JOURNAL OF COMPUTATIONAL PHYSICS 16, 371–832 (1974)

Numerical Treatment of Singular Integral Equations*

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Received December 12, 1973; May 23, 1974

We present a method for numerically solving a certain class of integral equations. We demonstrate that the technique is directly applicable to equations which have kernels with a particular type of singularity. We also show that this scheme allows one to find the unknown function directly, at any desired value of the argument, without resorting to interpolation. To illustrate the method, we apply it to an integral equation which arises in the theory of intrinsic viscosity of macromolecules. This equation has been dealt with elsewhere, and we compare our results to those already published.

I. INTRODUCTION

In this paper, we present a method for obtaining a numerical solution to an integral equation. It is applicable to equations in which the kernel satisfies

$$\lim_{x \to y} K(x, y) = \infty, \qquad \lim_{x \to y} (x - y) K(x, y) = \text{constant}. \tag{1}$$

We will consider two classes of kernels of the form $K(x - y)$. If the constant in Eq. (1) is zero, we call this a weak singularity. A strong (pole-type) singularity, such as might arise in integral equations obtained from dispersion relations, would yield a nonzero constant in Eq. (1). In this first paper, we consider weakly singular kernels.

Other techniques for solving weakly singular integral equations have been presented by Schlitt [1], Ullman [2], Ullman and Ullman [3], and Bellman *et al.* [4]. A weakly singular integral equation of this type arises in the theory of intrinsic viscosity developed by Kirkwood and Riseman [5]. This is the equation treated by Schlitt in [1]. We consider this equation as an illustrative example, comparing our results to those obtained by Schlitt. We also solve the equation using Ullman's technique [2] and compare these results to our own. For large values of a parameter

† Presented in partial fulfillment of the requirements for the Master of Science degree.

* Research partially supported by grants from the Research Corporation and institutional Grant #GU 3220.

in the equation, an analytic first approximation can be obtained. Our results are also compared to this analytic form. Corrections to this first approximation are also discussed.

II. Numerical Solutions

We consider the one-dimensional integral equation

$$\phi(x) = f(x) + \lambda \int_a^b K(x - y)\, \phi(y)\, dy, \tag{2}$$

with $f(x)$ and $K(x - y)$ known functions. There is a wide class of problems in physics, with kernels of this form, in which the limit a is finite, and b is either finite or infinite. In both instances, one can easily show that the integral equation can be cast into the form

$$\psi(z) = g(z) + \lambda' \int_{-1}^1 K(z - w)\, \psi(w)\, dw. \tag{3}$$

If both a and b are finite,

$$x = a + (b - a)(1 + z)/2; \qquad \psi(z) = \phi(x) \tag{4a}$$

transforms Eq. (2) into the form of Eq. (3). If b is infinite,

$$x = 2a/(1 + z); \qquad \psi(z) = (a/x)\, \phi(x) \tag{4b}$$

yields the stated form for $\psi(z)$. If $a = 0$, a simple translation preceding the transformation of Eq. (4b) yields the desired equation for $\psi(z)$. Thus, to study this class of integral equations, we need only consider

$$\phi(x) = f(x) + \lambda \int_{-1}^1 K(x - y)\, \phi(y)\, dy. \tag{5}$$

The usual method for solving an integral equation of the form

$$\phi(x) = f(x) + \lambda \int_{-1}^1 K(x, y)\, \phi(y)\, dy \tag{6a}$$

is to approximate the integral by a sum over quadrature points. Applying this to Eq. (6a), one would obtain

$$\phi(x) \simeq f(x) + \lambda \sum_{j=1}^N w_j K(x, y_j)\, \phi(y_j), \tag{6b}$$

where w_j and y_j are the weights and abscissas of some quadrature. Evaluating x at each y_i yields a matrix equation

$$\sum_{j=1}^{N} [\delta_{ij} - \lambda w_j K_{ij}]\, \phi_j = f_i ,$$

where $\phi_j \equiv \phi(y_j)$, $f_i \equiv f(y_i)$, and $K_{ij} \equiv K(y_i, y_j)$. The value of $\phi(x)$ at each quadrature point can then be obtained by straightforward matrix inversion.

One disadvantage to this standard method is that one is restricted to finding ϕ directly, only at the values of the quadrature abscissas, y_i. To find ϕ at other values of y, one must interpolate, or create a new quadrature, containing the desired new points as quadrature abscissas.[1]

A more serious problem arises if $K(x, y)$ becomes infinite for some values of x and y. Then, this direct method leads to infinite entries in the matrix, and the method can no longer be used. In the treatment that follows, we will deal with kernels of the form $K(x - y)$ which are singular (infinite) when $x = y$.

III. Solutions for Weakly Singular Kernels

For kernels with weak singularities, Ullman [2] has devised a technique which treats K_{ij} as if it were nonsingular when $K \neq \infty$. The elements of the kernel matrix that would be infinite are replaced by

$$\int_{y_i - w_i/2}^{y_i + w_i/2} K(x, y_i)\, dx.$$

This integrated form of $K(x, y)$ is no longer infinite.

The method used by many authors, and applied to this problem by Schlitt [1] (and henceforth called Schlitt's method), subtracts the unknown function at the singularity. That is, the integral equation in (6a) is rewritten:

$$\phi(x) = f(x) + \lambda \int_{-1}^{1} K(x, y)[\phi(y) - \phi(x)]\, dy + \lambda\phi(x) \int_{-1}^{1} K(x, y)\, dy.$$

Assuming $\phi(y)$ has a Taylor expansion around $y = x$,

$$\lim_{x \to y} K(x, y)[\phi(y) - \phi(x)] = 0,$$

and $\int_{-1}^{1} K(x, y)\, dy$ is finite. Thus, with the above manipulations, both the Ullman and Schlitt methods yield finite matrices, and a matrix inversion technique is used.

[1] The technique we propose, eliminates the need for either of these procedures. Our scheme allows one to insert any desired point into an already existing data set.

Our method involves writing the integral of Eq. (5) as a sum over small intervals. With $K(x, y) = K(x - y)$ we write

$$\phi(x) = f(x) + \lambda \sum_{j=1}^{N} \int_{\theta_j}^{\theta_{j+1}} K(x - y)\, \phi(y)\, dy. \tag{7}$$

We now write $\phi(y)$ as

$$\phi(y) = F_j(y)\, \phi(y_j), \qquad \theta_j < y < \theta_{j+1}.$$

As before, y_j is a point in the set of abscissas at which ϕ is to be found. The functions $F_j(y)$ are chosen to try to fit $\phi(y)$ in the interval $[\theta_j, \theta_{j+1}]$. The simplest choice for $F_j(y)$ is

$$F_j(y) = \begin{cases} 1, & \theta_j < y < \theta_{j+1}, \\ 0 & \text{otherwise.} \end{cases} \tag{8a}$$

That is,[2] $\phi(y) \simeq \phi(y_j) = \text{constant}$ for $\theta_j < y < \theta_{j+1}$. Thus, the integral in Eq. (7) becomes

$$\phi_j \int_{\theta_j}^{\theta_{j+1}} K(x - y)\, dy. \tag{8b}$$

Since the integral itself is never approximated by a sum, there is no need to choose a particular set of points (like the points in a set of quadrature abscissa) in this development.

If we now set x equal to each y_i in the chosen set of points, and use Eqs. (8a) and (8b), Eq. (7) becomes

$$\phi_i \simeq f_i + \lambda \sum_{j=1}^{N} \phi_j L_{ij}, \tag{9}$$

where ϕ_i and f_i are as previously defined, and

$$L_{ij} \equiv \int_{\theta_j}^{\theta_{j+1}} K(y_i - y)\, dy. \tag{10}$$

Since $K(x - y)$ has a weak singularity, L_{ij} is finite for all i and j.

[2] To insure the continuity of ϕ, one could choose a more complicated function $F_j(y)$ which satisfies $F_j(\theta_{j+1})\phi_j = F_{j+1}(\theta_{j+1})\phi_{j+1}$.

As a concrete example, we consider an integral equation derived by Kirkwood and Riseman [5] in the theory of intrinsic viscosity; namely,

$$\phi(x) = f(x) - \lambda \int_{-1}^{1} \phi(y) \mid x - y \mid^{-\alpha} dy, \qquad 0 < \alpha < 1. \tag{11}$$

As in [1], we will take $f(x) = x^2$ and $\alpha = \frac{1}{2}$.

Using a 20-point Gauss–Legendre quadrature, we obtain a numerical solution to this equation for four values of λ; namely, $\lambda = 0.5$, 5, 20, and 200, as in [1]. We compare these results to those obtained using Schlitt's method and Ullman's scheme. These data are presented in Tables I–IV at representative points. Since ϕ is symmetric about the origin, we need only list ϕ at positive values of x.

As can be seen, $\phi(x)$ decreases as λ increases. Thus, $\phi(x)$ can be written

$$\phi(x) = \sum_{n=1}^{\infty} \psi_n(x)\, \lambda^{-n}. \tag{12}$$

Substituting this into Eq. (11), with $f(x) = x^2$ and $\alpha = \frac{1}{2}$, we obtain

$$\sum_{n=1}^{\infty} \psi_n(x)\, \lambda^{-n} = x^2 - \sum_{n=1}^{\infty} \lambda^{-n+1} \int_{-1}^{1} \psi_n(y) \mid x - y \mid^{-1/2} dy. \tag{13}$$

Equating the coefficients of like powers of λ, we obtain, from the λ° term,

$$0 = x^2 - \int_{-1}^{1} \psi_1(y) \mid x - y \mid^{-1/2} dy. \tag{14}$$

Auer and Gardner [6] have shown how to solve equations of this type. They find

$$\psi_1(x) = (\sqrt{2}/3\pi)(4x^2 - 1) \cdot (1 - x^2)^{-1/4}. \tag{15a}$$

Thus, for large λ,

$$\phi(x) \simeq (\sqrt{2}/3\pi\lambda)(4x^2 - 1) \cdot (1 - x^2)^{-1/4}. \tag{15b}$$

In Table IV, we also include the values of $\phi(x)$ from Eq. (15b) for $\lambda = 200$.

As can be seen, all three methods agree with each other quite well, and from Table IV, they all agree well with the analytic result; ours being slightly better near the singularities of ϕ at ± 1 than the other two.

We can find a corrected value of ϕ for large, but finite λ, by taking the λ^{-1} term in the expansion of Eq. (13). We obtain

$$\psi_1(x) = -\int_{-1}^{1} \psi_2(y) \mid x - y \mid^{-1/2} dy, \tag{16}$$

TABLES I–IV

Selected Values of $\phi(x)$ Using a 20-Point Gauss–Legendre Quadrature as Obtained by Ullman's, Schlitt's, and Our Method for Various Values of λ

x	$\phi(x)$ Ullman	$\phi(x)$ Schlitt	$\phi(x)$ present method	$\phi(x)$ analytic for $\lambda \to \infty$ uncorr.	corr.
TABLE I. $\lambda = 0.5$					
.99313	.63303	.63130	.62997		
.96397	.55114	.54817	.54650		
.74633	.25311	.25121	.24995		
.51087	.06767	.06737	.06631		
.07653	−.07907	−.07790	−.07882		
TABLE II. $\lambda = 5.0$					
.99313	.19322	.19148	.19018		
.96397	.13553	.13346	.13112		
.74633	.04332	.04269	.04209		
.51087	.00358	.00369	.00332		
.07653	−.02496	−.02429	−.02456		
TABLE III. $\lambda = 20$					
.99313	.06127	.06049	.05998		
.96397	.03873	.03803	.02695		
.74633	.01135	.01174	.01099		
.51087	.00049	.00054	.00044		
.07653	−.00718	−.00697	−.00704		
TABLE IV. $\lambda = 200$					
.99313	.00671	.00661	.00655	.00646	.00639
.96397	.00404	.00396	.00382	.00395	.00393
.74633	.00115	.00113	.00111	.00113	.00113
.51087	.00003	.00004	.00003	.00004	.00005
.07653	−.00075	−.00073	−.00074	−.00073	−.00073

where $\psi_1(x)$ is given in Eq. (15a). Rather than attempting to solve this equation, we made a numerical estimate of ψ_2/λ^2, by solving Eq. (11) with $\lambda \to -\lambda$. Referring to Eq. (12), for large λ,

$$\psi_2(x)/\lambda^2 \simeq [\phi_\lambda(x) + \phi_{-\lambda}(x)]/2, \tag{17}$$

so that

$$\phi_\lambda(x) \simeq \psi_1(x)/\lambda + \psi_2(x)/\lambda^2. \tag{18}$$

This estimated corrected value of ϕ_λ is also listed in Table IV.

In [1], Schlitt has presented values for the above function at values of x contained in the 40- and 80-point Gauss–Legendre sets of integration points. We have noted that our method does not restrict the researcher to a fixed set of data points. To illustrate this, we solve the above problem using a data set constructed out of various points at which results already exist.

We first constructed a data set by embedding the five points reported in [1] (hereafter called the Schlitt points) into the 20-point Gauss–Legendre set. The results are presented in Tables V–VIII for $\lambda = 0.5$, 5, 20, and 200. As can be seen from these tables, the results compare reasonably well with Schlitt's and with the results reported in Tables I–IV. However, near the singularities of ϕ, the results tend to be somewhat inaccurate; these inaccuracies being larger for larger values of λ (see, for example, the results at $x = .99313$ for various values of λ). For this reason, in discussing improvements of the method, we will report results for $\lambda = 200$, only.

Our first attempt at removing these inaccuracies involved creating a data set starting with the Schlitt points. We then constructed other data points equally spaced between two adjacent Schlitt points. We found this method to be unsatisfactory. For example, in Table IX, we report the ϕ values obtained at the Schlitt points using the above data set with three additional, equally spaced points between the Schlitt points. Using a data set with seven equally spaced points between the Schlitt points yielded results essentially identical to those in Table IX. As can be seen, although the results are not extremely bad, they are not very accurate, particularly near $x = \pm 1$.

The results shown in the first nine tables indicate that, at least for this problem, using an augmented Gauss–Legendre data set is more accurate than an equally spaced set of points. The inaccuracies in Tables V–VIII are due to embedding points which are too close to the singularities in $\phi(x)$.

As a next attempt, we returned to the 20-point Gauss data set, embedding in it the four Schlitt points that were smaller than .99313 (the largest abscissa of the 20-point set). With this data set we obtained remarkably accurate results. This is illustrated in Table X.

Finally, we considered a data set created from the 40 Gauss–Legendre points. Into this, we embedded the five 20-point abscissas reported in Tables I–IV, plus the two smaller 80-point abscissas used by Schlitt. These excellent results are shown in Table XI. In particular, the reader should note the accuracy of this result near the singularity. We have also solved the problem with the largest 80-point

TABLES V–VIII

Selected Values of (x) Using Our Method with a Data Set Formed by Embedding the Schlitt Points into the 20-Point Gauss-Legendre Set, for Various Values of λ.

x	$\phi(x)$ Schlitt from [1], Tables I–IV	$\phi(x)$ our method: With Schlitt points in 20-point set	$\phi(x)$ our method: Without Schlitt points in 20-point set
		TABLE V. $\lambda = 0.5$	
.99955	.67454	.67256	
.99313	.63130	.62929	.62997
.96397	.54817	.54646	.54650
.77831	.28399	.28312	
.74633	.25121	.24952	.24995
.51087	.06737	.06679	.06631
.50280	.06254	.06149	
.11608	−.07376	−.07417	
.07653	−.07790	−.07847	−.07882
.01951	−.08100	−.08148	
		TABLE VI. $\lambda = 5.0$	
.99955	.25986	.25237	
.99313	.19148	.18483	.19018
.96397	.13346	.13059	.13112
.77831	.05028	.04998	
.74633	.04269	.04158	.04209
.51087	.00369	.00363	.00332
.50280	.00271	.00216	
.11608	−.02354	−.02363	
.07653	−.02429	−.02448	−.02456
.01951	−.02490	−.02503	

x	$\phi(x)$ Schlitt from [1], Tables I–IV	$\phi(x)$ our method: With Schlitt points in 20-point set	$\phi(x)$ our method: Without Schlitt points in 20-point set	
		TABLE VII. $\lambda = 20$		
.99955	.10163	.09459		
.99313	.06049	.05576	.05998	
.96397	.03803	.03676	.02695	
.77831	.01327	.01320		
.74633	.01174	.01080	.01099	
.51087	.00054	.00055	.00044	
.50280	.00027	.00008		
.11608	−.00677	−.00679		
.07653	−.00697	−.00703	−.00704	
.01951	−.00714	−.00717		
		Table VIII. $\lambda = 200$		
				corr. analytic value.
.99955	.01298	.01157		
.99313	.00661	.00585	.00655	.00639
.96397	.00396	.00381	.00382	.00393
.77831	.00135	.00134		
.74633	.00113	.00109	.00111	.00113
.51087	.00004	.00004	.00003	.00005
.50280	.00001	−.00001		
.11608	−.00071	−.00071		
.07653	−.00073	−.00073	−.00074	−.00073
.01951	−.00075	−.00075		

abscissa (.99955) added to this augmented 40-point data set. This is also reported in Table XI. We note that these results are also quite satisfactory.

A comparison of Tables X and XI also shows that our method converges to an accurate result quite well with an augmented 40-point data set. To illustrate this, we have compiled data from Tables IV and XI which present values of ϕ for

TABLE IX

$\phi(x)$ Using a Data Set with Equally Spaced Points between Schlitt Points, for $\lambda = 200$

x	$\phi(x)$ at Schlitt points from [1]	$\phi(x)$ at Schlitt points from equal spacing data set
.99955	.01298	.00853
.77831	.00135	.00129
.50280	.00001	−.00002
.11608	−.00071	−.00072
.01951	−.00075	−.00076

TABLE X

$\phi(x)$ using a Data Set Created by Embedding the Four Smaller Schlitt Points into the 20-Point Gauss–Legendre Set

x	$\phi(x)$ at Schlitt points from [1]	$\phi(x)$ using augmented 20-point Gauss set	$\phi(x)$ using 20-point Gauss set only
.99313	.00661	.00655	.00655
.96397	.00396	.00382	.00382
.77831	.00135	.00134	
.74633	.00113	.00109	.00111
.51087	.00004	.00004	.00003
.50280	.00001	−.00001	
.11608	−.00071	−.00071	
.07653	−.00073	−.00073	−.00074
.01951	−.00075	−.00075	

$\lambda = 200$ using a 20-point data set and an augmented 40-point data set. These are compared to the large λ analytic solution, corrected by addition of the second $(1/\lambda^2)$ term. As can be seen, the convergence of the method is quite good. Using the augmented 40-point data set, the results are essentially identical to the analytic solution. These data are presented in Table XII.

TABLE XI

$\phi(x)$ Using a Data Set Created by Embedding All 20-Point Abscissas Shown in Tables I–IV, and Some 80 Schlitt Points Embedded into 40-Point Gauss Set

x	$\phi_a(x)$	$\phi_b(x)$	$\phi_c(x)$	$\phi_d(x)$
.99955	.01298		.01301	
.99313	.00661	.00639	.00635	.00639
.96397	.00396	.00394	.00393	.00393
.77831	.00135	.00135	.00135	
.74633	.00113	.00113	.00113	.00113
.51087	.00004	.00004	.00004	.00005
.50280	.00001	.00001	.00001	
.11608	−.00071	−.00071	−.00071	
.07653	−.00073	−.00073	−.00073	−.00073
.01951	−.00075	−.00075	−.00075	

Note. ϕ_a is data taken from [1] and Table IV; ϕ_b is obtained with augmented data set with largest 80-point abscissa ommitted; ϕ_c is obtained with augmented data set including largest 80-point abscissa; ϕ_d is corrected analytic value taken from Table IV.

TABLE XII

A Comparison of ϕ Values Using a 20-Point and an Augmented 40-Point Data Set, Illustrating the Convergence of the Present Method of Solution

x	ϕ_{20}	$\phi_{40}+$	ϕ_{analytic}(with correction)
.99313	.00655	.00635	.00639
.96397	.00382	.00393	.00393
.74633	.00111	.00113	.00113
.51087	.00003	.00004	.00005
.07653	−.00074	−.00073	−.00073

IV. Summary and Conclusions

We have presented a method for solving linear integral equations which is directly applicable to weakly singular equations. The scheme has the advantage over other methods in that one can obtain the value of the unknown function, directly, at any desired point. In other methods, one is restricted to direct results only at values of abscissas contained in a predescribed data set.

It is also possible that a technique of this type is applicable to integral equations which have kernels with pole singularities. An investigation is currently under way with such equations. They will be reported when completely available.

Acknowledgment

One of us (HC) would like to express his appreciation for the hospitality shown him at the Stanford Linear Accelerator Center during the summer of 1974. In particular, he would like to thank Dr. Y. S. Tsai for many stimulating and informative conversations.

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