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A FAST ALGORITHM FOR SOLVING A CLOSE-COUPLED EQUATION

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A recent paper (Delves *et al.* 1979) described a Galerkin method for solving linear Fredholm integral equations of the second kind with weakly singular kernels, for which the total solution time using N expansion functions is $O(N^2 \ln N)$ compared with the standard Galerkin count of $O(N^3)$. We describe here the application of this method which retains this operations count to a close-coupled equation :

$$f(x) = g(x) + \int_{-1}^{1} dy\, K_1(x, y) \int_{-1}^{1} dz\, K_2(y, z)\, f(z).$$

The method provides error estimate which is cheap to compute.

1. Introduction

A recent paper (Delves *et al.* 1979) described a modified Galerkin algorithm to solve weakly singular integral equations of the second kind:

$$f(x) = g(x) + \int_{-1}^{1} \mu(x, y)\, Q(x, y)\, f(y)\, dy \qquad \ldots(1.1)$$

where μ is a smooth function and Q contains the singularity, using a Chebyshev expansion for the solution $f(x)$:

$$f(x) \simeq f_N(x) = \sum_{i=0}^{N} a_i T_i(x) \qquad \ldots(1.2)$$

and fast Fourier transform technique to evaluate the integrals appearing numerically; with operation count $O(N^2 \ln N)$ for setting up equations and $O(N^2)$ for solving the linear equations defining the coefficients a_i, $i = 0, 1, \ldots, N$. Also the algorithm provides an error estimate which is cheap to compute in the sense that it relates the estimate to quantities which are available during the course of the calculation. We show in this paper how this algorithm can be employed to solve integral equation of the form

$$f(x) = g(x) + \int_{-1}^{1} dy\, K_1(x, y) \int_{-1}^{1} dz\, K_2(y, z)\, f(z). \qquad \ldots(1.3)$$

This type of equation arises in quantum scattering (Horn and Fraser 1975) with infinite interval $[0, \infty]$ instead of $[-1, 1]$. Using the transformation

$$\xi = (\eta - \alpha)/(\eta + \alpha), \ \alpha \neq 0$$

the infinite interval $[0, \infty]$ can be converted to $[-1, 1]$. An error analysis of the method is given in section 3, while the efficiency and stability of the method have been tested numerically by an example given in section 4.

2. Description of the Method

The Galerkin method computes the numerical solution of eqn. (1.3) by computing the coefficients a_i of expansion (1.2) as the solution of set of $(N + 1)$ linear algebraic equations:

$$(\bar{D} - \bar{K})\,\mathbf{a} = \bar{\mathbf{g}} \qquad \ldots(2.1)$$

where $\bar{D}$ is $(N + 1 \times N + 1)$ diagonal matrix with elements

$$\bar{D}_{00} = 2, \ \bar{D}_{ii} = 1, \ 1 \leqslant i \leqslant N \qquad \ldots(2.2)$$

$\bar{\mathbf{g}}$ is an $(N + 1)$ vector with elements $\bar{g}_i$:

$$\bar{g}_i = \frac{2}{\pi} \int_{-1}^{1} dx\, g(x)\, T_i(x)/(1 - x^2)^{1/2}, \qquad i = 0, 1, \ldots, N \qquad \ldots(2.3)$$

and $\bar{K}$ is $(N + 1 \times N + 1)$ matrix with elements

$$\bar{K}_{ij} = \frac{2}{\pi} \int_{-1}^{1} dx\, T_i(x)/(1 - x^2)^{1/2} \int_{-1}^{1} dy\, K_1(x, y) \int_{-1}^{1} dz\, K_2(y, z)\, T_j(z),$$

$$i, j = 0, 1, \ldots, N. \qquad \ldots(2.4)$$

Define the two functions

$$B(x, y) = K_1(x, y)\,(1 - y^2)^{1/2} \quad \text{and} \quad C(y, z) = K_2(y, z)\,(1 - z^2)^{1/2}$$

with Chebyshev expansions

$$B(x, y) = \sum_{i,j=0}^{\infty}{}' \bar{B}_{ij} T_i(x)\, T_j(y) \qquad \ldots(2.5)$$

$$C(y, z) = \sum_{i,j=0}^{\infty}{}' \bar{C}_{ij} T_i(y)\, T_j(z) \qquad \ldots(2.6)$$

(Σ' denotes a sum whose first term is halved) with Chebyshev coefficients

$$\bar{B}_{ij} = \frac{4}{\pi^2} \int_{-1}^{1} dx\, T_i(x)/(1-x^2)^{1/2} \int_{-1}^{1} dy\, K_1(x, y)\, T_j(y) \qquad \ldots(2.7)$$

$$\bar{C}_{ij} = \frac{4}{\pi^2} \int_{-1}^{1} dy\, T_i(y)/(1-y^2)^{1/2} \int_{-1}^{1} dz\, K_2(y, z)\, T_j(z) \qquad \ldots(2.8)$$

and hence satisfy bounds of the form (see Bain and Delves 1977):

$$|\bar{B}_{ij}| \leqslant W_B \hat{i}^{-\alpha} \hat{j}^{-\beta} \qquad (i, j \geqslant 0) \qquad \ldots(2.9)$$

$$|\bar{C}_{ij}| \leqslant W_C \hat{i}^{-\gamma} \hat{j}^{-\delta} \qquad (i, j \geqslant 0) \qquad \ldots(2.10)$$

where

$$\hat{i} = \begin{cases} i, & i > 0 \\ 1, & i = 0 \end{cases}$$

and W_B, W_C are constants. The coefficients α, β and γ, δ depend on the analyticity properties (the smoothness) of $B(x, y)$ and $C(y, z)$ respectively, and so we should expect for smooth $K_1(x, y)$ and $K_2(y, z)$, α and γ are large but β and δ are small. Substituting eqns. (2.5) and (2.6) into (2.4) we thus have

$$\bar{K}_{ij} \simeq K_{ij} = {\sum_{r=0}^{N}}' \left(\frac{\pi}{2} \bar{B}_{ir}\right) \left(\frac{\pi}{2} \bar{C}_{rj}\right) \qquad \ldots(2.11)$$

hence

$$\bar{K} \simeq K = \bar{B} \,.\, \bar{C} \qquad \ldots(2.12)$$

where $\bar{B}$ and $\bar{C}$ are square matrices of order $(N+1)$ with elements defined by

$$\left(\frac{\pi}{2} \bar{B}_{ij}\right) \text{ and } \left(\frac{\pi}{2} \bar{C}_{ij}\right)$$

respectively. The solution of eqn. (1.3) may now be reduced into two parts : First, the evaluation of the coefficients $\bar{g}_i$ and $\bar{B}_{ij}$, $\bar{C}_{ij}$, $i, j = 0, 1, \ldots, N$ numerically and we refer to the fast algorithm (Delves *et al.* 1979) to effectively approximate the integrals (2.3), (2.7) and (2.8), it does this by considering the fact that $\bar{g}_i$ are Chebyshev coefficients in expansion:

$$g(x) = {\sum_{i=0}^{\infty}}' \bar{g}_i T_i(x) \qquad \ldots(2.13)$$

while relating $\bar{B}_{ij}$ to Chebyshev coefficients $\overline{K1}_{ij}$, $\bar{h}_i$ in expansions of

$$K_1(x, y),\ (1 - y^2)^{1/2},$$

and $\bar{C}_{ij}$ to Chebyshev coefficients $\overline{K2}_{ij}$, $\bar{h}_i$ in expansions of $K_2(y, z)$, $(1 - y^2)^{1/2}$ where

$$K_1(x, y) = \sum_{i,j=0}^{\infty}{}' \overline{K1}_{ij} T_i(x)\, T_j(y) \qquad \ldots(2.14)$$

$$K_2(y, z) = \sum_{i,j=0}^{\infty}{}' \overline{K2}_{ij} T_i(y)\, T_j(z) \qquad \ldots(2.15)$$

where

$$\overline{K1}_{ij} = \frac{4}{\pi^2} \int_{-1}^{1} dx T_i(x)/(1 - x^2)^{1/2} \int_{-1}^{1} dy K_1(x, y)\, T_j(y)/(1 - y^2)^{1/2}, \qquad \ldots(2.16)$$

$$\overline{K2}_{ij} = \frac{4}{\pi^2} \int_{-1}^{1} dx T_i(y)/(1 - y^2)^{1/2} \int_{-1}^{1} dz K_2(y, z)\, T_j(z)/(1 - z^2)^{1/2}, \qquad \ldots(2.17)$$

$$(1 - y^2)^{1/2} = \sum_{i=0}^{\infty}{}' \bar{h}_i T_i(y). \qquad \ldots(2.18)$$

Use the fast Fourier transform technique (FFT) with operation count $O(N^2 \ln N)$ to evaluate numerically $\overline{K1}_{ij}$ and $\overline{K2}_{ij}$, $i, j = 0, 1, \ldots, N$ and $O(N \ln N)$ to evaluate numerically $\bar{g}_i$, $i = 0, 1, \ldots, N$, while $\bar{h}_i$ can be estimated exactly (Delves *et al.* 1979); [$O(N^2 \ln N)$ operation count for setting up the matrix $\bar{D} - \bar{K}$]. Secondly, the solution of algebraic eqns. (2.1) and this we do using the iterative procedure (Delves 1977a) in $O(N^2)$ operations.

3. Error Analysis

The error in the numerical solution $e_N(x) = f(x) - f_N(x)$ contains three distinct components:

(a) The "truncation error" due to cutting off the expansion (1.2) at the Nth term and this is represented by $N \mid a_N \mid$ (see Delves 1977b).

(b) The "discretization error" which can be written as (see Delves 1977b)

$$\| \delta a \| \sim Q\, [\| \delta K \|\, \| \mathbf{a} \| + \| \delta \mathbf{g} \|]/[1 - Q \| \delta K \|] \qquad \ldots(3.1)$$

where $Q = \| (D - K)^{-1} \|$. From Delves (1977b) a rough estimate for Q can be taken to be

$$Q \sim \| \mathbf{g} \| / \| \mathbf{a} \| \qquad \ldots(3.2)$$

while δK is the error represented in the matrix $D - K$ and $\delta \underline{\mathbf{g}}$ is the error in the vector $\mathbf{g}$. In case of $\delta \underline{\mathbf{g}}$ it is a quadrature error while in case δK, it has two components:

(i) "product error", represented by δK_p, due to the multiplication of the two matrices B and C [eqn. (2.12)] having quadrature errors represented by δB and δC;

(ii) "truncation error", represented by δK_T, due to truncating the series (2.11) at the Nth term.

(c) There are also errors arising from the numerical solution of the linear equations, and from round off error. In practice the Galerkin equations are well conditioned, and may in any case be made arbitrarily small; we do not consider it further.

Hence from (a) and (b)

$$| e_N | \sim N \, | a_N | + \| \delta \underline{\mathbf{a}} \|. \qquad \ldots(3.3)$$

The truncation error of (a) and the quadrature error of (b) were previously considered explicitly in Delves (1977b) and Delves *et al.* (1979) in which discussion remains valid subject to the provision of appropriate estimates for the error norm $\| \delta K \|$ which we now consider explicitly.

(i) *Product error* δK_p

From eqn. (2.12)

$$\delta K_p = (B + \delta B)(C + \delta C) - BC \sim B \,.\, \delta C + C \,.\, \delta B$$

then

$$\| \delta K_p \| \sim \| B \| \, \| \delta C \| + \| C \| \, \| \delta B \| \qquad \ldots(3.4)$$

where from Delves *et al.* (1979),

$$\| \delta B \| \sim \frac{\pi}{2} N \, \| \bar{\mathbf{h}} \|_\infty \left(| K1_{N0} | + | K1_{0N} | \right) \qquad \ldots(3.5)$$

$$\| \delta C \| \sim \frac{\pi}{2} N \, \| \mathbf{h} \|_\infty \left(| K2_{N0} | + | K2_{0N} | \right) \qquad \ldots(3.6)$$

$\bar{\mathbf{h}}$ is an $(N + 1)$ vector with elements $\bar{h}_i$, $i = 0, 1, \ldots, N$.

(ii) *Truncation error* δK_T

From eqn. (2.11)

$$| (\delta K_T)_{ij} | \leqslant \frac{\pi^2}{4} \sum_{r=N+1}^{\infty} | \bar{B}_{ir} | \; | \bar{C}_{rj} |$$

using the bound given by (2.9) and (2.10)

$$| (\delta K_T)_{ij} | \leqslant \frac{\pi^2}{4} W_B W_C \hat{i}^{-\alpha} \hat{j}^{-\delta} \sum_{r=N+1}^{\infty} r^{-(\beta+\gamma)}$$

$$= \frac{\pi^2}{4} W_B W_C \hat{i}^{-\alpha} \hat{j}^{-\delta} N^{1-(\beta+\gamma)}/[(\beta + \gamma) - 1]$$

$$\| \delta K_T \|_\infty \leqslant \frac{\pi^2}{4} W_B W_C N^{1-(\beta+\gamma)} [2 + 1/(\delta - 1)]/[(\beta + \gamma) - 1]$$

$$\| \delta K_T \|_\infty \sim \frac{\pi^2}{2} N \, | B_{0N} | \; | C_{N0} | . \quad \ldots(3.7)$$

Adding (3.4) and (3.7) we compute approximation for $\| \delta K \|_\infty$, and hence an estimate for $\| \delta \underline{\mathbf{a}} \|_\infty$ is available provided $\| \delta \underline{\mathbf{g}} \|$ is taken to be either $| g_N |$ when $g(x)$ is smooth or $N \, | g_N |$ when $g(x)$ is not smooth (see Delves 1977b, Delves *et al.* 1979)

A Bound on the Elements of K

Finally, we derive the following bound on $| K_{ij} |$:

Lemma — For α, $\delta > 1$

$$| K_{ij} | \leqslant W_K \hat{i}^{-\alpha} \hat{j}^{-\delta} \qquad (i, j \geqslant 0) \quad \ldots(3.8)$$

where

$$W_K = \frac{\pi^2}{4} W_B W_C \{\tfrac{3}{2} + 1/[(\beta + \gamma) - 1)]\}. \quad \ldots(3.9)$$

PROOF : From (2.11) using the bound given by (2.9) and (2.10)

$$| K_{ij} | \leqslant \frac{\pi^2}{4} {\sum_{r=0}^{N}}' | \bar{B}_{ir} | \; | \bar{C}_{rj} |$$

$$\leqslant \frac{\pi^2}{4} W_B W_C \hat{i}^{-\alpha} \hat{j}^{-\delta} {\sum_{r=0}^{N}}' r^{-(\beta+\gamma)}$$

$$\leqslant \frac{\pi^2}{4} W_B W_C \hat{i}^{-\alpha} \hat{j}^{-\delta} \{\tfrac{3}{2} + 1/[(\beta + \gamma) - 1]\}$$

and hence lemma follows.

4. Numerical Example

In order to have an idea about the computational efficiency and stability of the method described in this paper, we consider as an example the integral eqn. (1.3) subject to

$$K_1(x, y) = x^2 + xy$$

$$K_2(y, z) = 2z^2 + 2z \sin(yz) + 1 + y \cos(yz)$$

$$g(x) = e^{x^2} - 4e\{x^2 + x(\sin(1) - \cos(1))\}$$

Solution: $f(x) = e^{x^2}$

The computed error σ_N are defined to be

$$\sigma_N = \left\{ \sum_{j=0}^{N} e_N^2(x_j)/N \right\}^{1/2} \approx \left\{ \int_{-1}^{1} e_N^2(x)\, dx \right\}^{1/2} \qquad \ldots(4.1)$$

where $x_j = \cos(j\pi/N)$, $j = 0, 1, \ldots, N$. The second and third column in the table represents two different ways to compute σ_N; while in the second column σ_N is computed directly by considering $e_N(x_j) = f(x_j) - f_N(x_j)$, in the third column eqn. (3.3) is used as an estimate for $|e_N|$.

Computed results for the numerical example

N	σ_N directly	σ_N using eqn. (3.3)
2	6.4×10^{-1}	—
3	6.3×10^{-2}	2.5×10^{-1}
4	1.3×10^{-1}	3.0×10^{0}
5	2.8×10^{-3}	6.8×10^{-2}
6	9.1×10^{-3}	9.4×10^{-3}
7	5.0×10^{-5}	3.2×10^{-4}
8	5.5×10^{-5}	8.7×10^{-4}
9	9.2×10^{-7}	2.6×10^{-7}
10	2.7×10^{-5}	2.2×10^{-5}
11	1.8×10^{-8}	1.5×10^{-8}
12	1.1×10^{-6}	8.4×10^{-7}
13	3.7×10^{-10}	3.3×10^{-9}
14	4.0×10^{-8}	3.0×10^{-8}
15	5.0×10^{-10}	1.8×10^{-9}
16	1.3×10^{-9}	2.5×10^{-9}

From the numerical results obtained, we can make the following comments:

(1) The very rapid convergence obtained shows that we indeed succeeded in applying Galerkin technique on an integral equation of "non standard" type given by (1.3).

(2) The error estimates obtained reflect the actual error extremely well.

(3) The method described in this paper takes operations count:

Set up equations: $O(N^2 \ln N)$

Iterative solution: $O(N^2)$

hence it takes total solution time $O(N^2 \ln N)$ while standard Galerkin calculation has an operations count of $O(N^3)$ for both setting up and solving the linear equations.

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