Reliable uncertainties in indirect measurements

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Abstract

In this article we present very intuitive, easy to follow, yet mathematically rigorous, approach to the so called data fitting process. Rather than minimizing the distance between measured and simulated data points, we prefer to find such an area in searched parameters’ space that generates simulated curve crossing as many acquired experimental points as possible, but at least half of them. Such a task is pretty easy to attack with interval calculations. The problem is, however, that interval calculations operate on guaranteed intervals, that is on pairs of numbers determining minimal and maximal values of measured quantity while in vast majority of cases our measured quantities are expressed rather as a pair of two other numbers: the average value and its standard deviation. Here we propose the combination of interval calculus with basic notions from probability and statistics. This approach makes possible to obtain the results in familiar form as reliable values of searched parameters, their standard deviations, and their correlations as well. There are no assumptions concerning the probability density distributions of experimental values besides the obvious one that their variances are finite. Neither the symmetry of uncertainties of experimental distributions is required (assumed) nor those uncertainties have to be ‘small.’ As a side effect, outliers are quietly and safely ignored, even if numerous.

Keywords: data analysis, reliable computations, guaranteed results, safety critical applications, scientific computations

1. Introduction

Practically all known data fitting procedures are based on minimization of distance between measured and simulated values. Yet there exist various, equally good, distances (metrics) in n-dimensional space $\mathbb{R}^n$. Besides the best known Euclidean distance there exist many other ones, like Manhattan (taxi driver) or Chebyshev distance. Those three produce exactly the same values of $d(x,y)$ when $n = 1$, but still another metrics, defined as

$$d(x,y) = c \log (1 + |x - y|/c)$$

(with any fixed $c > 0$) will differ.

The choice of this or other metrics is therefore not unique. Exactly for this reason we have various families of fitting procedures at our disposal, with (weighted) least squares regression (LSQ) being most popular.

However, the real question is: why at all we are resorting to distance–based routines? The results of individual measurements are conventionally reported in form $y_0 \pm \sigma_y$, with $y_0$ being the most likely numerical estimate of true value $\hat{y}$, and $\sigma_y$ its standard deviation. Such result is usually drawn as a section of a straight line $[y_0 - \sigma_y, y_0 + \sigma_y]$, when presented in graphs. This doesn’t mean that the true value $\hat{y} = y_0$, nor that $\hat{y}$ is even contained within the interval shown! Indeed, when $\hat{y}$ is normally distributed (a common but often unfounded assumption), the chance for its true value to be located outside this interval is roughly equal to 1/3 — rather far from being negligible. This simple observation makes all distance–based procedures questionable at least. Besides, we often fit our data after non-linear transformation, performed just to visualize them as forming a straight line in the new coordinate system. After such a transformation, the original center of uncertainty interval no longer corresponds to the center of its image, thus making the notion of distance even more dubious.

So, perhaps we should deal with intervals of type $[y_0 - \delta, y_0 + \delta]$ instead, where $\delta$ is maximal uncertainty of a measurement? This way the true value $\hat{y}$ is guaranteed to reside inside the interval shown. But is it indeed? No, at least not in experimental practice, when unpredictable interferences do happen (or just data storage/transmission errors). Additionally, under this approach, our task would be to find a set of curves passing through all the measured values expressed as guaranteed intervals. Informally speaking, we should find a ‘thick’ simulated curve and then evaluate somehow the uncertainties of all its fitted parameters. However, it is easy to see that a single outlier may make this task impossible. On the other hand, when the said outlier is ‘small’ enough, then the fitted curve will be unrealistically narrow, thus suggesting incredibly good precision of its parameters. No wonder that this approach didn’t gain much popularity in scientific laboratory practice (notable exceptions are proposals given by Zhilin3,4 or Kieffer5), nevertheless it is developed in the field of various engineering applications under the keywords like tolerance problem6,7, confidence regions8,9, or guaranteed state estimation10,11.

In many cases the LSQ approach leads to solving a set of linear equations. This is also true for interval versions of those procedures. It appears, however, that interval linear systems have definitely more specific features than their classical predecessors. Specifically, they may have solutions of many differ-
ent kinds. This fact was most likely first recognized by Shary, who also proposed a classification scheme for solutions of interval systems of linear equations (applicable to non-linear systems as well). The literature concerning linear interval equations is now quite impressive while non-linear systems are investigated less frequently and often presented at conferences only. Needless to say that majority of mentioned papers is of purely mathematical nature, without explicit relations to physical problems.

The combination of interval calculus with probability is tempting but certainly uneasy to satisfy. The papers in this area are appearing only recently and still remain scarce. Our approach, as presented below, tries to follow this trend but seems more general and at the same time generally easier to follow.

2. Bridging the gap between intervals, probability and statistics

2.1. Interval calculus

For some reasons, interval calculus remains still largely unknown to the general computing public. It is much younger than the idea of complex numbers but it is with us already since 1960 and proves to be very useful, especially in computer calculations. In fact, it was developed first of all to put under strict control the uncertainties of results produced by various computers operating with finite precision arithmetic, often with different machine word lengths and/or representations of real numbers, thus necessarily introducing rounding errors. Informally, interval arithmetic makes possible to compute guaranteed ranges of mathematical expressions when exact ranges of all their components are known. By guaranteed we mean that the obtained results contain true ranges with certainty. It doesn’t mean, however, that those ranges are equal. It happens quite often that interval result overestimates the true result – but never underestimates it.

For those completely unfamiliar with interval computations, we provide a brief introduction in Appendix A and Appendix B. Readers interested in more details are referred to classical books or to the nice Wikipedia page. Here we only mention the notation used in the rest of this article: symbols like \( x, p, \) or \( f \) are for real variables, parameters or functions, while their interval counterparts will be written in different font as \( \bar{x}, \bar{p}, \) or \( \bar{f} \), respectively. Greek letters always represent real quantities.

2.2. Connection with probability and statistics

At first sight, there cannot be any direct connection between interval calculus and probability or statistics. While intervals are always guaranteed to contain the true values then probability and statistics operate rather with imprecise quantities, describing them in terms of most likely (expected) values and estimating their standard deviations. On the other hand, the very existence of well known term confidence interval strongly suggests that such connection is possible.

One might also ask why not to simply rewrite well known procedures, like Least Squares Method, into their interval formulations? This is indeed possible when experimental uncertainties are known as guaranteed intervals (i.e. containing true values with probability equal exactly to unity). Doing so we are lead to system of interval equations. But even in the simplest case, when all equations are linear, we encounter few serious problems. First, we have to decide which kind of solutions we are looking for – as there are many possible classes to choose from. In what follows, we will consider only the so called united solutions set. United solution set is an interval generalization of ordinary set of solution of a system of equations. In usual arithmetics, the vector \( \bar{p} \) of unknowns belongs to the solution set if for all considered equations the following equality holds:

\[
L_i(\bar{p}) = R_i(\bar{p}),
\]

where \( L_i(\cdot) \) and \( R_i(\cdot) \) are left- and right-hand sides of equation \( i \), respectively.

However, when operating with intervals, both \( L_i(\cdot) \) and \( R_i(\cdot) \) are not just real numbers, but intervals, each containing infinitely many numbers. In this case a subset \( S \) of searched parameters space certainly does not belong to the united solutions set when

\[
L_i(S) \cap R_i(S) = \emptyset \quad \text{for at least one} \quad i
\]

(\( \emptyset \) is an empty set). It may be somewhat unexpected, but the opposite, i.e. \( L_i(S) \cap R_i(S) \neq \emptyset \) for all \( i \) does not guarantee that \( S \) contains at least one true solution of our system. In other words, \( S \) is only a set of possible solutions.

One more comment is in order here. It is rather unlikely that the solution set \( S \) is a single multidimensional interval. More often it is a rich composition of many ‘small’ intervals (boxes), sometimes counted in thousands. It is not a comfortable situation when computer memory (or disk space) required merely to store such a set greatly exceeds the storage needed for original data. Additionally, any simple operation on \( S \) becomes time-consuming task as it has to be performed on each member of set \( S \). This is probably the main reason why interval computations are still rare, even in cases when the observed data can be considered to be guaranteed intervals. Of course, one might use less precise description of solution set \( S \), say in form of intervals describing minimal and maximal values of each parameter in turn. The drawback is that set \( S \) will usually occupy only a very small part of so defined single big box.

In further consideration we will need only one fact from probability and statistics, namely the famous Chebyshev inequality (1874):

\[
\Pr \left( \left| x - E(x) \right| > \xi \sigma \right) \leq \frac{1}{\xi^2} \quad \text{valid for} \quad \xi > 1.
\]

It quantifies the probability of large deviations of measured value \( x \) from its expected value \( E(x) \). It is valid for any probability density function, if only \( E(x) \) and variance \( \sigma^2 \) both exist and are finite.
3. The algorithm

3.1. Preliminaries

As usually, we start with a set of $N$ uncertain measurements $y_1 \pm \sigma_1, y_2 \pm \sigma_2, \ldots, y_N \pm \sigma_N$, obtained at the corresponding values of control variables $x_1, x_2, \ldots, x_N$. Control variables, $x$'s, are often just real numbers but may be multidimensional entities and/or uncertain as well. We also have a model $f$, containing $k$ unknown parameters $p_1, p_2, \ldots, p_k$ and relating uniquely every $y_i$ with $x_i$. The relation $f$ most often takes the form of algebraic equation

$$y_i = f(x_i, p_1, p_2, \ldots, p_k), \quad i = 1, \ldots, N \quad (4)$$

(one equation for each individual measurement $y_i$, taken at always the same, fixed set of unknown parameters $p_1, p_2, \ldots, p_k$).

Sometimes our problem is more complicated and cannot be written in explicit form, as in (4), but rather as an implicit formula

$$f(x, y, p_1, p_2, \ldots, p_k) = 0, \quad i = 1, \ldots, N \quad (5)$$

For purely numerical reasons (see Appendix A) it may be desirable — if possible — to write relation (4) in still another, but equivalent form

$$f_L(x_i, y_i, p_1, p_2, \ldots, p_k) = f_R(x_i, y_i, p_1, p_2, \ldots, p_k) \quad (6)$$

where $f_L$ and $f_R$, treated separately, have all their (interval) arguments appearing at most once, i.e. without repetitions.

From now on, our measurements will be represented as intervals: $y_i \pm \sigma_i \rightarrow y_i = [y_i - \xi \sigma_i, y_i + \xi \sigma_i]$, with $\xi$, called extension factor, equal to one unless noted otherwise. Note that in interval calculus the above range should be guaranteed to contain the true value with probability equal to exactly one. This requirement is satisfied only when $\sigma_i$ is equal to maximum absolute deviation, as specified by measuring instrument maker, and $\xi = 1$. But even then, we may face the problem of outliers; either because our instrument is malfunctioning or due to undetected data transmission errors. In all other situations, when $\sigma_i$ is a standard deviation of measurement $y_i$, even for arbitrarily large $\xi$ we have

$$\Pr\{\text{true value of } y(x_i) \in [y_i - \xi \sigma_i, y_i + \xi \sigma_i]\} < 1 \quad (7)$$

and the inequality is sharp. This observation may suggest that interval calculus is completely unsuitable for the kind of calculations we would like to perform. It will be shown below that such a view is unjustified.

3.2. Main idea

Our idea is illustrated in Fig. 1 When presented a set of uncertain measurements supposed to lay on a straight line, we can quickly estimate its slope and offset by simply using a ruler. It is rather difficult to say which so obtained line is the ‘best,’ but after few trials we are able to estimate the sensible ranges of both relevant parameters. Our algorithm only formalizes those simple actions. Its main steps are:

0. Start with the box of all fitted parameters, large enough to contain the solution, and make it the first and only element of list $L$. Establish unit lengths for all searched parameters (for explanation see the end of section 3.3).
1. Pick the largest box $V$ from list $L$ and remove it from list.
2. Bisect the box $V$, by halving its longest edge, to obtain two offspring boxes, $V_L$ and $V_R$.
3. Perform admissibility tests on boxes $V_L$ and $V_R$. Discard box, if it appears certainly unsuitable, or append it to the list $L$ otherwise.
4. Stop when the list $L$ is empty or contains only elements being either small or certified boxes. Otherwise go to step 1.

![Figure 1: Straight line fitting by guess. Rectangles represent results of uncertain measurements $y_i$ taken at uncertain locations $x_i$. Not every trial line is equally good: two of them miss the measurement at $x = 10$, and two others do not intercept the uncertainty rectangle near $x = 6$. On the other hand, it is obvious that any line with negative slope (not shown) is much worse: it will cross 0, 1, or at most 2 rectangles.](image)

3.3. Details of operations

- **Bisecting** means halving the longest edge of the box $V$. More precisely: if $V^m$ is the center of the longest edge $m$ of the original box $V$ then $V_L^m = [V^m, V^m]$ and $V_R^m = [V^m, V^m]$, while all the remaining components ($\neq m$) are exact copies of those of parent box $V$. This way $V = V_L \cup V_R$, what means that no point within the original search area will ever be missed by the algorithm. On the other hand we also have $V_L \cap V_R \neq \emptyset$, since offspring boxes always share a common face. We will need this feature at later stages.

- **Testing** means counting ‘hits.’ By ‘hit’ we understand the event $f(x_i, V) \cap y_i \neq \emptyset$ (compare with formula (4)), or non-empty intersection of $f_L(x, y, V)$ and $f_R(x, y, V)$ — when formula (6) is at work. Box $V$ should pass the test, when number of hits exceeds number of misses (empty intersections). But we shouldn’t ignore constraints, if there are any. Violating of at least one constraint immediately invalidates the box, if only this violation is certain.
For example, if we require two unknown parameters $p_0$ and $p_*$ to be equal, then the investigated box $V$ should be discarded only when the intersection of its corresponding components is empty: $V = \emptyset$. Non-empty intersection means that our constraint has a chance to be satisfied in current box and therefore $V$ should be retained for further investigations (if there is no other certainly violated constraint within this box, of course).

It may happen, when the task is to satisfy formula (4), that in given box $V$ the following inclusion occurs: $(x_i, V) \subseteq y_i$, for $i = 1, 2, \ldots, N$, whenever $(x_i, V) \cap y_i = \emptyset$. Such a box may be safely called certified as it needs not to be bisected further. This is because any subset of $V$ also satisfies this inclusion. It is therefore a good idea to put such box aside and never test it again.

- **Small boxes** are those with diameter not exceeding unity. But how can we compare searched parameters of different nature, expressed in various units, like meters, degrees or seconds? For this we need to arbitrarily establish unit lengths, individually for each searched parameter. This way the lengths of all edges of our boxes will become dimensionless numbers. Adopted unit lengths should not exceed accuracies we expect to get, but making them too small will result in significant increase of computation time.

### 3.4. What next?

#### 3.4.1. $L$ is empty

We are done, but certainly not satisfied, when $L$ is empty. What could be the reason not to obtain any result at all? Apart from obvious mistake of processing data obtained from different experiment, or mistakenly searching parameters outside their true ranges, we can think about the validity of our formula $f$. Maybe our model $f$ is simply too rough and is therefore unable to replicate observed features? Maybe it is only applicable within some range of control parameters and not outside it?

Less obvious reason for emptiness of the list $L$ is perfectly adequate model evaluated on too precise data. By too precise data we mean those with grossly underestimated uncertainties, including the case when they are being presented as equal to zero to the algorithm. It is evident that cheating doesn’t pay.

Yet, the case of too precise data need not to be completely at lost. It is possible to get $L \neq \emptyset$ in another run, with significantly enlarged unit lengths. Of course, the standard deviations of so obtained results may be very disappointing. This is the price for poor quality/inconsistent measurements.

When none of the above mentioned cases applies and the list $L$ in nevertheless empty, then we can conclude that our model $f$ is certainly inadequate to the problem under investigations.

#### 3.4.2. $L$ is non-empty

In this case we should check whether the convex hull of all boxes has no common parts with any face of the initial search domain. The presence of some boxes at the original boundary usually means that either the initial search domain was too small (not covering all solutions) or the corresponding unit length was selected too large. The second possibility will certainly occur in ‘pathological’ cases, when we don’t want to evaluate some parameter(s) and therefore deliberately and forcibly fix their values by setting widths of their search intervals to zero. There exist still other possibilities, to be discussed later, but in any case the algorithm should issue a detailed warning after encountering such a situation.

So, there is at least one box present on the list $L$. Yet even a single box contains infinite number of solutions, what is in sharp contrast with results delivered by other point-type routines, Monte Carlo investigations, or even population-based approaches, like genetic algorithms. By the way, the list $L$ with exactly one member will be an exception rather than the rule. More often $L$ will consist of much more boxes, perhaps counted in thousands. How should we report our results?

#### 3.5. Reporting results

Well, first thing is to check how many solutions were found. The obtained boxes need not to make a simply connected set, they may form few disjoint clusters. Is it possible? Yes, think about fitting two non-overlapping spectral peaks (their positions, amplitudes and half-widths) located on noisy background. Without constraints we will get two solutions, showing exactly the same two peaks but in different order.

For this reason, the next step should be to recover the individual simply connected components, that is clusters of neighboring boxes. It is the place where the property $V_i \cap V_j = \emptyset$ will be exploited extensively. Indeed, this part of algorithm often appears the most time-consuming one. Only after this step is completed, it is possible to process/report each solution, one after another.

#### 3.5.1. Original uncertainties are guaranteed limits

In this case the final processing is rather simple. All we have to do is to compute the convex hull of each cluster. This way the guaranteed lower and upper limit of each searched parameter are determined, in full concordance with usual rules of interval computations. Final report will typically include extremal values for each parameter as well as centers of those intervals.

One can think about the hulls of certified boxes making each cluster. Looks like that by doing so, we may get ‘more accurate’ (tight) estimates of searched parameters, see Fig. 2. Unfortunately, this is a bad idea. First, the cluster might contain no certified boxes at all! This will almost certainly happen whenever adopted unit lengths are too large. Second, we will lose the rigor of interval computations.

In some applications it is essential to know guaranteed tolerances of searched parameters. If so, then we need as a solution the ‘biggest’ box covering certified boxes, and only those boxes. However, the solution having this property is not unique — it depends on what the word ‘biggest’ means in every particular case. In practice, some parameters may be easy to control, while others only with excessive cost, and so on. Thus it may be a matter of user preferences which solution is preferable. The
case of linear equations was extensively studied by Shary and similar problems – mostly related to robotics – were presented at numerous conferences. Nevertheless, this topic is out of scope of the current paper.

3.5.2. Original uncertainties and standard deviations

At first sight, the rigor of interval computations becomes doubtful, when we operate on data expressed in familiar form, i.e. as a pair: measurement result, \( y \), and its standard deviation, \( \sigma_y \). This is because no interval of type \([y - \xi \sigma_y, y + \xi \sigma_y]\) guarantees that the true value, \( \tilde{y} \), is located within these limits, no matter how large (but finite) is the positive extension factor \( \xi \).

In some cases we can find the exact value of probability of such event, most notably when the measured quantity, \( y \), follows normal (Gaussian) distribution, or — generally — when the probability distribution is known (preferably in analytical form). In all other cases we can use the already mentioned Chebyshev inequality \( \| \) to rigorously estimate probabilities of interest.

Before we proceed further, let us explain our point of view on data fitting process, to our best knowledge never presented before. In short: data fitting process is like a final step of any ordinary (direct) measurement. And here is why. During direct measurements, the measuring instrument, say a ruler, seems to transfer to our brain, which decides the final outcome of measurement. This complicated process may be formally described as a superposition of several transformations. So, being the last part in chain of transformations normally performed by measuring instrument. What remains, usually the experimenter’s task (and her computer, perhaps), is to derive simplest statistical properties of the bunch of measurements. But now finding expected values of searched parameters, their standard deviations, and correlation coefficients as well, is a next to trivial task. Best of all, it can be done without any tricks, or simplifications, just by following appropriate definitions.

In conclusion: for most popular types of measurements we are able to find and present not only the extremal values of fitted parameters but also highly desired, reliable estimates of their standard deviations and correlation coefficients, for every separate cluster in turn.

Final note. It is tempting to treat on unequal basis the boxes differing by number of hits. Assigning higher weights to points located in boxes with higher number of hits will certainly result in smaller values of standard deviations of fitted parameters – but is it well justified? At this moment this remains an open question.

4. The meaning of extension factor

Before the algorithm starts, it needs to know its input data in interval form. This is easy when input data are known within guaranteed limits. No extension factor is needed then, correct intervals are already known.

Let’s discuss all other cases now. As already mentioned, no value of extension factor \( \xi \) makes certain that true value is covered by so created interval. Assume that we know nothing about the distribution(s) ruling our measurements, except that its average value and variance do exist and are both finite. Our goal is to find such values of unknown parameters that resulting curve (or a hyper-surface in multidimensional case) hits more than half of our uncertain measurements. Suppose such set of parameters indeed makes sense (exists). If so, then hits are binomially distributed, with probability \( p \) of success in a single trial equal to the probability of true value being located within the inspected interval. One might think, that all what is needed to hit more than half of measurements is to set \( (\xi^2 = 2) \equiv (\xi = \sqrt{2}) \) in Chebyshev inequality. Unfortunately, this guess is correct only for a single measurement or for infinitely many measurements. In all other cases we need to find smallest \( 0 < p < 1 \) satisfying inequality:

\[
\sum_{k=0}^{\lfloor (N+1)/2 \rfloor - 1} \binom{N}{k} p^k q^{N-k} \leq \sum_{k=\lfloor (N+1)/2 \rfloor}^{N} \binom{N}{k} p^k q^{N-k} \tag{8}
\]

where \( N \) is the number of uncertain data points, \( q = 1 - p \), and \( \lfloor \cdot \rfloor \) means integer part of the argument. From Chebyshev inequality \( \| \) we immediately have \( 1 - p \leq 1/\xi^2 \) and thus the minimal value of extension factor \( \xi = 1/\sqrt{1-p} \).

This is exactly what our algorithm is doing, with the small exception that its ‘measurements’ are repeated infinitely many times. Thanks to this observation we can think about every point within the obtained cluster of boxes as being the result of a single measurement – why not? This way our algorithm becomes a last part in chain of transformations normally performed by measuring instrument. What remains, usually the experimenter’s task (and her computer, perhaps), is to derive simplest statistical properties of the bunch of measurements. But now finding expected values of searched parameters, their standard deviations, and correlation coefficients as well, is a next to trivial task. Best of all, it can be done without any tricks, or simplifications, just by following appropriate definitions.

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In order to satisfy the inequality (8), one has to resort to numerical calculations. The results, for \( N \leq 30 \), are presented in Table I, together with minimal required probability of success (hit) in single attempt \( (p = \text{min. Pr}) \). Somewhat unexpectedly, the sequence \( \{\xi_N\} \) appears to consist of two distinct subsequences: one for even and the other for odd \( N \), as illustrated in Fig. 3. Both subsequences are decreasing and converge to the same limit: \( \lim_{N \to \infty} \xi_N = \sqrt{2} \). For practical purposes extension factors may be approximated by

\[
\xi_N \approx \sqrt{2} \left( 1 + \frac{3}{2N} \right) \quad \text{for } N \text{ even} \tag{9}
\]

\[
\xi_N \approx \sqrt{2} \left( 1 + \frac{1}{N} \right) \quad \text{for } N \text{ odd} \tag{10}
\]

Both approximations are from below, with the ratio of true extension factor and its approximated value dropping below 1.0010 for \( N \geq 35 \), valid for normally distributed uncertainties. One might think that for normally distributed data it should make a sense to shrink their intervals (apply \( \xi < 1 \)) whenever \( N \geq 7 \). Unfortunately, this is not recommended, as in such case we are loosing the solid ground of Chebyshev inequality (3).

In effect, to avoid this unreasonable temptation, we leave the last column of Table I mostly unfilled.

Note also the unexpected relation

\[
\Pr(N - 1) > \Pr(N) < \Pr(N + 1) \tag{11}
\]

valid for odd \( N \). Analogous inequality is satisfied by \( \xi \), what suggests potentially more tight estimates for data sets containing odd number of measurements — at least when using the proposed approach. In fact, we are dealing here with the old truth: odd number of voters will never generate a tie what might happen when the number of voters is even. Another surprising observation is that the general idea more is better indeed works, but only for \( N \geq 4 \).

**Final remark:** Some measurements deliver not just a single number but rather few components at once, say two or three components of a vector. The extension factor, \( \xi \), should be modified in such situations accordingly. Namely, it should be replaced with \( \xi \leftarrow \xi^D \), where \( D \) is the number of individual components making single measurement. Not doing so will result in needlessly overestimated uncertainties of fitted parameters.

| \( N \) | \( N_{\text{min}} \) | \( \xi \text{ unknown} \) | \( \text{min. Pr} \) | \( \xi \text{ Gauss} \) |
|---|---|---|---|---|
| 1 | 1 | 1.000000 | 0.500000 |
| 2 | 2 | 1.847759 | 0.707107 | 1.051801 |
| 3 | 3 | 2.201664 | 0.793701 | 1.263802 |
| 4 | 3 | 2.507033 | 0.840896 | 1.408092 |
| 5 | 3 | 1.785116 | 0.686190 | 1.007259 |
| 6 | 4 | 1.944591 | 0.735550 | 1.159353 |
| 7 | 4 | 1.657220 | 0.635884 | |
| 8 | 5 | 1.766335 | 0.679481 | |
| 9 | 5 | 1.594986 | 0.606915 | |
| 10 | 6 | 1.678127 | 0.649490 | |
| 11 | 6 | 1.558150 | 0.588110 | |
| 12 | 7 | 1.625364 | 0.621471 | |
| 13 | 7 | 1.533792 | 0.574923 | |
| 14 | 8 | 1.590223 | 0.604557 | |
| 15 | 8 | 1.516488 | 0.565167 | |
| 16 | 9 | 1.565126 | 0.591773 | |
| 17 | 9 | 1.503560 | 0.557658 | |
| 18 | 10 | 1.546302 | 0.581774 | |
| 19 | 10 | 1.493535 | 0.551699 | |
| 20 | 11 | 1.531658 | 0.573738 | |
| 21 | 11 | 1.485532 | 0.546856 | |
| 22 | 12 | 1.519939 | 0.567140 | |
| 23 | 12 | 1.478997 | 0.542843 | |
| 24 | 13 | 1.510348 | 0.561625 | |
| 25 | 13 | 1.473559 | 0.539463 | |
| 26 | 14 | 1.502354 | 0.556947 | |
| 27 | 14 | 1.468964 | 0.536777 | |
| 28 | 15 | 1.495588 | 0.552929 | |
| 29 | 15 | 1.465029 | 0.534084 | |
| 30 | 16 | 1.489787 | 0.549441 | |

Table 1: Extension factor \( \xi \) vs. the number of collected measurements \( N \), valid for unknown distribution of their uncertainties. \( N_{\text{min}} = 1 + \lceil \sqrt{N/2} \rceil \) is the required minimal number of hits. The column marked as ‘min. Pr’ shows minimal probability of a single measurement to guarantee that \( \Pr(N_{\text{hit}} \geq N_{\text{min}}) > 1/2 \). The last column shows extension factors for normally distributed measurements. Values below unity are not shown.

5. **An example**

As an example we present how our algorithm deals with experimental data on Newton gravitational constant \( G \). This fundamental physical constant still remains the least precisely
6. Advantages and disadvantages

Advantages:

- recovering unknown parameters from implicit dependencies is equally easy as from explicit formulas
- robustness against outliers, up to 50 %
- obtained uncertainties (variances) are never underestimated
- no need to apply any ‘error propagation law,’ often questionable
- high flexibility. The same algorithm may be used for detecting outliers, hypotheses testing, solving systems of nonlinear equations, possibly containing uncertain parameters, or just for simulations of complex, implicit models with uncertain parameters. The presented approach may be also useful in metrology, for inter-laboratory comparisons.

- uncertainties in both coordinates do not pose any problem and are handled naturally, including non-linear and implicit cases. In fact, we have found in literature only two articles describing straight line fitting with uncertainties in both variables; general non-linear cases seem not to be discussed at all.

Disadvantages:

- worst case complexity is exponential in the number of fitted parameters, thus
- impractical when the number of unknowns is large
- the computed standard deviations may be overestimated by unknown factor.

7. Conclusions

It is hoped that the presented algorithm will soon replace a great deal of existing optimization procedures. In author’s opinion, interval computations deserve to become soon as familiar to experimentalists as are complex numbers to electrical engineers.

Appendix A. Brief introduction to interval computations

Appendix A.1. Some definitions and important properties

An interval \( x \) is a compact and finite subset of a real axis:

\[
x = [x, \bar{x}] = \{ x \in \mathbb{R} : x \leq x \leq \bar{x} \}
\]

where both \( x \) and \( \bar{x} \) are finite. It may be thought to be a representation of a real number, certainly located somewhere between \( x \) and \( \bar{x} \), inclusive, but unknown otherwise. A special case is \( x = [a, a] \) (a.k.a. thin interval or singleton), identified with the real number \( a \). The set of all intervals is usually denoted as \( \mathbb{I} \).

It is easy to define interval counterparts of ordinary arithmetic operations:

\[
\begin{align*}
x + y &= [x + y, \bar{x} + \bar{y}] \\
x - y &= [x - \bar{y}, \bar{x} - y] \quad (a \neq 0 \Rightarrow a - a \neq 0) \\
x \cdot y &= [\min \{x, \bar{x}\}, \max \{x, \bar{x}\}]
\end{align*}
\]

where \( Z \) is a four–element set:

\[
Z = [x, \bar{x}, y, \bar{y}] = \{ x \cdot y, x \cdot \bar{y}, \bar{x} \cdot y, \bar{x} \cdot \bar{y} \}.
\]

Division is defined, for \( y \neq 0 \) as:

\[
x/y = x \cdot \bar{y} \quad (1/y, 1/\bar{y}) = \begin{cases} 1/y, 1/\bar{y} & \text{if } y \neq 0, \\
\text{undefined otherwise} & \text{if } y = 0.
\end{cases}
\]

It may be checked that so defined arithmetic operations produce all possible results of \( x \square y \) for any pair \( (x, y) \) satisfying \( x \in X \) and \( y \in Y \), and only those results (here \( \square \) stands for any of \(+,-,\cdot,\div\)). However, more complicated arithmetic expressions may
happen to overestimate the true range. Specifically, we generally have: $x(y+z) \subseteq xy+xz$ for $x,y,z \in \mathbb{R}$, not the equality. Nevertheless, the following theorem holds:\footnote{Theorem (Fundamental Theorem of Interval Arithmetic)}

Let $f(x_1, x_2, \ldots, x_n)$ be an explicitly defined real function. Then evaluating $f$ in “interval mode” over any interval inputs $(x_1, x_2, \ldots, x_n)$ is guaranteed to give a set $f$ that contains the range of $f$ over those inputs.

The above theorem is true, but in practice we often obtain overestimated results, i.e. intervals wider than necessary. To avoid such undesired situations, we should — whenever possible — write complex interval expressions in form with each interval variable appearing exactly once. For example, to compute the resistance $R$ of two resistors $R_1$ and $R_2$, connected in parallel, we normally use the formula $R = R_1\cdot R_2/(R_1 + R_2)$. When $R_1$ and $R_2$ are uncertain, it is better to compute their equivalent resistance as $R = (1/(R_1 + 1/R_2))^{-1}$.

There is another subtlety, not mentioned until now. Our algorithm extensively exploits the ‘obvious’ property: $x \subseteq y \Rightarrow f(x) \subseteq f(y)$, which need not to be true. Functions $f$ satisfying these relations are called monotonously inclusive. At this place it is enough to say that all ordinary (‘calculator’) functions have this property. Nevertheless exceptions sometimes happen and among the suspected functions are those containing min and/or max.

When dealing with interval computations on a computer, that is with finite precision, it is also very important to properly round all the intermediate results, as well as the final one. Proper rounding means outwards rounding, i.e. lower (left) endpoint has to be rounded towards minus infinity, while the other one — towards plus infinity. Fortunately, the existing interval software packages have this feature built in. Sometimes, however, it is highly recommended to perform such an action explicitly.

Interval $n$-dimensional vectors, i.e. objects belonging to Cartesian product $\mathbb{R}^n = \mathbb{R} \times \mathbb{R} \times \ldots \times \mathbb{R}$, are often called boxes, for obvious reasons. We will need to know how large are our boxes. The box’s diameter is a real number, defined as the length of its longest edge:

$$\text{diam } (x_1, \ldots, x_N) = \max \left( |x_1 - \bar{x}_1|, \ldots, |x_N - \bar{x}_N| \right) \quad (A.4)$$

### Appendix B. Set theory operations on intervals

Intervals are sets and therefore also the set-theory operations may be performed on them. Here we sketch only two:

- **intersection**
  \[ a \cap b = \left[ \min (\bar{a}, \bar{b}), \ \max (\underline{a}, \underline{b}) \right] \quad (B.1) \]

  When $a$ and $b$ happen to be disjoint, then the above formula will necessarily produce illegal result, not an element of $\mathbb{R}$, i.e. the one with left endpoint value higher than right endpoint. If this is the case, then we should replace the so obtained result with an empty interval, see below.

- **convex hull**

  \[ \text{hull } (a, b) = \left[ \min (a, b), \ \max (\bar{a}, \bar{b}) \right] \quad (B.2) \]

  This operation is an interval counterpart of union of two sets, with result being again an element of $\mathbb{R}$. We always have $a \cup b \subseteq \text{hull } (a, b)$, with equality occurring only for arguments having non-empty intersection. Therefore we can say that interval hull possibly overestimates ordinary union of $a$ and $b$.

- **empty interval**

  It is easy to see that arbitrary illegal interval $a = [\bar{a}, \bar{a}]$ with $\bar{a} > \bar{a}$, doesn’t guarantee the satisfaction of the otherwise obvious property $a \cup b = \varnothing \cup b = b$, as one might expect. Therefore we need to define an empty interval in a special form, the one making possible to always obtain correct results during computer calculations. The suitable choice is

  \[ \varnothing = [\text{HUGE}, -\text{HUGE}] \quad (B.3) \]

  where $\text{HUGE} > 0$ is the largest machine number.

### Acknowledgments

Current author’s interest in interval computations started after Ramon E. Moore published the paper\footnote{R. Baker Kearfott, Vladik Kreininovich, Sergey P. Shary and Sergei I. Zhilin for words of encouragement and occasional email discussions on interval-related problems.} (1977) showing the power of interval Newton method applied to nonlinear equations. Author is deeply indebted to him as well as to R. Baker Kearfott, Vladik Kreininovich, Sergey P. Shary and Sergei I. Zhilin for words of encouragement and occasional email discussions on interval-related problems.

For long time the interval computations were developed with no visible link to physical problems, until the largely overlooked conference presentation\footnote{For long time the interval computations were developed with no visible link to physical problems, until the largely overlooked conference presentation in 2002. This article presents a working algorithm following the ideas sketched there.} given in 2002. This article presents a working algorithm following the ideas sketched there.

This work has been done as a part of author’s regular duties in the Institute of Physics, Polish Academy of Sciences, and was not funded otherwise.

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