Kuwait J. Sci. Eng. **30**(1) 2003

Topics in computer supported error control

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ABSTRACT

The concept of computer aided error control or verifying solutions is a new branch in scientific computing. Verification establishes, in addition to traditional numerical approximations, bounds for marginal errors. To secure enclosures we combine methods from functional analysis, automatic differentiation and interval analysis. Established are algorithms which ultimately control the accuracy of the computed solution. In this article we provide, in particular, a survey on enclosure methods for integral equations.

AMS subject classifications: 45B05; 45D05; 65G10; 65R20.

Key words: enclosure method; integral equation; safe bound.

1 - Problem Setting

The principal subject of this article is operator equations of the second kind

$$x = g + k(x) \ , \tag{1}$$

where k is either a Fredholm

$$k(x) := \int_a^b k(s,t)x(t)dt \quad , \quad a \le s \le b \quad , \tag{2}$$

or a Volterra

$$k(x) := \int_a^s k(s,t)x(t)dt \quad , \quad a \le s \le b \quad , \tag{3}$$

integral operator. We use the same notation for the operator as for the corresonding kernel. For clarity, verification schemes are derived for real kernels which depend on two variables; an extension to higher dimensions requires only minor technical adjustment: We consider $C(a, b)$, the pre-Hilbert space of continuous real valued functions where (.,.) denotes the canonical scalar product, and $\|.\|$ the maximum norm; $\Re$ denote the real numbers and $\aleph$ the natural numbers.

Definition 1 *A verification scheme is a numerical algorithm where mathematical assured error bounds are part of the result.*

Primarily considered are basic principles of self-validating numerics, then enclosure methods for Fredholm integral equations of the second kind are derived. Section 4 deals with Volterra equations.

2 - Basic principles of self-validating numerics

We begin with a concise survey of the elements of self-validating numerics.

2.1 Precise computer arithmetic

There is need for a precise formulation of basic floating point operations, summarized briefly by the requirement: "No floating point number lies between the exact and the rounded result of a single floating point operation". Therefore we adopt the exact scalar product as a fifth floating point operation to determine sums without cancellation. For extensive discussion of this mathematical theory of computer arithmetic we refer to Kulisch & Miranker (1981).

2.2 Interval analysis

Error tolerances are described by intervals

$$A - [A] = [\underline{A}, \overline{A}] = \{x \in \Re \,|\, \underline{A} \le x \le \overline{A}\} \quad , \quad \underline{A}, \overline{A} \in \Re \ , \tag{4}$$

$I\Re$ denotes all such intervals together with the basic arithmetic operations. Relations such as $=, \subseteq, \cup$ etc., are explained in a set theoretic manner (componentwise for vectors and matrices).

For $A \in I\Re$ the following definitions are of importance

$$\mathrm{mid}(A) := \frac{1}{2}(\underline{A} + \overline{A}) \ ,$$

$$\mathrm{diam}(A) := \overline{A} - \underline{A} \ ,$$

$$|A| := \max_{a \in A} |a| \ .$$

For intervals A, B, C instead of the distributive law only the subdistributive law is valid:

$$A(B + C) \subseteq AB + AD \quad . \tag{5}$$

When adding/subtracting two intervals then the diameter increases according to

$$\text{diam}(A \pm B) = \text{diam}(A) + \text{diam}(B) \quad . \tag{6}$$

In addition to Equation 5 and 6, the following so called inclusion monotonicity has important consequences for the construction of validation schemes:

$$\left.\begin{array}{r} a \in A, b \in B \Longrightarrow a * b \in A * B \quad , \\ A \subseteq C, B \subseteq D \Longrightarrow A * B \subseteq C * B \quad , \end{array}\right\} \begin{array}{l} * \in \{+, -, ., /\} \\ A, B, C, D \in I\Re. \end{array}$$

A real valued element of A is denoted with $\dot{A}$.

2.3 Function intervals

Let $S_n = span(\varphi_1, \varphi_2, ..., \varphi_n) \subseteq C(a, b)$ be an n-dimensional subspace, where $\{\varphi_i\}_{i \in \aleph}$ is dense in $C(a, b)$. In $C(a, b)$ a relation $\leq$ is defined according to

$$f \leq g :\Longleftrightarrow f(s) \leq g(s) \quad , \quad a \leq s \leq b \quad , \tag{7}$$

thus function intervals $F = [\underline{F}, \overline{F}]$ may be defined:

$$[\underline{F}, \overline{F}] = \{h \in C(a, b) \,|\, \underline{F} \leq h \leq \overline{F}\}. \tag{8}$$

We are particularly interested in intervals whose boundary functions pertain to S_n

$$I_n = \{|\,\underline{F}, \overline{F}] \,|\, \underline{F}, \overline{F} \in S_n\} \supseteq C(a, b) \quad .$$

Lemma 2 *The elements of I_n are closed, bounded and convex.*

Proof: Derives from the implications (Note $f, g \in C(a, b)$)

$$f \geq g \Longrightarrow \alpha f \geq \alpha g \quad , \quad \alpha > 0 \quad ,$$

$$f_n \geq 0 \quad , \quad \lim_{n \to \infty} \|f_n - f\| = 0 \Longrightarrow f \geq 0 \quad . \qquad \square$$

The arithmetic operations in I_n are defined so that I_n is algebraically closed, thus a rigorous error control is possible. Let $F, G \in I_n$ then $F * G, * \in \{+, -, ., /\}$ is characterized by the inclusion monotonicity

$$F * G = \{f * g \,|\, f \in F, g \in G\} \subseteq H \in I_n \quad . \tag{9}$$

Definition 3 *$F \in I_n$ is called enclosure of $f \in C(a,b)$ iff*

$$f(s) \in F(s) \quad , \quad a \leq s \leq b \quad . \tag{10}$$

The set of enclosures of f is denoted with $E(f)$.

Analogical enclosures for kernels and operators are explained.

We are now looking for efficient tools to determine enclosures with small diameters.

2.4 Automatic differentiation

An important tool to determine function enclosures is automatic differentiation; it provides the explicit computation of derivatives without symbolic manipulation of formulas. We consider a continuous differentiable function $k : \Re^2 \to \Re$ and we are seeking the function value and the gradient ∇k at an arbitrary but fixed point $(s_0, t_0) \in \Re^2$. For functions $u, v \in \Re^2 \to \Re$ and 3-tupels $U = (u_s, u_g), \; V = (v_s, v_g)$, with function values $u_s, v_s \in \Re$ and u_g, v_g value of the gradients at a particular point, a gradient arithmetic is defined according to

$$U \pm V = (u_s \pm v_s, u_g \pm v_g) \tag{11}$$

$$U.V = (u_s \,.\, v_s, u_s \,.\, v_g + u_g \,.\, v_s) \tag{12}$$

$$U/V = \left(\frac{u_s}{v_s}, \frac{u_g - \frac{u_s}{v_s} v_g}{v_s} \right) \quad . \tag{13}$$

The independent variables s, t are represented by the vectors $(s, 1, 0), (t, 0, 1)$ and constants c by $(c, 0, 0)$. Thus function values and values of gradients are computed step-by-step for arithmetic expressions. Formulas 11 to 13 can be extended to differentiate standard functions as well as higher order derivatives, thus for a given function $k(s, t), a \leq s, t \leq b$ a Taylor representation

$$k(s, t) = k_n(s, t) + k_r(\sigma, \tau) \tag{14}$$

is computable where k_n is the Taylor polynomial of n-th degree, k_r the corresponding remainder term and σ, τ intermediate values. Replacing σ, τ by the domain $[a.b]$,

$$K(s,t) = k_n(s,t) + k_r([a,b],[a,b]) \in E(k) \quad , \tag{15}$$

yields an enclosure for k.

2.5 Fixed point theorems

Fixed point theorems, formulated in a form suitable for computer applications, are another important skill in self-validating numerics. As illustration we offer two examples for such theorems.

Definition 4 *Let $F, G \in I_n$ and $\varepsilon > 0$ be given. Then G is said to be an ε-enclosure of F : $F \subseteq_\varepsilon G$, if there exists a closed ball $B_0(\varepsilon)$ with radius ε, centered at 0 so that*

$$F(s) + B_0(\varepsilon) \subseteq G(s) \quad , \quad a \leq s \leq b \quad . \tag{16}$$

Theorem 5 *Let $A \in \Re^{n\times n}, b \in \Re^n, \emptyset \neq X \in I\Re^{n\times n}$ so that*

$$Rb + (I - RA)\ X \subseteq_\varepsilon X,$$

then the linear system

$$Ax = b$$

has only one solution $\hat{x}$ and furthermore

$$\hat{x} \in X.$$

Proof: *see Kaucher & Miranker (1984).* □

Theorem 6 *Let $k : C[a,b] \to C[a,b]$ be an α-condensing operator and $K : I_n \to I_n$ an enclosure of k. If $\emptyset \neq X \in I_n$ fulfills*

$$K(X) \subseteq X \tag{17}$$

then the operator k has a fixed point $\hat{x}$ and furthermore

$$\hat{x} \in X. \tag{18}$$

Proof: For the definition of α-condensing operators we refer to Sadvoskij (1972); for the proof see Kaucher & Miranker (1984). □

3 - Enclosure methods for second kind Fredholm equations

We consider Fredholm integral equations of the second kind

$$x(s) = g(s) + \int_a^b k(s,t)x(t)dt \quad , \tag{19}$$

and derive enclosure concepts for this class of problems.

3.1 Decomposition technique

As previously demonstrated a decomposition and enclosure of k

$$k(s,t) = k_n(s,t) + k_r(s,t) \in K_n(s,t) + K_r(s,t), a \le s,t \le b, \tag{21}$$

can be obtained by automatic differentiation, here k_n and K_n denote the degenerate parts, p_i, q_i linear independent functions and P_i, Q_i their corresponding enclosures

$$k_n(s,t) = \sum_{i=1}^{n} p_i(s)q_i(t) \in \sum_{i=1}^{n} P_i(s)Q_i(t) = K_n(s,t). \tag{21}$$

K_r is an enclosure of the remainder $k_r = k - k_n$. Since the kernel is assumed to be at least continuous it can be represented by a convergent series, hence the parameter n can be chosen, so that k_r resp. K_r are contractive (see also Hammer *et al* 1993). We iterate in I_n according to

$$V^{(l+1)} = G + K_r(V^{(l)}) \quad , \quad G \in E(g) \quad , \quad l = 0, 1, \ldots \quad , \tag{22}$$

$$W_i^{(l+1)} = P_i + K_r(W_i^{(l)}) \quad , \quad i = 1, \ldots, n \quad , \quad l = 0, 1, \ldots \quad . \tag{23}$$

For simplicity we take the same iteration index l uniformly.

Theorem 7 *Let the enclosure conditions*

$$V := V^{(l+1)} \subseteq V^{(l)} \quad , \quad W_i := W_i^{(l+1)} \subseteq W_i^{(l)} \quad , \quad i = 1, \ldots, n, \tag{24}$$

be fulfilled for subsequent iterates $V^{(l+1)}, V^{(l)}, W_i^{(l)}, W_i^{(l+1)}, i = 1, \ldots, n,$ *of the schemes 22 and 23. If* $Y = (Y_1, \ldots, Y_n)$ *is an enclosure for the solution of the linear system*

$$AY = B \quad , \tag{25}$$

with A an interval square matrix

$$A := A(Q_j, W_i) := (\delta_{ji} - \int_a^b Q_j(t)W_i(t)dt)_{j,i=1,\ldots,n} \quad , \tag{26}$$

and B an interval vector

$$B := B(Q_j, V) := (\int_a^b Q_j(t)V(t)dt)_{j=1,\dots,n} \quad , \tag{27}$$

then the solution x of problem 19 exists and is enclosed within $X(s)$:

$$x(s) \in V(s) + \sum_{i=1}^{n} Y_i W_i(s) =: X(s) \quad , \quad a \le s \le b \quad . \tag{28}$$

Proof: The continuous, real valued quantities v and w_i are defined as solutions of the integral equations

$$v(s) = g(s) + \int_a^b k_r(s,t)v(t)dt \quad , \quad a \le s \le b \quad ,$$

$$w_i(s) = p_i(s) + \int_a^b k_r(s,t)w_i(t)dt \quad , \quad i = 1,\dots,n \quad , \quad a \le s \le b \quad ,$$

then the solution x of Equation 19 is given by

$$x(s) = v(s) + \sum_{i=1}^{n} y_i w_i(s) \quad , \quad a \le s \le b \quad ,$$

where the n-dimensional real vector $y = (y_1, \dots, y_n)$ satisfies the linear system

$$\dot{A}\dot{Y} = \dot{B}$$

$$\dot{A}(q_j, w_i)\dot{Y} = \dot{B}(q_j, v) \quad , \tag{29}$$

where the interval - valued functions in Equations 26 and 27 have to be replaced by the corresponding real quantities. Using the enclosure property (see Equation 10), we deduce

$$V \in E(v) \quad , \quad W_i \in E(w_i) \quad , \quad i = 1,\dots,n \quad ,$$

hence $\dot{A} \in A, \dot{B} \in B$ which implies $\dot{Y} \in Y$ and the enclosure estimation 28 follows. □

Remark 8 *In traditional schemes (cf. Delves & Mohamed 1985) the solution of Equation 19 is approximated using only k_n and truncating the remainder k_r. In this case a complete error control is not possible.*

Remark 9 *The validation process described above is also suitable for parallel processing. The entries of the matrix and the right hand side can be determined simultaneously.*

3.2 Direct enclosure

Next we outline a method which is based on the enclosure of the kernel k by a degenerate interval valued kernel. This ansatz does not require the decomposition of the kernel into a degenerate and a contractive part. Let K be a degenerate enclosure of k that is

$$k(s,t) \in K(s,t) = \sum_{i=1}^{n} P_i(s) q_i(t) \quad , \quad a \le s, t \le b \quad , \tag{30}$$

where $P_i \in I_n, q_i \in C(a,b), i = 1, ..., n$. Then the following enclosure statement is valid.

Theorem 10 *Let*

$$q_i(s) x(s) \neq 0 \quad , \quad a \le s \le b \quad , \quad i = 1, ..., n \quad , \tag{31}$$

and

$$A(q_j, P_i)^{-1} B(q_j, F) \subseteq Y = (Y_1, ..., Y_n) \quad , \quad F \in E(f) \quad ,$$

then no solution x of Equation 19 lies outside of the function set

$$X(s) = G(s) + \sum_{i=1}^{n} Y_i P_i(s) \quad , \quad a \le s \le b \quad ,$$

or equivalent

$$x(s) \in G(s) + \sum_{i=1}^{n} Y_i P_i(s) = X(s) \quad , \quad a \le s \le b \quad . \tag{32}$$

Proof: We write $y_j := \int_a^b q_j(t) x(t) dt$ and assume that a solution x of Equation 19 exists, then Equation 31 gives

$$\begin{aligned} X(x) &\in G(s) + \int_a^b \sum_{j=1}^{n} P_j(s) q_j(t) x(t) dt \\ &= G(s) + \sum_{j=1}^{n} P_j(s) \int_a^b q_j(t) x(t) dt \quad , \quad a \le s \le b \quad . \end{aligned}$$

Multiplication with $q_i, i = 1, ..., n$, and integration on both sides over $[a, b]$ leads to $y_j \in Y_j, J = 1, ..., m$, which completes the proof.

Remark 11 *An enclosure K of the form $K(s,t) = \sum_{i=1}^{n} p_i(s) Q_i(t)$, with $p_i \in C(a,b), Q_i \in I_n$, requires that the matrix $A(Q_j, p_i)$ of the linear system has a spectral radius less than one.*

Remark 12 *The nonsingularity of the matrix set $A(q_j, P_i)$ and the computation of its inverse are validated with enclosure algorithms based on Theorem 3 (cf Hammer et al 1993).*

Remark 13 *The methods previously mentioned do not work if Equation 19 is in the eigenvalue case. Here the equation must be reformulated as a problem in the noneigenvalue case, by prescribing the total distribution of the solution and using Wielandt's removal of an eigenvalue from the spectrum. For details we refer to Dobner (1999b).*

3.3 Numerical examples

The methods discussed in the previous sections are implemented in PASCAL XSC (cf. Hammer *et al* 1993). In the following table numerical results for some test problems are displayed. In the last column the verified number of correct digits is shown. Two types of basic functions are used. They are referred to as P_n and F_n respectively.

$$P_n = span(s^0, s^1, ..., s^n) \quad ,$$
$$F_n = span(1, \cos(s), ..., \cos(ns), \sin(s), ..., \sin(ns)) \quad .$$

Problem	Subspace S_n	Digits
$x(s) = 2s^2 + e^s \sin(s) + \int_{-1}^{1} \cos(s) e^{\sin(s)+\cos(t)} x(t) dt$	P_{40}	8
$x(s) = s^4 - \frac{1}{15}s^6 + \frac{1}{5}s - \frac{1}{6} + \int_0^1 \lvert s-t \rvert x(t) dt$	P_{20}	10
$x(s) = 2 + \frac{1}{2\pi}\int_0^{2\pi} k(s,t) x(t) dt$ $k(s,t) = \frac{1-(1/4)^2}{1-(1/4)^2 - \frac{1}{2}\cos(s+t)}$	F_{40}/F_{50}	4/6
$k(s,t) = -\frac{1-(1/4)^2}{1-(1/4)^2 - \frac{1}{2}\cos(s+t)}$ (eigenvalue case)	F_{50}	6
$x(s) = 2e^{-s} + \int_0^1 s e^{x(t)} dt$	F_{30}/F_{60}	3/9

Concerning accuracy, numerical experiments demonstrated that there is no significant difference between the methods of section 3.1 and section 3.2.

4 - Enclosure methods for second kind Volterra equations

Estimates for the solution of Volterra equations

$$x(s) = f(s) + \int_0^s k(s,t)x(t)dt \quad , \quad 0 \leq s \leq b \quad ,$$

are computable iteratively. Without restriction we can take $a = 0$ as lower integration bound in Equation 3.

4.1 Iteration technique

Theorem 14 *If for two iterates of the process*

$$X^{(l+1)}(s) = F(s) + K(X^{(l)}(s)), \quad l = 0, 1, ..., \; F \in E(f) \; , \; K \in E(k) \; , \tag{33}$$

the stopping criterion

$$X^{(l+1)} \subseteq X^{(l)} \quad , \tag{34}$$

is achieved, then it is assured that the solution x exists within the function tube $X^{(l+1)}$:

$$x(s) \in X^{(l+1)}(s) \quad , \quad 0 \leq s \leq b \quad . \tag{35}$$

Proof: This assertion is a consequence of Theorem 6 together with the enclosure property of F and K. □

If k is not a contraction, Equation 34 can not be fulfilled and a residual iteration must be applied. For this purpose let $\tilde{x}$ be an initial approximation for x and $\tilde{X} \in E(\tilde{x})$. If V denotes the residuum with respect to $\tilde{X}$, the iteration has the form

$$X^{(l+1)} = -\sum_{\mu=0}^{m} K^{\mu}(V) + K^{m+1}(X^{(l)}) \quad , \quad l = 0, 1, ... \quad , \quad m \in \aleph \quad , \tag{36}$$

here k^{μ} is the μ-th iterated kernel of k and $K^{\mu} \in E(k^{\mu})$.

Theorem 15 *If the stopping rule in Equation 34 holds for two subsequent iterates* $X^{(l)}, X^{(l+1)}$ *of Equation 36, then the estimation*

$$x \in \tilde{X}(s) + X^{(l+1)}(s) \quad , \quad 0 \le s \le b \quad , \tag{37}$$

is valid.

Proof: For proof we employ Theorem 6, the Newton scheme and the representation of the inverse of $(I-k) = (I-k)'$ by a Neumann series. The finite sum in Equation 36 is an approximation for $(I-k)^{-1}$. □

Remark 16 *The spectral radius of the Volterra operator is zero, therefore an integer m with* $\|k^m\| < 1$ *can be chosen. In practice Equation 36 is performed with an initial approximate for m, based on a rough and quick estimate for* $\|K^m\|$. *If after a prescribed number of iterations Equation 34 is not attained, then the iterations are restarted with an increased value for m.*

4.2 Some generalizations

Considered are now nonlinear Volterra equations of the form

$$x(s) = f(s) + \int_0^s k(s,t,x(t))dt \quad , \quad 0 \le s \le b \quad . \tag{38}$$

We assume that $k(s,t,x)$ and $\frac{\partial}{\partial x}k(s,t,x)$ are continuous functions. If $\tilde{x}$ is an approximation for x and $\cup$ is the convex union we have:

Theorem 17 *If for two iterates of the iteration scheme*

$$X^{(l+1)}(s) = F(s) + \int_0^s K(s,t,\tilde{X}(t))dt - \tilde{X}(s) \tag{39}$$

$$+ \int_0^s \frac{\partial}{\partial x} K(s,t,((X^{(l)} + \tilde{X}) \ \cup \ \tilde{X})(t))X^{(l)}(t)dt \quad ,$$

$$l = 0,1,\dots \quad , \quad K \in E(k) \quad , \quad 0 \le s \le b \quad ,$$

performed in I_n*, Equation 34 holds, then it is shown that the solution x of Equation 38 lies in the function tube determined by* $\tilde{X}$ *and* $X^{(l+1)}$

$$x(s) \in \tilde{X}(s) + X^{(l+1)}(s) \quad , \quad 0 \le s \le b \quad . \tag{40}$$

Proof: With the mean value theorem and Equation 34 we conclude that $\int_0^s k(s,t,x(t))dt - \tilde{x}(s)$ maps the closed, bounded and convex set X^l into itself, so that together with Theorem 6 the error estimation is deduced. □

Volterra equations of the first kind

$$\int_0^s k(s,t)x(t)dt = f(s) \quad , \quad 0 \le s \le b \quad , \tag{41}$$

can be recast under suitable prerequisities as the equivalent second kind equation

$$k(s,s)y(s) = f'(s) - \int_0^s \frac{\partial k(s,t)}{\partial s} y(t)dt \quad , \quad 0 \le s \le b \quad .$$

Therefore Equation 41 can also be treated with the validation techniques of section 4.1.

4.3 Numerical examples

Finally, we display some numerical results. For the notations we refer to section 3.3.

Problem	**Subspace**	**Digits**
$x(s) = \frac{1}{2}s^2e^{-s} + \int_0^s \frac{1}{2}(s-t)^2 e^{-(s-t)} x(t)dt \ , \ 0 \le s \le 1$	P_{10}/P_{10}	5/11
$\int_0^s (1+s-t)x(t)dt = 1+s-\sin(s)-\cos(s) \ , \ 0 \le s \le 1.2$	P_{10}/P_{20}	6/12
$x(s,t) = 1-2+t+\int_0^t \int_0^s (\tau y((\sigma,\tau) - x(\sigma,\tau))d\sigma \, d\tau$ $y(s,t) = -1 + \int_0^t (\tau y(s,\tau) - x(s,\tau))d\tau \quad , \quad 0 \le s,t \le 1$	P_{10}^2/P_{40}^2	6/10

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Submitted : *13 October 2001*
Revised : *4 April 2002*
Accepted : *14 April 2002*

موضوعات حول تحكم الخطأ باستعمال الحاسب

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خلاصة

إن مفهوم تحكم الخطأ أو التحقق من الحل بالاستعانة بالحاسب موضوع من الحساب العلمي. بإضافة إلى التقريب العددي المعروف فإن التحقق يحد من مجال الخطأ. سوف نستعمل طرق من التحليل الذالي والتفاضل الأوتوماتيكي والتحليل في الفترة لضمان العلاقات. إن بعض الخوارزميات لتحكم دقة الحل المحسوب متوفرة. في هذا المقال نوفر مسح لطرق العلاقات للمعادلات التكاملية.