

Rigorous Sensitivity Analysis for Parameter-Dependent Systems of Equations

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In this paper we construct rigorous and realistic enclosures for the solutions of parameter-dependent systems of equations $F(\bar{x}, \bar{t}) = 0$. The enclosure of the solution $\bar{x} = x(\bar{t})$ is given in the form $x^0 + S(\bar{t} - t^0)$ with interval vectors x^0 , t^0 and an interval matrix S . This allows a detailed analysis of the sensitivity of the solution $x(\bar{t})$ to small changes of \bar{t} and the influence of specific changes in selected parameters on the solution. The linear case is treated separately.

Für die Lösungsmenge eines parameterabhängigen linearen oder nichtlinearen Gleichungssystems $F(\bar{x}, \bar{t}) = 0$ werden garantierte und realistische Einschließungen berechnet. Die Darstellung der Lösung $\bar{x} = x(\bar{t})$ in der Form $x^0 + S(\bar{t} - t^0)$ mit Intervallvektoren x^0 , t^0 und einer Intervallmatrix S erlaubt eine detaillierte Sensitivitätsanalyse der Lösung für kleine Änderungen von \bar{t} . © 1989 Academic Press, Inc.

1. INTRODUCTION

Solving parameter-dependent systems of equations $F(\bar{x}, \bar{t}) = 0$ is an important part of scientific computation. Traditionally, this is done either by continuation methods which trace a particular solution curve (or solution manifold if the parameter \bar{t} is multidimensional), as in [2, 11, 13], or by linearizing the equations around a particular solution and to deduce from this linearization the effect on the solution of small changes in one or several parameters. The latter technique has become known under the name of *sensitivity analysis*. Because of the neglect of higher-order nonlinearities, traditional sensitivity analysis is valid only for "sufficiently small" changes, and it requires expert knowledge to assess which perturbations can still be considered as sufficiently small. In the present paper we modify the traditional approach, using interval analysis to quantify the effect of higher-order nonlinearities. This results in rigorous error bounds for the solution of perturbed equations; the error bounds derived are essentially linear in the perturbation (more precisely, they are sublinear in the

and for $x^0, x^1 \in x \in \mathbb{D}_0, t^0 \in t \in \mathbb{I}T_0$ we have

$$F[x^0, x^1](t^0) \in \partial_1 F(x, t),$$

$$F(x^0)[t^0, t^1] \in \partial_2 F(x, t).$$

We develop in Sections 2 and 3 a rigorous sensitivity analysis for the equations $F(\bar{x}) = \bar{b}$ ($\bar{b} \in b$) and $F(\bar{x}, \bar{t}) = 0$ ($\bar{t} \in t$), and prove in Section 4 a bound on the overestimation which implies the quadratic approximation property of the enclosure of Section 3. We shall need the following auxiliary result.

1.1. LEMMA. Let $a, b \in \mathbb{R}$, and $\langle a \rangle := \inf\{|\bar{a}| \mid \bar{a} \in a\}$. Then:

- (i) $0 \in ab \Rightarrow \rho(ab) = \sup(|a|\rho(b), \rho(a)|b|)$.
- (ii) $0 \in b \Rightarrow \rho(ab) \leq (\langle a \rangle + 2\rho(a))\rho(b)$.

Proof. Part (i) follows easily from Proposition 2.1 in Krawczyk and Neumaier [6] since $|a| = |\bar{a}| + \rho(a)$, and (ii) holds since $|a| \leq \langle a \rangle + 2\rho(a)$ and $|b| \leq 2\rho(b)$ (if $0 \in b$). ■

2. DEPENDENCY ON THE RIGHT-HAND SIDE

In this section we consider the problem of enclosing the solutions \bar{x} of the family of equations

$$F(\bar{x}) = \bar{b} \quad (\bar{b} \in b) \tag{1}$$

by bounds depending on \bar{b} ; here $F: D_0 \subseteq \mathbb{R}^n \rightarrow \mathbb{R}^n$ is assumed to be continuously differentiable, and $b \in \mathbb{R}^n$ is an interval vector specifying the range of interest for the right-hand side \bar{b} . We assume that a vector $x^0 \in D_0$ is known such that $F(x^0)$ is close to a vector in b , such an x^0 can be determined by standard numerical methods for systems of equations, e.g., by Newton's method.

2.1. THEOREM. Let D be a convex subset of D_0 and suppose that $A \in \mathbb{R}^{n \times n}$ is regular and satisfies

$$F[x^0, \bar{x}] \in A \quad \text{for all } \bar{x} \in D.$$

If $x \in \mathbb{R}^n$ is an enclosure of $x^0 + A^H(b - F(x^0))$ and $S \in \mathbb{R}^{n \times n}$ is an enclosure of A^{-1} then:

- (i) For $\bar{b} \in b$, every solution $\bar{x} \in D$ of $F(\bar{x}) = \bar{b}$ is in x and satisfies
$$\bar{x} = x^0 + \bar{S}(\bar{b} - F(x^0)) \quad \text{for some } \bar{S} \in S. \tag{2}$$

sense of [8]), and they are valid for all parameter values \bar{t} in an initially specified interval. We also prove that the bounds obtained are realistic for narrow ranges of the parameters.

We shall use the following notation. \mathbb{R}^n denotes the set of interval vectors with n components, and for $D \subseteq \mathbb{R}^n$, we write $\mathbb{D} := \{x \in \mathbb{R}^n \mid x \subseteq D\}$. $\mathbb{R}^{m \times n}$ denotes the set of interval $m \times n$ -matrices. The terms *vector* and *matrix* will be used synonymously to interval vector and interval matrix. The *midpoint*, *radius*, and *absolute value* of a matrix $A \in \mathbb{R}^{m \times n}$ are understood componentwise, and are denoted by $\bar{A} = \text{mid}(A)$, $\rho(A) = \text{rad}(A)$, and $|A|$, respectively. Similar definitions apply for vectors. The square matrix $A \in \mathbb{R}^{n \times n}$ is called *regular* if all $\bar{A} \in A$ are nonsingular; in this case $A^H B$ (where $B \in \mathbb{R}^{n \times p}$) denotes the hull of the solution set $\{\bar{X} \in \mathbb{R}^{n \times p} \mid \bar{A}\bar{X} = \bar{B}$ for some $\bar{A} \in A, \bar{B} \in B\}$ of the linear interval "equation" $AX = B$. Here the hull of a bounded set is the interval $\square S = [\inf(S), \sup(S)]$. The hull of the set $\{\bar{A}^{-1} \mid \bar{A} \in A\}$ of inverses is denoted by A^{-1} ; note that $A^H B \subseteq A^{-1}B$, with strict inequality in many cases.

If $F: D_0 \rightarrow \mathbb{R}^n$ is a continuously differentiable function and the line joining x_1, x_2 is in D_0 we define

$$F[x^0, x^1] := \int_0^1 F(x^0 + s(x^1 - x^0)) ds.$$

Clearly, $F[x^0, x^1] = F[x^1, x^0]$ and

$$F(x^1) = F(x^0) + F[x^0, x^1](x^1 - x^0);$$

thus $F[x^0, x^1]$ is a *slope* in the sense of Krawczyk and Neumaier [5], and for any interval extension of the derivative we have

$$F[x^0, x^1] \in F'(x) \quad \text{if } x^0, x^1 \in x \in \mathbb{D}_{D_0}.$$

Similarly, we define for functions $F: D_0 \times T_0 \rightarrow \mathbb{R}^n$ of two variables

$$F[x^0, x^1](t^0) := \int_0^1 \partial_1 F(x^0 + s(x^1 - x^0), t^0) ds,$$

$$F(x^0)[t^0, t^1] := \int_0^1 \partial_2 F(x^0, t^0 + s(t^1 - t^0)) ds.$$

Then

$$F(x^1, t^0) = F(x^0, t^0) + F[x^0, x^1](t^0) \cdot (x^0 - x^1),$$

$$F(x^0, t^1) = F(x^0, t^0) + F(x^0)[t^0, t^1] \cdot (t^0 - t^1),$$

This allows a simple assessment of the effects of changing \tilde{b} . The effects on linear combinations of the solution components can also be accurately described by

$$a^T \tilde{x} \in a^T x^0 + (a^T S)(\tilde{b}' - F(x^0)),$$

and

$$a^T \tilde{x} \in a^T x^0 + (a^T C)(\tilde{b}' - y).$$

The enclosures obtained in this way are usually considerably better than those obtained by multiplying an enclosure x of \tilde{x} by a^T .

3. THE GENERAL CASE

In this section we consider the problem of enclosing the solutions \tilde{x} of the family of equations

$$F(\tilde{x}, \tilde{t}) = 0 \quad (\tilde{t} \in I) \tag{4}$$

by bounds depending on \tilde{t} ; here $F: D_0 \subseteq \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}^n$ is assumed to be continuously differentiable, and $I \in \mathbb{IR}^m$ is an interval vector specifying the range of interest for the m -dimensional parameter vector \tilde{t} . Now we assume that a pair $(x^0, t^0) \in D_0$ is known such that $F(x^0, t^0) = 0$ and t^0 is in I . This is slightly unrealistic for finite precision calculation, but in practice one can take in place of x^0 any narrow enclosure of a solution of the equation $F(x^0, t^0) = 0$, and still get rigorous results. Such enclosures can be computed with standard interval methods for nonlinear systems: see, e.g., Alefeld and Herzberger [1] and Rump [12].

3.1. THEOREM. Let $D \times T$ be a convex subset of D_0 such that $x^0 \in D$, $t^0 \in T$, and suppose that $A \in \mathbb{IR}^{n \times n}$ is regular and satisfies

$$F[x^0, \tilde{x}](t^0) \in A \quad \text{for all } \tilde{x} \in D,$$

and that $B \in \mathbb{IR}^{n \times m}$ satisfies

$$F(\tilde{x})[t^0, \tilde{t}] \in B \quad \text{for all } \tilde{x} \in D, \tilde{t} \in T.$$

If $F(x^0, t^0) = 0$ and $S \in \mathbb{IR}^{n \times m}$ is an enclosure of $-A^{-1}B$, and if $x = x^0 + S(t - t^0)$ then:

(i) For $\tilde{t} \in T$, every solution $\tilde{x} \in D$ of $F(\tilde{x}, \tilde{t}) = 0$ is in x and satisfies

$$\tilde{x} = x^0 + \tilde{S}(\tilde{t} - t^0) \quad \text{for some } \tilde{S} \in S. \tag{5}$$

(ii) If $x \subseteq D$ and $x^0 \in \text{int}(D)$ then x (and hence D) contains for every $\tilde{b} \in b$ a solution \tilde{x} of $F(\tilde{x}) = \tilde{b}$.

Proof. Put $\tilde{S} = F[x^0, \tilde{x}]^{-1}$. Then $x^0 + \tilde{S}(\tilde{b} - F(x^0)) = x^0 + \tilde{S}(F(\tilde{x}) - F(x^0)) = x^0 + \tilde{S}F[x^0, \tilde{x}](\tilde{x} - x^0) = x^0 + (\tilde{x} - x^0) = \tilde{x}$, and since $\tilde{S} \in A^{-1} \subseteq S$, part (i) follows. Part (ii) is a simple consequence of Theorem 1 of Neumaier [9]. ■

At the expense of some loss of accuracy for \tilde{b} very close to $F(x^0)$ we can give a variation of the enclosure which is truly linear in \tilde{b} .

2.2. THEOREM. Under the first hypothesis of Theorem 1, let $C \in \mathbb{R}^{n \times n}$ be such that AC is regular. If $y \in \mathbb{IR}^n$ is an enclosure of $(AC)^H(F(x^0) + (AC - I)b)$ and $x = x^0 + C(b - y)$ then:

(i) For $\tilde{b} \in b$, every solution $\tilde{x} \in D$ of $F(\tilde{x}) = \tilde{b}$ is in x and satisfies

$$\tilde{x} = x^0 + C(\tilde{b} - \tilde{y}) \quad \text{for some } \tilde{y} \in y. \tag{3}$$

(ii) If $x \subseteq D$ and $x^0 \in \text{int}(D)$ then x (and hence D) contains for every $\tilde{b} \in b$ a solution \tilde{x} of $F(\tilde{x}) = \tilde{b}$.

Proof. If AC is regular then C is nonsingular, and $\tilde{y} := \tilde{b} - C^{-1}(\tilde{x} - x^0)$ satisfies $\tilde{x} = x^0 + C(\tilde{b} - \tilde{y})$. With $\tilde{A} = F[x^0, \tilde{x}] \in A$ we find $(\tilde{A}C)\tilde{y} = (\tilde{A}C)\tilde{b} - \tilde{A}(\tilde{x} - x^0) = (\tilde{A}C)\tilde{b} - F(\tilde{x}) + F(x^0) = F(x^0) + (\tilde{A}C - I)\tilde{b}$ so that $\tilde{y} = (\tilde{A}C)^{-1}(F(x^0) + (\tilde{A}C - I)\tilde{b}) \in y$ and $\tilde{x} = x^0 + C(\tilde{b} - \tilde{y}) \in x$. This implies (i), and (ii) follows by applying Theorem 1 in Neumaier [9] to $\phi(y) = F(x^0 + C(\tilde{b} - \tilde{y})) - \tilde{b}$ in place of $F(x)$. ■

In the linear case $F(\tilde{x}) = \tilde{A}\tilde{x}$, $D = \mathbb{R}^n$ we get:

2.3. COROLLARY. If $A \in \mathbb{IR}^{n \times n}$ and $C \in \mathbb{R}^{n \times n}$ are such that AC is regular, and $y \in \mathbb{IR}^n$ is an enclosure of $(AC)^H(Ax^0 + (AC - I)b)$ then $A^{-1}b \subseteq x^0 + C(b - y)$, and every \tilde{x} with $\tilde{A}\tilde{x} = \tilde{b}$ for some $\tilde{A} \in A$, $\tilde{b} \in b$ satisfies (3).

Remarks. 1. A good choice for C is the midpoint inverse \tilde{A} ; in finite precision calculation, the approximate inverse should be computed by applying Gauss elimination to the columns of the identity matrix (this gives a small residual $AC - I$ but possibly a large residual $CA - I$).

2. Equations (2) and (3) imply for $\tilde{b} \in b' \subseteq b$ that

$$\tilde{x} \in x^0 + S(b' - F(x^0)),$$

and

$$\tilde{x} \in x^0 + C(b' - y).$$

(ii) If $x \subseteq D$ and $x^0 \in \text{int}(D)$ then x (and hence D) contains for every $\tilde{t} \in t$ a solution \tilde{x} of $F(\tilde{x}, \tilde{t}) = 0$.

Proof. We have

$$\begin{aligned} 0 &= F(\tilde{x}, \tilde{t}) = F(\tilde{x}, t^0) + F(\tilde{x})[t^0, \tilde{t}] \cdot (\tilde{t} - t^0) \\ &= F(x^0, t^0) + F[x^0, \tilde{t}](t^0) \cdot (\tilde{x} - x^0) \\ &\quad + F(\tilde{x})[t^0, \tilde{t}] \cdot (\tilde{t} - t^0), \end{aligned}$$

and since $F(x^0, t^0) = 0$ we get (5) with

$$\tilde{S} = F[x^0, \tilde{x}](t_0)^{-1} F(\tilde{x})[t^0, \tilde{t}].$$

This proves part (i), and part (ii) follows by a trivial modification of the proof of Theorem 1 of Neumaier [9]. ■

If F is linear in x , a simple modification yields slightly better results.

3.2. THEOREM. Let $A: T \subseteq \mathbb{R}^m \rightarrow \mathbb{R}^{n \times n}$ and $b: T \rightarrow \mathbb{R}^n$ be continuously differentiable, and suppose that $t \in T$ is chosen such that $A(\tilde{t})$ is regular for all $\tilde{t} \in t$. Then every solution $\tilde{x} = A(\tilde{t})^{-1} b(\tilde{t})$ ($\tilde{t} \in t$) of the equation $F(\tilde{x}, \tilde{t}) := A(\tilde{t})\tilde{x} - b(\tilde{t}) = 0$ satisfies (5) with $x^0 = A(t_0)^{-1} b(t_0)$ and an $S \subseteq \mathbb{R}^{n \times m}$ satisfying

$$-A(\tilde{t})^{-1} F(x^0)[t^0, \tilde{t}] \in S \quad \text{for all } \tilde{t} \in t.$$

Proof. Now $0 = F(\tilde{x}, \tilde{t}) = F(x^0, \tilde{t}) + A(\tilde{t})(\tilde{x} - x^0) = F(x^0, t^0) + F(x^0)[t^0, \tilde{t}](\tilde{t} - t^0) + A(\tilde{t})(\tilde{x} - x^0)$, and the arguments of the previous proof apply. ■

Remarks. 1. Equation (5) implies for $\tilde{t} \in t \subseteq t$ that

$$\tilde{x} \in x^0 + S(\tilde{t} - t^0),$$

and for linear combinations of the solution components,

$$a^T \tilde{x} \in a^T x^0 + (a^T S)(\tilde{t} - t^0).$$

2. With interval extensions of the partial derivatives, we can satisfy the condition on S of Theorem 3.1 for boxes D with

$$S \supseteq \hat{c}_1 F(D, t^0)^H \hat{c}_2 F(D, t),$$

and the condition of Theorem 3.2 with

$$S \supseteq A(t)^H \hat{c}_2 F(x^0, t).$$

In the special case where F is linear in x and the parameters occur only in the right-hand side then $\hat{c}_2 F(x^0, t) = -b'(t)$, and we get

3.3. COROLLARY. Let $b: T \subseteq \mathbb{R}^m \rightarrow \mathbb{R}^n$ be continuously differentiable, and let $A \in \mathbb{R}^{n \times m}$ be regular. If $x^0 \in \mathbb{R}^n$ is an enclosure for $A^H b(t^0)$ and if $S \in \mathbb{R}^{n \times m}$ is an enclosure of $A^H b'(t)$ (where $b'(t)$ is an interval extension of the derivative of $b(t)$) then, for every $\tilde{A} \in A$ and every $\tilde{t} \in t$, the solution $\tilde{x} = \tilde{A}^{-1} b(\tilde{t})$ of $\tilde{A}\tilde{x} = b(\tilde{t})$ satisfies (5).

4. COMPUTABLE BOUNDS FOR THE OVERESTIMATION

In all interval calculations one must be aware of the danger of getting enclosures which are much wider than the true range of the solution of the problem considered. In the spirit of earlier work by Gay [4] we show here that our sensitivity analysis has the quadratic approximation property, i.e., for narrow parameter ranges of order $O(\varepsilon)$, the bounds produced have a radius which overestimate the true radius of the solution hull by only $O(\varepsilon^2)$. Since the true radius is generally of order $O(\varepsilon)$, this shows that for narrow parameter intervals our analysis gives excellent result, and unreasonable overestimation need not be feared. Moreover, since a bound for the overestimation can be computed explicitly, one can check a posteriori whether the input intervals are narrow enough for the overestimation to be negligible.

The overestimation results are based on the following improvement of Theorem 2 in Krawczyk and Neumaier [5].

4.1. THEOREM. Let $F: D_0 \subseteq \mathbb{R}^n \rightarrow \mathbb{R}^m$ be a function. If $\tilde{z} \in D \subseteq D_0$ and $S \in \mathbb{R}^{m \times n}$ are such that for all $\tilde{x} \in D$, a relation of the form

$$F(\tilde{x}) = F(\tilde{z}) + \tilde{S}(\tilde{x} - \tilde{z}) \quad \text{for some } \tilde{S} \in S \quad (6)$$

is valid, then, for every $x \in \mathbb{0}D$ containing \tilde{z} , the range

$$F^*(x) := \mathbb{0}\{F(\tilde{x}) \mid \tilde{x} \in x\}$$

is contained in the centered form

$$F_{\tilde{z}}(x) := F(\tilde{z}) + S(x - \tilde{z}), \quad (7)$$

and we have

$$0 \leq \text{rad}(F_{\tilde{z}}(x)) - \text{rad}(F^*(x)) \leq 2\rho(S)\rho(x). \quad (8)$$

Proof. Clearly (6) implies $F^*(x) \subseteq F_z(x)$ and thus the lower bound in (8). To get the upper bound in (8), we first show that

$$\text{rad } F^*(x) \geq P\rho(x) \quad \text{with } P = \inf\{|\tilde{S}| \mid \tilde{S} \in S\}. \quad (9)$$

Fix a row index i , and define two vectors $x^{(i)}, y^{(i)} \in x$ by putting

$$\begin{aligned} x_k^{(i)} &:= \bar{x}_k, & y_k^{(i)} &:= \underline{x}_k & \text{if } S_{ik} > 0, \\ x_k^{(i)} &:= \underline{x}_k, & y_k^{(i)} &:= \bar{x}_k & \text{if } S_{ik} < 0, \\ x_k^{(i)} &:= \bar{z}_k, & y_k^{(i)} &:= \bar{z}_k & \text{if } S_{ik} \ni 0. \end{aligned}$$

Then $x^{(i)}, y^{(i)} \in x$, and by hypothesis there are matrices $\tilde{S}, \tilde{T} \in S$ such that

$$F(x^{(i)}) = F(z) + \tilde{S}(x^{(i)} - z), \quad F(y^{(i)}) = F(z) + \tilde{T}(y^{(i)} - z).$$

Hence the i th component of $F(x^{(i)}) - F(y^{(i)})$ equals

$$\begin{aligned} & \sum_k \tilde{S}_{ik}(x_k^{(i)} - z_k) - \sum_k \tilde{T}_{ik}(y_k^{(i)} - z_k) \\ & \geq \sum_k P_{ik}(x_k^{(i)} - z_k) - \sum_k P_{ik}(y_k^{(i)} - z_k) \\ & = \sum_k P_{ik}(x_k^{(i)} - y_k^{(i)}) = \sum_k P_{ik}(\bar{x}_k - \underline{x}_k) \end{aligned}$$

by construction of $x^{(i)}, y^{(i)}$, and P , so that

$$\begin{aligned} (P\rho(x))_i &= \frac{1}{2} \sum_k P_{ik}(\bar{x}_k - \underline{x}_k) \leq \frac{1}{2} (F_i(x^{(i)}) - F_i(y^{(i)})) \\ & \leq \frac{1}{2} (\sup(F_i^*(x)) - \inf(F_i^*(x))) = \text{rad}(F_i^*(x)), \end{aligned}$$

and since i was arbitrary, (9) follows. Now Lemma 1.1(ii) implies

$$\begin{aligned} \text{rad}(F_z(x))_i &= \text{rad}(S(x - \tilde{z}))_i = \sum_k \rho(S_{ik}(x - \tilde{z})_k) \\ & \leq \sum_k (\langle S_{ik} \rangle + 2\rho(S_{ik}))(\rho(x_k - \tilde{z}_k)) \\ & = \sum_k (P_{ik} + 2\rho(S_{ik}))\rho(x)_k = ((P + 2\rho(S))\rho(x))_i, \end{aligned}$$

so that $\text{rad}(F_z(x)) \leq (P + 2\rho(S))\rho(x)$, which, together with (9), yields the upper bound in (8). ■

If we replace $F(\tilde{x})$ in Theorem 4.1 by a function $x(\tilde{t})$ defined implicitly by $F(x(\tilde{t})) = 0, x(\tilde{t}) \in D$, we get overestimation bounds for the enclosures constructed in Section 3.

4.2. COROLLARY. Under the hypothesis of Theorem 3.1, let $t' \in \mathbb{R}^n$ satisfy $t' \subseteq t$. Then the range

$$x^*(t') = \square\{\tilde{x} \in D \mid F(\tilde{x}, \tilde{t}) = 0 \text{ for some } \tilde{t} \in t'\}$$

is contained in

$$x(t') = x^0 + S(t' - t^0),$$

and we have

$$0 \leq \text{rad}(x(t')) - \text{rad}(x^*(t')) \leq 2\rho(S)\rho(t').$$

If F is given by an arithmetical expression, so that expressions for partial derivatives are available, and if x and t are narrow intervals with $\rho(x), \rho(t)$ of order $O(\varepsilon)$, then $A = \partial_1 F(x, t^0)$ and $B = \partial_2 F(x, t)$ will also have radii of order $O(\varepsilon)$, and the enclosure S of $-A^H B$ constructed by a standard preconditioning method will also have a radius of order $O(\varepsilon)$; see Miller [7], Gay [3], and Neumaier [10]. Since $t' \subseteq t$, the corollary now implies an overestimation bound of order $O(\varepsilon^2)$, as claimed.

Of course, similar remarks apply to the other enclosures of the present paper.

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