MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

T a g u n g s b e r i c h t 11/1990

Interval Methods for Numerical Computation

4.3. bis 10.3.1990

Die Tagung fand unter der Leitung von O.E. Lanford (Zürich) und A. Neumaier (Freiburg) statt.

Schwerpunkt der Thematik waren einerseits Fragen der Sensitivität, Parameterabhängigkeit und mehrdeutigen Lösbarkeit bei endlich-dimensionalen linearen und nichtlinearen Gleichungssystemen, andererseits gelöste und ungelöste Probleme bei der Verifikation der Existenz oder Nichtexistenz von Lösungen von Randwertproblemen und Funktionalgleichungen mit Komposition.
Mehrere Vorträge über Anwendungen in der mathematischen Physik und bei Ingenieurproblemen stellten den Bezug zur Praxis her.

VORTRAGSAUSZÜGE

G. ALEFELD:

Enclosure methods for the range of values with higher order of convergence

In this talk we consider the problem of approximating the range of real functions which admit a respresentation of the form $f(x) = p(x) + \ell(x)h(x)$. We show that this can be done by an interval extension of the form $f(X) = p(X) + \ell(X)h(X)$ and that under some assumptions on $p(X)$, $\ell(X)$ and $h(X)$ the Hausdorff distance between $f(X)$ and the range of f on X is of order $O(d(X)^k)$. This generalizes recent results on centered forms as well as on higher order centered forms and on remainder forms.

H. BAUCH

Accuracy, sensitivity and tolerance in scientific computation (computer arithmetic

The new methodology for scientific computation is based on the so-called advanced computer arithmetic by KULISCH, MIRANKER a.o. The combination of the three features optimal scalar product, interval arithmetic and residual correction guarantees high or even maximum accuracy.In order to describe set-valued data in a more precise way, so-called tolerance intervals are introduced. With the help of this new type of intervals, bounds and inner estimations of high accuracy are simultaneously computable. In this way a proper numerical treatment of the influence of direct (input-intervals) and indirect (computer arithmetic) tolerances in scientific computation becomes possible.

A. CELLETTI:

Computer-assisted KAM methods with applications to celestial mechanics

In nearly-integrable Hamiltonian systems of the form

$$H(\underline{y},\underline{x}) = h(\underline{y}) + \varepsilon f(\underline{x},\underline{y}), \ \underline{y} \in \mathbb{R}^{\ell}, \ \underline{x} \in (\mathbb{R}/2\pi\mathbb{Z})^2$$

the existence of invariant surfaces can be established by means of KAM theory. We implement a KAM theorem for the Hamiltonian describing the spin-orbit interaction in a satellite-planet-system. The existence of invariant surfaces is proved for "realistic" values of the perturbation parameter ε. However, since the amount of computations is very large we use a computer implementing the interval arithmetic to control the numerical errors.

J. DEMMEL:

Optimal error bounds in numerical linear algebra without interval arithmetic

One application of interval arithmetic is computing error bounds for problems in numerical linear algebra. Recent progress in perturbation theory, algorithm design and error analysis permits optimal error bounds to be computed for a variety of problems using neither interval arithmetic nor extra precision. By optimal we mean that there is a small relative uncertainty in each entry of the data (i.e. the original data consists of intervals I_j where the width of I_j is small compared to the smallest number in I_j), and that the error bounds are nearly attainable for some initial data in the intervals. This can be done, with some limitations, for linear equation solving, least squares, the bidiagonal SVD, the dense SVD, the symmetric tridiagonal eigenproblem, the dense positive definite symmetric eigenproblem, and the dense positive definite generalized eigenproblem. The algorithms are about as fast and sometimes faster than conventional algorithms which do not deliver error bounds. Many of these algorithms will be incorporated in the LAPACK linear algebra library.

J.-P. ECKMANN and O.E. LANFORD

The computer-assisted proof of the Feigenbaum conjectures

Our objective in this talk is to describe a concrete example of the use of interval arithmetic methods in the proof of a qualitative mathematical theorem. We consider the operator

$$T : f \mapsto \frac{1}{f(1)} f(f(f(1)x)) ,$$

acting on an appropriate domain in the space of even analytic mappings of the interval [-1,1] to itself which send 0 to 1. The Feigenbaum conjectures are

1. T has a fixed point, i.e., there is an analytic solution

$$g(x) \approx 1.0 - 1.5276 \cdots x^2 + 0.1048 \cdots x^4 + \cdots$$

of the *Feigenbaum-Cvitanović equation*

$$g(x) = -\frac{1}{\lambda} g(g(\lambda x)),$$

where $\lambda = -g(1) \approx 0.3995 \cdots$.

2. The linear operator $DT(g)$ has all its spectrum inside the open unit disk except for a single simple eigenvalue $\delta > 1$.

(For the applications, one also needs to know something about the global behavior of the (one-dimensional) unstable manifold for T at g, but we will not formulate the exact assertions here.)

In outline, the proof goes as follows:

1. Using a simplified version of Newton's method, we convert the original fixed point problem to a fixed point problem for a *contraction* Φ.

2. We study the fixed point problem for Φ in a Banach space of analytic functions, normed with the ℓ^1 norm of the Taylor coefficients. This norm has the advantage that it is relatively easy to make sharp estimates of norms of linear operators.

3. We introduce a data structure - in the spirit of the interval data structure - giving a finite representation for a large class of "balls" in this Banach space, and construct a set of procedures for "doing elementary operations on these balls". These procedures are based on interval arithmetic.

4. By stringing together calls to these procedures, we make a program which verifies that Φ is contractive on an explicit ball in the Banach space, and hence that an analytic fixed point exists.

5. It turns out to be possible to organize the estimates so that the assertion about the spectrum of DT at the fixed point follows from essentially the same calculations as are needed to prove its existence.

D.M. GAY

<u>Automatic differentiation of nonlinear AMPL models</u>

One can now express nonlinear constraints and objectives in AMPL (a modeling language for mathematical programming). Nonlinear expressions are translated to loop-free code, which makes analytically correct gradients and Jacobian matrices particularly easy to compute - static storage allocation suffices. Interval enclosures of gradients, Hessians, and Jacobian matrices should also be straightforward to compute, which invites using interval techniques to seek global optima of mathematical programs written in AMPL.

F. HEIZMANN:

Solution of parameter dependent systems of equations

Given a function $F : D \subseteq \mathbb{R}^n \rightarrow \mathbb{R}^m$, $n > m$, the concern is to find all zeros which F has within an a priori interval $x \subseteq D$.

A method is pointed out how an enclosure of the solution, consisting of finitely many sets of the form $\{Q\tilde{r} \mid \tilde{r} \in r\}$, can be computed, where $Q \in \mathbb{R}^{n \times n}$ and r is a n-dimensional interval, of which m components should be narrow.

It is shown how the existence of solutions within those sets can be numerically verified.

CH. JANSSON:

Sensitivity and error analysis for linear programming problems

A method for calculating guaranteed bounds for the solution of a linear programming problem is presented. All input data are allowed to vary between given lower and upper bounds. The method calculates very sharp and guaranteed error bounds and allows a rigorous sensitivity analysis. The sharpness of the computed bounds can be estimated.

R.B. KEARFOTT:

Splitting preconditioners for the interval Gauss-Seidel method

Interval Newton methods involve finding bounds on the solution set $\mathbf{X}_k$ to the linear interval equation

$$\mathbf{F}'(\mathbf{X}_k)(\tilde{\mathbf{X}}_k - X_k) = -F(X_k),$$

where $\mathbf{F}'(\mathbf{X}_k)$ is a suitable interval extension to the Jacobian matrix of the function F over the box $\mathbf{X}$, and where $X_k \in \mathbf{X}$; i.e. we find a box $\tilde{\mathbf{X}}_k$ for which

$$\mathbf{F}'(\mathbf{X}_k)(\tilde{\mathbf{X}}_k - X_k) \supset -F(X_k).$$

To obtain $\tilde{\mathbf{X}}_k$ which is as small as possible, we may multiply by a non-interval preconditioner matrix Y to obtain

$$YF'(\mathbf{X}_k)(\tilde{\mathbf{X}}_k - X_k) = - YF;$$

we the may obtain bounds $\tilde{\mathbf{X}}_k$ by formally applying the interval Gauss-Seidel method.

On strategy for obtaining Y is to make the widths of the coordinate intervals of $\mathbf{X}_k$ as small as possible; this has been investigated by the speaker and his associates. Another strategy is to force a division by a zero-containing interval in the interval Gauss-Seidel method, and to make the gap in the resulting extended interval as large as possible.We will analyze and discuss this possibility.

KELCH:

<u>Numerical quadrature with result verification</u>

Starting from Romberg-extrapolation the recursive implementation of the T-table elements T_{ik} is replaced by direct evaluation of an accurate scalar product representing a weighted sum of function values:

$T_{ik} = h_o \cdot \Sigma\, w_{ikj}\, f(x_{ij})$. Explicit formulas are derived for the weights.The weights can be represented precisely, are independent of the function and may be a priori computed and stored in a table.

An enclosure R´ of the remainder term R may be computed via automatic differentiation algorithms by $R' = c_m \cdot f^{(i)}([a,b])$, with a known constant c_m. The integral is then enclosed as $J \in T_{mm}+R'$. We consider different step size sequences and introduce a new one, called "decimal sequences". It is possible to compute a priori a list of optimal methods depending on the desired T-table-diagonal. A fast search algorithm determines that method of this list which requires the least computation effort while satisfying the requested accuracy.

Only after this computation of the optimal remainder term the appropriate T_{mm} is computed (directly without requiring any other T_{ik}).

Local adaptive refinement via bisection and increase of the approximation degree make it possible to reduce the global error efficiently to the requested size, since additional computation is done only where necessary.

It is just in case of difficult functions that the classical estimator often indicates an error being several orders smaller than it really is. Thus, reliability of this estimator and the quality of the approximation become doubtful. In contrast the new algorihm provides guaranteed intervals with narrow bounds.

L. KOLEV:

Interval methods for finding all solutions of quasilinear systems

We consider quasilinear systems of the form $f(a) = \ell(x)$ where $f: X^{(0)} \to R^n$ with $X^{(0)} \in I(R)$, $f_i(x) = f_i(x_i)$ and $\ell(x) = Hx+s$ with H and s being a constant matrix and a constant vector, respectively. The problem is to find all the solutions contained in $X^{(0)}$. Three methods for solving the problem considered are presented. The first two are due to Hansen and Sengupta (1981) and Alefeld and Herzberger (1983), respectively, and are applicable for the case where $f \in C^1$. The third method is valid for all continuous f. It is based on an iterative procedure making use of $F(X) \cap L(X)$ at each current step. A numerical example illustrates the efficiency of the three methods considered.

R. de la LLAVE:

Computer assisted proofs of stability of matter

In this talk I describe joint work with C. Fefferman. We study the behaviour of an arbitrarily large number of electrons interacting among themselves and with an arbitrarily large number of nuclei at fixed positions. We show that the energy per particle is bounded by a term proportional to the number of particles - and not to the number of particles raised to a higher power. Mathematically, this can be formulated as proving bounds of the form

$$\inf_{N,M,y_1,\dots,y_M} \inf_{\psi \in L^2_{\text{antisym}}} (\psi, H\psi) \geq C(N+M),$$

where

$$H = H(N,M,y_1,\dots,y_M) = \sum -\Delta_{x_i} + \alpha \left(\sum |x_i - x_j|^{-1} + \sum |y_k - y_l|^{-1} - \sum |x_i - y_k|^{-1}\right),$$

$i,j=1,\dots,N$, $k,l=1,\dots,M$, and L^2_{antisym} denotes the square integrable functions on $(\mathbf{R}^3)^N$ which are antisymmetric on the exchange of arguments.In this case, obtaining good values of the constant C is very important.

The model above can be controlled by showing that a similar model in which $-\Delta$ is replaced with $(-\Delta)^{1/2}$ is positive definite.

We show that this problem can be reduced to estimating a single singular integral operator and showing it is positive. This proof is accomplished using interval analysis in order to improve the constants.

One can hope that this is a prototype for the study of many analysis problems that can be reduced to obtaining estimates of concrete "maximal" operators.

R. LOHNER:

<u>Interval methods for ordinary differential equations</u>

Methods for the computation of bounds for the solution of ordinary initial and boundary value problems are presented, which were developed during the past 5-10 years. For initial value problems Taylor expansion is used where the remainder term is enclosed by use of interval arithmetic. Also special care is taken to reduce the "wrapping effect" which often severely blows up the enclosures of th global error. For boundary value problems single and multiple shooting methods are used to reduce the problem to a finite dimensional problem and the integration of initial value problems. Then existence of solutions of the boundary value problem can be shown within the computed bounds. All methods can be programmed on a computer in such a way that only the problem has to be entered in some mathematical form. The algorithm then works fully automatically.

G. MAYER:

Enclosure for the inverse algebraic eigenvalue problem

The inverse algebraic eigenvalue problem consists in finding real numbers $c_1, c_2, \ldots, c_n$ such that the $n \times n$-matrix $A(c_1, c_2, \ldots, c_n) := A_0 + \sum c_i A_i$ has prescribed eigenvalues $\lambda_1 < \lambda_2, \ldots < \lambda_n$, where the A_i, $i=1,\ldots,n$ are given $n \times n$-matrices. Based on Newton´s method, an algorithm is presented which verifies existence and uniqueness of the c_i within some small intervals $[c]_i$, $i=1,\ldots,n$.

F. MRAZ:

Solution function of an interval linear programming problem

A linear programming problem whose constraint coefficients are prescribed by intervals is investigated. Let A be an m by n interval matrix, let b be an interval m-vector.

Interval linear programming (abbr. ILP) problem is a family of linear programming problems

$$\max \{c^t x \mid Ax=b, x \geq 0\}, \qquad S(A,b)$$

where $A \in [A]$, $b \in [b]$. Let us denote by $f(A,b)$ the optimal value of a problem S(A,b). The function defined in this way is called a solution function of an ILP problem. Some algorithms for computing its supremum $f = \sup \{f(A,b) \mid A \in [A], b \in [b]\}$ are mentioned. A necessary condition for the infimum value f is proved and an algorithm for its computation is given. It terminates with the value f if the ILP problem is basis stable, and with a local minimizer of f in the general case.

E.A. MUSAEV:

Comparison of traditional, generalized and aposteriori interval analysis

The aposteriori interval method of Matijasevich has been extended to the case of arbitrary programs. Traditional, generalized and aposteriori interval arithmetic (IA) were implemented and a comparison of these three methods was made. It shows that:

1) by time and storage aposteriori IA is nearer to traditional IA than generalized one as predicted;

2) by precision aposterioriIA is nearer to generalized IA than to traditional one as predicted;

3) there are cases when traditional IA is most precise (especially when input errors are large);

4) nowadays aposteriori IA is applicable to arbitrary programs and shows good results for scientific computations, but suitable realizations are needed.

M.T. NAKAO:

A numerical verification method for the existence of solutions for partial differential equations

We propose a numerical method for the automatic proof of existence of weak solutions for elliptic and parabolic partial differential equations. First, for the linear Dirichlet problem, a verification condition based on Schauder´s fixed point theorem is formulated and, using the finite element approximation and its error estimates, we present a numerical verification algorithm by computer. Then the method is extended to the case of interval coefficient equations as well as more general linear problems. Moreover, we also consider the nonlinear Dirichlet problems. Finally, it is shown that these verification principles are applicable to the second order nonlinear parabolic initial boundary value problems. Some numerical examples are given.

A. NEUMAIER:

Inclusion algebras and numerical integration

As a natural and flexible setting for the calculation with regions in function space (describable by finitely many parameters), the concept of an inclusion algebra is introduced. After reviewing standard inclusion algebras related to interval polynomial and Taylor series, two new inclusion algebras for analytic functions and for asymptotic enclosures are defined. These are applied to adaptive integration with verification of integrals of the form

$$\int_a^b f(x)dx \quad \text{and} \quad \int_0^\infty k(x,t)f(x)dx.$$

Among the kernels treated are $k(x,t) = e^{-tx}$, $\cos(tx)$, $\sin(tx)$.

D . OELSCHLÄGEL:

Einige Interall-Optimierungsprobleme

Es wird ein Überblick über Anwendungen der Intervallmathematik in Merseburg und über die gewonnenen Ergebnisse gegeben. Eine besondere Rolle spielt dabei die Optimierung. Seit den siebziger Jahren werden Untersuchungen zur intervall-mathematischen Behandlung von konvexen Optimierungsproblemen mit Datenfehlern durchgeführt. Unter Benutzung der Kuhn-Tucker-Theorie wurden auf verschiedenen Wegen Einschließungen der Menge der Optimalpunkte und der Menge der optimalen Zielfunktionswerte gewonnen. Seit Beginn der achtziger Jahre werden Verfahren zur Lösung von Intervallanfangswertaufgaben entwickelt, die meist Polynomschrankenfunktionen für den Lösungsschlauch liefern. Durch Verwendung genügend hochgradiger Polynome wird ein evtl. auftretender wrapping-Effekt in seiner Wirkung hinausgezögert.

Rein praktische Anwendungen waren die intervallmathematische Untersuchung von Mehrschichtenströmungen, die Behandlung chemischer Fragestellungen mit Intervallinterpolation, intervallmathematische Trendrechnungen in der Metrologie, die intervallmathematische Behandlung von Massenbilanzierungen und die Fließschemasimulation in der Verfahrenstechnik.

G. REX:

Interval homotopy methods for zeros of systems of nonlinear equations

Let a system of nonlinear equations $f(\cdot) = 0$, $f: \mathbb{R}^n \to \mathbb{R}^n$ be given. By means of the homotopy concept there is a possibility for the computation of a zero x^* of $f(\cdot)$. The homotopy concept is generalized by defining an interval homotopy function and moving along a family of paths from a a given interval vector $X^0 \in I(\mathbb{R}^n)$ to x^*. This method is related to the global Newton method, and this process can be continued for the computation of other zeros. This practice can be advantageous to increase robustness of numerical procedures.

J. ROHN:

Linear interval equations with dependent coefficients

When solving a linear interval system by usual methods, it is assumed that the coefficients and the right-hand sides may range independently of each other over the prescribed intervals. In case of dependent coefficients (think e.g. of a symmetric matrix), this approach may lead to an unnecessary overestimation of the hull. We shall present a method which takes into account linear dependences among coefficients of a rather general type and, under certain assumptions concerning sign stability of some expressions, computes the exact hull by constructing two sequences of matrices whose diagonals converge to the upper and the lower bound of the hull, respectively.

S.M. RUMP:

Sensitivity analysis for systems of linear and nonlinear equations

Methods are presented for performing a rigorous sensitivity analysis for general systems of linear and nonlinear equations w.r.t. weighted perturbations in the input data. The weights offer the advantage that all or part of the input data may be perturbed, e,g, relatively or absolutely. System zeros may, depending on the application, stay zero or not. Estimations for the sensitivity come together with very sharp and guaranteed bounds for the solution.

L.A. SECO:

Computer assisted solutions to ordinary differential equations

Given the ODE, the problem consists in, first, producing good bounds for the solution to initial value problems, and, second, to use these bounds to produce information on boundary value or eigenvalue problems.
The particular ODE dealt with comes from a problem in atomic physics.

H.J. STETTER:

Some problems in the control of inclusion algorithms for ODEs (initial value problems)

We consider the Moore-Lohner approach (Taylor series, remainder term inclusion) and discuss some questions regarding the control of its parameters (order and step-size). The various contributions to the stepwise excess of the method are analyzed, analogies and distinctions with regard to appproximation methods are identified. Possibilities for local control mechanisms are suggested and their limitations are discussed. It appears that it will be advisable to collect information about the global behavior of the problem in a first pass over the interval (without inclusions) so that the expensive inclusion pass may be economically controlled.

V. WIEBIGKE:

Anwendung hochgenauer Algorithmen in der Systemverfahrenstechnik

Gegeben ist eine technische Anlage mit n Bausteinen (Reaktoren und Abscheider). Gesucht ist die Massenbilanzierung dieses technischen Systems, wobei der Massenstrom aus m Komponenten besteht. Die Modellierung dieses Problems führt zu einem linearen Gleichungssystem $Ax = b > 0$ der Dimension ($mn \times mn$). Den Techniker interessiert die Zusammensetzung der Massenströme, wobei bestimmte Koeffizienten in vorgegebenen Intervallen enthalten sind und für jeden Reaktor j die folgenden Bilanzbedingungen erfüllen müssen:

$$\sum_{i=1}^{m} \mu^{i}_{j} = 1, \quad \mu^{i}_{j} \geq 0, \quad \mu^{i}_{j} \in [\mu^{i}_{j}]. \qquad (*)$$

Die Koeffizientenmatrix A ist für jede technisch sinnvolle Konstellation (*) eine M-Matrix. Nach Einsetzen der Intervalle $[\mu^{i}_{j}]$ kann diese Eigenschaft für das Oberschrankenproblem $\bar{A}x = b$ verlorengehen. Die Einschließung aller technisch sinnvollen Konstellationen wird erreicht durch die Lösung reeller Randprobleme $\underline{A}x = b$ ($\underline{A}$ ist immer M-Matrix) und $\bar{A}x = b$ (falls $\bar{A}$ eine M-Matrix ist), wobei nur die Relation $1 \leq \sum_{i=1}^{m} [\mu^{i}_{j}]$ realisiert ist und damit eine Überschätzung der Lösung vorliegt. (Mitautoren: S. Kütscher, J. Schulze)

M.A. WOLFE:

The application of functional programming languages to interval arithmetic computation

The use of functional programming languages to create computational environments for the excution of interval arithmetic algorithms is illustrated using the language Miranda. The Miranda libraries utils, intfns, imolib, and pracks which will illustrate input-output functions, a naive implementation of real interval arithmetic, interval vector and interval matrix manipulation, and the manipulation of generic data structures are presented. The algorithms MN_p and MS_p (Alefeld and Potra, Computing 42 (1989)) are implemented using intfns. The value of functional programming languages for implementing parallel algorithms is discussed. Finally some work which we hoped to begin in the near future is described.

A.G. YAKOVLEV:

Interval computations in the USSR

In the last years, interval computations in the USSR were intensively developed. But as it follows from "Science Citation Index", Western specialists don't cite Soviet works. Reasons for such a situation are discussed. The report contains information concerning directions of research, publications, conferences, software development and other aspects of professional activity in this area in the USSR. Some proposals on strenghening of communications between Soviet and West specialists on interval computations are given.

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