On the Numerical Solution of Fredholm Integral Equations of the First Kind by the Inversion of the Linear System Produced by Quadrature*

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1. *Introduction*

In a recent paper Phillips [1] discussed the problem of the unwanted oscillations often found in numerical solutions to integral equations of the first kind and described a method whereby a controlled smoothing could be induced in the solution obtained by the inversion of the quadrature approximation to the integral equation. The purpose of the present note is to show how the same result can be obtained in a way which requires the inversion of only one matrix, whereas the method described by Phillips involves the inversion of two matrices. The method to be described also possesses the advantage that it allows solutions in cases where the matrix of quadrature coefficients is not square (i.e. the number of observations exceeds the number of unknowns).

2. *Method*

In any practical case the integral equation should be written

$$\int_a^b K(y, x)f(y)\, dy = g(x) + \epsilon(x)$$

since there will always be some error unless the integral is equated to an analytic function. If now the above equation is expressed as a quadrature, it becomes

$$Af = g + \epsilon \tag{1}$$

where A is the matrix of quadrature coefficients for the tabular points y_1, y_2, $\cdots$, y_m and x_1, x_2, $\cdots$, x_n, and ϵ_1, ϵ_2, $\cdots$, ϵ_m are the corresponding errors. As was well demonstrated by Phillips, the "exact" solution obtained when (1) is solved with ϵ set to zero is almost always poor and often disastrously so—in the sense that the solution oscillates or displays some other feature which conflicts with a priori knowledge. For example, the physics of a problem may demand a smooth, or even monotonic solution. Without such a priori knowledge, there is no reason for rejecting any solution, oscillatory or otherwise. But if the knowledge does exist, it should obviously be included, if possible, among the mathematical constraints. Phillips accomplished this by finding the smoothest acceptable solution—in the sense of minimizing the second-difference expression

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$\sum_i (f_{i-1} - 2f_i + f_{i+1})^2$ with the auxiliary conditions $Af = g + \epsilon$ and $\sum_i \epsilon_i^2 =$ constant. The quantity to be minimized was then

$$\sum_i (f_{i-1} - 2f_i + f_{i+1})^2 + \gamma^{-1} \sum_i \epsilon_i^2$$

and the solution obtained was

$$f = (A + \gamma B)^{-1} g, \tag{2}$$

γ being an undetermined multiplier, B a matrix with elements

$$\beta_{jk} = \alpha_{k-2,j} - 4\alpha_{k-1,j} + 6\alpha_{k,j} - 4\alpha_{k+1,j} + \alpha_{k+2,j}$$

and α_{kj} the element of the inverse matrix A^{-1}. Both the sum of the squares of the errors $\sum_i \epsilon_i^2$ and the smoothness of the solution depend on γ, and it is on these grounds that γ is selected—solutions are found for several values of γ, but some will exhibit values for $\sum_i \epsilon_i^2$ too large to be acceptable; the smoothest solution (i.e. the largest value for γ) is selected which still gives an acceptable value for $\sum_i \epsilon_i^2$.

If the expression to be minimized is differentiated with respect to the f_i rather than the ϵ_i there results

$$\gamma^{-1} \sum_j \epsilon_j a_{ji} + (f_{i-2} - 4f_{i-1} + 6f_i - 4f_{i+1} + f_{i+2}) = 0,$$

where α_{ji} is an element of A. This equation can be written in matrix form

$$A^* \epsilon + \gamma H f = 0 \qquad (A^* = \text{transpose of } A). \tag{3}$$

Here H represents the matrix

$$\begin{bmatrix} 1 & -2 & 1 & 0 & 0 & \cdot & \cdot & \cdot \\ -2 & 5 & -4 & 1 & 0 & \cdot & \cdot & \cdot \\ 1 & -4 & 6 & -4 & 1 & 0 & \cdot & \cdot \\ 0 & 1 & -4 & 6 & -4 & 1 & 0 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}.$$

Elimination of ϵ between (1) and (3) now gives the solution in a different form, which does not require that the matrix A be square:

$$f = (A^*A + \gamma H)^{-1} A^* g. \tag{4}$$

This solution involves only one matrix inversion. That it is equivalent to that of Phillips (equation (2)) can be shown directly. From the identity $A^*(A^{-1})^* = (A^{-1}A)^* = I^* = I$ there follows the alternate form for (4)

$$(A^*)^{-1} A^* A f + \gamma (A^*)^{-1} H f = g$$

or

$$Af + \gamma (A^{-1})^* H f = g,$$

which is Phillips' solution, since $(A^{-1})^* H$ is the matrix B of (2).

3. *Other Possibilities*

It is evident that the criterion of minimization of the second-difference expression is one of many possible constraints which may be used in this kind of treatment. The second difference expression $\sum_i (f_{i-1} - 2f_i + f_{i+1})^2$ is not always suitable—for example the solution might be known to possess one or more sharp bends, and the application of a criterion designed to eliminate such features as much as possible would hardly be realistic. However, if the general shape and order of magnitude of the solution is known, a trial solution could be constructed and the deviation of the ultimate solution from the trial solution minimized. Alternately, in other cases there might be grounds for minimizing the third rather than the second differences. Another possibility again is combining several such constraints, appropriate weights being given to each constraint. It can readily be shown that in all these cases one need only replace the matrix H by matrices similar in form. For example, if the solution is to minimize the sum of the squares of the departures from a trial solution p, then it is readily demonstrated by substituting $\sum_i (f_i - p_i)^2$ for $\sum_i (f_{i-1} - 2f_i + f_{i+1})^2$, that the identity matrix I need only be used for H and the vector γp added to g, to obtain a solution which is exactly equivalent to (4) except for the introduction of a different constraint:

$$f = (A^*A + \gamma I)^{-1}(A^*g + \gamma p). \tag{5}$$

To minimize the third, rather than the second differences, equation (4) may be applied if the following matrix is used in place of the former definition of H:

$$\begin{bmatrix} 1 & -3 & 3 & -1 & 0 & 0 & 0 & \cdot & \cdot & \cdot \\ -3 & 10 & -12 & 6 & -1 & 0 & 0 & \cdot & \cdot & \cdot \\ 3 & -12 & 19 & -15 & 6 & -1 & 0 & \cdot & \cdot & \cdot \\ -1 & 6 & -15 & 20 & -15 & 6 & -1 & \cdot & \cdot & \cdot \\ 0 & -1 & 6 & -15 & 20 & -15 & 6 & -1 & \cdot & \cdot \\ 0 & 0 & -1 & 6 & -15 & 20 & -15 & 6 & -1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}.$$

If H is defined in this way, (4) will give the solution which minimizes the third differences.

4. *Conclusions*

By a slight modification it is possible to derive a solution to the equation $Af = g$ which has the same property as that given by Phillips, but is simpler to compute and can be applied to an overdetermined system. This solution is one case of a group of solutions which may be written in the general form

$$f = (A^*A + \gamma H)^{-1}(A^*g + \gamma p).$$

For a number of minimal criteria this equation provides the solution when the appropriate values are used for H and p. It is thus possible to impose a number of constraints, separately or simultaneously, in addition to the minimization of the second differences which was the constraint selected by Phillips.

The examples given by Phillips are convincing demonstrations of the value of the method proposed by him, and since the solution given here for the criterion of minimization of second-differences has been shown to be completely equivalent to that of Phillips no purpose would be served by further examples of this kind. However, an example will be given of the application of the constraint of minimization of departures from a trial solution. The results are given in Table 1 and show the solutions obtained by four methods: solution as an exact system, solution as a least squares problem, solution by the second-difference method, and solution by the trial solution method. In this case the "true curve" showed a sharp upturn near one extremity: it is primarily for this reason that the second-difference method did not succeed in this case—the solution is not a smooth curve, but the physics of the problem requires a shape of this kind, and the trial solution method permits advantage to be taken of this physical knowledge. It was known that the solution must be monotonic, must take a zero or small positive value at $y = 0$, must take the value 1000 at $y = .21$ and must show a sharp upturn from values less than 100 somewhere between $y = .15$ and $y = .21$. The kernel of the integral equation was e^{-yx}, the integration limits $y = 0$ to $y = .21$, and the range of values of x employed in the inversion was 5 to 35. The matrix A was accordingly strongly skew-angular. It is of interest to note that

TABLE 1

f, true curve; f_1, "exact solution"; f_2, least squares solution;
f_3, solution for minimization of second differences (Phillips method);
f_4, solution for minimization of departures from trial curve; p, trial curve.

y	$f(y)$	f_1	f_2	f_3	f_4	p
0.0	0	−17.8	0.2	1.4	0.0	0
.01	1.0	18.9	−4.5	−7.2	2.4	6
.02	2.5	−7.1	17.8	−11.3	2.6	13
.03	5.0	7.3	−1.8	−5.6	2.9	22
.04	7.5	8.5	33.9	11.1	5.1	30
.05	10.0	19.3	85.7	34.8	8.9	40
.06	14.0	1.4	57.0	58.4	13.5	50
.07	17.5	−67.0	40.9	74.2	18.3	60
.08	20.0	141.0	111.3	75.6	22.5	75
.09	22.0	−254.4	−151.4	59.3	25.0	90
.10	25.0	380.5	229.2	25.8	26.9	170
.11	29.0	258.6	−170.0	−20.3	28.0	127
.12	32.5	−67.1	156.1	−70.6	29.1	150
.13	35.5	−141.9	66.3	−113.8	29.5	177
.14	38.0	−140.4	−131.3	−137.0	30.7	210
.15	40.5	−137.7	186.0	−127.0	32.3	250
.16	43.0	−550.7	−343.8	−71.8	40.2	300
.17	47.5	890.7	221.3	37.5	58.1	363
.18	59.0	−118.5	695.5	205.1	75.9	450
.19	125.0	1613.8	−463.6	429.3	174.5	565
.20	500.0	−911.5	557.9	700.4	360.3	745
.209	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0

the use of least-squares solution did not appreciably improve the solution obtained by "exact" solution. It is also a curious fact that the method designed to produce a smooth solution (i.e. the method of minimization of second differences) gave, in this case, a smooth but slowly undulating solution, while the solutions given by the method designed to minimize departures from the trial solution were monotonic throughout.

REFERENCE

1. Phillips, B. L. A technique for the numerical solution of certain integral equations of the first kind. *J. ACM 9* (1962), 84–97.