JOURNAL OF COMPUTATIONAL PHYSICS 37, 268–273 (1980)

Note

Improving the Convergence of Solutions to the Fredholm Integral Equation of the First Kind

I. INTRODUCTION

The equation,

$$g(y) \pm \varepsilon(y) = \int K(y, x) f_\epsilon(x)\, dx, \tag{1A}$$

comes up frequently in the measurement of physical quantities. The precise meaning of this equation is

$$g_0(y) + \delta(y) = \int K(y, x) f(x)\, dx, \tag{1B}$$

where $g_0(y)$ is the "true" unknown function, $g(y) = g_0(y) + \delta(y)$ is the average value as measured experimentally, the statistical average $\langle \delta(y) \rangle = 0$, and $\langle \delta^2(y) \rangle = \varepsilon^2(y)$. We denote by $f_\epsilon(x)$ the solution of Eq. (1) obtained with the experimental values of $g(y)$ and by $f_0(x)$ the presumed "exact" unknown which would be the solution if $\delta(y) = 0$ everywhere. We assume that $f_0(x)$ exists and is unique. We attempt to use $g(y)$ to obtain an approximation to $f_0(x)$.

If the "left-iterated kernel" K_L and the "right-iterated kernel" K_R are

$$K_L(x', x) = \int K(y, x')\, K(y, x)\, dy, \qquad K_R(y', y) = \int K(y', x)\, K(y, x)\, dx, \tag{2}$$

we may attempt to expand $f_0(x)$ and $g_0(y)$ in series of the eigenfunctions of K_L and K_R [1–3]:

$$\phi_n(x') = \mu_n \int K_L(x', x)\, \phi_n(x)\, dx, \qquad \xi_n(y') = \mu_n \int K_R(y', y)\, \xi_n(y)\, dy. \tag{3}$$

The $\phi_n(x)$ and $\xi_n(y)$ are orthonormal sets of functions and related by [2]

$$\phi_n(x) = \mu_n^{1/2} \int K(y, x)\, \xi_n(y)\, dy. \tag{4}$$

0021-9991/80/110268-06$02.00/0

The two expansions are related by

$$g_0(y) = \sum_n g_n^0 \xi_n(y),$$
$$f_0(x) = \sum_n f_n^0 \phi_n(x) = \sum \mu_n^{1/2} g_n^0 \phi_n(x), \tag{5}$$

where

$$g_n^0 = \int g_0(y)\, \xi_n(y)\, dy, \qquad f_n^0 = \int f_0(x)\, \xi_n(x)\, dx. \tag{6A}$$

For later convenience we define

$$\delta_n = \int \delta(y)\, \xi_n(y)\, dy. \tag{6B}$$

It is well known that a useful approximation $f_N(x)$ to $f_0(x)$ is given by [2]

$$f_N(x) = \sum_{N=1}^{N} \mu_n^{1/2} g_n \phi_n(x), \tag{7}$$

where $g_n = g_n^0 + \delta_n$ replaces the g_n^0 of Eq. (5), and where N is usually small. Now the sum in Eq. (5) must be infinite if the solution $f(x)$ is to be unique, but if the sum in Eq. (7) were extended to an infinite number of terms, it would not be likely to converge. Nonetheless, the finite sum, properly terminated, frequently gives a useful approximation to $f(x)$.

In fact, if the solution for f_0 is to be unique, there must be many large eigenvalues μ_n. If $g_0(y)$ and $f_0(x)$ are smooth, g_n^0 and f_n^0 will generally be largest for n corresponding to small μ_n. However, the measured $g(y)$ will not be smooth due to the experimental error, so g_n will not in general be small for all small μ_n; in other words, some g_n are dominated by the error. Unfortunately, the terms that are dominated by the error are given the largest weight in the solution due to the factor $\mu_n^{1/2}$ in Eq. (5). The solution is therefore unstable unless the sum is terminated before the error dominates. With the characteristic-function method it is easy to see when to terminate the series, which is probably the major advantage of the method.

An acceptable criterion for including or excluding terms from the sum in Eq. (7) is to exclude those terms for which δ_n in an appreciable fraction of g_n. An estimate of δ_n must be obtained. We define

$$\varepsilon_n^2 \equiv \langle \delta_n^2 \rangle = \int dy\, dy' \langle \delta(y)\, \delta(y') \rangle\, \xi_n(y)\, \xi_n(y'),$$

where $\langle \cdots \rangle$ denotes the statistical average. For many problems the correlation function $\langle \delta(y)\, \delta(y') \rangle$ vanishes very quickly as $y - y'$ increases. In fact, in practice we

know $g(y)$ experimentally only at a finite number of points, and the $\delta(y)$ are frequently essentially uncorrelated at the different points. It is therefore reasonable to approximate ε_n^2 as

$$\varepsilon_n^2 = \int dy \langle \delta^2(y) \rangle \xi_n^2(y) = \int dy \varepsilon^2(y)\, \xi_n^2(y). \tag{8}$$

We then omit terms from Eq. (7) for which ε_n is an appreciable fraction of g_n. In essence, we replace the unknown δ_n by an estimate of $\langle \delta_n^2 \rangle^{1/2}$.

The expected random variation in $f_N(x)$ is

$$\Delta_R^2 \equiv \int \langle [f_N(x) - f_N^0(x)]^2 \rangle\, dx = \int dx \left\langle \left[\sum_{n=1}^{N} \mu_n^{1/2}\, \delta_n \phi_n(x) \right]^2 \right\rangle,$$

where f_N^0 is obtained using g_n^0 in Eq. (7). Under the same approximations used to get Eq. (8),

$$\Delta_R^2 = \int dx\, dy\, \varepsilon^2(y) \left[\sum_n \mu_n^{1/2} \xi_n(y)\, \phi_n(x) \right]^2. \tag{9}$$

While exploring methods of solving the problem outlined in Section III, we found that when $K(y, x)$ is small for some values of x regardless of y, the approximations to f converge too slowly to be useful. The slow convergence, which causes an increased sensitivity to random error, is in part caused (roughly speaking) by an effort to determine f for values of x where inadequate information is available. This situation will be discussed further in Section II and a method for restoring stability (reducing sensitivity to the random error) to the solution established. In Section III we show the improvement obtained in our original problem when the method of Section II is used.

II. Properties of the Standard Solution

We first modify our functions in ways that will not change the form of Eq. (1) but will give us additional freedom in the process of solving the equation. Define

$$\bar{f}(x) = C(x)\, f(x), \qquad \bar{K}(y, x) = K(y, x)/[C(x)], \tag{10}$$

where $C(x)$ is an arbitrary positive function. Equation (1) becomes

$$g(y) \pm \varepsilon(y) = \int \bar{K}(y, x)\, \bar{f}(x)\, dx. \tag{11}$$

Since the form of Eq. (1) is unchanged, the expansions in Eq. (5) will still have the same form, although the functions will naturally be changed.

A feasible and useful procedure for choosing $C(x)$ is to use $C(x)$ to minimize the

random error Δ_R in the first term of the expansion for $\bar{f}(x)$. Keeping only the first term in Eq. (9), we vary

$$\Delta_R^2 = \bar{\mu}_1^2 \int dx \int \bar{\xi}_1^2(y) \left[\int \frac{K(y', x)\, \bar{\xi}_1(y')}{C(x)} dy' \right]^2 dy, \tag{12}$$

subject to the conditions that $\bar{\xi}_1(y)$ be the normalized eigenfunction of $\bar{K}_R$ and that $\int C^2(x)\, dx$ be constant:

$$\int \bar{\xi}_1(y) \frac{K(y, x)\, K(y', x)}{C^2(x)} \bar{\xi}_1(y')\, dy\, dy'\, dx = 1/\bar{\mu}_1,$$
$$\int \bar{\xi}_1^2(y)\, dy = 1, \qquad \int C^2(x)\, dx = 1. \tag{13}$$

The variation is to be taken with respect to $C^2(x)$ and with respect to $\bar{\xi}_1$ and $\bar{\mu}_1$ (which may be treated as independent of C^2 only by introducing the constraints in Eq. (14) through Lagrange multipliers λ_i). After taking the variations and undertaking some manipulation involving the last of Eqs. (13), we get a solution for $C^2(x)$ of

$$C^2(x) = C_0 \left\{ \frac{\lambda_1 \int dy\, dy'\, \xi_1(y)\, K(y, x)\, K(y', x)\, \xi_1(y')}{\lambda_1/\mu_1} \right\}^{1/2}$$
$$= C_0 \mu_1^{1/2} \int dy\, \xi_1(y)\, K(y, x). \tag{14}$$

(We have assumed the integral to be everywhere positive. If it is not, a sign factor must be carried along in the following argument.)

Equation (14) and the first of Eqs. (13) must be solved together for C and ξ_1. Equation (14) may be substituted directly into the first of Eqs. (13) to get $\xi_1(y) = (\sqrt{\mu_1}/C_0) \int dx\, K(y, x)$. If we apply the normalization condition for ξ_1 to this equation, we obtain μ_1, and then by substitution we get ξ_1 and C^2. It is convenient to choose the arbitrary C_0^2 to be $C_0^2 = \int K(y, x)\, K(y, x')\, dy\, dx\, dx'$. We get $\mu_1 = 1$ and

$$\xi_1(y) = \int K(y, x)\, dx \left\{ \int dy' \left[\int K(y', x)\, dx \right]^2 \right\}^{-1/2},$$
$$C^2(x) = \int K(y, x)\, K(y, x')\, dx'\, dy. \tag{15}$$

Thus, in the process of determining the weight function we also determine the first eigenvalue and associated eigenfunction. The solution is completed by using Eqs. (3) and (4) to obtain the remainder of the $\bar{\xi}_n$ and $\bar{\phi}_n$ and Eqs. (5), (6), and (7) to obtain the expansion of f. The point-to-point statistical error is given by the integrand of Eq. (9) (integration over dy retained).

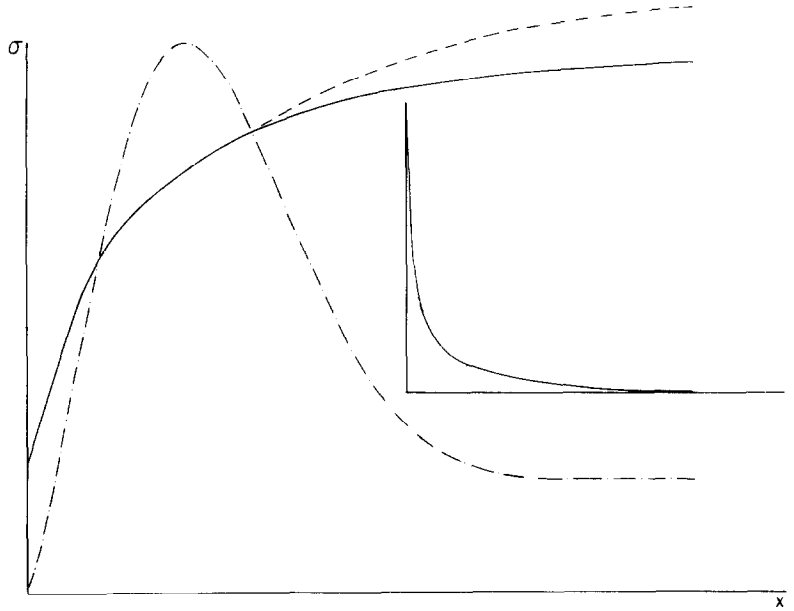

FIG. 1. Exact (model) cross section (solid curve) and solutions of the integral equation with (dashed curve) and without (dot–dash curve) weight functions, using data with 1 % artificial error as described in the text. The inset is the weight function $C(x)$. With the use of weight functions, four terms in the expansion could be kept, as opposed to only two in the unweighted solution.

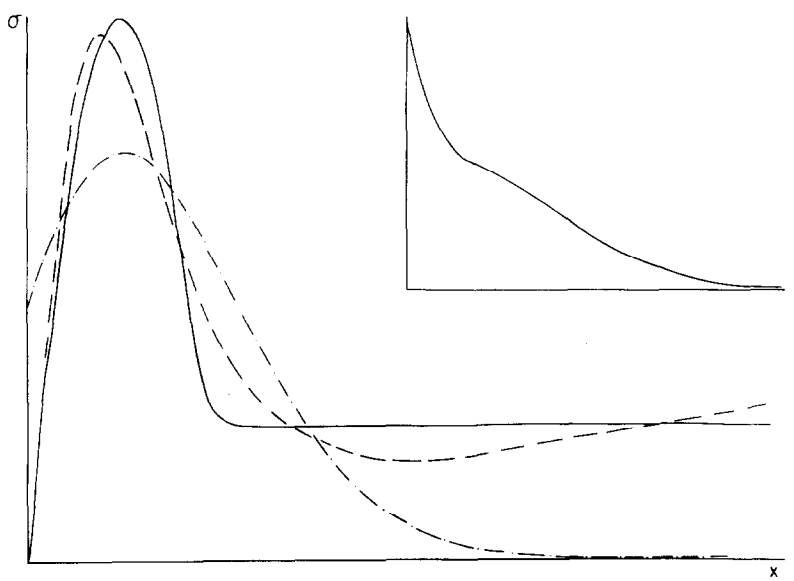

FIG. 2. Same as Fig. 1 with a different exact solution. Four terms could be kept in the weighted and three in the unweighted solution.

III. An Example

To show the improvement that can be obtained by using the weight functions, we display the results for a rather broad kernel of explicit physical interest. The reaction rate R of an ion with a molecule in a drift tube containing a constant electric field E is given by [4]

$$R(E) = \int_{v^*}^{\infty} vg(E, v)\,\sigma(v)\,dv, \tag{16}$$

where

$$g(E, v) = g_0 v\{\exp[-\mu(v - v_d)^2/(2kT_e)] - \exp[-\mu(v + v_d)^2/(2kT_e)]\}, \tag{17}$$

and where $v_d = ME$, $T_e = T_0 + T_1E^2$, and g_0, M, T_0, T_1, μ, and k are constants. As described in Ref. [4], artificial data were generated for Eq. (16) by assuming a $\sigma(v)$, calculating the resulting rate constants, and adding a random relative error of a specified standard deviation. We show in Figs. 1 and 2 typical results of attempting to solve Eq. (16) for σ by the characteristic-function method with and without the use of a weight function. A comparison of the two solutions shows that the improvement is substantial, largely because the use of weight functions permits the retention of a larger number of terms in the expansion. The inclusion of a weight function substantially improves the convergence of the characteristic-function method and in some problems is essential to the success of the method.

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Received: March 14, 1978; revised: May 16, 1979

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