will assume, that those intervals are indeed guaranteed, i.e. they contain the true values of control variables, and measured results respectively, with probability equal exactly to 1. We will search not for the most likely values of unknown parameters $a$, but for their possible values instead. For example, when fitting the straight line (extension for more complicated cases is immediate) $y = ax + b$, (parameters $a = (a, b)$), we will consider the set of relations:

$$\{(a x_j + b) \cap y_j \neq \emptyset \quad j = 1, 2, \ldots, N\}$$

In geometrical interpretation the above means that the straight line with slope in the interval $a$ and intercept in the interval $b$, both yet unknown, passes through every ‘uncertainty rectangle’ $x_i \times y_i$, $i = 1, 2, \ldots, N$. In purely algebraic terms:

$$((a x_j + b) \cap y_j \neq \emptyset) \iff (a x_j + b \leq y_j \land a x_j + b \geq y_j)$$  \hspace{1cm} (1)

This way the data themselves and their uncertainties, with no additional assumptions, determine the intervals for possible values of unknown parameters $a$ and $b$. Such a possibility was first pointed out by Walster [4] in 1988. To discover the intervals $a$ and $b$ we will use the following procedure:

1. start with initial box $V = (a, b)$ such that all inequalities (1) are possibly satisfied somewhere within $V$ but certainly not on their faces.
2. working with $V'$, the exact copy of $V$, and using box slicing algorithm, obtain its new version taking into account all the inequalities $a x_j + b \leq y_j$ only.
3. working with $V''$, another exact copy of $V$, and using box slicing algorithm again, obtain its new version when only the inequalities $a x_j + b \geq y_j$ are all satisfied.
4. if $V' \cap V'' \neq V$
   then $V \leftarrow V' \cap V''$
   if $V \neq \emptyset$ then goto step 2 else stop
   else stop

The last step illustrates very important and often used rule of interval calculations: if the result can be obtained on more than one way — do so and take the intersection of partial results as the final one. Sometimes at this step $V' \cap V''$ will be empty. If this ever happens, then we can be sure, that there are no solutions within the initial box $V$. This may mean one of two things:

- either our data set contains one or more outliers, or
- our mathematical model ($f$) is inadequate, the theory is invalidated by present observations.

The box slicing algorithm, reducing $p$-dimensional initial box $V$, is given below. Explicitly shown is the phase called slicing from the left. Slicing from the right is obtained using comments (surrounded by ’/*’ and ‘*/’ pair) instead of original text in lines marked as 2, 5 and 7. The complete algorithm consists of both phases, applied in any order.
for $j = 1$ to $p$ do
  $\xi \leftarrow 1$ /* $\xi \leftarrow 0$ */
  $k = 1$
  repeat
    $\xi \leftarrow \xi / 2$ /* $\xi \leftarrow (1 + \xi)/2$ */
    $k \leftarrow k + 1$
  consider box $V' = a_1 \times a_2 \times \ldots \times [a_j, \xi (\pi_j - a_j)] \times \ldots \times a_p$
  /* consider box $V' = a_1 \times a_2 \times \ldots \times [\xi (\pi_j - a_j), \pi_j] \times \ldots \times a_p$ */
  success $\leftarrow \text{not (all conditions/inequalities satisfied in } V')$
  if success then $V \leftarrow V \setminus V'$
  until (success or $k > M$)
end for

The number $M$ denotes simply the number of bits in floating point representations of real numbers used by a given processor/compiler pair; for example $M = 25$ for single precision reals and $M = 57$ for double precision type numbers in PC-compatible computers equipped with g77 or gcc compiler. The variable success is of type boolean.

It must be noted, that the procedure outlined in this article produces the interval hull of possible solutions. Not every point within the final box $V$ represents possible solution of the problem, but — on the other hand — no other point, outside $V$, is feasible. For graphical illustration see for example [5].

The ideas expressed here are closely related to the ones described in [6], [7], however they go much further: instead of producing just the interval version of well known least squares procedure, like in [8], we have developed completely different approach, much stronger. There are, of course, some drawbacks:

- the correlations between searched parameters are lost, and
- the relations of our method with the familiar confidence level and other statistical terms are still to be determined. Probably the famous Chebyshev inequality will be the only effective tool for this purpose.

And what are the advantages? Well, several:

- no assumptions are made concerning the distributions of experimental uncertainties, in particular they need not to be gaussian (Ockham’s razor principle at work),
- the results are always valid, no matter whether the experimental uncertainties are ‘small’ or not,
- it is easy to reliably identify outliers in collected data,
- uncertainties in both variables are handled naturally and easily,
- more data usually means less wide intervals for the searched parameters, in full accordance with common sense,
- possibly no solution will be obtained, if some uncertainties are underestimated, deliberately or otherwise,
- reliable bounds for searched parameters (their accuracies) are produced automatically, without the need for additional analysis. They are directly and precisely related to input uncertainties.

It is interesting to note, that in [5][b] we have found an example, when the ‘most likely’ least squares estimates for $a$ and $b$ are outside the bounds produced by our box slicing algorithm.
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VII. Historical note

First traces of ‘interval thinking’ might be attributed to Archimedes from Syracuse, Greece (287–212 b.c.), famous physicist and mathematician, who found two-sided bounds for the value of a number $\pi$: $\frac{223}{71} \leq \pi \leq \frac{22}{7}$ and a method to successively improve them. More than 2000 years later, the american mathematician and physicist, Norbert Wiener, published two papers: A contribution to the theory of relative position (Proc. Cambridge Philos. Soc. 17, 441-449, 1914) and A new theory of measurements: a study in the logic of mathematics (Proc. of the London Math. Soc., 19, 181–205, 1921), in which the two fundamental physical quantities, namely the position and the time respectively, were given an interval interpretation. Only after Second World War more papers on the subject were written. Here we have, probably among several others: chapter 2 of the book Linear Computations by Paul S. Dwyer (John Wiley & Sons, Inc., 1951, chapter Computation with Approximate Numbers) and Theory of an Interval Algebra and its Application to Numerical Analysis by Teruo Sunaga, (RAAG Memoirs, 2, 29–46, 1958). Facsimile of those and other early papers on interval analysis are freely available in the web at http://www.cs.utep.edu/interval-comp/early.html. Here we can also find two papers by polish mathematician Mieczyslaw Warmus: Calculus of Approximations (Bull. Acad. Pol. Sci. Cl. III, vol. IV (5), 253–259, 1956) and Approximations and Inequalities in the Calculus of Approximations. Classification of Approximate Numbers (Bull. Acad. Pol. Sci. math. astr. & phys., vol. IX (4), 241–245, 1961). And, finally, there are two technical reports from Lockheed Aircraft Corporation, Missiles and Space Division, Sunnyvale, California, Interval Analysis I by R.E. Moore with C.T. Yang, LMSD-285875, dated September 1959, and Interval Integrals by R.E. Moore, Wayman Strother and C.T. Yang, LMSD-703073, dated August 1960. R.E. Moore later developed more systematic studies in this area, with still more results presented in his Ph.D. Thesis (Stanford, 1962). He also wrote the first widely available monograph Interval Analysis (Prentice Hall, Englewood Cliffs, NJ, 1966) on this topic. Almost nobody was willing to make any progress in this direction until it was discovered, that the same problem, programmed in the same computer language, produces sometimes drastically different results when solved on different machines. Due to his accomplishments, R.E. Moore is regarded as a founding father of interval analysis. He is still (2003) active. Besides other things, we owe him the proof of convergence of interval Newton Method (A test for existence of solutions to nonlinear systems, SIAM J. Numer. Anal., 14 (4), 611–615, 1977). Since that time we observe growing interest into interval methods, not only within numerical analysis community.

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