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The collocation variational method for solving Fredholm integral equations and an application to potential scattering

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Abstract. We have formulated a simple method, the collocation variational method, to solve the Fredholm integral equations of the second kind and have proved its convergence. As applications, we have shown that the method can be usefully employed not only to solve the Fredholm equations, but also some other equations reducible to it, and, in particular, the Lippman–Schwinger equation in potential scattering.

1. Introduction

The problem of obtaining the solution $f(x)$, of the Fredholm integral equation of the second kind

$$f(x)-\lambda\int_a^b k(x, y)f(y)\,\mathrm{d}y=g(x) \tag{1}$$

arises in many areas of mathematics and physics and, in particular, in the theory of potential scattering. Equation (1) can be written as a functional equation

$$(1-\lambda K)f=g \tag{2}$$

in some function space H. We assume H to be the Hilbert space of square integrable functions of x_j; i.e. g is square integrable and a square integrable solution f of (2) exists.

A simple method, the collocation method (Noble 1973), to solve (1) stems from the original considerations of Fredholm (Riesz and Nagy 1971). In this method one solves the following set of algebraic equations:

$$f_i-\lambda\sum_{j=1}^{n}\omega_j k(x_i, y_j)f_j=g(x_i) \tag{3a}$$

where x_j and ω_j, $j=1$ to n, are the roots and weights of a suitable quadrature formula. For a compact K generated by a sufficiently smooth $k(x, y)$, it has been shown that f_i converge to $f(x_i)$, $i=1$ to n. The approximate value $f_n^{\mathrm{c}}(x)$ of $f(x)$ at points other than x_i, $i=1$ to n, is usually obtained from (Kantorovich and Kirylov 1964):

$$f_n^{\mathrm{c}}(x)=g(x)+\lambda\sum_{j=1}^{n}\omega_j k(x, y_j)f_j. \tag{3b}$$

The equation (3b) is naturally suggested by (1) itself. However, one may use any suitable interpolation formula to obtain an approximate value of $f(x)$ (Noble 1973).

The Bubnov–Galerkin method (BG) (Mikhlin 1964) attempts to solve (2) by solving the following set of equations:

$$\sum_{j=1}^{n} \alpha_j \langle \psi_i | (1-\lambda K) \psi_j \rangle = \langle \psi_i | g \rangle \qquad (4)$$

where $\{\psi_i\}$ is an orthonormal basis in H and $\langle \cdot | \cdot \rangle$ denotes the scalar product in H. The approximate value f_n^{v} of f in this method is given by $f_n^{\mathrm{v}} = \Sigma_{j=1}^{n} \alpha_j \psi_j$. For a compact K this method is known to yield a convergent process; i.e., $f_n^{\mathrm{v}} \xrightarrow[n\to\infty]{} f$ in the norm $\|\cdot\|$ of H (Mikhlin 1964). The operator norm in H will also be denoted by $\|\cdot\|$.

Although both of these methods provide convergent procedures to determine f, from the computational point of view they both have some disadvantages. The rate of convergence of the collocation method is rather slow. As a result one needs to solve quite large matrix equations in order to achieve a reasonable degree of accuracy (Walters 1971, Holt and Santoso 1973), which is, in turn, compromised in dealing with these large matrices. On the other hand, the rate of convergence of BG is usually quite rapid, but at the expense of evaluating the double integrals which appear in the left-hand side of (4). The labour involved in evaluating these double integrals is usually too much to justify the use of BG in many realistic problems. For this reason, for example, the Schwinger variational method in potential scattering, which is equivalent to BG (Singh and Stauffer 1974), has been unpopular and the less satisfactory Kohn method is preferred (Mott and Massey 1965).

For these reasons an intermediate method, which we shall call the collocation variational method (CV), has been found useful (Conkie and Singh 1969). In this method one takes a basis $\{\psi\}$ in H and solves the following set of equations:

$$\sum_{j=1}^{n} \tilde{\alpha}_j \left(\psi_j(x_i) - \lambda \int_a^b k(x_i, y) \psi_j(y) \, \mathrm{d}y \right) = g(x_i) \qquad (5)$$

and $f_n^{\mathrm{cv}} = \Sigma_{j=1}^{n} \tilde{\alpha}_j \psi_j$ is taken to be the approximate value of f. Computationally, the method is promising in that it appears to be almost as rapidly convergent as BG with the same basis set, and involves much less labour than either BG or the collocation method (Conkie and Singh 1969). However, no rigorous analysis of CV has been attempted yet. In the present paper we prove the convergence of CV in solving (1) and present some situations where the method can be usefully employed.

2. The convergence of the collocation variational method

Let C^n be the n-dimensional space of column vectors with complex components and norm $\|\cdot\|_n$ defined by $\|\alpha\|_n = (\Sigma_{j=1}^{n} |\alpha_j|^2)^{1/2}$ for each α in C^n. The norm of an operator A on C^n, $\sup \|A\alpha\|_n / \|\alpha\|_n$, will also be denoted by $\|A\|_n$. In the sequel we shall need the following well known results which are valid not only in C^n but also in any other Banach space with obvious replacements of definitions (Mikhlin 1964).

Result 1. Let $A, \epsilon: C^n \to C^n$, A^{-1} exists and $\|A^{-1}\epsilon\|_n < 1$. Then $(A+\epsilon)^{-1}$ exists and

$$\|(A+\epsilon)^{-1} - A^{-1}\|_n \leq \frac{\|A^{-1}\epsilon\|_n \|A^{-1}\|_n}{1 - \|A^{-1}\epsilon\|_n}.$$

As a simple consequence of this result, the following result is obtained.

Result 2. If $A\alpha=\beta$, where β is in C^n, has a solution, then $(A+\epsilon)\tilde{\alpha}=\beta+\delta$, where δ is in C^n, also has a solution.

From these two results one also has the following third result.

Result 3. Let ϵ_m, δ_l be the sequences of matrices and vectors respectively in C^n such that $\|\epsilon_m\|_n \xrightarrow[m\to\infty]{} 0$ and $\|\delta_l\|_n \xrightarrow[m\to\infty]{} 0$, then $(A+\epsilon_m)\tilde{\alpha}_{ml}=\beta+\delta_l$ has a solution for sufficiently large m and each l and $\|\tilde{\alpha}_{ml}-\alpha\|_n \xrightarrow[m,l\to\infty]{} 0$.

Now (4) can be written as a matrix equation in C^n as follows:

$$(1_n-\lambda B)\alpha=\beta \tag{6}$$

where 1_n is the $n\times n$ unit matrix, B is the matrix with elements $(B)_{ij}=\langle\psi_i|K\psi_j\rangle$, $i,j=1$ to n; α,β are vectors in C^n with components α_j and $\langle\psi_j|g\rangle$, $j=1$ to n, respectively. It is easy to check that $\lim_{n\to\infty}\|(1_n-\lambda B)^{-1}\|_n=\|(1-\lambda K)^{-1}\|$, i.e. $(1_n-\lambda B)^{-1}$ remains bounded in the limit of large n. Consider the following set of equations:

$$\sum_{j,k=1}^{n}\psi_i^*(x_k)w_k\left(\psi_j(x_k)-\lambda\int_a^b k(x_k,y)\psi_j(y)\,\mathrm{d}y\right)\tilde{\alpha}_j=\sum_{k=1}^{n}\psi_i^*(x_k)w_kg(x_k) \tag{7}$$

where x_k and w_k are the roots and weights of some 'reasonable' numerical quadrature formula by which we mean that $|\int_a^b f(x)\,\mathrm{d}x-\Sigma_{k=1}^n w_kf(x_k)|\leq M/n^{1+\epsilon}$, $M<\infty$ and $\epsilon>0$.

Equation (7) can aso be written as:

$$J^+W(J-\lambda C)\tilde{\alpha}=J^+WG \tag{8}$$

where J is a matrix with elements $(J)_{ij}=\psi_j(x_i)$, $i,j=1$ to n; W is a diagonal matrix with elements $(W)_{ij}=w_i\delta_{ij}$ and J^+ is the Hermitian conjugate of J. C is another $n\times n$ matrix with $(C)_{ij}=\int_a^b k(x_i,y)\psi_j(y)\,\mathrm{d}y$ and $G_j=g(x_j)$.

We may also write equation (7) as:

$$[1_n+\epsilon_n^1-\lambda(B+\epsilon_n^2)]\tilde{\alpha}=\beta+\delta_n \tag{9}$$

in analogy with equation (6), with ϵ_n^1 and ϵ_n^2 being $n\times n$ matrices and δ_n a vector in C^n. From equation (8) $\epsilon_n^1=J^+WJ-1_n$, $\epsilon_n^2=J^+WC-B$ and $\delta_n=J^+WG-\beta$.

By virtue of the rapid convergence of the quadrature formula, one has that $\lim_{n\to\infty}\|\epsilon_n^1\|_n=\lim\|\epsilon_n^2\|_n=\lim_{n\to\infty}\|\delta_n\|_n=0$. To show this, for example,

$$\|\epsilon_n^1\|_n^2\leq\mathrm{Tr}[\epsilon_n^{1+}\epsilon_n^1]=\sum_{i,j}|\epsilon_{ij}|_n^2\leq n^2\sup|\epsilon_{ij}|^2=n^2\left(\frac{M^2}{n^{2+2\epsilon}}\right)=\frac{M^2}{n^{2\epsilon}}.$$

Thus $\lim_{n\to\infty}\|\epsilon_n^1\|_n=0$. Similar demonstrations can be used for $\|\epsilon_n^2\|_n$ and $\|\delta_n\|_n$. We have the following lemma.

Lemma 1. For sufficiently large n, J^+W is invertible.

Proof. From equations (8) and (9) $J^+WJ=1_n+\epsilon_n^1$. Since $\|\epsilon_n^1\|_n \xrightarrow[n\to\infty]{} 0$ from result 1, $(1_n+\epsilon_n^1)^{-1}$ exists for n so large as $\|\epsilon_n^1\|_n<1$. Right inverse of $J^+W=J(1_n+\epsilon_n^1)^{-1}$ for $J^+WJ(1_n+\epsilon_n^1)^{-1}=(1_n+\epsilon_n^1)(1_n+\epsilon_n^1)^{-1}=1_n$. Since J^+W is a square matrix, $J(1_n+\epsilon_n^1)^{-1}$ is its left inverse also.

Theorem 1. If (2) has a solution f in H, K is compact and x_k, $k=1$ to n, are the roots of a 'reasonable' quadrature formula, then for sufficiently large n, the set of equations given by (5) has a solution f_n^{cv}, and $\|f-f_n^{cv}\| \xrightarrow[n\to\infty]{} 0$.

Proof. For a given $\epsilon > 0$ let n be so large as

(a) (4) has a solution and that $\|f-f_n^{v}\| < \frac{1}{2}\epsilon$;

(b) $\|(1_n-\lambda B)^{-1}(\epsilon_n^1-\lambda\epsilon_n^2)\|_n < 1$ and $\|\alpha-\bar{\alpha}\|_n < \frac{1}{2}\epsilon$;

(c) $\|\epsilon_n^1\|_n < 1$.

We know that (2) can be satisfied (Mikhlin 1964). Existence of $(1_n-\lambda B)^{-1}$ is implied by (a). The first part of (b) can be satisfied by observing that $\|(1_n - \lambda B)^{-1}\|_n$ has a bounded limit and $\|\epsilon_n^1\|_n$ and $\|\epsilon_n^2\|_n$ converge to zero. This implies that (9) has a solution $\bar{\alpha}$. The second part of (b) can now be obtained by using result 3. We can obtain (c) by observing, again, that $\lim_{n\to\infty}\|\epsilon_n^1\|_n = 0$. Thus n can be increased until (a), (b) and (c) are all satisfied.

Now one has that

$$\left\|f_n^{v}-\sum_{j=1}^{n}\bar{\alpha}_j\psi_j\right\| = \left\|\sum_{j=1}^{n}(\alpha_j-\bar{\alpha}_j)\psi_j\right\| = \|\alpha-\bar{\alpha}\|_n < \tfrac{1}{2}\epsilon.$$

It is now obvious that $\|f-\sum_{j=1}^{n}\bar{\alpha}_j\psi_j\| < \epsilon$.

From lemma 1 and (c), $(J^+W)^{-1}$ exists. Multiplying both sides of (9) by $(J^+W)^{-1}$ one has that (9) is identical with (5) with $\bar{\alpha}$ replacing $\tilde{\alpha}$. Thus the set of equations given by (5) has a solution for sufficiently large n and $\|f-f_n^{cv}\| < \epsilon$.

From the proof of the theorem it is clear that whenever BG is applicable and the roots of a reasonable numerical quadrature formula are available, then CV is also applicable. In particular, the domain of integration in (1) can be enlarged to infinitely large intervals and several dimensions, as long as the operator K defined by the kernal is compact.

In the following we give a few examples where CV can prove useful in solving an equation which, as such, is not a Fredholm equation of the second kind but is reducible to one.

3. Applications

For the first application, let

$$(T+A)f = g \tag{10}$$

be defined in H where T is a symmetric operator bounded below by a positive constant, and $T^{-1}A$ is compact in H. Define a scalar product: $[u|v] = \langle u|Tv\rangle$ for each u, v in $D(T)$ and complete $D(T)$ with respect to this scalar product. Thus, one obtains a complete Hilbert space H_0. Equation (10) reduces to the form of (2) in H_0 and can be solved by BG. It is now easy to check that (10) can also be solved by CV: i.e. f can be approximated by $\sum_{j=1}^{n}\alpha_j\psi_j$ where

$$\sum_{j=1}^{n}\alpha_j\{[(T+A)\psi_j](x_i)\} = g(x_i). \tag{11}$$

A useful example of an equation of the form of (10) is the Sturm–Liouville equation which can be solved by CV.

As another application we show that the problem of potential scattering can be treated by CV. In fact our interest in the method was motivated from this problem, for the application of the Schwinger variational method is tedious and other methods attempted proved unsatisfactory.

For the purpose of illustration we consider the Lippman–Schwinger equation for a partial wave:

$$\psi = \psi_0 - zG_0 v\psi \tag{12}$$

where ψ_0 is the free-state function, ψ the scattering-state standing-wavefunction, G_0 is the principal part of the free-particle Green function, $v>0$ is the interacting potential and z is the potential strength which could be positive or negative. If v is free from a long-range tail and from strong singularities then (12) can be cast in $H=L^2(R^+)$ as follows. Let $f=(\sqrt{v})\psi$, $g=(\sqrt{v})\psi_0$ and $K=(\sqrt{v})G_0(\sqrt{v})$. f, g are in H and K is a compact operator on H (Scadron *et al* 1964). By multiplying both sides of (12) with $\sqrt{v}$ one has that

$$(1+zK)f=g \tag{13a}$$

and the tangent t of the phase shift is given by

$$z^{-1}t = -\int_0^\infty \psi_0(r)v(r)\psi(r)\,\mathrm{d}r = -\langle g|f\rangle. \tag{13b}$$

(13a) can be solved by BG which is equivalent with the Schwinger variational method (Holt and Santoso 1973, Singh and Stauffer 1974). From the theorem it can also be solved by CV; i.e. by solving

$$\sum_{j=1}^{n} \alpha_i\left(\phi_j(r_i)+z\int_0^\infty [\sqrt{v(r_i)}]G_0(r_i,r_1)[\sqrt{v(r_1)}]\phi_j(r_1)\,\mathrm{d}r_1\right)=g(r_i) \qquad i=1,\ldots,n; \tag{14}$$

implies that $\|f-\Sigma_{j=1}^{n}\alpha_j\phi_j\| \xrightarrow[n\to\infty]{} 0$, and hence $z^{-1}t_n = -\langle g|\Sigma_{j=1}^{n}\alpha_j\phi_j\rangle \xrightarrow[n\to\infty]{} z^{-1}t$. Here r_i could be taken to be the roots of the Gauss–Legendre quadrature formula. Now let $\{\psi_i\}$ be a set such that $\{(\sqrt{v})\psi_i\}$ is a basis in H. Then (14) can be written as:

$$\sum_{j=1}^{n} \alpha_j\left([\sqrt{v(r_i)}]+z\int_0^\infty [\sqrt{v(r_i)}]G_0(r_i,r_1)v(r_1)\psi_j(r_1)\,\mathrm{d}r_1\right)=[\sqrt{v(r_i)}]\psi_0(r_i)$$
$$i=1,\ldots,n; \tag{15a}$$

and t_n is given by

$$z^{-1}t_n=\sum_{j=1}^{n}\alpha_j\int_0^\infty \psi_0(r)v(r)\psi_j(r)\,\mathrm{d}r. \tag{15b}$$

Since $v(r_i)>0$ for each i, (15a) reduces to

$$\sum_{j=1}^{n}\alpha_j\left(\psi_j(r_i)+z\int_0^\infty G_0(r_i,r_1)v(r_1)\psi_j(r_1)\,\mathrm{d}r_1\right)=\psi_0(r_i) \qquad i=1,\ldots,n. \tag{16}$$

Thus, t can be approximated by t_n which can be obtained by solving (16).

In the foregoing analysis we considered the case of an interaction of a definite sign. However, the procedure remains unmodified when v is indefinite, other conditions on it remaining the same. In that case v can be partitioned as $v=ACA$, where A is an invertible operator and C is bounded (Kato 1966), and one defines $f=A\psi$, $g=A\psi_0$ and $K=AG_0AC$. It is easy to check now that one still has to solve (16) and obtain t_n from (15b).

It is worth pointing out here that the convergence of the Schwinger variational method has as yet been established only for interactions of a definite sign (Singh and

Stauffer 1974, 1975). Attempts at proving the convergence of this method to solve (12) with indefinite v runs into trouble because of the appearance of C. However, a slight modification of the method can be used to obtain a solution. In that case one should use A explicitly in calculation and solve (13a) directly. Although no significant complications result because of this modification, the method is still as tedious as the Schwinger method for a v of a definite sign. On the other hand CV requires no modification in the computation procedure. In addition, CV can be used to evaluate the scattering amplitude. In that case one encounters multiple integrals in (16) and $\{r_i\}$ has to be replaced by $\{(\boldsymbol{r})_i\}$.

4. Discussion

We have shown that a simple method, the collocation variational method, is capable of handling the Fredholm integral equations of the second kind and some other equations related to it. The computational simplicity of the method indicates that it can be usefully employed to solve equations which are otherwise treated by the collocation method, or by the Bubnov–Galerkin method. In particular the method appears to be promising in solving the Lippman–Schwinger equation. This equation can be solved also by the Schwinger variational method, by the Kohn variational method or the collocation method. The rate of convergence of the collocation method is very slow. Although the Kohn method computationally is quite easy, convergence results known about the method are rather unsatisfactory (Singh and Stauffer 1974, Nuttal 1969). On the other hand the Schwinger method, or its modification presented in the present article, is computationally difficult. Thus, the present method has several advantages over the other methods used to solve potential scattering problems.

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