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BOUNDING SETS IN FUNCTION SPACES WITH APPLICATIONS TO NONLINEAR OPERATOR EQUATIONS*

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Abstract. We can compute with bounding sets of numbers, vectors, or functions using the techniques of interval mathematics. The techniques can be used to computationally verify sufficient conditions for existence, uniqueness, and convergence and to construct upper and lower bounds on solutions of nonlinear operator equations. Rounding errors are taken into account. We can compute with set-valued functions and operators on them. The techniques are also useful in search procedures for finding safe starting regions for iterative methods and for constructing natural stopping criteria.

1. Introduction. A body of techniques known as *interval analysis* [52] or *interval mathematics* [61], evolved over the past decade and a half, has useful applications to the kind of testing and bounding needed to verify conditions for existence, uniqueness, and convergence and determine upper and lower bounds to solutions of nonlinear operator equations. It is the purpose of this paper to survey some old and new results of this kind. The methods to be described are based on *computations with sets and set-valued functions*. While the list of references is not complete, it does represent a cross-section of work in this growing new field.

In order to make this paper reasonably self-contained, some basic concepts and notation will be presented in the remainder of this section.

We can perform arithmetic with *sets* of real numbers as follows. Let $I=[a, b]$, $a \leqq b$, and $J=[a, b]$, $a \leqq b$ be closed bounded *intervals* on the real line. If $*$ is an arithmetic operation $+, -, \cdot, /$ on pairs of real numbers, it can be extended to pairs of intervals I, J by

$$I*J=\{x*y : x \in I, y \in J\}.$$

In fact, $I*J$ is again a closed bounded interval unless $0 \in J$ when the operation $*$ is division (in which case, we do not define $I*J$). We have

$$\begin{aligned}
[a, b]+[c, d]&=[a+c, b+d],\\
[a, b]-[c, d]&=[a-d, b-c],\\
[a, b]\cdot[c, d]&=[\min(ac, ad, bc, bd), \max(ac, ad, bc, bd)],\\
[a, b]/[c, d]&=[a, b]\cdot[1/d, 1/c] \quad \text{for } 0 \notin [c, d].
\end{aligned}$$

Note that we can test the condition $0 \in [c, d]$ on a computer for machine numbers c and d.

The arithmetic system thus defined is called *interval arithmetic* [49], [52]. By testing signs of a, b, c, and d, the endpoints of the product of two intervals can be reduced to a single multiplication each, except for one out of nine cases. By rounding right endpoints up, and left endpoints down, when necessary, the resulting intervals will *contain* the exact results as defined. This is called *rounded interval arithmetic*. This

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system can be implemented on any computer [6], [18], [22], [43], [49], [50], [52], [55] and forms a basis for computations with bounding sets and set-valued functions.

If f is a function of n real variables given by a *rational* expression for its values $f(x_1, \cdots, x_n)$, then we can attempt to evaluate f in rounded interval arithmetic beginning with intervals $X_1, \cdots, X_n$. If we succeed, then *the range of values of f is bounded by the result* for $x_1 \in X_1, \cdots, x_n \in X_n$. Otherwise, if division by zero occurs, f may not be defined over the chosen region. If overflow occurs, f may have values outside the range of machine numbers used.

Mathematically equivalent expressions for the value $f(x_1, \cdots, x_n)$ do not necessarily produce identical numerical bounds on the range of values by evaluations in rounded interval arithmetic. The excess width of the numerical bounds can be kept small when the intervals $X_1, \cdots, X_n$ are themselves narrow by using the *centered form* for the evaluation. This amounts to expanding the function about the midpoints of the intervals $X_1, \cdots, X_n$ [28], [52], [57]. See also Hansen [61, pp. 7–18]. At the Numerisk Institut of the Technical University of Denmark a computer program has been written in Stanford ALGOL W which can produce the centered form for a given rational expression [personal communication]. See also Ratschek [78].

Arbitrarily sharp upper and lower bounds on the range of values of a bounded rational function over an n-dimensional rectangle described by intervals $X_1, \cdots, X_n$ *can* be computed using rounded interval arithmetic on subdivisions of the region regardless of the width of $X_1, \cdots, X_n$. There are various ways to avoid having to evaluate the function on every part of a subdivision. The important question of how to bound most efficiently the range of values of a rational function of n variables over an arbitrary n-dimensional rectangle is discussed in [57]. Further work on this problem remains to be done.

We can program computations for the ranges of values of various special functions of a single variable ranging over an interval: x^n, a^x, $\log_a x$, $\sin x$, $\arctan x$, etc. Functions of several variables which are representable as compositions of such unary functions and rational operations can then be bounded over n-dimensional rectangles [49], [50], [52].

Functions of complex variables can be bounded over circular discs or rectangles in the complex plane using either *circular arithmetic* [17], [30], [38] or interval arithmetic on real and imaginary parts [67]. This technique has been discussed in [54] as a way of bounding quadrature errors for analytic functions, using also [14].

Still other arithmetic systems for families of sets have been considered, in particular, for *ellipsoids* and for *polytopes* [32], [33], [34], [72].

Computations involving *matrices with interval coefficients* (matrix inversion, solution of linear systems, etc.) have been studied and special methods for such problems have been developed, [5], [6], [22], [23], [24], [25], [29], [36], [52], [70]. Matrix methods are *used in interval versions of Newton's method in n dimensions*, [6], [15], [19], [37], [42], [45], [49], [50], [52], [55], [57], [58], [59], [60], [64].

In addition to their application to nonlinear operator equations, interval versions of Newton's method are finding applications in *nonlinear mathematical programming* problems [16], [46], [47], [66].

We will need the following *notation*. For an interval $[a, b]$, $a \leqq b$, define

$$|[a, b]| = \max(|a|, |b|),$$

$$w([a, b]) = b - a, \quad \text{the } \textit{width} \text{ of } [a, b],$$

$$m([a, b]) = (a + b)/2, \quad \text{the } \textit{midpoint} \text{ of } [a, b].$$

For an *interval vector* $X=(X_1, X_2, \cdots, X_n)$, define

$$\|X\|=\max_i |X_i|,$$

$$w(X)=\max_i w(X_i),$$

$$m(X)=(m(X_1), \cdots, m(X_n)).$$

For an *interval matrix* A, with interval coefficients A_{ij}, define

$$\|A\|=\max_i \sum_{j=1}^{n} |A_{ij}|,$$

$$w(A)=\max_{i,j} w(A_{ij}),$$

$$m(A)=\text{the real matrix with components } m(A_{ij}).$$

For intervals $[a, b]$ and $[c, d]$ define

$$[a, b]\cap[c, d]=\begin{cases}\phi, \text{ the empty set,} & \text{if } b<c \text{ or } d<a,\\ [\max(a, c), \min(b, d)] & \text{otherwise.}\end{cases}$$

(This is the ordinary *intersection* of two intervals.) If two intervals intersect, then their union $[a, b]\cup[c, d]$ is again an interval and can be easily computed:

$$[a, b]\cup[c, d]=[\min(a, c), \max(b, d)].$$

We write $[a, b]\subseteq[c, d]$ if $[a, b]$ is *contained* in $[c, d]$, $c\leqq a\leqq b\leqq d$. Finally,

$$[a, b]=[c, d] \quad \text{means} \quad a=c \quad \textit{and} \quad b=d.$$

For two interval vectors X and Y, define

$$X\cap Y=(X_1\cap Y_1, \cdots, X_n\cap Y_n).$$

If $X_i\cap Y_i$ is empty for any i, then so is $X\cap Y$.

2. Bounding sets in function spaces. Suppose we have found that the operator equation

$$P(x)=0$$

with $P: S_1\to S_2$, (S_1, S_2 normed linear spaces), has a solution x approximated by $y\in S_1$, and we have found an error bound of the form $\|x-y\|_{S_1}\leqq r$, $r>0$. We can then say that the solution x lies in the *set* $N(y, r)=\{u: u\in S_1, \|u-y\|_{S_1}\leqq r\}$ in S_1.

If S_1 is a space of real vector-valued functions $u: D_1\to R^n$, and if

$$\sup_{t\in D_1}\|u(t)\|_{R^n}\leqq\|u\|_{S_1}, \quad \text{with } \|p\|_{R^n}=\max|p_i|, \quad i=1, 2, \cdots, n,$$

then $|x_i(t)-y_i(t)|\leqq r$ for all $i=1, 2, \cdots, n$ and all t in D_1. We can also express this as

$$x(t)\in Y(t) \quad \text{for all } t \text{ in } D_1, \tag{2.1}$$

where $Y(t)=(Y_1(t), Y_2(t), \cdots, Y_n(t))$ with $Y_i(t)=y_i(t)+[-r, r]$. Thus each $Y_i(t)$ is an interval and $Y(t)$ is an n-dimensional rectangle. We can abbreviate (2.1) by the notation $x\in Y$.

More generally, if Y is any *set-valued* function, $Y: D_1 \to S(R^n)$ where $S(R^n)$ is the set of subsets of R^n, we define $y \in Y$ to mean $y(t) \in Y(t)$ for all t in D_1. Similarly, we denote by $Z \subseteq Y$, the relation $Z(t) \subseteq Y(t)$ for all t in D_1.

We will survey some methods for constructing set-valued functions which contain solutions to nonlinear operator equations. If $Y(t)$ is an interval vector and $x \in Y$ for $P(x) = 0$, then

$$|x_i(t) - m(Y_i(t))| \leqq \tfrac{1}{2} w(Y(t)) \tag{2.2}$$

for $i = 1, 2, \cdots, n$ and for all t in D_1, (see § 1 for notation).

If $x \in Y$, we can also write

$$\begin{aligned} &\underline{Y}_i(t) \leqq x_i(t) \leqq \bar{Y}_i(t), \\ &\text{where } \underline{Y}_i(t) = m(Y_i(t)) - \tfrac{1}{2} w(Y_i(t)), \quad \bar{Y}_i(t) = m(Y_i(t)) + \tfrac{1}{2} w(Y_i(t)). \end{aligned} \tag{2.3}$$

As we shall see, we can often obtain an expression for $Y(t)$ directly without first obtaining $\underline{Y}_i(t)$ and $\bar{Y}_i(t)$ explicitly.

An *interval polynomial*

$$Y(t) = A_0 + A_1 t + \cdots + A_q t^q \tag{2.4}$$

in a real variable t with interval coefficients $A_i = [\underline{A}_i, \bar{A}_i]$ contains a whole *set* of real-valued functions. For example the *constant* inverval polynomial $Y(t) \equiv [-1, 1]$ contains every function f in $C[0, 1]$ for which $\|f\| \leqq 1$.

By substituting an interval of values $[a, b]$ for the real variable t, in an interval polynomial $Y(t)$, we can evaluate $Y([a, b])$ and can bound the range of values over $[a, b]$ of all functions contained in Y.

In the following sections we will illustrate the usefulness of interval polynomials and other interval-valued functions in the computational verification of sufficient conditions for existence and uniqueness of solutions to nonlinear operator equations and in the construction of upper and lower bounds.

We can formally integrate the interval polynomial (2.4)

$$\int_0^t Y(s)\, ds = A_0 t + A_1 \frac{t^2}{2} + \cdots + A_q \frac{t^{q+1}}{q+1}.$$

If f is a continuously differentiable real-valued function and if $f'(t) \in Y(t)$ for $0 \leqq t \leqq T$, then

$$f(t) \in f(0) + \int_0^t Y(s)\, ds \quad \text{for } 0 \leqq t \leqq T.$$

We can formally differentiate the interval polynomial (2.4) as well;

$$Y'(t) = A_1 + 2A_2 t + \cdots + qA_q t^{q-1}.$$

However, it is *not* true that $f \in Y$ implies $f' \in Y'$ [65].

On the other hand, if $f'(t) \in Y(t)$ for $0 \leqq t \leqq T$, with $Y(t)$ given by (2.4), we *can* formally differentiate the interval polynomial

$$P(t) = f(0) + A_0 t + A_1 \frac{t^2}{2} + \cdots + A_q \frac{t^{q+1}}{q+1}$$

obtained by formal integration of $Y(t)$. The interval polynomial $P(t)$ is called *derivative*

More generally, if Y is any *set-valued* function, $Y: D_1 \to S(R^n)$ where $S(R^n)$ is the set of subsets of R^n, we define $y \in Y$ to mean $y(t) \in Y(t)$ for all t in D_1. Similarly, we denote by $Z \subseteq Y$, the relation $Z(t) \subseteq Y(t)$ for all t in D_1.

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for $i = 1, 2, \cdots, n$ and for all t in D_1, (see § 1 for notation).

If $x \in Y$, we can also write

$$\begin{gathered} \underline{Y}_i(t) \leqq x_i(t) \leqq \bar{Y}_i(t), \\ \text{where } \underline{Y}_i(t) = m(Y_i(t)) - \tfrac{1}{2} w(Y_i(t)), \quad \bar{Y}_i(t) = m(Y_i(t)) + \tfrac{1}{2} w(Y_i(t)). \end{gathered} \tag{2.3}$$

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We can formally differentiate the interval polynomial (2.4) as well;

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$$P(t) = f(0) + A_0 t + A_1 \frac{t^2}{2} + \cdots + A_q \frac{t^{q+1}}{q+1}$$

obtained by formal integration of $Y(t)$. The interval polynomial $P(t)$ is called *derivative* *compatible* (ableitungsverträgliche [35], [39], [54], [65]). We have, formally,

$$P'(t) = A_0 + A_1 t + \cdots + A_q t^q = Y(t)$$

with $f \in P$ and $f' \in P'$.

Similarly, if $f^{(k)} \in Y$, we can obtain a k-fold derivative compatible interval polynomial enclosure of f by k-fold formal integration of $Y(t)$. The resulting interval polynomial, say P, satisfies $f \in P$, $f' \in P', \cdots, f^{(k)} \in P^{(k)}$. For this, exact values of $f^{(k-1)}(0), \cdots, f(0)$ are not required but it is sufficient to have intervals B_j, $j = 0, 1, 2, \cdots, k-1$ such that $f^{(j)}(0) \in B_j$.

If Y is a continuous interval-valued function [49], [52] of a real variable t with $Y(t) = [\underline{Y}(t), \bar{Y}(t)]$ we define the *interval integral* [49], [52]

$$\int_a^b Y(t)\,dt = \left[\int_a^b \underline{Y}(s)\,ds, \int_a^b \bar{Y}(s)\,ds\right]. \tag{2.5}$$

We must exercise care when integrating interval polynomials over intervals $[a, b]$ which contain both positive and negative numbers. Formal integration is no longer valid. This is because the upper and lower end points of the coefficients $A_i = [\underline{A}_i, \bar{A}_i]$ will be switched upon multiplication by t^i for t negative and i odd. For instance, for the interval polynomial (2.4), we have, with $s_1, s_2 > 0$,

$$\begin{aligned} \int_{-s_1}^{s_2} Y(t)\,dt &= \int_0^{s_1} Y(-t)\,dt + \int_0^{s_2} Y(t)\,dt \\ &= A_0 s_1 - A_1 \frac{s_1^2}{2} + \cdots + (-1)^q A_q \frac{s_1^q}{q} + A_0 s_2 + A_1 \frac{s_2^2}{2} + \cdots + A_q \frac{s_2^q}{q}. \end{aligned} \tag{2.6}$$

Now, however,

$$-A_1 = [-\bar{A}_1, -\underline{A}_1] \qquad (\textit{not } [-\underline{A}_1, -\bar{A}_1]);$$

thus for $Y(t)$ given by (2.4), and for $a < 0 < b$ we have

$$\int_a^b Y(t)\,dt = T_0 + T_1 + T_2 + \cdots + T_q \tag{2.7}$$

with

$$T_i = \begin{cases} A_i\left(\dfrac{b^{i+1}}{i+1} - \dfrac{a^{i+1}}{i+1}\right), & i \text{ even}, \\[2ex] \left[\underline{A}_i \dfrac{b^{i+1}}{i+1} - \bar{A}_i \dfrac{a^{i+1}}{i+1}, \bar{A}_i \dfrac{b^{i+1}}{i+1} - \underline{A}_i \dfrac{a^{i+1}}{i+1}\right], & i \text{ odd}. \end{cases}$$

When a and b have the *same sign*, we have the usual formal integration formula

$$\int_a^b (A_0 + \cdots + A_q t^q)\,dt = A_0(b-a) + \cdots + A_q\left(\frac{b^{q+1} - a^{q+1}}{q+1}\right). \tag{2.8}$$

Note that when the coefficients are degenerate intervals (real numbers) with $\underline{A}_i = \bar{A}_i$, then (2.7) reduces to the usual formula (2.8).

The use of interval polynomials with iterative methods for solving operator equations can lead to rapid increase in the degrees of successive iterates. An important device for *degree reduction* (at the cost of some coarsening—"Vergröberung"—of bounds) is due to F. Krückeberg (see [9], [26], [39], [54]). To illustrate, we can enclose the polynomial $Y(t)$ of (2.4) for instance for $0 \leqq t \leqq T$ in an interval polynomial of degree 4, when $q > 4$, by making use of the following. We have

$$0 \leqq \left(\frac{t}{T}\right)^i \leqq \left(\frac{t}{T}\right)^4 \quad \text{for } i > 4 \quad \text{and} \quad 0 \leqq t \leqq T;$$

and so $t^i \in [0, T^{i-4}]t^4$ for $i > 4$ and $t \in [0, T]$. In fact, we have $Y(t) \subseteq P_4(t)$ for all t in $[0, T]$ where

$$P_4(t) = A_0 + A_1 t + A_2 t^2 + A_3 t^3 + \{A_4 + A_5[0, T] + \cdots + A_q[0, T]^{q-4}\}t^4.$$

Sharper methods for degree reduction based on Chebyshev approximation and economization procedures are discussed in [9].

We can combine the techniques we have discussed so far. For example,

$$\sin t \in t - \frac{t^3}{3!} + [-1, 1]\frac{t^5}{5!} \subseteq t - \frac{t^3}{3!} + \frac{[-1, 1][0, T^2]}{5!} t^3.$$

Thus, for t in $[0, .5]$ we have

$$\sin t \in t - (\tfrac{1}{6} + [-.0021, .0021])t^3, \qquad \sin t \in t - [.164, .169]t^3.$$

Expanding this polynomial in centered form about $t = .5$, we obtain

$$\sin t \in P(t) = [.247359, .24744] + [.9683, .9693](t - .25)$$
$$- [.123, .127](t - .25)^2 - [.164, .169](t - .25)^3.$$

From this we can find, for instance, that

$$\max_{t \in [0, .5]} |\sin t| \leqq |P([0, .5])| < .47952.$$

Derivative compatible generalized interval polynomials and Hermite interpolation are discussed in [35]. Two dimensional interval spline functions have been used by Appelt [8].

Taylor series expansions provide an important tool for the construction of interval polynomials and piece-wise interval polynomial functions containing nonpolynomial functions and functions defined by *initial value problems* in differential equations [11], [40], [44], [49], [50], [51], [52], [72], [73]. The Taylor coefficients can be generated recursively with interval bounding of error by computer programs (see [52, Chap. 11] and also [11], [13], [19], [20], [55]). The remainder term in a finite Taylor expansion can be bounded by interval computation resulting in an interval coefficient for the last term of the resulting polynomial. This can also be used for rigorous error bounding with *quadrature methods* [20]. See also [2], [49], [50], [52], [55].

3. Inclusion monotonicity and interval integration. A very general and obvious property of mappings (functions, operators, etc.) is *inclusion monotonicity* [49] (or the *subset property*). Suppose S_1 and S_2 are any two sets and

$$f: S_1 \to S_2$$

is a mapping which assigns to each element x in S_1 a unique element $f(x)$ in S_2.

If X is a subset of S_1 we denote by $\bar{f}(X)$ the *image* of X under the mapping f, $\bar{f}(X) = \{f(x) : x \in X\}$.

If X and Y are subsets of S_1, then $\bar{f}$ has the property

(3.1) $$X \subseteq Y \quad \text{implies} \quad \bar{f}(X) \subseteq \bar{f}(Y).$$

It is crucially important for many of the techniques to be discussed in the following sections that the interval functions and operators we use have the property (3.1). The basis for this is the *inclusion monotonicity* of interval arithmetic [49], [50], [52]: if I, J, K, L are intervals, then it follows from the definitions of the interval arithmetic operations that

$$\begin{aligned} &I \subseteq K, \quad J \subseteq L \quad \text{implies} \\ &I + J \subseteq K + L, \\ &I - J \subseteq K - L, \\ &IJ \subseteq KL, \\ &I/J \subseteq K/L \qquad (0 \notin L). \end{aligned}$$

From this, it follows that a rational interval function $F(X_1, X_2, \cdots, X_n)$ is also inclusion monotonic. If $F(X_1, X_2, \cdots, X_n)$ is defined and $Y_i \subseteq X_i$, $i = 1, 2, \cdots, n$, then $F(Y_1, \cdots, Y_n)$ is also defined and $F(Y_1, Y_2, \cdots, Y_n) \subseteq F(X_1, X_2, \cdots, X_n)$ [52].

Interval integration preserves inclusion monotonicity [52]. If F and G are interval-valued functions of a real variable with $F(t) \subseteq G(t)$ for t in $[a, b]$, then

$$\int_a^b F(t)\, dt \subseteq \int_a^b G(t)\, dt.$$

The integration of interval-valued functions defined by (2.5) is equivalent to

$$\int_a^b Y(s)\, ds = \bigcap_{n=1}^{\infty} \sum_{i=1}^{n} Y(S_i^{(n)}) \frac{b-a}{n}, \tag{3.2}$$

with $S_i^{(n)} = a + [i-1, i]((b-a)/n)$, where

$$Y(S) = \bigcup_{s \in S} Y(s)$$

It follows that

$$\int_a^b Y(s)\, ds \subseteq \sum_{i=1}^{n} Y(S_i^{(n)}) \left(\frac{b-a}{n}\right)$$

for any $n = 1, 2, \cdots$. For instance

$$\int_a^b Y(s)\, ds \subseteq Y([a, b])(b-a).$$

If we can compute the values of $Y^*(S)$ (for instance, if Y^* is a rational interval function) and if $Y(S) \subseteq Y^*(S)$, then we can compute intervals containing the integral, namely

$$\int_a^b Y(s)\, ds \subseteq \sum_{i=1}^{n} Y^*(S_i^{(n)}) \left(\frac{b-a}{n}\right). \tag{3.3}$$

Denote by IF$[D]$ the set of all interval-valued functions with domain D. For $X, Y \in$ IF$[D]$, we write $X \subseteq Y$ if

$$X(t) \subseteq Y(t) \quad \text{for all } t \text{ in } D.$$

We call an *interval operator*

$$P: M \subseteq \mathrm{IF}[D] \to \mathrm{IF}[D]$$

inclusion monotone if for all

$$X, Y \text{ in } M, \qquad X \subseteq Y \text{ implies } P(X) \subseteq P(Y).$$

For example, an interval operator defined by

$$P(Y)(t) = h(t) + \int_a^t F(t, s, Y(s))\, ds, \tag{3.4}$$

is inclusion monotone on the set of interval functions for which the integral exists. The corresponding real operator is *not*, in general, "monotone" in any usual sense (e.g. inverse isotone, [69]).

A useful result is the following.

THEOREM 3.1 [56]. *If* $P: M \subseteq \mathrm{IF}[D] \to M$ *is inclusion monotone and if* $P(Y_0) \subseteq Y_0$ *for some* Y_0 *in* M, *then the sequence defined by*

$$Y_{k+1} = P(Y_k), \qquad k = 0, 1, 2, \cdots, \tag{3.5}$$

has the following properties:

1) $Y_{k+1} \subseteq Y_k$, $k = 0, 1, 2, \cdots$,

2) *for every* t *in* D, *the limit*

$$Y(t) = \bigcap_{k=0}^{\infty} Y_k(t) \tag{3.6}$$

exists and Y *is in* $\mathrm{IF}[D]$ (*but not necessarily in* M).

3) $Y \subseteq Y_k$, $k = 0, 1, 2, \cdots$.

COROLLARY 1. *Assume the hypotheses of Theorem* 3.1. *Let* M_r *be a set of real-valued functions. If* $M_r \subseteq M$ *and* $p: M_r \to M_r$ *is a real operator for which* P *is an* interval majorant,

$$p(y) \in P(Y) \quad \text{for } y \in Y,$$

then any fixed point of p, $y = p(y)$, *which is in* Y_0 *is also in* Y_k *for all* $k = 0, 1, 2, \cdots$ *and in the limiting interval function,* Y, *as well.*

COROLLARY 2. *If the limiting function* Y *in* (3.6) *is real valued and* $Y \in M_r$ *and if* $P(Y)$ *is real valued, then* $y = p(y)$ *has a unique solution in* Y_0, *namely* Y.

Remarks on Theorem 3.1.

1) The same results also hold for n-dimensional vector-valued functions.

2) We can verify that the limiting interval function Y is real valued if we can show that there exists a real number θ, $0 \leqq \theta < 1$, such that

$$\sup_{t \in D} w(P(Y_k)(t)) \leqq \theta \sup_{t \in D} w(Y_k(t)).$$

In this light, Theorem 3.1 is seen as a contraction mapping theorem.

Suppose we are given an operator equation in the form

$$y = p(y) \tag{3.7}$$

to solve for a real (or vector) -valued function y (a *fixed point* of p), an inclusion monotone interval majorant of p, say P, and an interval (or interval vector) -valued function Y_0 on which P is defined. If Y_0 contains a solution of (3.7), then so does $P(Y_0)$ because

$$y \in Y_0 \quad \text{implies} \quad y = p(y) \in P(Y_0).$$

Therefore, any solution y of (3.7) in Y_0 is also in the intersection $Y_0 \cap P(Y_0)$; that is, $y(t) \in Y_0(t) \cap P(Y_0)(t)$ for all t in D.

THEOREM 3.2. *If there is a solution y to* (3.7) *in* Y_0, *then the algorithm*

$$Y_{k+1}(t) := Y_k(t) \cap P(Y_k)(t) \tag{3.8}$$

defines a nested sequence $\{Y_k\} \subseteq \mathrm{IF}[D]$, *with*

$$y(t) \in Y_{k+1}(t) \subseteq Y_k(t)$$

for all t in D and all $k = 0, 1, 2, \cdots$. *Furthermore*

$$Y(t) = \bigcap_{k=0}^{\infty} Y_k(t)$$

exists for all t in D and $y \in Y$. (See also [26], [53], [54], [56].)

Thus, we also have the following *exclusion principle*.

THEOREM 3.3. *If* $Y_0(t) \cap P(Y_0)(t)$ *is empty for some t in D, then there is no solution to* (3.7) *in* Y_0.

4. Computational verification of hypotheses and construction of bounds. Interval methods can be useful for the computational verification of sufficient conditions for existence, uniqueness, and convergence and for the construction of upper and lower bounds.

Example 1. Consider the initial value problem

$$y' = f(x, y), \qquad y(0) = y_0 \tag{4.1}$$

with f continuous.

Define the interval operator

$$P(Y)(x) = y_0 + \int_0^x f(t, Y(t))\, dt. \tag{4.2}$$

Suppose Y_0 is an interval function such that

$$P(Y_0)(x) \subseteq Y_0(x) \quad \text{for all } x \text{ in } [0, T]. \tag{4.3}$$

And suppose that, for some $0 \leqq \theta < 1$, we have

$$\max_{x \in [0,T]} w(P(Y)(x)) \leqq \theta \max_{x \in [0,T]} w(Y(x)) \tag{4.4}$$

for all $Y \subseteq Y_0$. Then the sequence $\{Y_k\}$ defined by $Y_{k+1} = P(Y_k)$ converges to a real-valued function and so (4.1) has a unique solution for x in $[0, T]$.

For example, for the problem

$$y' = x^2 + y^2, \qquad y(0) = 0 \tag{4.5}$$

we have

$$P(Y)(x) = \int_0^x (t^2 + Y^2(t))\, dt. \tag{4.6}$$

Let $Y_0(x) \equiv [0, b]$ for $x \in [0, T]$. Then

$$P(Y_0)(x) = \int_0^x (t^2 + [0, b^2])\, dt = \frac{x^3}{3} + [0, b^2]x.$$

The inclusion condition (4.3) will be satisfied if $\frac{1}{3}[0, T]^3+[0, b^2][0, T]\subseteq[0, b]$. This will be the case if $\frac{1}{3}T^3+b^2T\leqq b$. We can take $b=(\frac{1}{12})^{1/4}$ and $T\leqq(12)^{1/4}/2$.

In order to satisfy (4.4), we find, from (4.6),

$$w(P(Y)(x))=\int_0^x w(Y^2(t))\,dt\leqq\int_0^x 2bw(Y(t))\,dt$$

whenever $Y\subseteq Y_0$, for $Y_0(x)\equiv[0, b]$. Thus we can satisfy (4.4) with $\theta=2bT<1$. Putting these results together, we find that (4.5) has a unique solution for values of x at least up to $(12)^{1/4}/2$. Furthermore, the solution (for $x\in[0,(12)^{1/4}/2]$) is contained in the interval functions

$$Y_0(x)\equiv\left[0, \left(\frac{1}{12}\right)^{1/4}\right]$$

$$Y_1(x)=P(Y_0(x))=\frac{x^3}{3}+[0, b^2]x=\frac{x^3}{3}+\left[0, \frac{1}{2\sqrt{3}}\right]x.$$

$$Y_2(x)=P(Y_1)(x)=\left[\frac{12}{36}, \frac{13}{36}\right]x^3+\left[0, \frac{1}{15\sqrt{3}}\right]x^5+\frac{x^7}{63}\quad\text{etc.}$$

We can use the technique of degree reduction (see § 2) on any one of these iterates, if desired, to produce a polynomial of desired degree still containing the solution. For instance,

$$Y_2(x)\subseteq\left[0, \frac{1}{56\sqrt{3}}\right]\quad x+\left[\frac{12}{36}, \frac{13}{36}\right]x^3\quad\text{for } x \text{ in }\left[0, \frac{(12)^{1/4}}{2}\right].$$

We can, of course, continue the solution, if it exists, beyond $x=(12)^{1/4}/2$ by restarting there, say with the interval initial condition

$$Y\left(\frac{(12)^{1/4}}{2}\right)=Y_2\left(\frac{(12)^{1/4}}{2}\right).$$

Example 2 (A two point boundary value problem arising in chemical reactor theory, [62], [63]). Consider the differential equation

$$\text{(4.7)}\qquad y''+\frac{1}{x}y'+\beta\exp\left\{\frac{-1}{|y|}\right\}=0,\qquad 0<x<1,$$

with boundary values $y'(0)=0$, $y(1)=\tau$, for $\tau, \beta>0$.

We can rewrite (4.7) as

$$(xy')'=-\beta x\exp\left\{\frac{-1}{|y|}\right\}.$$

Integrating twice and incorporating the boundary values, we obtain

$$y(x)=\tau+\beta\int_x^1\frac{1}{s}\int_0^s t\exp\left\{\frac{-1}{|y(t)|}\right\}dt\,ds.$$

We define the interval operator

$$\text{(4.8)}\qquad P(Y)(x)=\tau+\beta\int_x^1\frac{1}{s}\int_0^s t\exp\left\{\frac{-1}{|Y(t)|}\right\}dt\,ds.$$

Let $Y_0(x) \equiv [\tau, T]$ for x in $[0, 1]$. Call $A_0 = \exp\{-1/|Y_0|\} = [\exp\{-1/\tau\}, \exp\{-1/T\}]$; then we have

$$P(Y_0)(x) = \tau + \beta A_0\left(\frac{1-x^2}{4}\right). \tag{4.9}$$

Now $P(Y_0)(x) \subseteq Y_0(x)$ for all x in $[0, 1]$ if

$$\tau + \frac{\beta}{4} \exp\left\{\frac{-1}{T}\right\} \leqq T,$$

or if

$$\beta \leqq 4(T-\tau) \exp\left\{\frac{1}{T}\right\}. \tag{4.10}$$

Clearly we can satisfy (4.10) for *any* $\beta, \tau > 0$ by taking T large enough. In fact, as $T \to \infty$, we obtain

$$P(Y_0)(x) \to \tau + \beta\left[\exp\left\{\frac{-1}{\tau}\right\}, 1\right]\left(\frac{1-x^2}{4}\right).$$

Now, any solution of (4.7) satisfies $y'(x) \leqq 0$ for x in $[0, 1]$ and so every solution $y(x)$ satisfies

$$\tau = y(1) \leqq y(x) \quad \text{for } 0 \leqq x \leqq 1.$$

Furthermore, every solution is necessarily bounded in $[0, 1]$. Therefore every solution $y(x)$ of (4.7) satisfies

$$y(x) \in \tau + \beta\left[\exp\left(\frac{-1}{\tau}\right), 1\right]\left(\frac{1-x^2}{4}\right) \quad \text{for all } x \text{ in } [0, 1]. \tag{4.11}$$

We could find conditions on τ and β for which P given by (4.8) is a contraction satisfying (4.4) in the region defined by (4.11). This would give us a region or regions in the τ, β plane in which there is a unique solution. Parter et al. [62], [63] have made a remarkably detailed study of the dependence on τ and β of the number of solutions to (4.7). They find regions in the τ, β plane for which there is a unique solution and other regions and curves in which there are exactly three solutions, two solutions, etc.

We consider next the well-known *Newton–Kantorovich* method for solving nonlinear operator equations (see, e.g. [64]). Interval methods can be used to computationally verify the conditions for existence and uniqueness of a solution and convergence of the sequence of Newton iterates and to construct rigorous global error bounds. Talbot [73] considers the problem

$$\begin{aligned} &y''(x) = f(x, y), \qquad a < x < b, \\ &y(a) = y(b) = 0 \end{aligned} \tag{4.12}$$

where the function f is allowed to be an interval extension of a real function which is twice continuously differentiable in $[a, b] \times [-l, l]$ (for some l to be determined).

Talbot shows that instead of dealing with the operator P given by

$$P(y)(x) = y''(x) - f(x, y(x)) \tag{4.13}$$

as a mapping from the Banach space $C_0^2[a, b]$ with a norm such as

$$\|y\| = \max_{a \leqq x \leqq b} \{|y(x)| + |y''(x)|\};$$

it is better computationally, resulting in sharper error bounds, to treat P as a mapping from the normed linear space

$$X=\{y : y\in C^2[a, b], y(a)=y(b)=0\}$$

with norm $\|y\|=\max_{a\leqq x\leqq b}|y(x)|$ into the Banach space $C[a, b]$ with the same norm. In this case X is *not* a Banach space (it is not complete with respect to the chosen norm). However, Talbot is able to derive a new version of the Kantorovich theorem on the convergence of Newton's method in this computationally preferable setting.

THEOREM 4.1 [73]. *Suppose that* y_0 *is in* X, $[P'(y_0)]^{-1}$ *exists; and* m_0, η_0, β_0, K *are constants such that*

$$y_1=y_0-[P'(y_0)]^{-1}P(y_0), \tag{4.14}$$

with

$$\|[P'(y_0)]^{-1}\|\leqq\beta_0, \tag{4.15}$$

$$\|y_1-y_0\|\leqq\eta_0, \tag{4.16}$$

$$\|P^{(2)}(y)\|\leqq K \quad \textit{for } y \textit{ in } N_{2\eta_0}(y_0)=\{y : \|y-y_0\|\leqq 2\eta_0\}, \tag{4.17}$$

$$h_0=\beta_0\eta_0K\leqq 1/2, \tag{4.18}$$

as in the Kantorovich conditions and, in addition, that

$$\max_{a\leqq x\leqq b}|f_y(x, y_0(x))|\leqq m_0, \tag{4.19}$$

and

$$j_0=(m_0\beta_0+1)K\eta_0+h_0<1. \tag{4.20}$$

Then there exists y^* *in* X *such that* $P(y^*)=0$ *and*

$$\|y^*-y_1\|\leqq\frac{h_0\eta_0}{1-h_0}. \tag{4.21}$$

The various quantities in Theorem 4.1 are bounded as follows. The interval $[a, b]$ is partitioned as $a=x_0<x_1<\cdots<x_n=b$. The equation (4.13) is then discretized for this partition and a discrete numerical solution is obtained using Newton's method in E^{n-1}. Cubic spline interpolation then is used to provide a twice continuously differentiable approximate solution $y_0(x)$ on $[a, b]$. Actually, the spline (piece-wise cubic polynomial) coefficients are found using rounded interval arithmetic so that (a piece-wise cubic interval polynomial) $Y_0(x)$ is found, rather than $y_0(x)$, such that

$$y_0(x)\in Y_0(x) \quad \text{for } x \text{ in } [a, b].$$

Next, the existence of $[P'(y_0)]^{-1}$ is determined by using interval methods to solve the initial value problem

$$s''(x)=f_y(x, y_0(x))s(x), \qquad a\leqq x\leqq b,$$
$$s(a)=0, \qquad s'(a)=1.$$

If $s(b)$ can be shown not equal to zero, say $S(x)$ is an interval function (e.g., interval polynomial) containing $s(x)$ and $S(b)$ does not contain zero, then $[P'(y_0)]^{-1}$ exists as a bounded linear operator from $C[a, b]$ into X and is given by

$$[P'(y_0)]^{-1}z(x)=\int_a^b g(x, t)z(t)\,dt, \tag{4.22}$$

with

$$g(x,t)=\begin{cases}\dfrac{1}{s(b)}s(x)w(t), & a\leqq x\leqq t\leqq b,\\[2ex] \dfrac{1}{s(b)}s(t)w(x), & a\leqq t\leqq x\leqq b,\end{cases}$$

and where w is determined by

$$w''(x)=f_y(x, y_0(x))w(x), \qquad a\leqq x\leqq b,$$
$$w(b)=0, \qquad w'(b)=1.$$

Next, y_1, satisfying (4.14) is sought as the solution of

$$\begin{aligned}&y_1''(x)=f_y(x, y_0(x))(y_1(x)-y_0(x))+f(x, y_0(x)),\\ &y_1(a)=y_1(b)=0.\end{aligned} \tag{4.23}$$

The solution of (4.23) can be found as a linear combination of solutions of the initial value problems

$$\begin{aligned}&u_1''(x)=f_y(x, y_0(x))(u_1(x)-y_0(x))+f(x, y_0(x)),\\ &u_1(a)=0, \qquad u_1'(a)=1,\end{aligned} \tag{4.24}$$

and

$$s''(x)=f_y(x, y_0(x))s(x), \qquad a\leqq x\leqq b,$$
$$s(a)=0, \qquad s'(a)=1.$$

In fact,

$$y_1(x)=u_1(x)-\frac{u_1(b)}{s(b)}s(x).$$

It has already been determined, in connection with (4.22), that $s(b)\neq 0$.

Again, using interval methods to solve (4.24), an interval function $U_1(x)$ is obtained such that $u_1(x)\in U_1(x)$ for x in $[a, b]$ and so

$$y_1(x)\in Y_1(x)=U_1(x)-\frac{U_1(b)}{S(b)}S(x). \tag{4.25}$$

Next, the constants m_0, η_0, β_0, and K are constructed to satisfy (4.15), (4.16), (4.17) and (4.19) making repeated use of the following:

if G is an interval extension of g then

$$\max_{a\leqq x\leqq b}|g(x)|\leqq \max(|G_1|, |G_2|)$$

where $G([a, b])=[G_1, G_2]$.

If the resulting constants satisfy (4.18) and (4.20) then (4.21) holds and, taking

$$\tilde{y}(x)=\text{midpoint of } Y_1(x)$$

one obtains

$$|y^*(x)-\tilde{y}(x)|\leqq\frac{h_0\eta_0}{1-h_0}+\frac{1}{2}\text{width of } Y_1(x) \tag{4.26}$$

for x in $[a, b]$.

Illustrative numerical results were obtained by Talbot [73] on the CDC 1604 computer using the method just described. If we call the maximum of the right hand side of (4.26) the *global error bound*; the following results were obtained:

Equation 1.

$$y''(x) = (y+\alpha)(y+\alpha-2)[1+2x^2(y+\alpha-1)],$$
$$y(-1) = y(1) = 0,$$
$$\alpha \in [.5378828427201, .5378828427493],$$
$$\textit{Global error bound}: \quad 1.3 \cdot 10^{-8}.$$

Equation 2.

$$y''(x) = e^{y(x)},$$
$$y(0) = y(1) = 0,$$
$$\textit{Global error bound}: \quad 2 \cdot 10^{-9}.$$

Equation 3.

$$y''(x) = e^{-y(x)},$$
$$y(0) = y(1) = 0.$$

This problem has two solutions [13], [73]. The "smaller" of the two results was

$$\textit{Global error bound}: \quad 1.7 \cdot 10^{-9}.$$

For the "larger" solution, a "shooting technique" was used (i.e., trying various *initial* conditions for $y'(0)$ until an approximate solution to the initial value problem $y''(x) = e^{-y(x)}$, $y(0) = 0$, $y'(0) = \alpha$ yielded a function $y_0(x)$ leading to the "larger" solution to the two-point boundary value problem). The results were:

$$\textit{Global error bound}: \quad 3.2 \cdot 10^{-4}.$$

Lee [44] has generalized the procedure of [73] to handle the problem

$$y'' = f(x, y, y'), \qquad a < x < b, \quad y(a) = y(b) = 0. \tag{4.27}$$

(and also systems of such equations with general boundary conditions). At the same time, the new method [44] gives sharper bounds for the special cases covered by the previous method.

Wauschkuhn [74], [75] has used interval methods to determine the existence of *periodic solutions* to systems of ordinary differential equations and to construct bounds. The "3-process-method" of Krückeberg [40] for bounding solutions to initial value problems is an important tool for this.

Interval methods have been used in conjunction with *defect methods* especially for operator equations where the operator has some type of monotonicity (inverse monotone, antitone, isotone, quasimonotone, etc.; see, e.g. Schröder [69]). Examples of this for partial differential equations can be found in [8], [41]. In [48], Marcowitz makes use of theoretical results of Schröder [69] together with interval computations to construct bounds for a control theory problem connected with the *re-entry* of an Apollo type space ship.

5. Safe starting points. A good initial approximation is required, in general, for the convergence of an iterative method of the Newton–Kantorovich type (including the interval versions of Talbot and Lee). For a two-point boundary value problem for a second order differential equation such as (4.27) a twice-differentiable function which closely approximates a solution is required as a *safe starting point* for the convergence of the iterative method. In this section we will describe some recent work on the problem of finding safe starting points for iterative methods.

If we can first find a good *discrete* approximation to a solution $y(x)$ of (4.27), say $(y_1, y_2, \cdots, y_n)$ with $y_i \approx y(x_i)$ for

$$a \leqq x_1 < x_2 < x_3 < \cdots < x_n \leqq b;$$

then we can construct a twice-differentiable function on $[a, b]$, say a cubic spline $y_0(x)$, which may well approximate $y(x)$ for all x in $[a, b]$. One way to do this for a problem such as (4.27) is to *discretize* the operator equation, approximating derivatives by difference quotients and integrals by finite sums. We then have to solve a system of n nonlinear equations in n unknowns. Again, we can use an iterative method, such as a Newton type method in n-dimensions, to solve such a system. See, e.g. [19], [42], [64]. We are still left with the problem of *finding a safe starting point for the convergence of an iterative method for finite nonlinear system of equations.*

Little work seems to have been done on this important problem. Recently, however, Moore and Jones [59] have introduced an interval search procedure which can find safe starting regions in n dimensions for iterative methods. In particular the search procedure works well with a specific iterative interval method [58] which is a modification of a method due to Krawczyk [37]. We will now describe the iterative method and the search procedure. We refer to § 1 of this paper for notation.

Consider the equation $f(x)=0$ where $f: D \subseteq R^n \to R^n$ is continuously differentiable in the open set D. Let F_i, F'_{ij} be inclusion monotonic interval extensions of f_i and $f'_{ij} = \partial f_i / \partial x_j$.

An iterative algorithm for producing a sequence of interval vectors $\{X^{(k)}\}$ from a *given* initial interval vector $X^{(0)}$ is as follows:

$$X^{(k+1)} = X^{(k)} \cap K(X^{(k)}) \tag{5.1}$$

where

$$K(X^{(k)}) = m(X^{(k)}) - Y^{(k)} F(m(X^{(k)})) + R^{(k)}(X^{(k)} - m(X^{(k)}))$$

with

$$R^{(k)} = I - Y^{(k)} F'(X^{(k)})$$

where I is the $n \times n$ identity matrix and the real matrices $Y^{(k)}$ are defined by

$$Y^{(k)} = \begin{cases} Y, & \text{an approximation to } [m(F'(X^{(k)}))]^{-1}, \\ & \text{if } k=0 \text{ or if } k>0 \text{ and } \|I - YF'(X^{(k)})\| \leqq \|R^{(k-1)}\|; \\ Y^{(k-1)}, & \text{if } k>0 \text{ and } \|I - YF'(X^{(k)})\| > \|R^{(k-1)}\|. \end{cases}$$

The algorithm (5.1) does not require the inversion of interval matrices but only the approximate inversion of real matrices. It has been shown to have the following properties [37], [58], [59]:

1) $X^{(k+1)} \subseteq X^{(k)}$ for all $k = 0, 1, 2, \cdots$;
2) if $X^{(k+1)} = X^{(k)} \cap K(X^{(k)})$ is empty, then there is no solution to $f(x)=0$ in $X^{(k)}$;
3) if $K(X^{(k)}) \subseteq X^{(k)}$ then there *is* a solution to $f(x)=0$ in $X^{(k)}$;
4) if $K(X^{(0)}) \subseteq X^{(0)}$ and $\|R^{(0)}\| < 1$, then there is a unique solution x to $f(x)=0$ in $X^{(0)}$. Furthermore, $x \in X^{(k)}$ for all $k \geqq 0$ and $\{w(X^{(k)})\} \to 0$.

In 4) the convergence is at least linear and under reasonable conditions it is quadratic [59]. The algorithm (5.1) has the computationally verifiable sufficient conditions 4) for existence, uniqueness and convergence.

In order to find a *safe starting region* $X^{(0)}$, satisfying $K(X^{(0)}) \subseteq X^{(0)}$ and $\|R^{(0)}\| < 1$, we can use the following *search procedure* [59]:

Let B be an *arbitrary* n-dimensional rectangle (interval vector) in the domains of F and F'. We would choose B *large* enough so that it *may* well contain at least one solution.

We do *not* require the nonsingularity of the Jacobian matrix f' in B.

The search procedure to be given will do one of three things:

(i) find a safe starting region $X^{(0)} \subseteq B$ for the convergence of the algorithm (5.1);

(ii) discover that there are no solutions in B;

(iii) terminate with a list of small subregions of B which may still contain solutions; higher precision machine arithmetic might be required to continue the search or slightly *enlarge* the small subregions in case a solution might fall exactly on a boundary.

The procedure, which creates a list of subregions of B yet to be tested, is as follows [59]:

(5.2) *Search procedure.*

Step 1. (Initialization) set list to empty; set X to B

Step 2. Compute $F(X)$

Step 3. (Exclusion) if $0 \notin F(X)$, go to Step 11

Step 4. Compute $Y \approx [m(F'(X))]^{-1}$; if not possible, go to Step 9

Step 5. Compute $\|R\|$ and $K(X)$

Step 6. (Exclusion) if $X \cap K(X)$ is empty, go to Step 11

Step 7. (Existence) if $K(X) \subseteq X$, then X (and also $K(X)$) contains a solution, continue; if not, go to Step 9

Step 8. (Convergence) if $\|R\| < 1$, then X is a safe starting region $X^{(0)}$ for the algorithm (5.1)—terminate search—; otherwise set B to $K(X)$ and go to Step 1

Step 9. (Bisection) choose a coordinate direction for bisection of X according to the following:

(1) find a pair i, j for which $w(F'(X)_{ij}) = w(F'(X))$

(2) bisect X, if possible, in each of the coordinate directions in turn which occur in the expression for $F'(X)_{ij}$ and *choose* the first coordinate direction for which $w\{F'(X^{(1)})_{ij} \cup F'(X^{(2)})_{ij}\}$ is a minimum, where $X = X^{(1)} \cup X^{(2)}$ and where $X^{(1)}$, $X^{(2)}$ are the halves of X resulting from the above trial bisections; having chosen a bisection direction, select one of the halves $X^{(h)}$, $h = 1, 2$, for which

$$\sum_{j=1}^{n} |m(F_j(X^{(h)}))| \quad \text{is minimum;}$$

if not possible, indicate "possible solution in X" and go to Step 11

Step 10. Set X to half region $X^{(h)}$ selected in Step 9; add remaining half region to head of list; go to Step 2

Step 11. (Test list) if list is empty, B contains no solution (unless previously indicated otherwise), terminate; otherwise (if the list is not empty) set X to region at head of list; delete this region from list; go to Step 2

The search procedure (5.2) and iterative method (5.1) have been tried on a number of examples of dimension up to $n = 20$. Numerical results as well as theoretical considerations indicate that the search procedure (5.2) is more powerful than continuation methods [59]. The bisection rules in Step 9 are based on heuristics and can probably be modified in various ways to produce a more efficient search procedure. As is, the procedure required 17 bisections to find a safe starting region for the algorithm (5.1) for a certain system of 10 nonlinear equations in 10 unknowns [59]. The region B searched was the 10-dimensional interval vector with all components $B_i = [-2, 2]$. The safe starting region found (for algorithm (5.1)) was

$$X^{(0)} = ([0, 0.5], [0, 1], [0, 1], [0, 1], [0, 1], [0, 1], [0, 1], [-2, 2], [-2, 2], [0, 1]).$$

For a simpler example, of dimension 2, namely

$$\begin{aligned} f_1(x_1, x_2) &:= x_1^2 + x_2^2 - 1 = 0, \\ f_2(x_1, x_2) &:= x_1^2 - x_2 = 0, \end{aligned} \tag{5.3}$$

we searched the rectangle $B = ([-1, 1], [0, 1])$ using the procedure (5.2) and found (after 6 bisections) the safe starting region (for algorithm (5.1)),

$$X^{(0)} = ([.75, 1], [.5, .75]).$$

From $X^{(0)}$, the algorithm (5.1) produces, in *four* iterations, an interval vector $X^{(4)}$ of width $1.5 \cdot 10^{-8}$ which contains a solution of (5.3).

By contrast a certain continuation algorithm (see [59]) fails to produce a safe starting point for Newton's method applied to (5.3) from the point (.75, .75) in our safe starting region $X^{(0)}$.

6. Stopping criteria. An iterative n-dimensional interval method of the form

$$X^{(k+1)} = X^{(k)} \cap M(X^{(k)}) \tag{6.1}$$

(for instance (5.1) of § 5) produces a nested sequence of interval vectors. Suppose the computation is carried out using inclusion monotonic, *rounded* interval arithmetic (see § 1); then we obtain, instead, a sequence $\{\bar{X}^{(k)}\}$ defined by

$$\bar{X}^{(k+1)} = \bar{X}^{(k)} \cap \bar{M}(\bar{X}^{(k)}) \tag{6.2}$$

where $\bar{M}$ is a properly rounded version of M,

$$M(\bar{X}^{(k)}) \subseteq \bar{M}(\bar{X}^{(k)}).$$

Thus, (6.2) produces interval vectors $\bar{X}^{(k)}$ whose components

$$\bar{X}_i^{(k)} = [a_i^{(k)}, b_i^{(k)}], \qquad i = 1, 2, \cdots, n,$$

are machine representable numbers $a_i^{(k)}, b_i^{(k)}$. By induction, $X^{(0)} \subseteq \bar{X}^{(0)}$ implies $X^{(k)} \subseteq \bar{X}^{(k)}$ for all $k \geqq 0$. In fixed precision machine arithmetic, there are only finitely many machine representable numbers. Therefore, since $\bar{X}^{(k+1)} \subseteq \bar{X}^{(k)}$, we will, after some finite number of iterations, reach the relation

$$\bar{X}^{(k+1)} = \bar{X}^{(k)}, \tag{6.3}$$

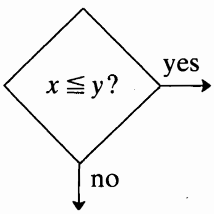
after which there is *no further change* in the iterates [77]. This is called *numerical convergence.*

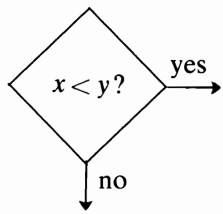
The width, $w(\bar{X}^{(k)})$, of the converged result will not, of course, be zero in general but will have some positive value which can be made arbitrarily small only by going to arbitrarily high precision on the computer.

The relation (6.3) is a *natural stopping criterion* for iterative interval methods in *n*-dimensions of the form (6.1) when carried out using fixed precision, rounded interval arithmetic (say "single-precision, floating point").

Wisskirchen [76] has obtained the remarkable result that, for inclusion monotonic rounded interval arithmetic (as usually realized on computers), interval total-step methods (like Jacobi iteration) based on iteration of inclusion monotone interval vector functions converge to the *same interval vector* as the corresponding single-step methods (like Gauss–Seidel iteration), providing only that the iterations start with the same initial vector. This is true in spite of rounding errors and in spite of the fact that completely different intermediate results occur during computation.

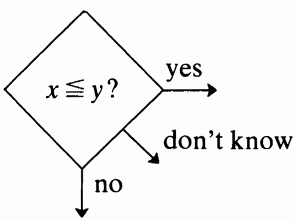
By using rounded interval arithmetic and *three valued logic* we can modify any computer program in such a way that the interval results contain the corresponding *infinite precision* (real arithmetic) results. To do this, we replace, in the program, any quantity which is subject to rounding error by an interval; replace all arithmetic operations on such quantities by the corresponding rounded interval arithmetic operations; and replace all conditional branches involving such quantities, such as

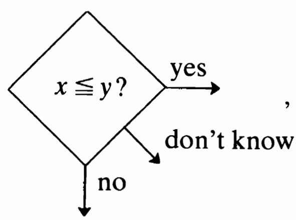




, etc.,

by corresponding three-valued branches of the forms:





, etc.

There are only *two* possible answers to the question

$$x \leqq y?$$

for *real numbers* x and y; there are, however, *three* possible answers to the question if all we know about x and y is that $x \in [a_1, a_2]$ and $y \in [b_1, b_2]$. These are:

1) *yes*, if $a_2 \leqq b_1$,
2) *no*, if $b_2 < a_1$,
3) *don't know*, otherwise.

Upon machine execution of a computer program which has been modified to incorporate rounded interval arithmetic and three valued logic, we will obtain intervals containing the corresponding infinite precision results (i.e. the results the machine would get from the program if it used infinite precision arithmetic) *as long as there are no conditional jumps* to "don't know". What to do in case such a jump does occur would depend, of course, on the intentions of the original program. (See also [55, §§ 1.2–1.4]).

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