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Fundamentals of Numerical Computation (Computer-Oriented Numerical Analysis)

Edited by G. Alefeld and R. D. Grigorieff
in cooperation with
R. Albrecht, U. Kulisch, and F. Stummel

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Preface

This volume contains mainly a collection of the invited lectures which were given during a conference on "Fundamentals of Numerical Computation", held in June, 5 – 8, 1979, on the occasion of the centennial of the Technical University of Berlin. About hundred scientists from several countries attended this conference.

A preceding meeting on "Fundamentals of Computer-Arithmetic" was held in August, 1975, at the "Mathematisches Forschungsinstitut Oberwolfach". The lectures of this conference have been published as Supplementum 1 of Computing (Editors R. Albrecht, U. Kulisch).

After a period of four years of active research the purpose of the Berlin-Conference was to give a broad survey of the present status of the closely connected topics Interval Analysis, Mathematical Foundation of Computer Arithmetic, Rounding Error Analysis and Stability of Numerical Algorithms and to give prospects of future activities in these fields. Besides the invited lectures 35 short communications, each of 20 minutes length, were given.

We gratefully acknowledge the support of the President of the Technical University and of his Aussenreferat as well as of the Department of Mathematics. Besides these institutions financial support was given by AEG-Telefunken, Berlin, Allianz Lebensversicherungs A.G., Stuttgart, CDC, Hamburg/Berlin, DATA 100, München, Gesellschaft von Freunden der TU Berlin e.V., Berlin and Siemens AG., Berlin. Finally we express our thanks to Mrs. G. Froehlich and Mrs. B. Trajanović, who managed the paper work before, during and after the conference.

Berlin, February 1980 G. Alefeld and R. D. Grigorieff

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On Methods for the Construction of the Boundaries of Sets of Solutions for Differential Equations or Finite-Dimensional Approximations with Input Sets*

E. Adams, Karlsruhe

Abstract

Collections of linear or nonlinear operator equations $Au = f$ are considered which may represent (i) differential or integral equations or (ii) finite-dimensional approximations. Input sets of coefficients a or data f are admitted. The envelope of the set of solutions is to be constructed where this boundary refers (i) to the range of values of the solutions or (ii) to a finite-dimensional space. The construction employs either topological boundary mapping or truncated Taylor expansions. Estimates of the local procedural errors are due to suitable a priori sets and interval mathematics. The relation between local and global error estimates is due to boundary mapping or an auxiliary inverse-monotone operator $\hat{B}$. The operator $\hat{B}$ is constructed for the case of arbitrary linear ordinary differential equations with boundary or initial conditions, provided the admitted A satisfy a mild condition.

1. Outline of the Problem

Collections of operator equations

$$Au = f \tag{1.1}$$

are considered which may represent (i) differential or integral equations with the usual side conditions or (ii) finite-dimensional approximations. The following types of input sets are admitted in (1.1): (*a*) sets S_f of data f and (*b*) sets S_a of coefficients a where "coefficient" refers to any input in A. An envelope ∂S_u of the set of solutions is to be approximated. The envelopes ∂S_a, ∂S_f, and ∂S_u either (*i*) refer to sets in finite-dimensional spaces if this is true for (1.1) or (*ii*) represent the upper and the lower envelopes of the ranges of the respective functions in (1.1). The existence of the solution of (1.1) will not be discussed.

The consideration of input sets S_a or S_f is motivated as follows:

Case (I) (Applied Mathematics). $A = A_0$ and $f = f_0$ are fixed:

(*1*) The execution of numerical methods requires that the solution u_0 of $A_0 u = f_0$ is well-conditioned with respect to neighboring coefficients and data;

(*2*) if a neighboring problem $A_v w = f_v$ can be solved, ∂S_u is of interest if S_a contains both a and a_v and if S_f contains both f and f_v;

(*3*) sets may appear in the analysis due to error estimates.

---

* This paper is dedicated to Prof. Dr. H. Görtler on the occasion of his 70th birthday. – The research was supported by the NATO Senior Fellowship Award SA.5-2-03B(112)961(78)MDL.

Case (II) (Applications of Mathematics). S_a and S_f are prescribed:

(*4*) The range of the solutions is to be bracketed as, e.g., for the case of a collection of loads in problems in civil engineering;

(*5*) mathematical models of real world problems have imprecisely known input.

With the possible exception of (4), input sets are usually "small", e.g., an input interval possesses a small span. The motivations (1)–(4) generally admit input sets with fixed deterministic envelopes; stochastic envelopes in the case of (5) will not be discussed here.

2. Ordinary Linear Initial Value Problems with Initial Sets

The solution of the linear ordinary ivp (initial value problem)

$$u' - A(t)u = g(t) \quad \text{for} \quad t \in J := (0, T], u(0) \in \mathbb{R}^n,$$
$$u: J \to \mathbb{R}^n, \quad A: J \to L(\mathbb{R}^n), \quad A, g \in C(\bar{J}) \tag{2.1}$$

can be represented as follows [11, p. 139–141]:

$$u(t) = X(t)\left[u(0) + \int_0^t (X(s))^{-1} g(s)\, ds\right] \quad \text{for } t \in J, \tag{2.2}$$

where X is the fundamental matrix of $u' - Au = 0$. A compact initial set $E(0) \subset \mathbb{R}^n$ is admitted. Then, (2.2) represents a bijective affine mapping with parameter t of $E(0)$ onto $E(t)$, the set of solutions at any $t \in J$, such that $\partial E(0)$ is mapped onto $\partial E(t)$. For the case of (2.1), this *Boundary Mapping* was recognized independently in 1977 by K. Nickel [18] and R. Lohner [14], [15].

The theory of differential inequalities ([13] or [23]) may be employed to construct an interval $I(t) = [\underline{u}(t), \bar{u}(t)] \subset \mathbb{R}^n$ such that $E(0) \subseteq I(0)$. Provided the off-diagonal elements of A are nonnegative, the ivp are inverse-monotone, i.e.,

$$u' - Au \geqslant w' - Aw \quad \text{for } t \in J \qquad \text{and} \qquad u(0) \geqslant w(0) \Rightarrow u(t) \geqslant w(t) \quad \text{for } t \in J. \tag{2.3}$$

Then, $\underline{u}, \bar{u}$ such that $\underline{u} \leqslant u \leqslant \bar{u}$ for $t \in J$ and every solution of (2.1) with $E(0)$ are solutions of $\bar{u}' - A\bar{u} = \underline{u}' - A\underline{u} = g$ on J and $\underline{u} \leqslant u \leqslant \bar{u}$ for $t = 0$ and every $u(0) \in E(0)$. If A does not possess this property, then

$$\left\{\begin{aligned} &\bar{u}_i' - a_{ii}\bar{u}_i - \operatorname*{Max}_{u \in \hat{I}(t)} \sum_{\substack{j=1 \\ j \neq i}}^{n} a_{ij} u_j = g_i(t) \\ &\underline{u}_i' - a_{ii}\underline{u}_i - \operatorname*{Min}_{u \in \hat{I}(t)} \sum_{\substack{j=1 \\ j \neq i}}^{n} a_{ij} u_j = g_i(t) \end{aligned}\right\} \quad \begin{aligned} &\text{for } t \in J, \underline{u}_i(0) \leqslant u_i(0) \leqslant \bar{u}_i(0), \\ &i = 1(1)n. \end{aligned} \tag{2.4}$$

Due to Max or Min, $\hat{I}(t) := [\underline{u}(t), \bar{u}(t)]$ generally exceeds the set $E(t)$.

Example 2.1. If

$$E(0) = [0.9, 1.1] \times [-0.1, 0.1] \subset \mathbb{R}^2 \quad \text{and} \quad A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \; g = 0, \tag{2.5}$$

then $\bar{u}_i(t) - \underline{u}_i(t) = 0.2\,e^t$ for $i = 1$ or 2 even though $E(t)$ is uniformly bounded with respect to every $t \in J$ for $T \to \infty$.

Since I or $\hat{I}$ at t completely determine I or $\hat{I}$ at $t + dt$, (2.3) and (2.4) are interval methods. The overestimates due to (2.4) make it desirable to look for a constructive execution of boundary mapping in the case of (2.1).

Example 2.2. The ivp (2.1), (2.5) is reconsidered. The superscript $k = 1(1)4$ denotes the four corners of the set $E(0)$. By use of $v := u_1$ and $w := u_2$ and the trapezoidal rule, the representation of the ivp by Volterra integral equations can be discretized as follows:

$$v_{j+1}^{(k)} = v_j^{(k)} + (h/2)[w_j^{(k)} + w_{j+1}^{(k)}] - (h^3/12)w''(\alpha_j)$$
$$\text{for } j = 0(1)N-1,\ h = T/N,\ \alpha_j \in [t_j, t_{j+1}],$$
$$w_{j+1}^{(k)} = \cdots \tag{2.6}$$

Since $v'' + v = w'' + w = 0$, a suitably selected a priori interval $\tilde{I}_{j+1}^{(k)} = \tilde{V}_{j+1}^{(k)} \times \tilde{W}_{j+1}^{(k)} \subset \mathbb{R}^2$ may be employed to estimate the remainder term in the truncated Taylor expansion

$$w^{(k)}(t) = w_j^{(k)} - (t - t_j)v_j^{(k)} - \tfrac{1}{2}(t - t_j)^2 w_j^{(k)} - \tfrac{1}{6}(t - t_j)^3 \underbrace{v_j^{(k)}(\beta_j)}_{\in \tilde{V}_{j+1}^{(k)}} \overset{!}{\in} \tilde{W}_{j+1}^{(k)}$$

$$\text{for } t \in [t_j, t_{j+1}],\ \beta_j \in [t_j, t_{j+1}], \tag{2.7}$$

of the function $w^{(k)}$ where ! denotes a condition. If the corresponding condition $v^{(k)}(t) \overset{!}{\in} \tilde{V}_{j+1}^{(k)}$ for $t \in [t_j, t_{j+1}]$ is also satisfied, $w''(\alpha_j)$ may be replaced by $\tilde{W}_{j+1}^{(k)}$ in (2.6). Then (2.6) is a linear algebraic interval system with a fixed matrix whose solution is a parallelogram, $P_{j+1}^{(k)}$, which can be enclosed by the smallest interval $I_{j+1}^{(k)}$. The four intervals $I_{j+1}^{(k)}$ with $k = 1(1)4$ then can be enclosed by the smallest quadrilateral $\tilde{E}(t_{j+1})$ which is an outer approximation of $E(t_{j+1})$ such that the four corners of $\tilde{E}(t_{j+1})$ are the starting vectors for the continuation of the construction. Due to the numerical results by E. Gerdon (Karlsruhe), $\partial E(t_j)$ and $\partial \tilde{E}(t_j)$ deviate by less than $1.5(10^{-6})t_j$ for $t_j \in (0, 20\pi]$ where $h = 10^{-2}$ was used and the CPU-time was 56 sec on the UNIVAC 1108 at the University of Karlsruhe.

Remark. As compared with Example 2.1, here the "interval-coarsening" is restricted to the small local procedural error and its transfer to the corresponding global error due to the outer approximation.

Remark. By use of the domain invariance theorem of topology ([12] or [19]), boundary mapping holds for nonlinear ordinary ivp provided a uniqueness condition is satisfied, e.g., [12] or [19]. Boundary mapping also holds for suitable linear operators in Banach spaces with infinite dimensions, e.g., [8].

3. Ordinary Linear Boundary Value Problems with Sets of Data and Coefficients

The following collection of linear ordinary Sturm-Liouville bvp (boundary value problem) is considered:

$$Au = f \Leftrightarrow \begin{cases} Pu := u'' - a(x)u = -g(x) \quad \text{for } x \in I := (0,1), \\ Ru := u = 0 \quad \text{for } x \in \partial I; \quad u \in U := C^2(\bar{I}); \; \gamma := a \text{ or } g, \\ \forall \gamma \in S_\gamma := [\underline{\gamma}, \bar{\gamma}] \cap C(\bar{I}). \end{cases} \tag{3.1}$$

It is assumed that there exists $a_0 \in S_a$ such that Green's function G_0 is explicitly known for the operator A_0 pertaining to a_0. Each individual admitted bvp can be represented equivalently by

$$Bu := u(x) - \int_0^1 K(x,\xi)u(\xi)\,d\xi = -\int_0^1 G_0(x,\xi)g(\xi)\,d\xi =: g^*(x) \quad \text{for } x \in \bar{I},$$

$$\forall \gamma \in S_\gamma,\; K(x,\xi) := G_0(x,\xi)[a(\xi) - a_0(\xi)] \quad \text{for } (x,\xi) \in \bar{I} \times \bar{I}. \tag{3.2}$$

Auxiliary kernels are introduced:

$$K^+(x,\xi) := K(x,\xi) \quad \text{if } K(x,\xi) \geqslant 0 \text{ locally and } K^+(x,\xi) = 0 \text{ otherwise},$$

$$K^-(x,\xi) := K(x,\xi) - K^+(x,\xi) \quad \text{on } \bar{I} \times \bar{I}. \tag{3.3}$$

The values of the set of solutions of $Bu = g^*$ can be bracketed by use of an interval $[\underline{u}, \bar{u}](x)$ for $x \in \bar{I}$ which solves the following interval extension of $Bu = g^*$

$$[\underline{u}, \bar{u}](x) = \int_0^1 ([\underline{K}^-, \bar{K}^-] + [\underline{K}^+, \bar{K}^+])(x,\xi)[\underline{u}, \bar{u}](\xi)\,d\xi = \int_0^1 [\underline{G_0 g}, \overline{G_0 g}]\,d\xi$$

for $x \in \bar{I}$, where $\underline{K}^- := \operatorname{Min}_{a \in S_a} K^-$ and $\underline{G_0 g} := \operatorname{Min}_{g \in S_g} G_0 g$ locally at every

$(x,\xi) \in \bar{I} \times \bar{I}$, etc. (3.4)

Generally, the relation between the input a, g and the corresponding solution u is lost as $Bu = g^*$ is replaced by (3.4). By use of the rule of interval multiplication, rearrangement of terms in (3.4) yields the "extended operator equation" with

$$\hat{B}\hat{u} := \bar{u} - \int_0^1 \left[\begin{pmatrix} (\operatorname{Max}_{a \in S_a} K^+)\bar{u} \text{ if } \bar{u} \geqslant 0 \text{ locally} \\ (\operatorname{Min}_{a \in S_a} K^+)\bar{u} \text{ if } \bar{u} < 0 \text{ locally} \end{pmatrix} + \begin{pmatrix} |\operatorname{Max}_{a \in S_a} K^-|(-\underline{u}) \text{ if } \underline{u} \geqslant 0 \text{ locally} \\ |\operatorname{Min}_{a \in S_a} K^-|(-\underline{u}) \text{ if } \underline{u} < 0 \text{ locally} \end{pmatrix} \right] d\xi,$$

$$:= (-\underline{u}) - \int_0^1 \left[\begin{pmatrix} (\operatorname{Min}_{a \in S_a} K^+)(-\underline{u}) \text{ if } \underline{u} \geqslant 0 \text{ locally} \\ (\operatorname{Max}_{a \in S_a} K^+)(-\underline{u}) \text{ if } \underline{u} < 0 \text{ locally} \end{pmatrix} + \begin{pmatrix} |\operatorname{Min}_{a \in S_a} K^-|\bar{u} \text{ if } \bar{u} \geqslant 0 \text{ locally} \\ |\operatorname{Max}_{a \in S_a} K^-|\bar{u} \text{ if } \bar{u} < 0 \text{ locally} \end{pmatrix} \right] d\xi,$$

for $x \in \bar{I}$ with $\hat{u}(x) := (\bar{u}(x), -\underline{u}(x))$ and $\hat{u} : \bar{I} \to \mathbb{R}^2$. (3.5)

The execution of the operators Max or Min yields (1) $\mathrm{Min}_{a\in S_a} K^+ = \mathrm{Max}_{a\in S_a} K^- = 0$ if $a_0(x)\in(\underline{a}(x), \bar{a}(x))$ for every $x\in\bar{I}$ and (2) discontinuous functions $a_x(\xi)$ whose values for any fixed $x\in\bar{I}$ are either $\underline{a}(\xi)$ or $\bar{a}(\xi)$; $\hat{B}$ is nonlinear unless $\underline{a} = \bar{a} = a_0$.

In order to show that $\hat{B}$ is inverse-monotone with respect to $\hat{u}$, it is required that there exists a test element $\hat{v} = (v, v)$ with $v\in C(\bar{I})$ and $v(x) > 0$ on $\bar{I}$ such that $\hat{B}\hat{v} > 0$ on $\bar{I}$. This inequality is trivially satisfied by the choice of $v(x) = 1$ for $x\in\bar{I}$ provided there holds

$$1 - \int_0^1 [(\operatorname*{Max}_{a\in S_a} K^+) + |\operatorname*{Min}_{a\in S_a} K^-|](x,\xi)\,d\xi \geqslant 1 - (\|\bar{K}^+\|_\infty + \|\underline{K}^-\|_\infty) \overset{!}{>} 0. \quad (3.6)$$

Theorem 3.1. *The operator $\hat{B}$ is inverse-monotone with respect to u if there exists a test element $\hat{v}\in C(\bar{I})$ such that $\hat{v} > 0$ and $\hat{B}\hat{v} > 0$ on $\bar{I}$.*

The *proof* as presented in [2] follows the one in [1].

Theorem 3.2. *The system of Fredholm integral equations*

$$\begin{aligned}
\hat{B}\hat{u} = \hat{f} :=\ & \int_0^1 \operatorname*{Max}_{g\in S_g}(-G_0 g)\,d\xi = -\int_0^1 G_0 \begin{Bmatrix} \underline{g}\,d\xi \text{ if } G_0 \geqslant 0 \text{ locally} \\ \bar{g}\,d\xi \text{ if } G_0 < 0 \text{ locally}\end{Bmatrix} \\
=:\ & \int_0^1 G_0 \breve{g}_x(\xi)\,d\xi, \\
:=\ & -\int_0^1 \operatorname*{Min}_{g\in S_g}(-G_0 g)\,d\xi = \int_0^1 G_0 \begin{Bmatrix} \bar{g}\,d\xi \text{ if } G_0 \geqslant 0 \text{ locally} \\ \underline{g}\,d\xi \text{ if } G_0 < 0 \text{ locally}\end{Bmatrix} \\
=:\ & \int_0^1 G_0 \underset{\smile}{g}_x(\xi)\,d\xi,
\end{aligned} \quad (3.7)$$

(1) possesses a unique solution $\underline{u}, \bar{u}\in C(\bar{I})$ such that

$$\underline{u}(x) \leqslant u(x) \leqslant \bar{u}(x) \text{ for } x\in\bar{I} \text{ and every solution } u\in C(\bar{I}) \text{ of (3.2)}, \quad (3.8)$$

provided (3.6) is satisfied; (2) $\underline{u}, \bar{u}$ are sharp bounds if (i) $\underline{a} = \bar{a} = a_0$ or (ii) $G_0 \geqslant 0$ on $\bar{I}\times\bar{I}$ and $\underline{a} = a_0$ on $\bar{I}$.

Proof. (*1*) This follows from Theorem 3.1 and the uniform convergence of the Neumann sequence of successive approximations; (*2*) this follows from a theorem by Arzela (e.g., [9, p. 772]) since the discontinuous functions $g_x(\xi)$ with values $\underline{g}(\xi)$ or $\bar{g}(\xi)$ for any fixed $x\in\bar{I}$ can be approximated with arbitrary accuracy by a sequence of functions $g_x^{(v)}(\xi)\in C(\bar{I})$, e.g., by use of the L_1-norm. □

For every collection (3.1) with $\|G_0\|_\infty\|\bar{a} - \underline{a}\|_\infty$ sufficiently small, (3.6) is satisfied; then, an interval $[\underline{u}, \bar{u}](x)$ can be constructed by use of the inverse-monotone extended operator $\hat{B}$. Hansen (e.g., [3, p. 232]) recognized the advantage of premultiplying a system of linear algebraic interval equations, $Au = f$, by A_0^{-1}.

Remark. The ivp (2.1) can be treated analogously.

Example 3.1. The operator equation $Au = f$ in (3.1) is reconsidered with a and g fixed. It is assumed that there exists a neighboring coefficient a_0 such that (*i*)

Green's function is (explicitly) known for (3.1) with a_0 instead of a and (*ii*) (3.6) is satisfied for functions $\underline{a}, \bar{a}$ such that $a, a_0 \in [\underline{a}, \bar{a}]$ on $\bar{I}$. Cubic Spline functions (e.g., [22, p. 81])

$$u_s := u_{sj} := u_j\left(\frac{x_{j+1} - x}{h}\right) + u_{j+1}\left(\frac{x - x_j}{h}\right) + \frac{M_j}{6}h^2\left[\left(\frac{x_{j+1} - x}{h}\right)^3 + \left(\frac{x - x_j}{h}\right) - 1\right] + M_{j+1}(h^2/6)[\cdots]$$

$$\text{for } x \in [x_j, x_{j+1}],\ x_j = jh,\ j = 0(1)n + 1,\ h = (n + 1)^{-1},\ x_0 = 0, \tag{3.9}$$

with any fixed $n \in \mathbb{N}$, are employed to construct an approximate solution of (3.1) for the case of fixed a and g. The composite Spline function $u_s \in C^2(\bar{I})$ yields a residual $r := Au_s - f$. A correction z is defined by use of $Az = -r$ such that $A[u_s + z] = f$. Analogous to (3.2) and (3.5), the equation $A_0^{-1}Az = A_0^{-1}r =: r^*$ gives rise to $\hat{B}\hat{z} = \hat{r}$. This yields the quantitative error estimates $z \in [\underline{z}, \bar{z}]$ and

$$u(x) \in [u_s(x) + \underline{z}(x), u_s(x) + \bar{z}(x)] \quad \text{for } x \in \bar{I}. \tag{3.10}$$

The standard error estimate of linear discrete analogies involves a constant $c \in \mathbb{R}^+$ which usually is not known quantitatively since c majorizes the norm of the inverse matrices for *every* $n \in \mathbb{N}$, [21, p. 9].

Remark. Linear elliptic bvp can be treated analogously by use of the Spline functions developed in [20] provided a Green's function G_0 is known.

4. Linear Ordinary Initial Value Problems with Sets of Coefficients

With reference to procedural or rounding errors, a complete conditioning (or sensitivity) analysis of a mathematical model requires a quantitative comparison of a "basic solution" $u(x, \gamma_0)$ with neighboring solutions $u(x, \gamma)$ where x stands for the independent variables and γ, γ_0 denote every data and coefficient. Interval mathematics *seems* to suggest that $\|u(x, \gamma) - u(x, \gamma_0)\|_\infty$ is majorized for $\gamma = \underline{\gamma}$ or for $\gamma = \bar{\gamma}$ provided $\gamma \in [\underline{\gamma}, \bar{\gamma}]$. This generally is *not true* unless the problem is inverse-monotone and γ stands for data only. The subsequent discussion of this topic cannot employ boundary mapping since each admitted data g defines a separate operator A of the ivp to be discussed.

Example 4.1. The following collection of ivp is considered:

$$u'' + u = g(t) \quad \text{for } t \in J := (0, T],\ u(0) = u_0,\ u'(0) = u_1 \text{ with fixed}$$
$$u_0, u_1 \in \mathbb{R},\ g \in S_g := [\underline{g}, \bar{g}] \cap C(\bar{J}). \tag{4.1}$$

For any fixed forcing function $g \in S_g$, the solution of (4.1) is as follows:

$$u(t) = \sigma(t) + \int_0^1 G(t, s)g(s)\,ds$$

$$\text{where } G := (\sin t)(\cos s) - (\cos t)(\sin s) = \sin(t - s),$$

$$\sigma := u_0 \cos t + u_1 \sin t. \tag{4.2}$$

Analogous to (3.7), the upper envelope of the values of the set of solutions of (4.1) is given by

$$\bar{u}(t) = \sigma(t) + \int_0^t \operatorname*{Max}_{g \in S_g} (G(t,s)g(s))\, ds = \sigma(t) + \int_0^t G(t,s)g_t(s)\, ds \quad \text{for } t \in J,$$

$$g_t(s) := \begin{cases} \bar{g}(s) \text{ if } G(t,s) \geqslant 0 \text{ locally} \\ \underline{g}(s) \text{ if } G(t,s) < 0 \text{ locally} \end{cases} \begin{cases} \text{for } t \in J \text{ fixed and} \\ \text{every } s \in [0,t]. \end{cases} \tag{4.3}$$

The lower envelope $\underline{u}$ is determined correspondingly; g_t may be interpreted as a control function whose choice majorizes the interval $[\underline{u}, \bar{u}](t)$. For the special choice of $\delta := -\underline{g} = \bar{g} \in \mathbb{R}^+$, obviously, $\bar{u} = \sigma + S$ and $\underline{u} = \sigma - S$ where $S := \delta \int_0^t |G|\, ds$. This yields

$$\bar{u}(m\pi) = \sigma(m\pi) + 2[\delta m] \quad \text{for } t = m\pi \text{ with every } m \in \mathbb{N}. \tag{4.4}$$

For comparison, (4.1) is considered for the "resonance case" of $g = \delta \sin t$:

$$u(m\pi) = \sigma(m\pi) + (\pi/2)[\delta(-1)^{m+1}m] \quad \text{for } t = m\pi \text{ with every } m \in \mathbb{N}. \tag{4.5}$$

Therefore, (*i*) the operator Max in (4.3) causes the selection of a forcing function g with the "resonance frequency", 1, (*ii*) the interval $[\underline{u}, \bar{u}](t)$ is almost covered by solutions of physical relevance, (*iii*) the interval $[\underline{u}, \bar{u}](t)$ is determined by functions $g_t(s) \notin S_g$ such that each g_t can be approximated with arbitrary accuracy by a sequence of functions $g_t^{(\nu)}(s) \in S_g$ whose values are *not* given by those of $\underline{g}$ and $\bar{g}$ only. Even if $\delta \in \mathbb{R}^+$ is arbitrarily small, (4.1) is unstable for $T \to \infty$ and ill-conditioned for any sufficiently large $T \in \mathbb{R}^+$. The unbounded increase of $|\bar{u}|$ and $|\underline{u}|$ can be avoided if there is a sufficiently large damping constant $b \in \mathbb{R}^+$ in the altered equation $u'' + bu' + u = g$ for $t \in J$.

As $t \to \infty$, a corresponding unbounded increase of $\bar{u}(t) - \underline{u}(t)$ occurs in the case of

$$u'' + a(t)u = 0 \quad \text{for } t \in J := (0, T];\ u(0), u'(0) \in \mathbb{R} \text{ fixed,}$$
$$a \in S_a := [\underline{a}, \bar{a}] \cap C(\bar{J}). \tag{4.6}$$

This "parameter-resonance" is well known in mechanics, e.g., [7, p. 225].

5. Partial Differential Equations with Input Sets

The discussions of ordinary (linear) ivp apply immediately to (linear) parabolic or hyperbolic pde with the usual side conditions and input sets, provided approximate solutions are constructed by use of the longitudinal line method, e.g., [23]. Elliptic pde with the usual side conditions and input sets can be treated approximately by use of discrete analogies, compare Section 6 and Example 3.1.

6. On Truncated Taylor Expansions for the Approximate Solution of Problems with Sets of Constant Input Properties

The collection of operator equations $Au = f$ in (1.1) is considered. In many cases, an algorithm for the exact or the approximate solution of (1.1) employs or yields a function from one finite-dimensional space into some other such space; e.g., the solution of a discrete analogy is such a function which depends on constant input parameters. Due to the motivations listed in Sect. 1, these real numbers may take values in certain input sets. The range of such a function then is to be determined precisely or to be approximated with sufficient accuracy. In many cases, interval methods are non-existent for these purposes or they yield unacceptable over-estimates.

This will be achieved by use of truncated Taylor expansions of the unknown function $\hat{F}$ representing the solution in terms of every constant input parameter (and the independent variables); $\hat{F}$ is assumed to be sufficiently smooth. Because of Sect. 7, first an interval polynomial will be treated.

Example 6.1. The following collection of functions $F\colon \mathbb{C} \to \mathbb{C}$ is considered:

$$F(z;a,b) := z^2 + 2az + b = 0, \quad z \in \mathbb{C}, \quad a \in [0.9, 1.1], \quad b \in [1.9, 2.1]. \tag{6.1}$$

Here, only the root $z = -a + i\sqrt{b - a^2}$ will be discussed further. For the special choice of $a_0 = 1$ and $b_0 = 2$, the root $z_0 := z(a_0, b_0) = -1 + i$ is obtained *from the nonlinear equation* (6.1). By use of $z = x + iy$, $\sigma = 1$, $\tau = i$, the root $z(a, b)$ of $F = 0$ defines the functions $\check{F}(a, b; \sigma, \tau) := F(x(a, b) + iy(a, b); a, b)$ and $\hat{F}(a, b) := \check{F}(a, b; \sigma, \tau)$ where $\hat{F}\colon D \to \mathbb{R}$ with $D := [0.9, 1.1] \times [1.9, 2.1] \subset \mathbb{R}^2$ and $\hat{F}(a, b) \equiv 0$. By use of recombining real quantities into complex quantities, differentiation of the last identity yields the following *linear decoupled equations* for the partial derivatives of z with respect to a or b:

$$\begin{aligned} \frac{\partial \hat{F}}{\partial a} &\equiv 0 \Rightarrow v := \frac{\partial z}{\partial a} = \frac{-z}{z+a} \Rightarrow v_0 = \frac{-z_0}{z_0 + a_0} = -1 - i, \\ \frac{\partial \hat{F}}{\partial b} &\equiv 0 \Rightarrow w := \frac{\partial z}{\partial b} = \frac{-1}{2(z+a)} \Rightarrow w_0 = \frac{-1}{2(z_0 + a_0)} = \frac{i}{2}, \\ \frac{\partial^2 \hat{F}}{\partial a^2} &\equiv 0 \Rightarrow \alpha := \frac{\partial^2 z}{\partial a^2} = \frac{-2v - v^2}{z+a}, \ldots \end{aligned} \tag{6.2}$$

The derivatives of z of any order exist if $z + a \neq 0$. A linear truncated Taylor expansion of $z(a, b)$ with respect to (a_0, b_0) is introduced:

$$\tilde{z} := z_0 + (a - a_0)v_0 + (b - b_0)w_0 = -a + i[1 - (a - a_0) + (b - b_0)/2]. \tag{6.3}$$

By use of the a priori set

$$\tilde{S}_z := [-1.2, -0.8] + i[0.8, 1.1] \qquad \text{with } z_0 \in \tilde{S}_z, \tag{6.4}$$

the following estimates are obtained: $|\partial^2 z/\partial a^2| \leqslant 10.3$, $|\partial^2 z/\partial a\,\partial b| \leqslant 2.36$, $|\partial^2 z/\partial b^2| \leqslant 0.49$, and $|R_2| \leqslant 0.1551/2$ where R_2 denotes the remainder term of the truncated expansion (6.3). The following table compares results for $\tilde{z}$ and the exact root $z = -a + i\sqrt{b - a^2}$:

Table 1

a	b	$\tilde{z}$	z	a	b	$\tilde{z}$	z
1.1	2.1	$-1.1 + 0.95i$	$-1.1 + 0.942i$	0.9	2.1	$-0.9 + 1.15i$	$-0.9 + 1.100i$
1.1	1.9	$-1.1 + 0.85i$	$-1.1 + 0.830i$	0.9	1.9	$-0.9 + 1.05i$	$-0.9 + 1.000i$

In each case, $|\tilde{z} - z| < 0.1551/2$. These results and the monotonicity of $\tilde{z}(a, b)$ confirm that $\tilde{z} \in \tilde{S}_z$ is valid for every admitted $(a, b) \in \mathbb{R}^2$.

Remarks. If the intervals for a and b admit double roots $z(a, b)$, (6.3) is still valid if (a_0, b_0) is selected so as to ensure that $z(a_0, b_0) + a_0 \neq 0$. Since $v, w, \alpha, \ldots$ are determined from decoupled (linear) equations, interval polynomials of any degree may be treated in this way. The books by Alefeld and Herzberger [3] and by Moore [16] on interval mathematics do not discuss the subject of interval polynomials.

The following example treats truncated Taylor expansions for a problem where an input set appears only due to embedding the operator equation into a collection of such equations.

Example 6.2. A nonlinear system in $\mathbb{R}^n$ is considered:

$$F(u) = 0 \text{ with } F\colon D \to \mathbb{R}^n \text{ and } D \subset \mathbb{R}^n;\ F \text{ possesses a continuous Frechet derivative } DF(u) \text{ on } D \text{ such that } (DF(u))^{-1} \text{ exists.} \tag{6.5}$$

This system is embedded in the following collection:

$$F(u) = b \quad \text{with } b \in S_b \subset \mathbb{R}^n. \tag{6.6}$$

It is assumed that this system possesses a real or complex root $u(b)$ for every $b \in S_b$. A function $\hat{F}(b) := F(u(b)) - b$ is defined such that $\hat{F}\colon S_b \to \mathbb{R}^n$ and $\hat{F}(b) \equiv 0$, which implies that $\partial \hat{F}_i/\partial b_j \equiv 0$ for $i, j = 1(1)n$. The last identities yield the matrix $(\partial u_i/\partial b_j) \in L(\mathbb{R}^n)$. Due to

$$(\partial F_i/\partial u_k)(\partial u_k/\partial b_j) = I \Rightarrow (\partial u_k/\partial b_j) = (DF(u))^{-1}, \tag{6.7}$$

where I is the identity matrix. By use of a superscript k to be explained subsequently, a linear truncated Taylor expansion of $u(b)$ at $b^{(k)} = F(u^{(k)})$ is introduced, which employs a free vector $\tilde{b}^{(k+1)} \in \mathbb{R}^n$:

$$u^{(k+1)} = u^{(k)} + (\partial u_i/\partial b_j)(\tilde{b}^{(k+1)} - b^{(k)}) \quad \text{with } k + 1 \in \mathbb{N} \text{ and } b^{(k)} = F(u^{(k)}). \tag{6.8}$$

If $\tilde{b}^{(k+1)} = 0$, this is the classical Newton method, whose divergence can be avoided if $d_i^{(k+1)} := |\tilde{b}_i^{(k+1)} - b_i^{(k)}|$ is sufficiently small for $i = 1(1)n$. A check on the choice of the individual $\tilde{b}_i^{(k+1)}$ is possible by use of the $u_j^{(k+1)}$, as following from (6.8), and $|\tilde{b}_m^{(k+1)} - b_m^{(k+1)}|$ for $j, m = 1(1)n$ where $b^{(k+1)} = F(u^{(k+1)})$. For the special choice of $n = 2$ and

$$F_1 := u_1^2 u_2^3 - 0.5 \qquad \text{and} \qquad F_2 := u_1 u_2 - 1.0, \tag{6.9}$$

the classical Newton method diverges if $u_i^{(0)} = 2$ for $i = 1$ and 2. The choice of

$$\tilde{b}_1^{(k+1)} := \begin{cases} b_1^{(k)} - 0.1 & \text{if } |b_1^{(k)}| \geqslant 0.2, \\ 0 & \text{otherwise,} \end{cases}$$

$$\tilde{b}_2^{(k+1)} := \begin{cases} b_2^{(k)} - 0.01 & \text{if } |b_2^{(k)}| \geqslant 0.1, \\ 0 & \text{otherwise,} \end{cases} \tag{6.10}$$

yielded a slow linear convergence (of 307 iteration cycles) and, subsequently, a rapid quadratic convergence of only 3 iteration cycles when $\tilde{b}_i^{(k+1)} = 0$ was reached for both $i = 1$ and $i = 2$. The solution, thus approximated, is $u_1 = 2$ and $u_2 = 0.5$.

Remark. Modified Newton methods (e.g., [22, p. 208]) usually employ a parameter $\lambda_k \in \mathbb{R}$ in

$$u^{(k+1)} = u^{(k)} - \lambda_k (DF(u^{(k)}))^{-1} F(u^{(k)}) \quad \text{with } k+1 \in \mathbb{N}. \tag{6.11}$$

Even though convergence can be enforced under rather general conditions, the determination of the λ_k is rather involved.

Next, $Au = f$ in (1.1) is assumed to represent a collection of systems of linear algebraic equations with $f \in \mathbb{R}^n$ fixed and a set of matrices $A \in L(\mathbb{R}^n)$; (1.1) then may be the discrete analogy of a differential equation with side conditions and a set of coefficients. The smallest interval enclosing the set of solutions, S_u, of $Au = f$ can be determined if every admitted matrix is an M-matrix, e.g., [5, p. 156]. This condition is not required in the following example, where ∂S_u is approximated for the case of $n = 2$.

Example 6.3. The collection of systems

$$Au - f = 0 \Leftrightarrow \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} \quad \text{with } a_{ij} \in [\underline{a}_{ij}, \bar{a}_{ij}] \text{ and } f \in \mathbb{R}^2 \text{ fixed} \tag{6.12}$$

is considered. A special matrix $A_0 = (a_{ij}^{(0)})$ is selected from the admitted set such that A_0^{-1} exists. The subsequent results are optimal with respect to the choice of A_0 if there holds

$$a_{ij}^{(0)} := \underline{a}_{ij} + \tfrac{1}{2}(\bar{a}_{ij} - \underline{a}_{ij}) \quad \text{for } i, j = 1 \text{ or } 2. \tag{6.13}$$

An auxiliary vector $\beta := (a_{11}, a_{12}, a_{21}, a_{22}) \in S_\beta := \prod_{i,j=1}^{2} [\underline{a}_{ij}, \bar{a}_{ij}] \subset \mathbb{R}^4$ is introduced. A function $F(u, A) := Au - f$ is defined. Since a sufficient condition for the existence of one and only one solution $u(\beta)$ is implied in the following, it may be assumed that a unique solution $u(\beta)$ exists for every $\beta \in S_\beta$. The function $\hat{F}(\beta) := F(u(\beta), A(\beta))$ has the properties $\hat{F}\colon S_\beta \to \mathbb{R}^2$ and $\hat{F}(\beta) \equiv 0$. The following notations are introduced:

$$v_k^{(i,j)}(\beta) := \frac{\partial u_k(\beta)}{\partial a_{ij}} \quad \text{and} \quad w_k^{(i,j;\sigma,\tau)}(\beta) := \frac{\partial^2 u_k(\beta)}{\partial a_{ij} \partial a_{\sigma\tau}}; k, i, j, \sigma, \tau = 1 \text{ or } 2. \tag{6.14}$$

By use of differentiating the identity $\hat{F}(\beta) \equiv 0$, four systems of linear algebraic equations with the identical matrix $A(\beta)$ are obtained for the four vectors $v^{(i,j)} \in \mathbb{R}^2$. In these systems, β is now replaced by $\beta_0 := (a_{11}^{(0)}, \ldots, a_{22}^{(0)}) \in S_\beta$. This defines the special solution $u(\beta_0) = A_0^{-1} f$ and the Taylor coefficients $v_0^{(i,j)} \in \mathbb{R}^2$ in the following linear truncated Taylor expansion:

$$\tilde{u}(\beta) = u(\beta_0) + \sum_{i,j=1}^{2} (a_{ij} - a_{ij}^{(0)}) v_0^{(i,j)} \quad \text{where } A_0 v_0^{(1,1)} = \begin{pmatrix} -u_1(\beta_0) \\ 0 \end{pmatrix}, \text{ etc.,} \tag{6.15}$$

i.e., the existence of A_0^{-1} implies the existence of the $v_0^{(i,j)}$. The validity of the following matrix representation is implied by the Neumann series for $A^{-1}(\beta)$:

$$\tilde{u}(\beta) = A_0^{-1}[f - B(\beta)u(\beta_0)] \qquad \text{where } A_0^{-1} = A^{-1}(\beta_0)$$

$$\text{and} \quad B(\beta) := ((a_{ij} - a_{ij}^{(0)})) \in L(\mathbb{R}^2). \tag{6.16}$$

Since $f - B(\beta)u(\beta_0) =: I(\beta) \subset \mathbb{R}^2$ is an interval, $A_0^{-1}I(\beta)$ is a parallelogram $P \subset \mathbb{R}^2$ such that (*i*) $\partial I \leftrightarrow \partial P$ due to (affine bijective) boundary mapping and (*ii*) ∂P is an approximation of ∂S_u where S_u is the set of solutions of (6.12). The theory of the Neumann series implies that the terms of the second order,

$$\Gamma_2 := \tfrac{1}{2} \sum_{i,j,\sigma,\tau=1}^{2} (a_{ij} - a_{ij}^{(0)})(a_{\sigma\tau} - a_{\sigma\tau}^{(0)}) w^{(i,j:\sigma,\tau)}(\beta), \tag{6.17}$$

in an extension of the expansion (6.15), admit the following matrix-representation:

$$\Gamma_2 = A^{-1}(\beta)B(\beta)A^{-1}(\beta)B(\beta)u(\beta). \tag{6.18}$$

The 10 vectors $w^{(i,j:\sigma,\tau)} \in \mathbb{R}^2$ in (6.17) are the solutions of 10 systems with the identical matrix $A(\beta)$. By use of (6.18), the remainder term, R_2, of the linear truncated expansion (6.15) can be estimated as follows by use of a suitably selected a priori set $\tilde{S}_u \subset \mathbb{R}^2$:

$$\|R_2\|_\infty \leqslant \operatorname*{Max}_{\beta \in S_\beta} \operatorname*{Max}_{u \in \tilde{S}_u} \|\Gamma_2\|_\infty \leqslant [\operatorname*{Max}_{\beta \in S_\beta} \|B(\beta)\|_\infty^2]\gamma^2[\operatorname*{Max}_{u \in \tilde{S}_u} \|u\|_\infty] =: \rho,$$

$$\text{where } \gamma := \frac{\|A_0^{-1}\|_\infty}{1 - \|A_0^{-1}\|_\infty \|(\bar{a}_{ij} - a_{ij}^{(0)})\|_\infty} \quad \text{if } \|A_0^{-1}\|_\infty \|(\bar{a}_{ij} - a_{ij}^{(0)})\|_\infty \overset{!}{<} 1. \tag{6.19}$$

Here, γ is due to a well-known estimate in Numerical Analysis, e.g., [6, p. 65]. If the condition denoted by ! is satisfied, then every admitted matrix is invertible, compare (3.6). For ∂P to be a sufficiently accurate approximation of the set of solutions, S_u, of (6.12), ρ as defined in (6.19) should be very much smaller than a characteristic geometric extension of P. The selected a priori set, $\tilde{S}_u$, is sufficiently large if $\partial\tilde{S}_u$ is an outer approximation of ∂P whose distance exceeds ρ. This construction has been applied to the following system:

$$A(\varepsilon)u - \mu I u = f \quad \text{with } \mu = 1.5, f \in S_f := [0.8, 1.2] \times [0.8, 1.2] \subset \mathbb{R}^2,$$

$$\varepsilon = (\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4) \in S_\varepsilon \subset \mathbb{R}^4,$$

$$A(\varepsilon) :\in \begin{pmatrix} [-3 - \varepsilon_1, -3 + \varepsilon_1] & [1 - \varepsilon_2, 1 + \varepsilon_2] \\ [-4 - \varepsilon_3, -4 + \varepsilon_3] & [2 - \varepsilon_4, 2 + \varepsilon_4] \end{pmatrix} \quad \text{with } |\varepsilon_i| \leqslant \bar{\varepsilon} \text{ for } i = 1(1)4. \tag{6.20}$$

The admitted matrices are not M-matrices; $A(0)$ possesses (*a*) the eigenvalues -2 and 1 and (*b*) the eigenvectors (1, 1) and (1, 4). The numerical results in Fig. 1 reveal that the set of solutions possesses roughly the direction of the eigenvector (1, 4) since $\mu = 1.5$ is close to the eigenvalue 1. J. Steckelberg (Karlsruhe) has computed the numerical results in Fig. 1 which hold for the two fixed choices of $\bar{\varepsilon} = 0.01$ and $\bar{\varepsilon} = 0.05$. The dashed parallelogram represents the set of solutions $A^{-1}(0)S_f$. The solid quadrilateral encloses $3^4 = 81$ parallelograms $A^{-1}(\varepsilon)S_f$ with 81 different fixed choices of $\varepsilon \in S_\varepsilon$ such that $|\varepsilon_i| \leqslant \bar{\varepsilon}$. Therefore, the solid boundary of this quadrilateral encloses the set of solutions, $S_u(\bar{\varepsilon})$, with a high degree of approximation. The double solid lines for the case of $\bar{\varepsilon} = 0.01$ are due to an application of the estimate denoted

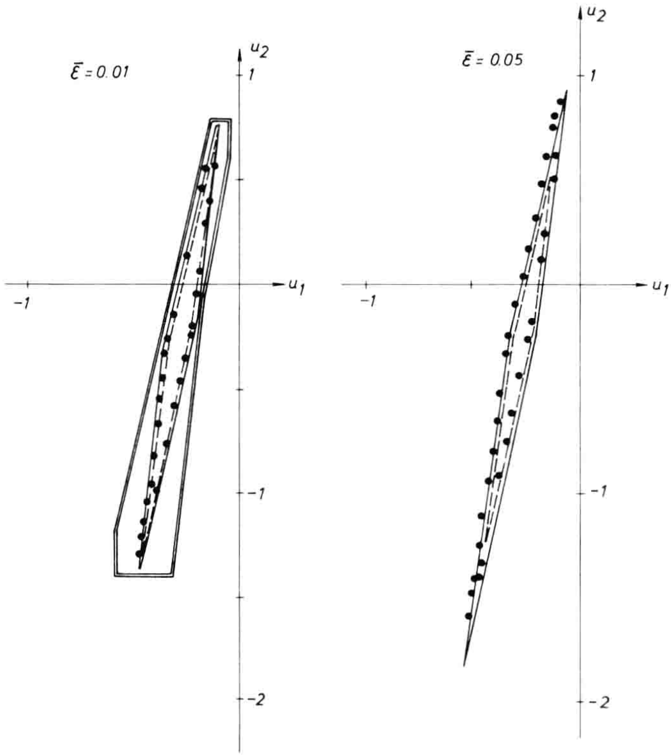

Fig. 1. The set of solutions for the collection (6.20) of systems of linear algebraic equations. The symbols are explained subsequent to (6.20)

by γ in (6.19) to selected fixed vectors $f \in S_f$. The linear truncated Taylor-expansion (6.15) was employed separately for (*i*) the two choices of $\bar{\varepsilon}$ and (*ii*) fixed choices of $f \in \partial S_f$ in a discretization of ∂S_f. The resulting parallelograms $P(\bar{\varepsilon}, f)$ are enclosed by the dots in Fig. 1 which define a quadrilateral $\partial S_T(\bar{\varepsilon})$. Due to (6.15), each $P(\bar{\varepsilon}, f)$ is determined by $A^{-1}(0)f$ and four vectors $v_0^{(i,j)} \in \mathbb{R}^2$ which are the solutions of systems with the identical matrix $A(0)$. Inspection of Fig. 1 reveals that $\partial S_T(\bar{\varepsilon})$ is a highly accurate approximation of the envelope $\partial S_u(\bar{\varepsilon})$ of the set of solutions for both $\bar{\varepsilon} = 0.01$ and $\bar{\varepsilon} = 0.05$. The number $\rho(\bar{\varepsilon})$ in (6.19) was determined by use of an a priori set $\tilde{S}_u(\bar{\varepsilon})$ with the following properties: (*i*) $S_T(\bar{\varepsilon}) \subset \tilde{S}_u(\bar{\varepsilon})$ and (*ii*) the distance of $\partial S_T(\bar{\varepsilon})$ and $\partial \tilde{S}_u(\bar{\varepsilon})$ exceeds a chosen number $d(\bar{\varepsilon})$:

$$\begin{aligned} \bar{\varepsilon} = 0.01: \quad & d(0.01) = 0.06 \quad \Rightarrow \rho(0.01) = 0.01619 \leqslant d(0.01), \\ \bar{\varepsilon} = 0.05: \quad & d(0.05) = 1.3266 \Rightarrow \rho(0.05) = 2.67 \quad \nleqslant d(0.05), \end{aligned} \tag{6.21}$$

i.e., the chosen a priori set $\tilde{S}_u(0.05)$ is too small. By construction, an expansion of each side of the dotted quadrilateral $\partial S_T(\bar{\varepsilon})$ by the distance $\rho(\bar{\varepsilon})$ yields an outer approximation of the set of solutions, $S_u(\bar{\varepsilon})$. For $\bar{\varepsilon} = 0.05$, the estimate $\rho \geqslant \|R_2\|_\infty$ exceeds considerably the distance between the solid quadrilateral and the dotted $\partial S_T(\bar{\varepsilon})$. Without a knowledge of the solid quadrilateral, a truncated Taylor