Interval straight line fitting

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Abstract. I consider the task of so called curve fitting or experimental data fitting commonly encountered in various branches of scientific research. Unlike the traditional approach I do not try to minimize any functional based on available experimental information, instead the minimization problem is replaced with constraint satisfaction procedure, which produces the interval hull of solutions of desired type. The method, called box slicing algorithm, is described in details. The results obtained this way need not to be labeled with confidence level of any kind, they are simply certain (guaranteed). Additionally, the memory requirements for the presented method are very conservative. The approach is directly applicable to other experimental data processing problems like outliers detection and finding the straight line, which is tangent to the experimental curve.

keywords: experimental data fitting, curve fitting, interval enclosures, experimental uncertainty, linear regression, constraint satisfaction, box slicing, outlier identification, asymptotes

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1 Stating the problem

In many branches of science the so called problem of experimental data fitting is often encountered. Its short description is following:

Given the data set, i.e. the set of experimental observations, called also measurements, \( \{(x_j, y_j)\}_{j=1}^{n} \), and the model, find appropriate parameters of this model, which adequately describe the data.

In the following I will assume that:

- the values of both coordinates for each measurement may be uncertain, i.e. for each \( x_j \) (respectively \( y_j \)) we know the interval, \([x_j, x_j]\) = \( x_j \) (resp. \([y_j, y_j]\) = \( y_j \)), containing \( x_j \) (resp. \( y_j \)) and guaranteed to contain the true, unknown value of the measured or controlled physical quantity,
- we are searching for parameters of a linear model relating \( x \) with \( y \):

\[
y = ax + b
\]

The further considerations are directly applicable to many other two-parameter models. The extension for even more complicated cases is also straightforward. I choose the linear model since it is very important, widely used and, at the same time, probably the simplest one.

Shortly: the goal is to find the bounds for two parameters, called hereafter \( a \) and \( b \), which describe reliably the experimental data. There are many procedures to solve such a problem, all depending on the exact meaning what is the best solution, the LSQ (least squares method) and LAD (least absolute deviations) being among the most popular. Yet, even the interval counterparts of those methods do not deliver the results expected by experimentalists. Often encountered is the “cluster problem” (see \( \text{[1]} \) and \( \text{[2]} \)), which makes the precise location of a global extremum difficult. Additionally, as a consequence of clustering, the enclosures for physically interesting parameters are usually very pessimistic, up to the point of complete unusability. So why bother at all with one more interval method?

2 Deficiencies of existing methods

Most popular and commonly used fitting methods are nowadays the ones based on probabilistic grounds. This is because the results of measurements are treated as random variables. There is nothing wrong with such an assumption, however further treatment of the experimental data is most often than not based on, rarely explicitly stated, additional assumptions concerning the distributions of measured quantities. It is assumed, and almost never checked, that the distributions are normal (Gaussian). However, contrary to common belief, they usually aren’t normal. Today the vast majority of measurements is performed with
digital measuring devices, so even if the investigated phenomenon is normally distributed, then the set of its measurements, consisting of discrete values only, cannot be normally distributed.

There is also one more hypothesis being used, namely that the uncertainties (errors) are small. This is never checked, and indeed cannot be checked, since there is no possibility to influence the uncertainties of measurements once they had been performed.

Finally, all such methods, explicitly or implicitly, make use of the Central Limit Theorem, without ever bothering, that the conclusions drawn on those grounds are only asymptotically valid, in the limit of infinite number of measurements.

The estimates of interesting parameters, obtained this way, are given as a pair of numbers meaning: either the most probable value and its standard deviation (again silently assuming the normal distribution!) or — less often — as the confidence interval. The choice of the so called confidence level, which is then a third number, remains arbitrary. Needless to say, that the confidence level is only very loosely related, if at all, to the performed measurements.

### 3 Interval point of view

In this paper we are going to find the tight and guaranteed bounds for both parameters \( a \) and \( b \). According to this aim, we will search for the intervals, \( a = [a, \overline{a}] \) and \( b = [b, \overline{b}] \), containing with certainty the true values of \( a \) and \( b \) respectively. This is equivalent with finding the solutions of the following system of equations:

\[
\begin{align*}
ax_1 + b &= y_1 \\
\vdots & \quad \vdots \\
ax_n + b &= y_n
\end{align*}
\]

It is a system of linear equations with \( n > 2 \) equations and only 2 unknowns. Since the number of available data exceeds the number of unknowns, then the system (1) is overdetermined and therefore generally has no solutions in the usual sense. Nevertheless, we will find such intervals \( a \) and \( b \), that the equations (1) and the experimental data will be in some sense consistent. According to Shary [3], there are many ways of saying what kinds of solutions are of interest to us. To count them all let us rewrite the system (1) in standard matrix form:

\[
\begin{pmatrix}
  x_1 & 1 \\
  x_2 & 1 \\
  \vdots & \vdots \\
  x_n & 1 \\
\end{pmatrix}
\begin{pmatrix}
  a \\
  b
\end{pmatrix}
= 
\begin{pmatrix}
  y_1 \\
  y_2 \\
  \vdots \\
  y_n
\end{pmatrix}
\]

To define a particular set of solutions, we have to assign one of two available quantifiers, \( \forall \) or \( \exists \), to each entry of the matrix of coefficients of equations and to each component of the right hand side vector (for details see [3] and the following
discussion). This makes $2^{2n} \times 2^n = 2^{3n}$ possible assignments corresponding to this many various solutions sets. Fortunately, this rather huge number can be substantially reduced. First, the second column of the matrix of coefficients consists of simple real numbers only, not intervals. There is no point in assigning any quantifier to the numbers originating from the degenerate interval $[1, 1]$, since there is exactly only one number contained in it. Secondly, we do not want to distinguish any particular measurement from among others. This means, that the quantifiers have to be assigned in a special way: all $x$’s should be connected with the same quantifier. The same can be said about $y$’s. Taking all this into account we arrive with only 4 kinds of solutions of the system \(1\). They are following:

solutions in the usual sense:

$$\{(a, b) : \forall_{k=1 \ldots n} \forall_{x \in x_k} \forall_{y \in y_k} \ ax + b = y\}$$  \(3\)

This set is unbounded when there is only one experimental point, exact or not. When the number of measurements is equal 2 and the measurements are exact (and different, i.e. \(x_1 \cap x_2 = \emptyset\)), then it reduces to the single point. For two inexact measurements it is bounded, when the measurements are disjoint, and unbounded otherwise. It is usually empty, when we have 3 or more measurements, since it is impossible to draw a straight line connecting three or more arbitrarily chosen points, each belonging to its own rectangle \(x_k \times y_k\), even if each of those rectangles consists of only one point. The solutions in usual sense are then of no interest for the experimentalists except, perhaps, the case \(n = 2\), which is described later. For now let’s assume that \(n > 2\).

united solutions:

$$\{(a, b) : \forall_{k=1 \ldots n} \exists_{x \in x_k} \exists_{y \in y_k} \ ax + b = y\}$$  \(4\)

This set, if non-empty, consists by definition of all straight lines having at least one common point with each of the rectangles \(x_1 \times y_1, x_2 \times y_2, \ldots x_n \times y_n\). In set theory language the above may be expressed as

$$\forall_{k=1 \ldots n} (ax_k + b) \cap y_k \neq \emptyset$$  \(5\)

Of course, not every pair \((a, b) \in (a, b)\) is the member of the set of solutions. Indeed, whenever we say “solutions”, then we really mean “interval hull of the solution set”. The same comment applies to the two remaining cases described below.

controllable solutions:

$$\{(a, b) : \forall_{k=1 \ldots n} \exists_{x \in x_k} \forall_{y \in y_k} \ ax + b = y\}$$  \(6\)

Treating intervals as sets, we can write the relation satisfied by interval hull of solutions of this kind as

$$\forall_{k=1 \ldots n} ax_k + b \supseteq y_k$$  \(7\)
Finally, we should consider

tolerable solutions:

\[ \{(a, b) : \forall k=1 \ldots n \forall x \in x_k \exists y \in y_k \ a x + b = y \} \]  \hspace{1cm} (8)

which are contained in the box \((a, b)\), for which the relation

\[ \forall k=1 \ldots n \ ax_k + b \subseteq y_k \]  \hspace{1cm} (9)

holds.

All the above relations should hold for every measurement; the names of various sets of solutions are used after Shary [3].

In the strictly mathematical sense we have covered all kinds of solutions. Experimentalists may be interested in one more type of “solutions”, which will be called here crude solutions. These are defined in almost the same way as the united solutions, except that the relations (9) are required to hold for majority of measurements, not necessarily for all of them. This way every united solution is, of course, a crude solution as well. Such “solutions” might be useful, when analyzing data containing outliers. Let us refrain from further discussion of crude solutions now, leaving it to the later part of this paper. Instead consider still another set, defined as the smallest one satisfying the conditions

\[ \forall k=1 \ldots n \ \forall x \in x_k \ a x + b \supseteq y_k \]  \hspace{1cm} (10)
Figure 2: Geometric interpretation of the tolerable solution. The straight line shown belongs to the set of tolerable solutions, since it passes through all, arbitrarily chosen, short vertical sections inside each experimental rectangle. It does not cross any horizontal edge of any rectangle.

which are very similar to those for the interval hull of controllable solutions. Simply stating, the set just defined has the intuitively simple property, that the graph of the expression \( y = ax + b \) covers all experimental uncertainty rectangles in the \( xy \) plane. I shall show now, that the set (10) is unbounded in \( \mathbb{R}^2 \):

Suppose that we have fixed parameter \( a = [a, a] \in \mathbb{R} \) as a thin (degenerate) interval being equal to the arbitrary real number. It is easy to adjust the parameter \( b = [b, b] \in \mathbb{R} \) such that (10) holds; it is enough to put

\[
\bar{b} \leq \min_k \left( y_k - ax_k \right) \tag{11}
\]

and

\[
\underline{b} \geq \max_k \left( y_k - ax_k \right) \tag{12}
\]

The smallest \( b \) corresponds, of course, to the situation, when we have equalities in (11) and (12). But, since \( a \) was arbitrary, then the entire set is unbounded in \( \mathbb{R}^2 \), and so must be its convex (interval) hull. Thus we have shown, that the smallest set of type (10), in the sense that it is contained in any other having required properties, does not exist.

We will not explore the idea of finding the box with minimal volume, since this might lead to unplausible or even unphysical results. Consider the poor quality
experimental data, (for sake of simplicity we assume that both variables are
dimensionless, so the inequality below makes sense) for which

\[
\text{width} \left( \bigcup x_k \right) < \text{width} \left( \bigcup y_k \right)
\]

and \( \bigcup \) denotes the convex hull. For such data it may easily happen, that the
“fitted” line will be perpendicular to the expected direction in the \( xy \) plane!

In conclusion, we will not discuss further the solutions of type (10). There is no
hope, that they would constitute good starting point for subsequent refinement
to other types of solutions, more tight. It may even happen, that the randomly
selected set of “solutions” with property (10) has no common elements with the
united solutions set.

4 Properties and usability of remaining types of solutions

First note that the following inclusions are always true:

\[
\text{tolerable solutions} \subseteq \text{united solutions}
\]

and

\[
\text{controllable solutions} \subseteq \text{united solutions}
\]

This means, that the set of united solutions is the “largest” one among all of
the true solutions (we exclude the crude solutions, since they are not true in the
sense, that they do not hold for every experimental point).

The natural question arises, which kind of solutions (and why) is the one, which
should be used by experimentalists? The quick answer is \textit{they all deserve our
attention}. Looking at Fig.3, we can see that the sets of tolerable and/or con-
trollable solutions deliver potentially better, i.e. more accurate (tight) and thus
tempting estimates of unknown parameters. Yet, for the experimentalist they
are unreliable. Suppose that after some time the new experimental result is
available, obtained with much better accuracy. It may place itself within the
one of the already known uncertainty rectangles but \textit{outside} the domain marked
with letter T (or C) in Fig.3. It is obvious, that in such circumstances the
tolerable (or controllable) solution set will be empty. No definite conclusion
can be drawn whether or not our knowledge had really increased as a result of
this new measurement. Driven by the widely accepted paradigm that increase
of knowledge is nothing else as decrease of ignorance, (and this should never
increase after new, correctly performed measurement) we would rather prefer
the united solutions’ set. Indeed, the choice between various kinds of solutions
is rather limited, since usually either tolerable or controllable solutions will be
available, if any, but not both. It is quite obvious, that significant progress,
i.e. better bounds for unknown parameters, can only be achieved when new
measurements, of similar accuracy, are taken off the already investigated range of controlled parameter $x$. Repeating measurements, within already explored range, is unlikely to improve significantly the bounds of searched parameters, unless they are definitely more accurate.

Summarizing the above considerations I propose to interpret various sets of solutions in a following uniform way:

- **if united solutions exist**, then the available data are in agreement with the model in use; there is no apparent contradiction between theory and data. The wording “fair”, “satisfactory”, “good” or “excellent agreement” is a matter of taste rather than anything else. Using of such phrases may be only justified by comparison with similar results, especially concerning the widths of intervals $a$ and $b$, obtained by different method(s) or by other authors.

- **if no united solution exist** (two other sets of solutions are then empty too) then either of the following happened:
  - one or more points are unreliable, i.e. their error bounds are underestimated, perhaps even all of them, or
  - one or more points are outliers. This may be the result of malfunctioning apparatus, errors in data transmission, or simply human
mistake when writing down the instrument’s readings or typing them into computer.

– the linear model is not applicable to the phenomenon under investigation.

The latter may happen to be true quite easily in physical sciences, where the approximate, linearized models are used frequently. They are usable only as long as newer and better, more accurate, results become available. Then it might be the time to revise, correct or even reject the current theory.

We can also see the united solution set from other perspective: if it is empty, then we have a proof, that our model is not adequate for the observed data. Inadequacy of the model may be bad news, but, on the other hand, the proof of this fact is much more valuable than the result of any statistical test. For this to be true, we have to be sure, that the uncertainties of all our data were estimated correctly, never underestimated.

Few words should be said concerning two other types of solutions. The existence of either tolerable or controllable solutions, in addition to the united set of solutions, has no peculiar meaning, at least for experimentalists. The lack of tolerable solutions may suggest that the uncertainties connected with variable $x$, which is usually under control, are either overestimated or should be reduced in further experiments, perhaps with better apparatus. The tolerable solutions may only exist, when those uncertainties are small enough. When all $x$’s are exact, then tolerable solutions are simply united solutions. Similarly, the controllable solutions exist only when the tolerances for all $y$’s are tight enough. Again, when those tolerances are equal to zero, then the controllable solutions are simply united solutions. So, the existence or lack of existence of tolerable or controllable solutions may be regarded only as a hint of how well the measurements were performed. As the final outcome of an experiment we should, however, use only the intervals $a$ and $b$ derived from a united solution set, no matter that the solutions of other kind usually look better.

5 The algorithm

In this section I present the general strategy of finding the interval enclosure of every kind of solutions of (1). It may be regarded as a functional counterpart of the interval functions $\text{ZERO1}$ and $\text{ZERO2}$ defined by van Emden in [4]. The method is called box slicing or box peeling algorithm.

The first step is to convert (1) into equivalent set of conditions, usually in a form of inequalities. We also need to determine an initial box $V$, containing all the potential solutions of desired type. Let’s defer the discussion on the exact forms of those conditions and the choices of initial box for later. Our goal is to find the smallest interval box $(a, b) \in \mathbb{R}^2$, containing all pairs $(a, b)$, for
which appropriate conditions are satisfied. The general outline of the algorithm is following:

| Input |
|-------|
| Initial box $V \in \mathbb{R}^2$ containing all solutions. |

| Algorithm |
|----------|
| For each unknown interval in turn do the following: |
| • try to slice the box $V$ from the left; replace $V$ with new box, if slicing was successful |
| • try to slice the box $V$ from the right; replace $V$ with new box, if slicing was successful |
| If any slicing, in any unknown, was successful, then repeat the procedure. |

| Output |
|--------|
| Tight interval hull $(a, b)$ for parameters $a$ and $b$. |

5.1 What is slicing?

Suppose that the current box is $V = (p_1, p_2, \ldots, p_r) \in \mathbb{R}^r$ and we are currently working with parameter $p_k$. Slicing from the left is described as a sequence of steps:

1. $\xi \leftarrow 1$
2. $\xi \leftarrow \xi/2$
3. divide $V$ into two parts, by cutting it with the plane $p_k = p_\xi$, where $p_\xi = p_k + \xi \left(p_k - p_{\xi}\right)$. Call the newly created subboxes slice ($p_k \leq p_\xi$) and rest ($p_k \geq p_\xi$).
4. probing slice means determining, whether or not the subbox slice fails the considered system of inequalities.
   If slice fails the system of inequalities then
   • $V \leftarrow$ rest (discard slice)
   • finish slicing from the left with parameter $p_k$; exit with flag success
   else (probe thinner slice)
• if termination criteria are not met then goto 2 else finish slicing from the left with parameter $p_k$; exit with flag \textit{no success}.

Slicing from the right is similar, except that at the beginning $\xi$ is set to 0 and the later updates have the form: $\xi \leftarrow (1 + \xi)/2$.

Few comments are in order. As seen from the description, at the beginning the algorithm probes large chunks of the initial box $V$. Indeed, the first slice has the same volume as the remaining part of box $V$, while the subsequent slices are smaller and smaller. We stop slicing in the direction of the current parameter at first success and then immediately switch to the next parameter, according to van Emden’s suggestions \footnote{1}.

What is the termination criterion? The most obvious should be the one based on width of a slice. Unsuccessful slicing should stop, at the latest, when the width of a slice, in direction of currently processed parameter, becomes small, comparable with the machine accuracy. One might think, that we should terminate slicing in a given direction even earlier, at some predefined threshold $\varepsilon$: slicing ceases, when $\xi \leq \varepsilon$ (slicing from the left) or $1 - \xi \leq \varepsilon$ (slicing from the right), where $\varepsilon$ is small, arbitrarily chosen, positive number, usually in range $10^{-6} - 10^{-3}$. This choice, however, does not guarantee obtaining the tightest possible bounds for searched parameters. Nevertheless, it may be practical in terms of of CPU time, and quite sufficient when processing experimental data.

Concluding, we may estimate the temporal complexity of a single cycle of slicing all unknowns, in the worst case, as being proportional to $m$ — the number of unknowns, and to $n$ — the number of experimental points: $C_t = 2Knmu$; effectively $C_t \sim O(n)$, since $m = 2$ is fixed. The factor 2 comes from the fact, that slicing is always two-sided. $K$, the proportionality constant, is roughly equal to the number of bits in mantissa plus twice the largest exponent used in floating point representation of real numbers. One must remember, however, that a single iteration, involving all unknowns in turn, only rarely will suffice. Fortunately, in the linear case considered here, all necessary intervals, even if calculated in a natural way (“naive”), have sharp ends, see Hansen’s \footnote{2} theorems on sharpness. That is why the computed interval enclosures are tight, also in the case of multivariate linear or linearized models. The above statement is not necessarily true, when the model is nonlinear.

The spatial complexity of box slicing algorithm is very attractive. At any stage of the calculations we are working with at most 3 interval boxes (original, slice and rest), each of size proportional to the number of unknowns ($m = 2 = const$), so $C_s \sim O(1)$.

### 5.2 Probing

The purpose of probing is to determine whether the given box contains the points with required properties, in our case – the solutions. The boxes, which
Figure 4: The bounding box denotes initial search domain in the plane ab. The target, slightly oversized, is a rectangle located near the center of figure. Two remaining lines, solid and dashed, divide the initial box into parts, for which some conditions are, or are not, met. The region bounded by dashed line is labelled as I, the region bounded by solid line has the label II. The details concerning the remaining domains III — VII are given in text.

certainly do not contain at least one interesting point, are eliminated from further considerations.

Proving the existence of solutions within the probed domain is, generally, not straightforward. Therefore, during probing, we will rather seek every opportunity to discard the (sub)box under study. The tests (“questions”) we are going to use during probing have to be carefully selected, since

\[\ldots \text{probing has a logic of its own.}\]

M.H. van Emden in [4]

Suppose that $p < q$ and we have obtained for some system of inequalities $\mathcal{I}$:

- $\mathcal{I}$ is non-failed for $x \leq q$ and
- $\mathcal{I}$ is non-failed for $x \geq p$.

Can we say anything about the localization of the solutions of $\mathcal{I}$, especially within the interval $[p, q]$? No, but on the other hand the result:
(I is failed for $x \leq q$) and (I is failed for $x \geq p$)

is a proof, that $I$ has no solutions at all, while

(I is failed for $x \geq q$) and (I is failed for $x \leq p$)

implies, that the solutions, if any, must be located within the interval $[p, q]$ (there are no solutions outside this interval).

Consider the Fig. 4. Think of the situation shown there as applicable to just one experimental point, say first, and to all the inequalities, in which this point is explicitly involved. For sake of simplicity from now on we drop the index numbering experimental points. Let’s concentrate first on the united solution set. We are going to find such $a$ and $b$ that

$$(ax + b) \cap y \neq \emptyset \quad (16)$$

for any pair $(x, y) \in (x, y)$. The opposite condition, when intervals $ax + b$ and $y$ are disjoint, is of better value for our purposes. It may be written in conventional interval notation as

$$(ax + b < y) \lor (ax + b > y) \quad (17)$$

The alternative (17), written above, provides us with the correct answer to the question whether the condition (16) is failed. Boxes $(a, b)$, for which (17) is true, can be safely discarded from further considerations, since all points belonging to them violate (16). All such boxes are localized outside the regions marked as I and II in Fig. 4, i.e. they may be found in regions III, IV or VII. So, the alternative (17) may be used as a rejection criterion by box slicing algorithm. Think, however, what will happen, if the united set of solutions is empty? In such case we will finish with very small box, still not sure whether or not there are any solutions in it. In contrast to ordinary point calculations, we cannot check it with a single calculation — there is still uncountable number of points belonging to such a box.

The solution of this dilemma is quite simple. Starting with initial box $V$ we discard those its parts, which satisfy the first term of the alternative (17), obtaining in result the box $V_d \subseteq V$. The box $V_d$ covers the region I in Fig. 4. Then we repeat the procedure, again starting with $V$, but this time using the second term of (17) as a rejection criterion. Now the resulting box is $V_u \subseteq V$, covering the domain II in Fig. 4. The solutions, if any, must be located in the intersection $V_d \cap V_u$. This intersection, if not empty, becomes the new initial box for another iteration. Continuing this process we obtain better and better interval hulls of regions marked as $V$ and VI in Fig. 4. Procedure terminates (“eventually stabilizes” in language of [6]), when $V_u = V_d = V$, or, in other words, when the slicing becomes idempotent operation. Empty intersection of $V_u$ and $V_d$, at any stage of calculations, constitutes a proof that the set of solutions is empty.

So, asking the proper questions during probing is not a trivial thing. The main difficulty lies in construction of appropriate rejection tests. Only the tests $Q$
with property \((V \subset W \in \mathbb{IR}^n)\):

\[
\left( Q(V) \text{ is non-failed} \right) \implies \left( Q(W) \text{ is non-failed} \right)
\] (18)

are appropriate. This is because we usually start with severely overestimated initial box known to contain solutions. We don’t want to have it rejected as a whole, in result of the first applied test.

5.3 Rejection tests and search regions for various kinds of solutions

5.3.1 United solutions

In case of just two different measurements \((m = 2, x_1 \cap x_2 = \emptyset)\) the problem may be quickly solved “analytically”:

\[
a = \frac{y_2 - y_1}{x_2 - x_1}
\] (19)

\[
b = (y_1 - ax_1) \cap (y_2 - ax_2)
\] (20)

Author cannot resist the temptation to comment on the elegance of the expression (20) – both measurements are treated in a perfectly symmetric manner. Despite this elegance, the expression for \(b\) does not necessarily produce the tight interval enclosure for \(b\), while the enclosure (19) for \(a\) is tight (sharp in Hansen’s terminology, see [5]). This is due to the well known dependency problem, which is unavoidable here; namely \(b\) is expressed by, among other, \(a, x_1\) and \(y_1\), while \(a\) was already calculated using the same variables. The lack of tightness is not a real problem here, we can rectify it using the box slicing algorithm, which, by its construction, always produces tight interval enclosures in linear case.

The construction given by formulae (19) and (20) can be used for establishing the bounds for the initial box \(V\), in which we will search for solutions (of any kind) of the original linear problem. It is sufficient to set

\[
V = (a, b) = \bigcup_{j,k} (a_{jk}, b_{jk})
\] (21)

where \(a_{jk}\) and \(b_{jk}\) are intervals obtained using values from measurements \(j\) and \(k\). The convex hull written above covers results for all pairs \((j, k)\) of experimental data satisfying \(x_j \cap x_k = \emptyset\). Calculation of (21) has thus the complexity \(O(n^2)\), what may seem excessive, especially when the number of measurements is large. Instead we may start with initial box defined as \(V = ([-\omega, +\omega], [-\omega, +\omega])\), where \(\omega\) is some sufficiently large number, say \(10^{40}\), at a price of increased number of iterations later.

In summary: in order to find united solutions we need the initial box given by (21) and a pair of rejection rules given in (17).
5.3.2 Tolerable solutions

Those, if exist, are a subset of united solutions. For this reason the initial box might be constructed the same way as for united solutions, see (21). What we need are the rejection rules appropriate for this case. Rules (17) are not sufficient. We need to discard boxes having no common parts with any tolerable solution, not just with the experimental points. Then we have to find at least one tolerable solution. Unfortunately, this is bad idea. Driven by such a condition, the procedure will converge not to the convex hull of tolerable solutions, but to this single, specific solution instead. Besides, we still don’t know how to find the first tolerable solution.

Let us start with calculating

\[ V_{tol} = (a_{tol}, b_{tol}) = \bigcap_{jk} a_{jk} \cap \bigcap_{jk} b_{jk} \]  

(22)

what can be done in the same loop, in which (21) is calculated. The box \( V_{tol} \), if not empty, contains all straight lines having common points with each experimental rectangle. If it is empty, then the tolerable solutions cannot exist. Let’s also calculate the auxiliary intervals, one for each measurement

\[ y'_k = a_{tol} x_k + b_{tol} \]  

(23)

Now the rejection rules may be expressed as follows. Reject box \((a, b)\), if for at least one measurement, say \(k\),

\[ (ax_k + b_k) \cap y'_k = \emptyset \]  

(24)

When calculating \( V_d \) reject also boxes satisfying the condition

\[ (ax_k + b < y_k) \lor (ax_k + b > y_k) \]  

(25)

for at least one measurement, while for \( V_u \) use as a rejection criterion

\[ (ax_k + b > y_k) \lor (ax_k + b < y_k) \]  

(26)

5.3.3 Controllable solutions

Controllable solutions, if exist, are subset of united solutions. So, the starting box can be constructed using (21) again. Following the prescription (22) we construct

\[ V_{con} = (a_{con}, b_{con}) \]  

(27)

and then the auxiliary intervals

\[ y'_k = a_{con} x_k + b_{con} \]  

(28)
If $V_{\text{con}} = \emptyset$ then the controllable solutions cannot exist. We discard all boxes $(a, b)$ satisfying (24) for at least one measurement. Additionally, when dealing with $V_d$ we use

$$\min (ax_k + b, ax_k + b) > y_k$$  \hspace{1cm} (29)$$

and when slicing $V_u$ the following condition

$$\max (ax_k + b, ax_k + b) < y_k$$  \hspace{1cm} (30)$$

as a rejection criterion. It happens quite often that initially $V_{\text{con}} \neq \emptyset$, but the set of controllable solution is empty anyway.

6 An Example

Using a FORTRAN program, described in [7], I have fitted an artificial data set consisting of 10 points, with uncertainties in both variables. As the uncertainties for each experimental measurement, $\sigma_x$ and $\sigma_y$, I have used third parts of radii of the corresponding intervals, i.e. $\frac{1}{6}$th of their widths. The data are listed in Table 1 and the results in Table 2.

Table 1: Data used in exemplary calculations. $\sigma_x$ and $\sigma_y$ were taken as rounded third parts of the corresponding radii.

| center of x | radius of x | $\sigma_x$ | center of y | radius of y | $\sigma_y$ |
|-------------|-------------|------------|-------------|-------------|------------|
| 0.9         | 0.1         | 0.333      | 3.65        | 0.45        | 0.150      |
| 1.9         | 0.1         | 0.333      | 4.60        | 0.40        | 0.133      |
| 2.9         | 0.1         | 0.333      | 5.65        | 0.22        | 0.073      |
| 3.9         | 0.1         | 0.333      | 6.60        | 0.40        | 0.133      |
| 5.4         | 0.1         | 0.333      | 8.00        | 0.50        | 0.167      |
| 5.9         | 0.1         | 0.333      | 8.55        | 0.35        | 0.117      |
| 6.9         | 0.1         | 0.333      | 9.60        | 0.50        | 0.167      |
| 8.7         | 0.1         | 0.333      | 11.30       | 0.50        | 0.167      |
| 9.1         | 0.1         | 0.333      | 12.75       | 0.55        | 0.183      |
| 10.1        | 0.1         | 0.333      | 13.70       | 0.30        | 0.100      |

Table 2: Results produced by program taken from [7], as recorded from computer screen, without any rounding.

| parameter | value        | parameter | value        |
|-----------|--------------|-----------|--------------|
| $a_{\text{LSQ}}$ | 1.08530271  | $\sigma_a$ | 0.0136506381 |
| $b_{\text{LSQ}}$ | 2.43730211  | $\sigma_b$ | 0.0823259652 |

I have also obtained an interval hull of united solution set for this problem, using full uncertainties for both variables. The result is (rounded outwards to
five significant figures):

$$(a, b) = ([1.02270, 1.13159], [2.06840, 2.96827])$$

As expected, $a_{LSQ} \in a$ and $b_{LSQ} \in b$. Using those values, the Table 3 was then prepared. In order to calculate the “corridor of errors” ($y_{LSQ} - 3\sigma$ and $y_{LSQ} + 3\sigma$ in Table) for LSQ results, I have mechanically adopted the widely used formula, taking as $\sigma$ the following quantity:

$$\sigma = \sqrt{|\frac{\partial y}{\partial a} \sigma_a|^2 + |\frac{\partial y}{\partial b} \sigma_b|^2} = \sqrt{|x\sigma_a|^2 + |\sigma_b|^2}$$

(31)

Table 3: Results of exemplary calculations. The intervals were rounded outwards to two significant figures, while the numbers labeled as $y_{LSQ} \pm 3\sigma$, resulting from point calculations, were rounded conventionally. The last column contains the ratio of widths of corresponding uncertainty estimates: interval to that produced by Least SQares method. First and last row do not correspond to any measurement, they are included to illustrate the extrapolation behavior of both approaches.

| $x$ | $y$ | $y_{fit}$ | $y_{fit} - y_{LSQ}$ | $y_{LSQ} - 3\sigma$ | $y_{LSQ} + 3\sigma$ | $\frac{w_{INT}}{w_{LSQ}}$ |
|-----|-----|-----------|---------------------|---------------------|---------------------|-------------------|
| 0.0 | 2.06| 2.97      | 2.434               | 2.441               | 120                 |
| 0.8 | 3.20| 3.88      | 3.105               | 3.506               | 2.494               |
| 1.0 | 4.10| 4.10      | 3.272               | 3.773               | 2.016               |
| 1.8 | 4.20| 5.01      | 3.943               | 4.839               | 1.239               |
| 2.0 | 5.00| 5.24      | 4.111               | 5.105               | 1.137               |
| 2.8 | 5.43| 6.14      | 4.781               | 6.171               | 0.871               |
| 3.0 | 5.87| 6.37      | 4.949               | 6.438               | 0.833               |
| 3.8 | 6.20| 7.27      | 5.620               | 7.503               | 0.701               |
| 4.0 | 7.00| 7.50      | 5.787               | 7.770               | 0.681               |
| 5.3 | 7.50| 8.97      | 6.877               | 9.502               | 0.568               |
| 5.5 | 8.50| 9.20      | 7.045               | 9.768               | 0.555               |
| 5.8 | 8.20| 9.54      | 7.296               | 10.168              | 0.536               |
| 6.0 | 8.90| 9.76      | 7.464               | 10.434              | 0.525               |
| 6.8 | 9.10| 10.67     | 8.135               | 11.500              | 0.490               |
| 7.0 | 10.10| 10.89    | 8.302               | 11.767              | 0.482               |
| 8.6 | 10.80| 12.70    | 9.644               | 13.898              | 0.433               |
| 8.8 | 11.80| 12.93    | 9.811               | 14.165              | 0.429               |
| 9.0 | 12.20| 13.16    | 9.979               | 14.431              | 0.425               |
| 9.2 | 13.30| 13.38    | 10.147              | 14.698              | 0.420               |
| 10.0| 13.40| 14.29    | 10.817              | 15.763              | 0.404               |
| 10.2| 14.00| 14.52    | 10.985              | 16.030              | 0.400               |
| 20.0| 22.52| 25.60    | 19.200              | 29.086              | 0.312               |

As can be seen from the Table 3, within the range, where the experimental points were taken, the results are comparable. However, if one examines the
behavior of both methods outside this domain, then the predictive power of
the interval method is clearly superior. The LSQ uncertainty estimate for \( y \) at
\( x = 0 \) seems at least unrealistic, while for \( x = 20 \) it is more than three times
wider comparing with the extrapolation based on interval result.

It should be noted that the problem of interpolation of interval valued experi-
mental data has already been investigated in [8] (Lagrange interpolating poly-
nomials) and in [9] (essentially the decomposition into set of basis functions —
generalized polynomials). In both cases the uncertainty appeared only in one
(dependent) variable. No conclusions concerning physical meaning or validity
of obtained parameters could be drawn.

7 Other applications in experimental sciences

7.1 Detection of outliers

Suppose, that we are trying to find the convex hull of united solutions for some
linear problem and it appears empty. This means, that one or more data points
are outliers. There are several methods, heuristic as well as based on probability
calculus, which make possible the identification of outliers. Note, that contrary
to the interval methods, the LSQ method always produces some estimates of
unknown parameters, regardless of the presence of outliers. Outliers can be most
easily spotted when the data and the best fitted line are plotted simultaneously
on the same graph. This is rather tedious task, if performed manually. In
control applications, either industrial or in laboratory, when the environment is
noisy, the misreadings or data transmission errors may occur quite frequently
and go undetected. This may seriously affect the quality and reliability of the
control procedures, sometimes leading to disastrous effects or even fatalities.

The advantage of interval methods over traditional LSQ method is then evident:
no outlier can go unnoticed. Nevertheless, the question of its identification still
remains. We should mention here, that other methods usually fail, when the
data set contains more than a single outlier, or there are just two outliers located
one next to the other.

Proposed is the following procedure for outlier detection: repeat finding the
united solution set for the experimental data using relaxed conditions (\( \mathfrak{g} \)), i.e.
with dropped requirement, that the condition is true for every measurement. In
other words, we will search for \textbf{crude} solutions mentioned earlier. In order to
find this set we will discard boxes \((a, b)\), which fail condition (\( \mathfrak{g} \)) for at least
\( k \) measurements, where index \( k \), initially set to zero, numbers the consecutive
trials. The value of index \( k \), at which we succeed for the first time, tells us
whether there are any outliers in the investigated data set and, eventually, how
many of them are there. Their identification is immediate: they all do not
satisfy the condition (\( \mathfrak{g} \)), evaluated with most recently obtained intervals \( a \) and
\( b \). Note, that there is no need for a priori knowledge, \textit{which} measurements are
suspected.
The method, outlined above, should be very robust—it should be able to detect and identify quite large number of outliers, even if they constitute up to 50% of all measurements. I have performed only a very limited number of tests, with only one or two outliers. The tests show, that the method is working as expected. It is obvious, that it always terminates, when only two measurements remain, at the latest.

7.2 Finding the asymptotic straight line

Sometimes we need to find, based on experimental information, the equation of a line, which is asymptotic or tangent to the investigated curve. The interval methods, described in this paper, may be of some help in eliminating the subjectivity of the person processing this sort of experimental data. Nowhere in the literature I was able to find a prescription on how to deal with problems of this kind. Yet they are important and so is the reliable determination of their relevant parameters, including the uncertainties. Consider, for example, the process described by formula:

\[
y(t) = A_0 + \sum_{j=1}^{k} A_j \exp \left( -\frac{t}{\tau_j} \right)
\]  

(32)

where the number of various subprocesses, \(k\), need not to be known precisely in advance and the unknown relaxation times \(\tau_j\)'s are well separated and ordered in increasing order. Recording such a process, especially near \(t = 0\), we obtain

\[
y(t) \approx y(0) - \frac{A_1}{\tau_1} t
\]

that is, the equation of a straight line, providing that the entire process is initially dominated by subprocess with shortest relaxation time. This is an equation commonly considered when studying (photo)chemical reaction’s kinetics, radioactive decay, multilevel relaxation and many other processes. Similar expressions can be obtained for the initial permeability of ferromagnetic materials or susceptibility of paramagnetics. In all such cases the interesting physical parameters are hidden in the slope of the corresponding straight line being tangent to the experimental curve. How can we obtain the reliable values of parameters for such a line?

Suppose, that we have found the interval hull of united solutions describing first \(n\) experimental points \((a_n, b_n)\). Observe now, what should happen when we enrich the data set with one more measurement and try to find united solutions again (and the experimental points follow the straight line!). It is obvious, that \((a_{n+1}, b_{n+1}) \subseteq (a_n, b_n)\), if only the measurements are correct. This simple observation is a basis for the proposed method. Starting with two first measurements (in this case the united solutions always exist), keep finding the united solutions, enlarging the set of measurements by one at every next trial. Finish when either \((a_{n+1}, b_{n+1}) \not\subseteq (a_n, b_n)\) or \((a_{n+1}, b_{n+1}) = \emptyset\), whatever
happens first. The solution is then \((a_n, b_n)\). Of course, the data should be properly ordered first, either as increasing or decreasing sequence of \(x\)’s.

8 Summary

I have demonstrated how the interval analysis can be helpful in objective and reliable processing of experimental data. I have discussed various types of possible solutions of linear systems, which may be useful and desired under different circumstances. The methods presented here easily handle classical cases, when the uncertainties affect only the dependent variable, the values of independent variable being exact, as well as those with uncertainties in both variables. There is no need for, always more or less arbitrary, weighting the experimental data.

9 Acknowledgments

The approach presented here was been inspired in great extent by the work of Krzysztof R. Apt \[6\]. After reading his paper author did realize, that the partial order existing in \(\mathbb{IR}\), the one generated by the inclusion, is the fundamental property of this set. Interval methods should depend on it, as is the case with the well known interval Newton algorithm. The interval part of presented numerical results was obtained using INTLIB \[10\] – free interval library written in FORTRAN 77.

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