

Guaranteed Nonlinear Parameter Estimation via Interval Computations

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Abstract

The problem of estimating the parameters of a nonlinear model from prior knowledge, experimental data and collateral requirements is viewed as one of set inversion, which is solved in an approximate but guaranteed way with the tools of interval analysis. It is, for instance, possible to characterize the set of all parameter vectors that are consistent with the data in the sense that the errors between the data and corresponding model outputs fall within known prior bounds. Any collateral requirements that can be expressed as a series of inequalities to be satisfied by the parameters can be taken into account. This is illustrated by asymptotic stability requirements for time-invariant models whose outputs are linear in their inputs, even if nonlinear in their parameters. The characterization of optimal confidence region in a Bayesian context can also be formulated in the framework of set inversion.

Keywords: Bayesian estimation, interval analysis, nonlinear estimation, parameter bounding, parameter uncertainty, robust stability, set estimation.

1 Introduction

The purpose of this paper is to briefly present some results recently obtained in the field of parameter estimation with the help of interval analysis and so far only published in the field of automatic control theory. For the sake of brevity, we have neither detailed the theoretical properties of the algorithms nor provided examples, these can be found in the references.

Building mathematical models to understand, predict and/or control the behavior of a system is a basic activity in most fields of pure and applied science. Frequently, prior knowledge is not sufficient to allow a complete derivation of models, and experimental data collected on this system must be used together with available prior knowledge (such as prior ranges or prior probability density functions) and collateral requirements (such as that the residuals be sufficiently

uncorrelated or that the model be asymptotically stable) in the modeling process.

A model structure may have to be selected among several candidates, each of which may involve a vector of *a priori* unknown parameters. The procedure employed then usually consists of estimating the parameters associated with each possible model structure and selecting the simplest structure with acceptable performances (see e.g. [14, 27]). Parameter estimation for a given structure is thus at the core of modeling, even when several structures are being considered.

The most classical approach for parameter estimation (see e.g. [4, 14, 21, 26]) is to look for the value of the parameter vector θ that is best in the sense of a given scalar criterion j . One may for instance look for the value of θ that minimizes the (weighted) least squares criterion

$$j(\theta) = \sum_{i=1}^n w_i (y(t_i) - y_m(t_i, \theta))^2,$$

where $y(t_i)$ is the i th experimental datum, $y_m(t_i, \theta)$ is the corresponding model output and w_i ($w_i \geq 0$) is the weight associated with the i th error. Many other criteria have also been considered, such as (weighted) least moduli, or any of the criteria generated by the maximum likelihood or bayesian approaches under various hypotheses on the noise corrupting the data, prior probability density function for the parameters and cost of assuming an erroneous value for the parameters [4, 14, 26].

In very special cases, such as when the criterion is quadratic in an error affine in the parameters, explicit formula are available to compute the optimal parameter vector. Most often, however, (e.g. when the model output is nonlinear with respect to the parameters, a situation that is the rule for models based on prior physical knowledge, no explicit formula can be provided for the best value of the parameter vector in the sense of the criterion chosen. A *local* optimization is then usually performed iteratively, starting from some initial value for the parameters and computing displacements in the parameter space aimed at improving the value of the criterion (see e.g. [26]). Such a local optimization of a scalar criterion has several drawbacks:

1. The choice of the initial value for the parameters relies largely on guess-work.
2. No guarantee of convergence to the global optimum of the criterion can be provided.
3. If there are several values of the estimated parameters that correspond to the same value of the criterion, a situation that may for instance result from the fact that the parameters are not globally identifiable (see e.g. [29]), the algorithm picks one of them without indicating that there are others.

4. In a large number of practical problems, such as the estimation of physical parameters from uncertain data in physics, chemistry, biology..., one is not actually interested in *the* optimal value of the parameters in the sense of a (somewhat artificial) scalar criterion but would rather like to characterize the *set* of *all* values that are acceptable in a sense to be specified.
5. Uncertainty on the estimate is evaluated (if at all) by use of asymptotic properties of the estimator that rely on a succession of dubious assumptions, so that no reliable evaluation is provided of the precision with which the estimated value of θ is obtained.

A possible way out of difficulties 1 to 3 is to use deterministic global optimization methods such as those described in [6, 24], but this still leaves difficulties 4 to 5 to be addressed. This is why we shall follow a different route, and look for the set of all models that are acceptable instead of looking for the model that is optimal in the sense of a given criterion. The first step is then to list all the properties that the model should have to be acceptable. Acceptability will be defined here by a set of (possibly nonlinear) inequalities to be satisfied by the parameters. This is a very realistic assumption in a large number of engineering problems, where acceptability is defined in terms of tolerances with respect to some nominal specifications. It makes it easy to incorporate collateral requirements as well as experimental data and prior information. Once these conditions of acceptability have been defined, one is interested in characterizing the set S of all parameter vectors such that the model is acceptable. This can be formulated as a problem of set inversion, which must be solved globally in order to avoid difficulties 1 to 3. Starting from some prior feasible set for the parameter vector under the form of some (possibly very large) axis-aligned box in the parameter space, we wish to characterize —approximately but in a guaranteed way— the posterior feasible set for the parameters, i.e. the set of all values of the parameter vector that are consistent with the prior feasible set and satisfy all conditions for acceptability. This will be performed with the help of an algorithm for set inversion described in Section 2.

A first example of acceptability conditions is that the residuals between the data $y(t_i)$, $i = 1, \dots, n$, and corresponding model outputs $y_m(t_i, \theta)$, $i = 1, \dots, n$, lie between some known bounds that express the confidence interval attached to individual measurements. This is the problem of bounded-error estimation, considered in Section 3. Other acceptability conditions not directly related to the errors could be considered as well. Section 4, for instance, addresses the computation of guaranteed stability domains, which can be seen as a problem of parameter estimation from collateral requirements only. The characterization of optimal confidence regions in a Bayesian context can also be cast in the framework of set inversion, as indicated in Section 5.

2 Set inversion via interval analysis

Our algorithm for set inversion via interval analysis (SIVIA) [8, 9] is aimed at characterizing the set

$$\mathcal{X} = \mathbf{f}^{-1}(\mathcal{Y}) \subset \mathcal{R}^p$$

from the knowledge of the set $\mathcal{Y} \subset \mathcal{R}^q$ and the vector function \mathbf{f} . Let us first very briefly recall the few notions of interval analysis (see e.g. [19]) needed to present it.

A *vector interval* (or *box*) in a p -dimensional space is the Cartesian product of p scalar intervals

$$[\mathbf{x}] = [x_1^-, x_1^+] \times \cdots \times [x_p^-, x_p^+].$$

The *width* $w([\mathbf{x}])$ of a box $[\mathbf{x}]$ is the length of its largest side(s). \mathcal{F} is an *inclusion function* of the vector function \mathbf{f} if for any $[\mathbf{x}]$, $\mathcal{F}([\mathbf{x}])$ is a box such that

$$\mathbf{f}([\mathbf{x}]) \subset \mathcal{F}([\mathbf{x}])$$

and

$$w([\mathbf{x}]) \longrightarrow 0 \implies w(\mathcal{F}([\mathbf{x}])) \longrightarrow 0.$$

The last equation is only needed to ensure convergence of SIVIA, and could be relaxed to account for numerical errors due to rounding. It means that the smaller the box $[\mathbf{x}]$ is the better the approximation provided by the inclusion function is going to be. The analysis of the space of interest will be performed by building sets of non-overlapping boxes with nonzero width (or *subpavings*).

SIVIA applies to any function \mathbf{f} for which an inclusion function \mathcal{F} can be computed. Exploration is limited to an initial box of interest $[\mathbf{x}](0)$, which is split by the algorithm into smaller boxes whenever needed until either a conclusion can be reached or the width of the box considered becomes smaller than some tolerance parameter ϵ_r to be specified by the user. Interval analysis provides us with two basic tests for deciding whether a given box $[\mathbf{x}]$ is included in \mathcal{X} :

$$\mathcal{F}([\mathbf{x}]) \subset \mathcal{Y} \implies [\mathbf{x}] \subset \mathcal{X} \text{ (i.e. } [\mathbf{x}] \text{ is } \textit{feasible}).$$

$$\mathcal{F}([\mathbf{x}]) \cap \mathcal{Y} = \emptyset \implies [\mathbf{x}] \cap \mathcal{X} = \emptyset \text{ (i.e. } [\mathbf{x}] \text{ is } \textit{unfeasible}).$$

In all other cases, $[\mathbf{x}]$ is *indeterminate*. SIVIA computes two subpavings iteratively, namely \mathcal{K}_{in} , containing all boxes that were proved feasible, and \mathcal{K}_i , consisting of all indeterminate boxes. From these subpavings, it is easy to bracket the portion of \mathcal{X} contained in $[\mathbf{x}](0)$ as

$$\mathcal{K}_{in} \subset [\mathbf{x}](0) \cap \mathcal{X} \subset \mathcal{K}_{out} := \mathcal{K}_{in} \cup \mathcal{K}_i.$$

Since \mathcal{K}_{out} is a finite union of boxes guaranteed to contain the portion of \mathcal{X} of interest, it is very convenient for implementing set-theoretic manipulations [7]. For another practical situation where interval computational methods can

be used to bracket a set of interest, see [3]. A stack will be used to store the boxes still under consideration. Initialization is performed by setting

$$k = 0, \text{ stack} = \emptyset, \mathcal{K}_{in} = \emptyset, \mathcal{K}_i = \emptyset.$$

Iteration k is as follows

1. If $\mathcal{F}([\mathbf{x}](k)) \subset \mathcal{Y}$, append $[\mathbf{x}](k)$ to the subpaving of feasible boxes \mathcal{K}_{in} and go to Step 4.
2. If $\mathcal{F}([\mathbf{x}](k)) \cap \mathcal{Y} = \emptyset$, discard $[\mathbf{x}](k)$ as unfeasible and go to Step 4.
3. If $w([\mathbf{x}](k)) \leq \epsilon_r$, then append $[\mathbf{x}](k)$ to the subpaving of indeterminate boxes \mathcal{K}_i , else bisect $[\mathbf{x}](k)$ and stack the two resulting boxes.
4. If the stack is not empty, then unstack into $[\mathbf{x}](k+1)$, increment k by one and go to Step 1, else stop.

Upon completion of SIVIA, no indeterminate box will have a width larger than ϵ_r . Moreover, under a few realistic technical conditions, \mathcal{K}_{in} and \mathcal{K}_{out} will tend to \mathcal{X} (respectively from within and from without) when ϵ_r tends to zero [9]. When the dimension of \mathcal{X} is less than four, the set \mathcal{K}_{in} of all boxes that have been proved to be feasible (or the union \mathcal{K}_{out} of this set with that of all boxes for which we have failed to prove anything) can be plotted in the parameter space. When the dimension of the parameter space is larger than three, the algorithm obviously still applies, but the results are obtained under the form of lists of boxes, easier to interpret with the help of a computer than graphically. A first example of a situation where parameter estimation can be cast in the framework of set inversion and solved by SIVIA is considered in the next section.

3 Bounded-error estimation

Bounded-error estimation (or membership set estimation) is becoming increasingly popular in mathematical modeling, automatic control and signal processing (see e.g. [30], the surveys [13, 17, 22, 32] and the references therein, as well as no less than 25 papers in [1]).

To simplify exposition, we shall only consider output errors:

$$e(t_i, \theta) = y(t_i) - y_m(t_i, \theta), \quad i = 1, \dots, n.$$

but other types of errors could be considered as well. It is assumed that these errors should satisfy

$$e_-(t_i) \leq e(t_i, \theta) \leq e_+(t_i), \quad i = 1, \dots, n.$$

to be acceptable, where $e_-(t_i)$ and $e_+(t_i)$ are known prior bounds. These prior bounds may result from hard facts, such as the performances of sensors as expressed in their technical specification sheets, or merely indicate how far we are

prepared to go in accepting discrepancies between our data and model outputs. Let \mathbf{y} be the vector of all data $y(t_i), i = 1, \dots, n$, collected on a system, and $\mathbf{y}_m(\boldsymbol{\theta})$ be the vector of all corresponding model outputs $y_m(t_i, \boldsymbol{\theta})$. The vector of all output errors can then be written as

$$\mathbf{e}(\boldsymbol{\theta}) = \mathbf{y} - \mathbf{y}_m(\boldsymbol{\theta}).$$

Define the *feasible set for the errors* \mathcal{E} as the set of all error vectors \mathbf{e} that satisfy

$$\mathbf{e}_- \leq \mathbf{e} \leq \mathbf{e}_+,$$

where the i th component of \mathbf{e}_- and \mathbf{e}_+ is respectively $e_-(t_i)$ and $e_+(t_i)$. To be acceptable, $\boldsymbol{\theta}$ must satisfy

$$\mathbf{e}(\boldsymbol{\theta}) \in \mathcal{E}.$$

The (*posterior*) *feasible set* for $\boldsymbol{\theta}$ is therefore given by

$$\mathcal{S} = \mathbf{e}^{-1}(\mathcal{E}).$$

Characterizing \mathcal{S} is thus a problem of set inversion, which can be solved with the help of SIVIA. Here, \mathcal{S} stands for \mathcal{X} , \mathbf{e} for \mathbf{f} and \mathcal{E} for \mathcal{Y} . The box $[\mathbf{x}](0)$ then corresponds to the prior feasible set for the parameters.

Most of the work so far has been devoted to models with outputs linear in their parameters, i.e.,

$$y_m(t_i, \boldsymbol{\theta}) = \mathbf{r}^T(t_i)\boldsymbol{\theta}, \quad i = 1, \dots, n,$$

where the regressor $\mathbf{r}(t_i)$ is a vector of known numbers. In this case, \mathcal{S} is a convex polyhedron, which is bounded if trivial identifiability conditions are satisfied. It can then be characterized exactly and recursively as the convex hull of its vertices (see e.g. [31]), or approximately but simply by computing outerbounding ellipsoids (see e.g. [2, 23]), boxes [15, 16] or parallelotopes [28].

By contrast, very few *guaranteed* results are available for nonlinear models, except the signomial approach advocated in [18]. Use of interval analysis is an alternative approach, independently suggested in [8, 9] and [20], to obtain such guaranteed results. Note that \mathcal{E} may be any prior feasible set for the errors defined by a finite set of inequality constraints. Collateral requirements are easily taken into account, provided that they can also be expressed as a series of nonlinear inequalities to be satisfied by the parameters. It then suffices to append these inequalities to those resulting from the bounded-error data. The next section shows, for instance, how stability requirements can be cast in the framework of set inversion.

4 Characterization of stability domains

Consider a time-invariant continuous-time model, described by an ordinary differential equation. (Transposition to discrete-time models is trivial.) Assume

that the output of this model is linear in its inputs, which does not imply that it is linear in its parameters. A necessary and sufficient condition for this model to be asymptotically stable is that all terms of the first column of the Routh table associated with its characteristic polynomial have the same sign [25]; and an early version of interval analysis was developed by S. Faedo [5] to derive sufficient conditions for stability by using this criterion. Assume that the characteristic polynomial to be considered depends on some uncertain parameter vector \mathbf{p} , so that it can be written as

$$P(s, \mathbf{p}) = \sum_{k=0}^n a_k(\mathbf{p})s^k.$$

In what follows, the coefficient $a_n(\mathbf{p})$ of the leading monomial is normalized to 1. The vector \mathbf{p} may consist of parameters of the model of the process, but may also include parameters of a controller. We wish to characterize the set \mathcal{P} of all values of \mathbf{p} such that the resulting model is asymptotically stable. Here, a_k may be any computable function of \mathbf{p} , so that the situation considered is much more general than with Kharitonov's celebrated theorem [10] and its extensions. If $\mathbf{f}(\mathbf{p})$ is the vector of all entries of the first column of the Routh table that are not identically equal to one, then the system with parameter vector \mathbf{p} will be asymptotically stable if and only if

$$\mathbf{f}(\mathbf{p}) > 0.$$

In other words, the system will be asymptotically stable at \mathbf{p} if and only if

$$\mathbf{f}(\mathbf{p}) \in \mathcal{Y},$$

where

$$\mathcal{Y} =]0, +\infty[^{\times(n)}.$$

Finding \mathcal{P} is thus again a problem of set inversion, since

$$\mathcal{P} = \mathbf{f}^{-1}(\mathcal{Y}).$$

This problem can readily be solved with SIVIA. The prior set for the parameters is then decomposed into subboxes to be tested for stability, an idea that can also be found in the work by Kiendl and coworkers (see e.g. [11]), where a Lyapunov function is used to establish the stability of subboxes. The analysis of the stability of polynomials with coefficients depending on interval parameters is also being considered by Kolev [12].

More traditional statistically-based approaches for parameter estimation can also be formulated as problems of set characterization, as evidenced by the next section.

5 Bayesian estimation

In Bayesian estimation, the parameters are assumed to be random variables, with known prior *probability density function* (*pdf*). A formal expression of their posterior *pdf* $\pi_{post}(\theta)$ (i.e. their distribution when the data and noise characteristics have been taken into account) is computed using Bayes' rule (see e.g. [4, 26]). The posterior *pdf* for the parameters thus obtained is often difficult to use in practice, and rules have been suggested to compute point estimates from it. The simplest of these rules is to compute the *maximum a posteriori* estimate, i.e. the value of θ that maximizes $\pi_{post}(\theta)$. If the cost of believing that the parameters have the value θ when their actual value is θ^* can be evaluated, it is also possible to compute a *minimum risk* estimate, i.e. the value of θ that maximizes the cost averaged over all possible values of θ^* , given that y has been observed. Whatever the rule for computing a point estimate, it must be noted that the optimization of the resulting scalar criterion is usually far from simple and that the information about the uncertainty on θ that was contained in the posterior *pdf* is lost, so that the difficulties alluded to in Section 1 about the lack of a reliable assessment of the uncertainty on the parameter estimates are still present. This is why we would rather compute an *optimal confidence region* at level α , denoted by \mathcal{S}_α and defined as the compact set with smallest volume such that $\theta \in \mathcal{S}_\alpha$ with probability α . Equivalently, \mathcal{S}_α can be defined as

$$\mathcal{S}_\alpha = \pi_{post}^{-1}([s_\alpha, +\infty[),$$

where s_α is a threshold level, to be chosen so as to ensure that the posterior probability of \mathcal{S}_α satisfies $\Pi_{post}(\mathcal{S}_\alpha) = \alpha$. SIVIA does not apply to finding \mathcal{S}_α , because the additional threshold parameter s_α is unknown. For that purpose, assume that the following are available (i) a paving \mathcal{K} of the prior feasible set for the parameters (i.e. a subpaving such that the prior feasible set \mathcal{K} is equal to the union of all its boxes); (ii) a pair of functions (π^+, π^-) such that $\pi^-(\theta) \leq \pi_{post}(\theta) \leq \pi^+(\theta)$ and that their values are constant over any box of \mathcal{K} ; (iii) a numerical procedure to compute the posterior probability $\Pi_{post}([\theta])$ for any box $[\theta]$ of \mathcal{K} . Interval analysis can be used to obtain (π^+, π^-) from π_{post} . To find a pair (s^-, s^+) of positive real numbers that bracket s_α , the following two relations can then be used:

$$\Pi_{post}((\pi^-)^{-1}([s^-, +\infty[)) > \alpha \implies s^- < s_\alpha,$$

$$\Pi_{post}((\pi^+)^{-1}([s^+, +\infty[)) < \alpha \implies s^+ > s_\alpha.$$

The procedure for computing s^- is as follows.

1. Sort all boxes of \mathcal{K} by decreasing values of π^- .
2. Set $[\theta]$ equal to the first box of \mathcal{K} . Compute $\alpha^+ = \Pi_{post}([\theta])$.

3. While $\alpha^+ \leq \alpha$, set $[\theta]$ equal to the next box of \mathcal{K} ,
set $\alpha^+ = \alpha^+ + \Pi_{post}([\theta])$.
4. Set $s^- = \pi^-([\theta])$.

The value of α^+ is equal to sum of the probabilities of all boxes explored so far. When the loop ends, $\alpha^+ > \alpha$, so that $s^- < s_\alpha$. The same type of algorithm can be used to compute s^+ . Once s^- and s^+ have been obtained, it is possible to bracket \mathcal{S}_α by setting

$$\mathcal{K}_{in} := \{[\theta] \in \mathcal{K} \mid \pi^-([\theta]) \geq s^+\},$$

$$\mathcal{K}_{ext} := \{[\theta] \in \mathcal{K} \mid \pi^+([\theta]) \leq s^-\} \cup \{[\theta] \in \mathcal{K} \mid \Pi_{post}([\theta]) = 0\}.$$

Then

$$\mathcal{K}_{in} \subset \mathcal{S}_\alpha \subset \mathcal{K}_{out} := \mathcal{K} - \mathcal{K}_{ext}.$$

The finer \mathcal{K} is the more accurate the bracketing will be, and the following procedure will be used for recursively improving \mathcal{K} and the quality of the bracketing.

1. Set $\mathcal{K} = \{[\theta](0)\}$.
2. Repeat
 - (a) select a box $[\theta]$ of \mathcal{K} that maximizes $\Pi_{post}([\theta])$,
 - (b) bisect it along a principal plane into $[\theta_1]$ and $[\theta_2]$,
 - (c) set $\mathcal{K} = \mathcal{K} - [\theta] + [\theta_1] + [\theta_2]$,
 - (d) compute s^- and s^+ ,
 - (e) compute \mathcal{K}_{in} and \mathcal{K}_{out} ,

until $\Pi_{post}(\mathcal{K}_{out}) - \alpha \leq \epsilon$ (where ϵ is a suitably small positive real number).

When this procedure ends, $\mathcal{K}_{out} \subset \mathcal{S}_{\alpha+\epsilon}$.

6 Conclusions

A very large number of problems of practical interest can be formulated as that of finding all values of a parameter vector that are acceptable in the sense that a finite set of (possibly nonlinear) inequalities are satisfied. The methods classically used for that purpose are random sampling and systematic exploration over a grid in the parameter space. Even after intensive computations, no definitive conclusion can be drawn with these approaches, because a very small subset of the parameter space may always have escaped attention.

By contrast, the set-inversion techniques advocated in this paper provide guaranteed results (even if approximate) with a finite number of operations.

Large portions of the prior parameter space can be very quickly eliminated, before concentrating on the indeterminate region. Theoretical results concerning the complexity of SIVIA—in terms of memory and computing time—can be found in [8]. The required memory for the stack remains surprisingly limited, even if the number of parameters becomes quite large. As could be expected, the number of boxes in the subpavings increases quickly when the number of parameters increases or when the tolerance parameter ϵ_r is decreased. Since the characteristics of these boxes can be stored on disks, problems of realistic size (say with less than ten parameters) can be considered. The main limitation of the algorithm is that the computing time increases exponentially with the dimension of the parameter space.

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