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Abstract

Interval arithmetic, numbers which are aff ways provides reliable numerical algorithms (that the exact result the computed tolerance cases these bounds mathough the statement spractice worthless, recently introduced a sibility of successionance. Furthermore, the exact of the solution is prove the solution t

These methods combine analysis with the con Kulisch and Miranker. point theorems and a essential for their in

0. <u>Introduction</u>

In [8] a mathematical what we call "Compute the algebraic structube described in temprocess of truncation achine representation the real numbers.

We will summarize some

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 \mathbb{R} , V_nS , M_nR , M_nS } an ordered set $\}$, i.e. the set $|a \le x \le b|$ properties of see [1],[6]).

from [4].

Occasionally, we will denote a member of an interval A by $\mbox{\mbox{\it A}}.$

For two intervals A,B \in T an arithmetic operation $\circ \in \{+,-,\cdot,\cdot\}$ is defined by $A \circ B := \{a \circ b \mid a \in A, b \in B\}$

 $\begin{picture}(20,20) \put(0,0){\line(0,0){10}} \put(0,$

 $A \ \underline{\cup} \ B := \{x \in S \mid \exists a \in A, b \in B : a \le x \le b \ \forall b \le x \le a\}$

 $d(\cdot)$ diameter of an interval, i.e. $A = [a,b] \in IS \implies d(A) := b-a$

♦:PR→IS rounding from PR into IS with the property

$$\bigwedge_{A \in PR} \Diamond A = \bigcap \{X \in IS \mid A \subset X\}$$

For vectors and matrices this definition applies componentwise

 $\begin{array}{ll} \diamondsuit\,,\diamondsuit\,,\quad\dots&\text{interval operations in IS,IV}_nS\text{ and IM}_nS\\ \diamondsuit\,,\diamondsuit&\text{defined for }T\in\{S,V_nS,M_nS\}\text{ by} \end{array}$

$$\bigwedge_{A,B\in IT} \bigwedge_{\circ\in\{+,-,\cdot,\prime\}} A \otimes B = \Diamond(A \circ B)$$

Throughout this paper we consider the following problem:

"Let $f: D \to V_n \mathbb{R}$ be a continuously differentiable function, $D \subset V_n \mathbb{R}$. We seek an $\hat{\mathbf{x}} \in V_n \mathbb{R}$ with $f(\hat{\mathbf{x}}) = 0$, or more practically, we ask for an inclusion $X \in IV_n \mathbb{R}$ of $\hat{\mathbf{x}}$, where the diameter d(X) is sufficiently small."

We restrict ourselves to the case where the components of f are arithmetic expression with operations +,-,*,/ and integer exponentiation. The algorithm to be introduced determines an inclusion X of the solution $\hat{\mathbf{x}}$ and performs an automatic verification of conditions such as the existence and uniqueness of a zero $\hat{\mathbf{x}}$ of f within X. These methods are called E-methods (E is the first letter of the three German words "Existenz" for existence, "Eindeutigkeit" for uniqueness, and "Einschlie β ung" for inclusion.

For this purpose, the problem of finding a zero x of f is transformed into a fixed point equation g(x) = x (see [7], [11], [12]). An inclusion of the solution of this fixed-point problem is computed iteratively in the space $IV_n\mathbb{R}$ starting with an approximate solution $x \in V_n\mathbb{R}$. By use of residual correction techniques the diameter of the resulting interval is diminished more and more.

Theoretical foundations

We summarize some theorems from [7], [11], [12] concerning the existence and uniqueness of a solution of a system of equations. At first, we need the following

Lemma 1: (Schauder's fixed point theorem)

> Let $f : X \to V_n \mathbb{R}$ be a continuous function on $X \subseteq V_n \mathbb{R}$, X nonempty, convex and compact. If $f(X) \subseteq X$, then, the equation f(x) = x has at least one solution x in X.

see [5], e.g. Proof: \Box

From this lemma we have immediately

Theorem 1: Let $f: X \to V_n \mathbb{R}$ be a continuous function on $X \in \mathbb{N}_n\mathbb{R}$, and $F : \mathbb{P}X \to \mathbb{P}V_n\mathbb{R}$

 $\bigwedge_{A \in \mathbb{P}X} \bigwedge_{x \in A} f(x) \in F(A).$ (1.1) If $F(X) \subseteq X$, then the equation f(x)=x

has at least one solution x in X and

$$\bigwedge_{k \geq 0} \hat{x} \in F^k(X)$$

where $F^{o}(X) := X$, $F^{k}(X) := F(F^{k-1}(X))$.

From $X \in IV_n\mathbb{R}$ we have: $X \neq \phi$, X compact Proof: and convex. From the definition we have $f(X) := \{f(x) \mid x \in X\} \subseteq F(X) \subseteq X$ Therefore, Lemma 1 delivers the existence of a solution $x \in X$ of f(x) = x. The rest is shown by induction.

F may be arbitrarily chosen to satisfy (1.1). In practical applications F will be any interval extension of f.,

Theorem 1 allows no conclusion about the uniqueness of the solution. For this purpose we define

$$\bigwedge_{A,B\in IR} A \subseteq B : \iff A \subseteq B \land A \neq B$$

We also need the following two lemmata from [15]:

Lemma 2: Let $A = ((a_{i,j})) \in M_n \mathbb{R}$, $x = (x_i) \in V_n \mathbb{R}$ and x>0. Then for the spectral radius,

$$\max_{\substack{i \leq i \leq n}} \frac{\sum_{j=1}^{n} |a_{ij}| x_{j}}{x_{i}}$$

ho

Lemma 3: Le: and $0 \le |B| \le A$. Then, o(4) .

From this we

Theorem 2: Le - C € IMnR.

> $\mathbf{A} \subseteq \mathbf{X}$, (1.2)wh. s defined componentwise.

Th.

(C) < 1.

Proof: Ob (X) > 0. Furthermore, we $(Z + C \cdot X) < d(X)$

> $\begin{array}{l} \operatorname{d}(X)\,, \\ \operatorname{tve} \quad \operatorname{d}(C \, \bullet \, X) \, \geq \, \left| C \right| \bullet \operatorname{d}(X) \\ \leqslant \operatorname{d}(X) \quad , \qquad \qquad (1.3) \\ \operatorname{d}(X)\,. \text{ Then by lemma 2} \end{array}$ \mathbf{F}_{Γ} ⇒

> > $\frac{y_i}{d(X_i)} \stackrel{\text{(1.3)}}{\leftarrow} \frac{d(X_i)}{d(X_i)} = 1.$

Th, € C we have

> $P(|\mathcal{D}|) \leq P(|\mathcal{C}|) < 1$ emma 3 twice.

> > llowing theorem which is a

rify the existence and the ion of a system of equa-

by a

Now we can pr constructive uniqueness of tions.

 $X \in V_n \mathbb{R}, f : X \cup \tilde{x} \to V_n \mathbb{R},$ Theorem 3: Le **f** € :). For arbitrary but fixed $\mathbf{Y} = \mathbf{t}$ let J(Y)∈IM_nR and assume

th. very set of n vectors \mathbf{y}_1 .

ho? : $\mathbb{P}X \to \mathbb{P}V_n\mathbb{R}$ be defined by

G(`:` $(x) + (I-R \cdot J(x \underline{U} Y)) \cdot (Y-x)$ X, where R ∈ MnR is an for

fixed matrix.

Ιf **G**(''' holds, one and $\hat{\mathbf{x}} \in G^{\mathbf{k}}$ Proof: Consider $g : X \cup x$ From the that for exists a . g(y) Theorexiste. Furthe. -**R**f(:.) Hence. for all " the eigand M . it foll a fur mean ·

In practical appl e matrix R will be an approximation c Theorem 3 has be computers. In c computer applic for any G*: x t ch satisfies

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The definition

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equation f(x) = 0 has solution x in X and

tinuous) function $g(x) = -R \cdot f(x).$ alue theorem we have C X and y \in Y there (x U Y) such that $(x)+M(Y)\cdot(y-x)$ (y-x) + $(I-R\cdot M(y))\cdot (y-x)$

1.4) then delivers the fixed point x of f. 1 (1.4) we have [(x U X)) • (X-x) ⊊ X-x : implies $\rho(I-R \cdot M) < 1$ of I-R.M we see that R r. With $x-R \cdot f(x) = x$, $f(\hat{x}) = 0$. Let $\hat{y} \in X$ be tion. The generalized rem implies the exis-€ J(x U X) with $) + M(\hat{y}) \cdot (\hat{y} - \hat{x}) .$ ar and hence $\Rightarrow y = x$.

e of the Jacobian J(x). ed for application on pproach the goal of st observation is that $\subset G^*(Y)$

- Y implies G(Y) ⊊ Y.

ert that theorem 3 reed by S and G(Y) by an on of G, i.e.

$$(\overset{\sim}{\mathbf{x}})$$
 $\overset{\smile}{\mathbf{U}}$ $\overset{\smile}{\mathbf{Y}})) \diamondsuit (\overset{\smile}{\mathbf{Y}} \diamondsuit \overset{\sim}{\mathbf{x}})$.

 $f : V_n \mathbb{R} \to IV_n S$ with

r product

requires an exact summation algorithm as stated in [8]. With such a tool the critical residual term \Diamond (I - R · J(x \underline{U} Y)) may be evaluated with only one rounding in each component.

Next, a theorem can be formulated directly applicable on computers. For a better understanding of the following corollary it should be remarked that, in practical application, the inclusion of the absolute error x - x of an approximate solution x leads to better results than an inclusion for x itself. This is summarized in the following

Corollary: Let $x \in V_nS$, $Z \in IV_nS$, $f \in C^1((x \otimes Z) \ \underline{U} \ x)$. For every arbitrary but fixed Y C $(x \Leftrightarrow Z) \cup x$, let $J(Y) \in$ $IM_{n}S$ and assume that for every set of \boldsymbol{n} vectors $y_1, \dots, y_m \in Y$,

$$\begin{pmatrix} \frac{\partial f_1}{\partial x_1} (y_1) & \cdots & \frac{\partial f_1}{\partial x_n} (y_1) \\ \vdots & & \vdots \\ \vdots & & \vdots \\ \frac{\partial f_n}{\partial x_1} (y_n) & \cdots & \frac{\partial f_n}{\partial x_n} (y_n) \end{pmatrix} \in J(Y)$$

holds. Let $H : \mathbb{P}Z \to IV_nS$ be defined as

$$H(Y) := -R \diamondsuit \diamondsuit f(\tilde{x}) \Leftrightarrow \\ \diamondsuit (I-R \cdot J(\tilde{x} \ \bigcup \ (\tilde{x} \Leftrightarrow \diamondsuit Y))) \diamondsuit \diamondsuit Y$$

for Y ∈ PZ, where R ∈ MnS is an arbitrary but fixed matrix. If

$$H(Z) \subseteq Z$$
, (1.6)

then the equation f(x) = 0 has one and only one solution x in $x \oplus Z$ and $x - x \in$ $H^{(k)}(Z)$, k > 0.

Equation solving with error control

The corollary provides the second of the two basic steps in computing verified bounds for the solution of a system of equations:

- 1) an approximation step to determine a sufficiently good estimate x.
- an inclusion step to determine the enclosure Z of the absolute error x - x with respect to x.

In this chapter we will discuss some implementation aspects of these two points. Let us start with the inclusion step.

2.1 Implementation of the inclusion step

According to [11] we define an ϵ -inflation for an interval $A \in IS$ by

$$A^{\circ} \epsilon := \begin{cases} A + [-1, 1] \cdot \epsilon \cdot d(A) & \text{for } d(A) \neq 0 \\ A + [-\eta, +\eta] & \text{for } d(A) = 0 \end{cases}$$

Here η is the smallest positive floating-point number of the computer in use. For interval vectors this definition applies componentwise. ϵ -inflation is indispensable to assure the convergence of the interval iteration. In practice, 0.1 turned out to be a good value for ϵ .

Using the corollary, a verified inclusion may be obtained by performing the following iteration in the space IV_nS :

$$Y := 0$$
; count := 0;
repeat
count := count + 1;
 $Z := Y \circ \epsilon$;
 $Y := -R \diamondsuit \diamondsuit f(x) \diamondsuit \Leftrightarrow \diamondsuit (I-R \cdot J(x \cup (x \diamondsuit Z))) \diamondsuit Z$
until $(Y \subsetneq Z) \text{ or } (\text{count} = \text{count_max})$;

If the termination criterion Y \subseteq Z is satisfied, then by corollary 1 it is verified that the exact solution \hat{x} lies in $\hat{x} \otimes Z$ and that no other solution lies between these bounds. (The integer variable count is used to prevent infinite looping in cases where the iteration is not convergent).

2.2 Performing the approximation step

There are a large number of different methods for obtaining an approximation for \hat{x} (see e.g. [9]). In the following any of those principles may be used. Here we describe only the "classical" Newton's method

$$x^{(k+1)} := x^{(k)} - (f'(x^{(k)}))^{-1} \cdot f(x^{(k)})$$
 (2.6)

since the problem of evaluating the function f at a point $\mathbf{x}^{(k)}$ with high accuracy is common to all methods. If it is not possible to compute the residual term $f(\mathbf{x}^{(k)})$ accurately, we have no measure how near we are to the exact solution.

As stated above, the components f_i of f are considered as arithmetic expressions. The computation of $f_i(x)$ is usually done on a computer step by step, i.e. using an algorithm which performs one operation in the formula after the other. The results of the operations are stored in some intermediate variables z_1, \ldots, z_n , say.

Example: The

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$$(x_3+x_4)/(x_5-x_6)$$
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We will state way to arrive at a highly accurate the function values:

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(In [2] and [3] and onlinear system was transformed into a second linear equations by using term rewriting also has triang the principles and can be solved with

We assume $\mathbf{g}_{\mathbf{k}}$ entiable in terms of $\mathbf{z}_1,\dots,\mathbf{z}_k$. Let $\hat{\mathbf{z}}$ enthe approximations and $\hat{\mathbf{z}}_1,\dots,\hat{\mathbf{z}}_n$ the \mathbf{e}

We define

$$\Delta z_{j} := \hat{z}_{j}$$
 , $j = 1, ..., n$
and seek an inc the correction $\Delta z_{j} \in \Delta$, $j = 1, ..., n$

$$\mathbf{g}_{\mathbf{k}}(\hat{\mathbf{z}}_1, \dots, \hat{\mathbf{z}}_{\mathbf{k}}) = \mathbf{g}_{\mathbf{k}}(\hat{\mathbf{z}})$$

$$\begin{array}{c} \overset{\cdot}{(\hat{z}_1,\hat{z}_2,\ldots,\zeta_k)} \cdot \Delta z_k \\ \\ \text{with} \quad \zeta_k \in \overset{\cdot}{z}_k \ \cup \ \overset{\cdot}{z}_k \end{array}.$$

Continuing this property results in

$$\begin{aligned} \mathbf{g}_{k}(\hat{\mathbf{z}}_{1}, \dots, \hat{\mathbf{z}}_{k}) &= \mathbf{g}_{k}(\hat{\mathbf{z}} \\ &+ \sum_{j=1}^{k} \frac{\partial}{\partial \mathbf{z}_{j}} \mathbf{g}_{k}(\hat{\mathbf{z}}) \end{aligned}$$

Since
$$\hat{z}_1, \dots, \hat{z}_k$$

 $g_k(\hat{z}_1, \dots, \hat{z}_k) = 0$.

$$\Delta z_{k} = \begin{bmatrix} -g_{k}(\tilde{z}) & \dots \\ -g_{j=1} & \frac{\partial}{\partial z_{j}} & \ddots \end{bmatrix}$$

$$\begin{bmatrix} \mathbf{z}_{j+1}, \dots, \mathbf{z}_{k} \end{bmatrix} \wedge \Delta \mathbf{z}_{j} \end{bmatrix} \wedge \frac{\partial}{\partial \mathbf{z}_{k}} \mathbf{g}_{k} (\mathbf{\hat{z}}_{1}, \dots, \mathbf{\hat{z}}_{k-1}, \zeta_{k})$$

$$\frac{1}{\zeta_k} \mathbf{g}_k(\hat{\mathbf{z}}_1, \dots, \hat{\mathbf{z}}_{k-1}, \zeta_k) \neq 0.$$

Via induction we

$$\Delta z_k \in \Delta Z_k := -g$$

$$-\frac{\mathbf{k}-1}{\mathbf{\Sigma}} \frac{\partial}{\partial \mathbf{z_j}} \mathbf{g_k} = \mathbf{1}^{+1}$$

$$\frac{\partial}{\partial \mathbf{z_j}} \mathbf{g_k} = \mathbf{1}^{+1}$$

$$\begin{array}{c} \Delta Z_{\mathbf{j}})^{\prime} \widetilde{z}_{\mathbf{j}} \widetilde{z}_{\mathbf{j}+1}, \ldots) \cdot \Delta Z_{\mathbf{j}} \bigg] / \\ \widetilde{z}_{\mathbf{k}-1}^{\prime} + \Delta Z_{\mathbf{k}-1}, (\widetilde{z}_{\mathbf{k}}^{\prime} + \Delta Z_{\mathbf{k}}) \underline{\cup} \widetilde{z}_{\mathbf{k}}^{\prime}) \end{array}$$

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$$\frac{\partial}{\partial z_k} g_k$$

ty of
$$g_k = 0$$
 for z_k in $(\hat{z}_1, \dots, \hat{z}_k)$.

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The last $\frac{\partial}{\partial z_k}$ \mathbf{g}_k does not

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is always true for all arising from arithmetic and the example above).

- The

 (z_1, \ldots, z_k) must be of

high accuracy to guarantee a sufficiently sharp inclusion. This is also possible for systems arising from arithmetic expressions by applying the exact scalar product as developed in [8]. For this purpose a "division equation" $z_k = z_i / z_j$ has to be transformed into $z_k \cdot z_j = z_i$.

In most cases it is not necessary to compute the value of the partial derivatives with the same effort as the function value since the success of (2.6) mainly depends on the accuracy of $f(x^{(k)})$. Nevertheless, it is also possible to determine the partial derivatives with comparable accuracy. (For the technique of computing the partial derivatives of a function we refer to [10]).

With the methods for linear systems from [7], each Newton step may be performed with high accuracy since each step is the solution of a system of linear equations

$$f'(x^{(k)}) \cdot (x^{(k)} - x^{(k+1)}) = f(x^{(k)})$$

The methods from [7] are specializations of the method described here, and so this way of performing a Newton step may be considered as a recursive call of the procedure in this paper. The possibility to do that is important in the cases where the Jacobian is ill-conditioned.

2.3 An algorithm for the solution of a system of nonlinear equation with maximum accuracy

We use the following notations: \hat{x} denotes the exact solution of the system of nonlinear equations f(x) = 0, b is the base of the floating-point system in use, t the length of the mantissa.

The approximation of \hat{x} in the k-th step is $\sum_{i=0}^{k} \hat{x}^{(i)}$

where $x^{(i)} \in S$, i=1,...,n. This form of our approximation x is usually called a "staggered correction form" of x since all values $x^{(i)}$ are actually stored and the summation will be done when we have finished. To this approximation we compute an inclusion Z of the next correction

$$\mathbf{x}^{(\mathbf{k})} := \mathbf{\hat{x}} - \mathbf{\sum_{i=0}^{k-1} \mathbf{x}^{(i)}}.$$

In step (N3) of this algorithm, least bit accuracy is forced. This may be weakened if t is replaced by some positive integer $t_0 < t$. In case one of the components of the exact solution is zero, some refined termination criterion may replace the one stated here. This should be done since the computation of an inclusion $[-\eta,\eta]$ of zero is rather expensive.

$$\begin{array}{lll} k:=0\;; & \{ \; \operatorname{correction} \; \operatorname{counter} \; \} \\ k-1 \sim (i) + x^{(k)} \} = 0 \\ & \operatorname{i=o} \\ & \operatorname{approximately} \; \operatorname{for} \; \operatorname{the} \; \operatorname{unknown} \; x^{(k)} \\ & \operatorname{using} \; \operatorname{Newton's} \; \operatorname{method} \; (2.6) \; \operatorname{with} \; \\ & \operatorname{formula} \; \operatorname{evaluation} \; \operatorname{technique}; \; \operatorname{in} \; \operatorname{ill-conditioned} \; \operatorname{cases} \; \operatorname{perform} \; \operatorname{each} \; \operatorname{step} \; \\ & \operatorname{with} \; \operatorname{high} \; \operatorname{accuracy} \; \operatorname{using} \; \operatorname{the} \; \operatorname{linear} \; \\ & \operatorname{techniques} \; \operatorname{from} \; [7]; \; \operatorname{call} \; \operatorname{the} \; \operatorname{appro-ximation} \; x^{(k)}; \\ (N2) \;\;\; \operatorname{Compute} \; \operatorname{an} \; \operatorname{approximation} \; R \; \operatorname{of} \; & & \\ & k \sim (i) > -1; \\ & \operatorname{i=o} \; & \operatorname{j:=0} \; ; \; \operatorname{i=o} \; \operatorname{counter} \; \} \\ & Z:= \; Y: \; X:= \diamondsuit (\sum x^{(i)}) \; ; \\ & z:= \; Y: \; X:= \diamondsuit (\sum x^{(i)}) \; ; \\ & z:= \; Y: \; x:= \diamondsuit (\sum x^{(i)}) \; ; \\ & \operatorname{success} \; := \; (Y \subseteq Z) \; ; \\ & \operatorname{until} \; \operatorname{success} \; \operatorname{or} \; \; (j=10); \\ (N3) \;\;\; \underset{1}{\operatorname{if}} \; \operatorname{success} \; \\ & \underset{1}{\operatorname{then}} \; \operatorname{dm} \; := \; \operatorname{d}(X \otimes Z) \; ; \\ & \underset{1}{\operatorname{if}} \; \operatorname{dm} \; \langle \; | X \otimes Z| \; \cdot \; \operatorname{b}^{-t+1} \; \operatorname{goto} \; (N4) \\ & \underset{2}{\operatorname{else}} \; \\ & k := \; k+1 \; ; \\ & \underset{1}{\operatorname{if}} \; k > 10 \\ & \underset{2}{\operatorname{else}} \; \operatorname{goto} \; (N1) \\ \\ (N4) \;\;\; \operatorname{Result:} \; \hat{x} \in X \otimes Z \\ \end{array}$$

3. Examples of application

The following two examples demonstrate the typical behaviour of the equation solver presented above. They will show the need of an exact scalar product and, furthermore, a formula evaluation technique using this scalar product.

Example 1:

We define the following system of equations for an unknown vector $\mathbf{x} \in V_n \mathbb{R}$:

$$f(x) := \alpha(H \cdot x + \psi(x)) = 0$$

where $H \in M_n\mathbb{R}$ is the Hilbert matrix of degree n, i.e. $H = ((h_{ij}))$, $h_{ij} := 1/(i+j-1)$, i, j = 1, ..., n. $\psi : V_n\mathbb{R} \to V_n\mathbb{R}$ is defined by

The whole multiplic an exact easily s solution. ϵ_i , the the solu teristic : s 68000 mic. decimal a : the ϵ_i γ . values, 🗤 ponent x. Newton st 4 answer: mation in accuracy. sion stel always the

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-1	3	no	2
12	3	no	2
7-12	4	no	2
7-11	8	yes	2
3−12	13	yes	2
3-04	27	yes	2
`-03	34	yes	2
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Example 2:

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