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A MATRIX METHOD FOR THE SOLUTION OF A LINEAR SECOND ORDER DIFFERENCE EQUATION IN TWO VARIABLES

by

M.L. Potters

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1. Introduction.

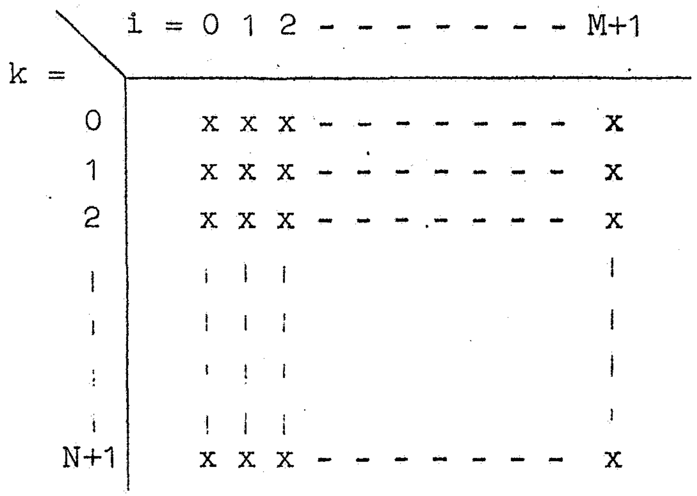
In practical analysis it often happens that a problem leads to a difference equation which cannot be solved in an analytical way.

There are various methods to handle these equation numerically, the relaxation method being a well-known one of them.

Since, however, iterative methods are in some cases very discouraging to the computer because of their slow convergence, in this report a method is offered where the solution is obtained by a direct computation. The equation treated will be a linear second order difference equation in two variables with some types of boundary conditions. As this problem frequently is originated by a differential equation, an example in this field is given.

2. The problem.

A function $f_{i,k}$ of two discrete variables i and k will be defined on the domain $i = 0(1)M+1$, $k = 0(1)N+1$, which can be represented by a rectangle of lattice points:



The function must satisfy a given linear second order difference quation:

$$a_{i,k}^{(-1)} f_{i-1,k-1} + b_{i,k}^{(-1)} f_{i,k-1} + c_{i,k}^{(-1)} f_{i+1,k-1} + \qquad \begin{pmatrix} i=1\ldots M \\ k=1\ldots N \end{pmatrix}$$

$$+ a_{i,k}^{(0)} f_{i-1,k} + b_{i,k}^{(0)} f_{i,k} + c_{i,k}^{(0)} f_{i+1,k} + \qquad (2,1)$$

$$+ a_{i,k}^{(+1)} f_{i-1,k+1} + b_{i,k}^{(+1)} f_{i,k+1} + c_{i,k}^{(+1)} f_{i+1,k+1} + d_{i,k} = 0.$$

In general, the nine coefficients $a_{i,k}^{(j)}$, $b_{i,k}^{(j)}$, $c_{i,k}^{(j)}$ $(j = -1,0,+1)$ nd the inhomogeneous term $d_{i,k}$ may depend on the variables i and k.

The boundary values $f_{i,k}$ where i=0, or M+1 or k=0 or N+1, are rescribed. The function values in the interior of the domain have o be determined. Between these MN unknowns the MN equations (2,1) old, so the solution is unique, unless the system is dependent or alse. We shall assume such algebraical difficulties not to be present.

Description of the method.

Consider the N function values $f_{i,k}$, (k=1..:N) as the elements a vector $\bar{f}_i$, (i=0(1)M+1):

$$\bar{f}_i = \begin{bmatrix} f_{i,1} \\ \vdots \\ f_{i,N} \end{bmatrix}$$

ote: square matrices will be indicated by capitals; vectors (column atrices) by barred lower case letters.

The equations (2,1) for a fixed i and k=1(1)N then can be written n an adequate matrix notation

$$A_i\bar{f}_{i-1} + B_i\bar{f}_i + C_i\bar{f}_{i+1} + \bar{d}_i = 0 \qquad (i = 1(1)M) \qquad (3,1)$$

f one defines the matrix A_i by

$$A_i = \begin{bmatrix} a_{i,1}^{(0)} & a_{i,1}^{(1)} & 0 & & 0 \\ a_{i,2}^{(-1)} & a_{i,2}^{(0)} & a_{i,2}^{(+1)} & & \\ 0 & & & \ddots & \\ & a_{i,N-1}^{(-1)} & a_{i,N-1}^{(0)} & a_{i,N-1}^{(+1)} \\ 0 & 0 & a_{i,N}^{(-1)} & a_{i,N}^{(0)} \end{bmatrix},$$

the matrices B_i and C_i analogously to A_i, and the vector $\bar{d}_i$ by

$$\bar{d}_i = \begin{bmatrix} a_{i,1}^{(-1)}f_{i-1,0} + b_{i,1}^{(-1)}f_{i,0} + c_{i,1}^{(-1)}f_{i+1,0} + d_{i,1} \\ d_{i,2} \\ \vdots \\ d_{i,N-1} \\ a_{i,N}^{(+1)}f_{i-1,N+1} + b_{i,N}^{(+1)}f_{i,N+1} + c_{i,N}^{(+1)}f_{i+1,N+1} + d_{i,N} \end{bmatrix}$$

Now suppose that for some i the vector $\overline{f}_{i-1}$ can be expressed linearly into $\overline{f}_i$ according to

$$\overline{f}_{i-1} = P_i\overline{f}_i + \overline{q}_i \tag{3,2}$$

where the matrix P_i and the vector $\overline{q}_i$ are known quantities. For i=1, indeed, this supposition is right; inserting $P_1=0$ and $\overline{q}_1 = \overline{f}_0$ into (3,2) one gets an identity and $\overline{f}_0$ is a known vector. Then substitute (3,2) into (3,1). One finds

$$A_iP_i\overline{f}_i + A_i\overline{q}_i + B_i\overline{f}_i + C_i\overline{f}_{i+1} + \overline{d}_i = 0$$

or

$$\overline{f}_i = -(B_i + A_iP_i)^{-1} C_i\overline{f}_{i+1} -(B_i + A_iP_i)^{-1}(A_i\overline{q}_i + \overline{d}_i).$$

Writing

$$\begin{aligned} P_{i+1} &= -(B_i + A_iP_i)^{-1} C_i \\ \overline{q}_{i+1} &= -(B_i + A_iP_i)^{-1} (A_i\overline{q}_i + d_i) \end{aligned} \tag{3,3}$$

one sees that one obtains an expression like (3,2) in which i has been replaced by i+1. Because of the induction principle the matrices P_i and the vectors $\overline{q}_i$ can be found for each i, from i=1 up to i = M+1 step by step. But in

$$\overline{f}_M = P_{M+1}\overline{f}_{M+1} + \overline{q}_{M+1}$$

$\overline{f}_{M+1}$ is not any longer an unknown vector. It is clear that with (3,2) each vector $\overline{f}_i$ from i = M down to i = 1 now can be determined, with which the solution of (2,1) has been found.

Resuming and writing the preceding formulae in a suitable form we have the following procedure:

1) Find P_i (i = 1(1)M+1) using

$$\begin{aligned} P_1 &= 0 \\ P_{i+1} &= -R_i^{-1}C_i \\ R_i &= B_i + A_iP_i \end{aligned}$$

2) Find $\overline{q}_i$ (i = 1(1)M+1) using

$$\begin{aligned} \overline{q}_1 &= \overline{f}_0 \\ \overline{q}_{i+1} &= -R_i^{-1}\overline{s}_i \\ \overline{s}_i &= A_i\overline{q}_i + \overline{d}_i \end{aligned}$$

3) Find $\overline{f}_i$ (i = M(1)1) using

$$\overline{f}_{i-1} = P_i\overline{f}_i + \overline{q}_i$$

4. Special case: Poisson's Equation.

When the difference equation (2,1) is analogous to the equation of Poisson in differential calculus the formulae at the end of section 3 are simplified as follows.

The coefficients are constant with respect to the variables i and k, viz.

$$a_{i,k}^{(-1)} = a_{i,k}^{(+1)} = c_{i,k}^{(-1)} = c_{i,k}^{(+1)} = 0$$

$$a_{i,k}^{(0)} = c_{i,k}^{(0)} = -\alpha$$

$$b_{i,k}^{(-1)} = b_{i,k}^{(+1)} = -\beta \qquad \text{where} \qquad 2\alpha + 2\beta = 1$$

$$b_{i,k}^{(0)} = 1$$

Taking the inhomogeneous term $d_{i,k} = 0$ one gets the "potential equation".

The matrices A_i, B_i and C_i become:

$$A_i = C_i = -\alpha I \qquad (I = \text{unit matrix of order } N)$$

$$B_i = B = \begin{bmatrix} 1 & -\beta & 0 & - & - & - & 0 \\ -\beta & 1 & -\beta & & & & \vdots \\ 0 & -\beta & 1 & -\beta & & & \vdots \\ \vdots & & & \ddots & \ddots & & \vdots \\ \vdots & & & & \ddots & \ddots & \vdots \\ 0 & - & - & - & & -\beta & 1 \end{bmatrix}$$

and the vector $\overline{d}_i$

$$\overline{d}_i = \begin{bmatrix} -\beta f_{i,0} + d_{i,1} \\ d_{i,2} \\ \vdots \\ d_{i,N-1} \\ -\beta f_{i,N+1} + d_{i,N} \end{bmatrix}$$

Further

$$R_i = B - \alpha P_i$$

$$P_{i+1} = \alpha R_i^{-1} = \alpha (B - \alpha P_i)^{-1}$$

$$\overline{s}_i = -\alpha \overline{q}_i + \overline{d}_i$$

$$\overline{q}_{i+1} = R_i^{-1}(\alpha \overline{q}_i - \overline{d}_i) = P_{i+1}\left(\overline{q}_i - \frac{\overline{d}_i}{\alpha}\right).$$

5. Special case: One Dimensional Problem.

In the case of a linear recurring sequence of the second order, with given initial and final terms one can apply the method of section 3, taking N=1. Now the "matrices" are scalars. The difference equation (2,1) becomes)

$$a_i f_{i-1} + b_i f_i + c_i f_{i+1} + d_i = 0$$

The matrix sequence P_i and the vector sequence $\overline{q}_i$ turn to number sequences p_i and q_i, satisfying

$$p_{i+1} = \frac{-c_i}{b_i + a_i p_i}$$

$$q_{i+1} = - \frac{a_i q_i + d_i}{b_i + a_i p_i}$$

with $p_1 = 0$, $q_1 = f_0$.

Using $f_{i-1} = p_i f_i + q_i$ one finds all terms from f_M to f_1.
Note, that p_i can be developed in a continued fraction.

$$p_i = \cfrac{-c_{i-1}}{b_{i-1} + a_{i-1} \cfrac{-c_{i-2}}{b_{i-2} + a_{i-2} \cfrac{-c_{i-3}}{\ddots \cfrac{-c_2}{b_2 + a_2 \cfrac{-c_1}{b_1}}}}}$$

6. The Boundary Conditions.

So far as boundary conditions for the function $f_{i,k}$ the function values were given on the four sides of the rectangle. However, it is possible to apply other types of boundary conditions without changing the procedure essentially.

We shall investigate to which variations will lead prescribing first differences instead of function values.

The following notation is adopted:

difference in i-direction: $\delta_{i+\frac{1}{2},k} = f_{i+1,k} - f_{i,k}$

$$\delta_{i,k} = \tfrac{1}{2}\,(\delta_{i+\frac{1}{2},k} + \delta_{i-\frac{1}{2},k}) ,$$

difference in k-direction: $\varepsilon_{i,k+\frac{1}{2}} = f_{i,k+1} - f_{i,k}$

$$\varepsilon_{i,k} = \tfrac{1}{2}\,(\varepsilon_{i,k+\frac{1}{2}} + \varepsilon_{i,k-\frac{1}{2}}) .$$

(i) On the upper side the mean first vertical difference $\varepsilon_{i,1}$ may be given.

Then

$$f_{i,0} = f_{i,2} - 2\,\varepsilon_{i,1}$$

This can be substituted in (2,1). The effect is a slight variation in the first row of the matrices A_i, B_i, C_i and of the vectors $\bar{d}_i$ in section 3:

$$A_i = \begin{bmatrix} a^{(0)}_{i,1} & a^{(+1)}_{i,1} + a^{(-1)}_{i,1} & 0 & & \\ a^{(-1)}_{i,2} & a^{(0)}_{i,2} & a^{(+1)}_{i,2} & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & a^{(0)}_{i,N} \end{bmatrix}$$

B_i and C_i analogous.

The first element of $\bar{d}_i$ becomes

$$-2a^{(-1)}_{i,1}\,\varepsilon_{i-1,1} - 2b^{(-1)}_{i,1}\,\varepsilon_{i,1} - 2c^{(-1)}_{i,1}\,\varepsilon_{i+1,1} + d_{i,1}$$

For the rest one can use the procedure of section 3.

Of course if one fixes the difference on the lower side, a similar modification appears in the last rows of the matrices.

(ii) Prescription of differences on the left hand boundary of the rectangle will change the initial terms of the sequences P_i and $\overline{q}_i$.

Suppose the mean first horizontal differences $\delta_{i,k}$ $(k=1(1)N)$ are given. Now we define the vector $\overline{\delta}_i$ as follows:

$$\overline{\delta}_i = \begin{bmatrix} \delta_{i,1} \\ \vdots \\ \delta_{i,N} \end{bmatrix}$$

then it holds

$$\overline{f}_0 = \overline{f}_2 - 2\overline{\delta}_1 ,$$

which substituted in (3,1) yields for i=1

$$A_1(\overline{f}_2 - 2\overline{\delta}_1) + B_1\overline{f}_1 + C_1\overline{f}_2 + \overline{d}_1 = 0 ,$$

or

$$\overline{f}_1 = -B_1^{-1} (A_1 + C_1)\overline{f}_2 + B_1^{-1} (2A_1\overline{\delta}_1 - \overline{d}_1).$$

Starting with

$$P_2 = -B_1^{-1}(A_1+C_1)$$
$$\overline{q}_2 = B_1^{-1}(2A_1\overline{\delta}_1-\overline{d}_1) ,$$

we can perform again the same calculations.

When, however, the difference vector $\overline{\delta}_{\frac{1}{2}}$ is given, then

$$\overline{f}_0 = \overline{f}_1 - \overline{\delta}_{\frac{1}{2}} ,$$

and it is clear, that $P_1 = I$, $\overline{q}_1 = -\overline{\delta}_{\frac{1}{2}}$ are the correct initial terms.

(iii) Finally, the differences on the right hand side may be given, e.g. the mean differences $\delta_{M,k}$ $(k=1(1)N)$.

Having determined the P_i and $\overline{q}_i$ in the ordinary way, one has the relations

$$\overline{f}_M = P_{M+1} \overline{f}_{M+1} + \overline{q}_{M+1}$$

$$\overline{f}_{M-1} = P_M \overline{f}_M + \overline{q}_M .$$

Of course,

$$\overline{f}_{M+1} - \overline{f}_{M-1} = 2\overline{\delta}_M$$

and from these three equations we find

$$\overline{f}_M = (I - P_M P_{M+1})^{-1}(P_{M+1}\overline{q}_M + 2P_{M+1}\overline{\delta}_M + \overline{q}_{M+1})$$

which is the initial term of the sequence f_i $(i=M(1)1)$.

Less complicated is the case with given $\tau_{M+\frac{1}{2}} = \bar{r}_{M+1} - \bar{r}_M$.
Then we have

$$\bar{r}_M = (I - P_{M+1})^{-1}(P_{M+1}\,\delta_{M+\frac{1}{2}} + \bar{q}_M).$$

It may be useful to draw attention to the fact that the matrices P_i (i=1(1)M+1) do neither depend on the boundary conditions of the function $f_{i,k}$ nor on the inhomogeneous term $d_{i,k}$, but only on the coefficients $a^{(j)}_{i,k}$, $b^{(j)}_{i,k}$, $c^{(j)}_{i,k}$ (j=-1,0,+1) of the difference equation (3,1).

Solving a problem over the same domain, with the same difference equation but with changed boundary values (of the same type of course) can be done therefore without tedious inverting of the matrices R_i. Only the vectors $\bar{d}_i$, $\bar{s}_i$, $\bar{q}_i$ and $\bar{r}_i$ have to be determined anew.

In the example of section 8 an application is made.

7. The numerical work.

In this section we shall consider the computational work, necessary for the solution of the boundary value problem. Only multiplications with non-zero numbers will be taken into consideration.

The following operations must be performed (cf the end of Section 3).

(i) The matrix x matrix multiplications A_iP_i and $R_i^{-1}C_i$. Both A_i and C_i have only 3N-2 non-zero elements; so each of these matrix multiplications requires (3N-2)N multiplications.

(ii) The matrix x vector multiplications $A_i\bar{q}_i$, $R_i^{-1}\bar{s}_i$ and $P_i\bar{r}_i$. The first one requires 3N-2, the latter two each N^2 multiplications.

(iii) The inversion of R_i. The number of multiplications depends somewhat on the used method. A method of Fox 1) and a method of Crout 2) both require N^3 multiplications for the inversion of a matrix having no special symmetry properties.

As each of these operations is done for M values of i, we find a total of about $MN^2(N+8)$ multiplications.

Of course, one will choose the i and k directions in such a way that $N \leqslant M$.

In the case of Poisson's equation with given boundary values there is a little reduction. In (i) the matrix x matrix multiplications disappear as A_i and C_i are scalar multiples of the unit matrix; only N^2 multiplications are required. In (ii) we keep $2N^2$.

For the inversion of (iii) we can use the notion of a "chain - matrix", introduced by Burgerhout 3). Matrices of this kind are determined by the elements of their first column. Since it can be shown that in this case all matrices to be inverted are chain matrices, the inversion reduces to solving N equations with N unknowns. Applying Gauss' method this requires $\frac{1}{6}N^2(N+9)$ multiplications 4), so that the whole procedure costs $\frac{1}{6}MN^2(N+33)$ multiplications.

8. An example.

A solution of the potential equation

$$\Delta f(x,y) \equiv \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = 0 \qquad (8,1)$$

is wanted in the region $0 \leqslant x \leqslant 1,\ 0 \leqslant y \leqslant 1$,

$f(x,y)$ being given on the boundaries $x=0$, $y=0$, $x=1$, $y=1$. For convenience we shall turn the problem and take a known function, satisfying (8,1), compute its boundary values and then forget the function and try to refind it by our matrix method.

We choose

$$f(x,y) = 0.2\{g(x,y) + 1\}, \qquad (8,2)$$

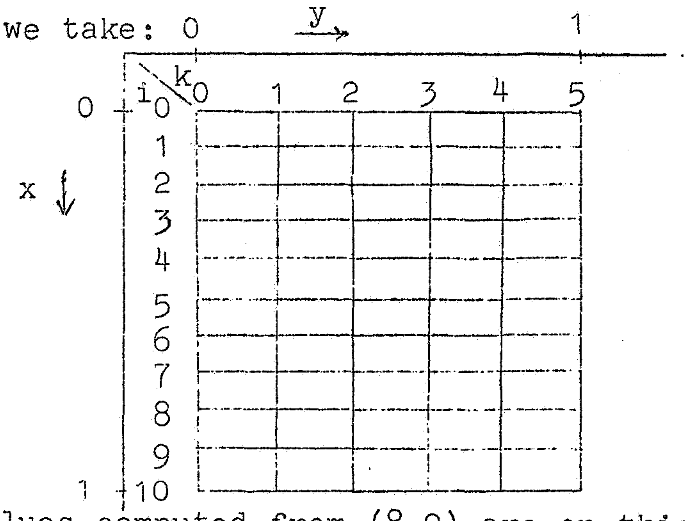
where

$$g(x,y) = \mathrm{Re}\ e^{z^2} = e^{x^2-y^2}\cos 2xy,$$

$$(z = x + iy).$$

so that $0 < f(x,y) < 1$.

As lattice we take:



The function values computed from (8,2) are on this lattice:

x \ k = 0, y = 0	1 .2	2 .4	3 .6	4 .8	5 1.0
0	.40000000	.39215789	.37042876	.33953527	.30545848	.27357589
.1	.40201003	.39393386	.37159104	.33992408	.30515783	.27283398
.2	.40816215	.39936034	.37511841	.34106723	.30419029	.27053354
.3	.41883486	.40874220	.38113391	.34288889	.30235031	.26644352
.4	.43470217	.42261913	.38984708	.34524200	.29926471	.26015512
.5	.45680508	.44181733	.40156025	.34787276	.29434201	.25104415
.6	.48666588	.46753130	.41667561	.35036115	.28669142	.23821370
.7	.52646324	.50144699	.43570097	.35202512	.27499907	.22041290
.8	.57929618	.54592394	.45924928	.35176828	.25734304	.19592564
.9	.64958160	.60426368	.48802291	.34783800	.23091837	.16242263
1.0	.74365637	.68110635	.52276568	.33744091	.19162949	.11677063

Now the derivatives in the lattice points can be developed in terms of differences:

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_{i,k} = \frac{1}{w_x^2}\left\{ \quad \delta''_{i,k} - \frac{1}{12}\delta^{IV}_{i,k} + \dots \quad \right\}$$

$$\left(\frac{\partial^2 f}{\partial y^2}\right)_{i,k} = \frac{1}{w_y^2}\left\{ \quad \varepsilon''_{i,k} - \frac{1}{12}\varepsilon^{IV}_{i,k} + \dots \quad \right\}$$

In these formulae w_x denotes the interval in x-direction
w_y " " " " y "
$\delta_{i,k}$ " the differences in x-direction
$\varepsilon_{i,k}$ " " " " y "

Substituting this in the equation and neglecting fourth and higher order differences one gets the second order difference equation

$$\frac{1}{w_x^2}\,\delta''_{i,k} + \frac{1}{w_y^2}\,\varepsilon''_{i,k} = 0 \qquad \begin{matrix} i = 1(1)9 \\ k = 1(1)4 \end{matrix}$$

or, with a normalising factor $-\dfrac{w_x^2 w_y^2}{2(w_x^2+w_y^2)}$.

$$-\frac{w_y^2}{2(w_x^2+w_y^2)}\,\delta''_{i,k} - \frac{w_x^2}{2(w_x^2+w_y^2)}\,\varepsilon''_{i,k} = 0 \qquad \begin{matrix} i = 1(1)9 \\ k = 1(1)4 \end{matrix} \qquad (8,3)$$

Since $\delta''_{i,k} = f_{i-1,k} - 2f_{i,k} + f_{i+1,k}$

$$\varepsilon''_{i,k} = f_{i,k-1} - 2f_{i,k} + f_{i,k+1} \quad ,$$

this leads to a set of equations, similar to (2,1) with coefficients (cf section 4)

$$a^{(-1)}_{i,k} = c^{(-1)}_{i,k} = a^{(+1)}_{i,k} = c^{(+1)}_{i,k} = 0$$

$$a^{(0)}_{i,k} = c^{(0)}_{i,k} = -\frac{w_y^2}{2(w_x^2+w_y^2)} = -\alpha$$

$$b^{(-1)}_{i,k} = b^{(+1)}_{i,k} = -\frac{w_x^2}{2(w_x^2+w_y^2)} = -\beta$$

$$b^{(0)}_{i,k} = 1$$

$$d_{i,k} = 0$$

As in our lattice $w_y = 2w_x$ we have $\alpha = 0.4; \beta = 0.1$.

In this way one obtains the solution:

i \ k	0	1	2	3	4	5
0	.40000000	.39215789	.37042876	.33953527	.30545848	.27357589
1	.40201003	.39405210	.37163205	.33984111	.30503539	.27283398
		2	2	2	1	
2	.40816215	.39956188	.37517811	.34090069	.30396125	.27053354
		-1	0	1	-1	
3	.41883486	.40901752	.38119758	.34262579	.30200916	.26644352
		0	0	0	-1	
4	.43470217	.42297380	.38990502	.34486211	.29879434	.26015512
		0	0	0	-1	
5	.45680508	.44226518	.40160600	.34735464	.29372237	.25104415
		0	0	1	0	
6	.48666588	.46808638	.41670503	.34969242	.28591189	.23821370
		-1	0	0	0	
7	.52646324	.50210802	.43571188	.35122217	.27408082	.22041290
		0	0	0	0	
8	.57929618	.54663989	.45924212	.35091482	.25638138	.19592564
		0	0	0	0	
9	.64958160	.60485714	.48800474	.34715901	.23016251	.16242263
		-1	-1	1	0	
0	.74365637	.68110635	.52276568	.33744091	.19162949	.11677063

The residuals $r_{i,k}$= left hand member of (2,1) in the interior points are written under the function (in units of the 8th decimal). As one sees, the stability of the procedure in this case is very satisfactory, the residuals being nearly zero in as many digits as were carried in the computation.

However, comparison with the "original" function shows a deviation of several units in the fourth decimal. This is due to neglecting of the fourth and higher differences.

According to a method of Fox 5) it is possible to improve the solution by taking the fourth and higher differences into account in the following way.

Instead of (8,3) we try to solve an equation that is a better approximation of the differential equation (8,1) namely

$$-\frac{w_y^2}{2(w_x^2+w_y^2)}\,\delta''_{i,k}-\frac{w_x^2}{2(w_x^2+w_y^2)}\,\varepsilon''_{i,k}+d_{i,k}=0 \qquad (8,4)$$

in which

$$d_{i,k}=\frac{w_y^2}{2(w_x^2+w_y^2)}\left(\frac{1}{12}\,\delta^{IV}_{i,k}-\frac{1}{90}\,\delta^{VI}_{i,k}\right)+$$

$$+\frac{w_x^2}{2(w_x^2+w_y^2)}\left(\frac{1}{12}\,\varepsilon^{IV}_{i,k}-\frac{1}{90}\,\varepsilon^{VI}_{i,k}\right).$$

If we could consider $d_{i,k}$ as a known inhomogeneous term we would find us in the case of section 6 and could compute a new solution only by multiplications matrix x vector.

Unfortunately, $d_{i,k}$ consists of the differences of the wanted function $f_{i,k}$. However, when we take the differences of the function computed above the error is not large and the new approximated function will be better than without any difference correction.

This procedure can be repeated until we find a constant function $f_{i,k}$.

We stress the point that these iterations are considerably simpler than the first solution since all matrices concerned are the same in all iterations.

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C O N T E N T S

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