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Analytical solution of the generalized discrete Poisson equation

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Abstract. We present an analytical solution to the generalized discrete Poisson equation, a matrix equation which has a tridiagonal matrix with fringes having an arbitrary value for the diagonal elements. The results are of relevance to a variety of physical problems, which require the numerical solution of the Poisson equation. As examples, the formula has been applied to the solution of the electrostatic problem of tunnelling junction arrays with two and three rows.

Many physical problems require the numerical solution of the Poisson equation on a rectangle [1–3]. In general, one uses the finite-difference method [1–3], where the rectangle is replaced by an $N \times k$ grid, and the Poisson equation is solved in the finite-difference representation. In this way, the problem is reduced to the discrete Poisson equation (DPE) on an $N \times k$ grid, a matrix equation having a tridiagonal matrix with fringes [1] (see equations (1) and (2)). Here we present a study of the *generalized* DPE, a matrix equation which has a tridiagonal matrix with fringes having an arbitrary value for the diagonal elements, since there are many other problems [4–7] which involve such equations. In the literature [1–4], many numerical methods have been developed to solve the generalized DPE. Here we report an analytical way to solve these equations.

The generalized DPE on an $N \times k$ grid has the following form [1–3]

$$\mathbf{A}u = \rho \tag{1}$$

where u is the discrete potential column, ρ is the column related to the source, and $\mathbf{A}$ is a $k \times k$ symmetric tridiagonal block matrix (the so-called 'tridiagonal matrix with fringes' [1]) given by

$$\mathbf{A} = \begin{pmatrix} \mathbf{M}_N & \mathbf{1}_N & \mathbf{0}_N & \dots & \dots & \mathbf{0}_N & \mathbf{0}_N & \mathbf{0}_N \\ \mathbf{1}_N & \mathbf{M}_N & \mathbf{1}_N & \dots & \dots & \mathbf{0}_N & \mathbf{0}_N & \mathbf{0}_N \\ \mathbf{0}_N & \mathbf{1}_N & \mathbf{M}_N & \dots & \dots & \mathbf{0}_N & \mathbf{0}_N & \mathbf{0}_N \\ \dots & & & \dots & \dots & & & \dots \\ \dots & & & \dots & \dots & & & \dots \\ \mathbf{0}_N & \mathbf{0}_N & \mathbf{0}_N & \dots & \dots & \mathbf{M}_N & \mathbf{1}_N & \mathbf{0}_N \\ \mathbf{0}_N & \mathbf{0}_N & \mathbf{0}_N & \dots & \dots & \mathbf{1}_N & \mathbf{M}_N & \mathbf{1}_N \\ \mathbf{0}_N & \mathbf{0}_N & \mathbf{0}_N & \dots & \dots & \mathbf{0}_N & \mathbf{1}_N & \mathbf{M}_N \end{pmatrix}. \tag{2}$$

Here in (2), $\mathbf{M}_N$ is the $N \times N$ symmetric tridiagonal matrix [5], with the same arbitrary constant D as diagonal elements and the same constant 1 as off-diagonal elements.

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In addition, $\mathbf{1}_N$ and $\mathbf{0}_N$ are the $N \times N$ unit and null matrix, respectively. Thus, the matrix A consists of $k \times k$ submatrices, each submatrix consisting of $N \times N$ elements. We note that an important special case of (2) is $D = -4$, which is the matrix form for the Poisson equation on a rectangle arising from the difference method [1–3]. Also, we note that for $D = -4 - C_0/C$, one can easily check that (1) and (2) appear as the matrix equation for the electrostatic problem of two-dimensional (2D) arrays of tunnel junctions [4] having the same junction capacitances C and stray capacitances C_0. In this case, there are N rows of junctions and k columns of junctions for the rectangular 2D arrays being studied.

Our analytic inversion of the block tridiagonal matrix A of (2) consists of three steps: (i) by applying the results of [5], we formally invert the block matrix A into another block matrix A^{-1}, (ii) we find the eigenvalues and eigenfunctions for the submatrices of the block matrix A^{-1}, (iii) we evaluate analytically each of the individual elements in the inverted matrix A^{-1} by the Schur decomposition [8] scheme.

First, it is apparent that the inverted block matrix A^{-1} of the $k \times k$ block matrix A is a $k \times k$ block matrix. By applying the results of [5], it is straightforward to show that the (i, j)th submatrix $\{\mathsf{A}^{-1}\}_{ij}$ in the inverted block matrix A^{-1} has the form

$$\{\mathsf{A}^{-1}\}_{ij} = -\frac{\cosh(k+1-|i-j|)\mathbf{\Theta}_N - \cosh(k+1-i-j)\mathbf{\Theta}_N}{2\sinh\mathbf{\Theta}_N \sinh(k+1)\mathbf{\Theta}_N} \qquad \text{for } i, j = 1, 2, \ldots, k \tag{3}$$

where the $N \times N$ matrix $\mathbf{\Theta}_N$ is defined by the following functional relation

$$-2\cosh\mathbf{\Theta}_N = \mathsf{M}_N \tag{4}$$

where M_N is the same as in (2). It is clear that the submatrix $\{\mathsf{A}^{-1}\}_{ij}$ in the inverted block matrix A^{-1} is itself an $N \times N$ matrix.

Next, we will find the eigenvalues and eigenfunctions for the submatrices $\{\mathsf{A}^{-1}\}_{ij}$ of the block matrix A^{-1}. This can be done by studying in turn the matrices M_N and $\mathbf{\Theta}_N$. For this purpose, we first identify the eigenvalues and the eigenfunctions for the matrix M_N, which is a standard procedure [8]. After some algebra, we obtain the eigenvalues $\{\Lambda_m\}$ for the matrix M_N as

$$\Lambda_m = D + 2\cos\frac{m\pi}{N+1} \qquad \text{for } m = 1, 2, \ldots, N \tag{5}$$

and the corresponding orthogonal eigenfunctions $\{x_m^{(n)}\}$ as

$$x_m^{(n)} = \sqrt{\frac{2}{N+1}} \sin\frac{mn\pi}{N+1} \qquad \text{for } n = 1, 2, \ldots, N. \tag{6}$$

We note that it is not difficult to deduce that since $\mathbf{\Theta}_N$ is a function of the matrix M_N, its eigenfunctions should be the same as (6) and its eigenvalues are directly related to that of M_N by the functional form as determined by (4). Defining the mth diagonal element of $-2\cosh\mathbf{\Theta}_N$ as $-2\cosh\lambda_m$, we obtain from (4) and (5)

$$\Lambda_m = -2\cosh\lambda_m = D + 2\cos\frac{m\pi}{N+1} \qquad \text{for } m = 1, 2, \ldots, N. \tag{7}$$

Thus, by means of (6) and (7), we readily obtain the eigenvalues and eigenfunctions for the submatrices $\{\mathsf{A}^{-1}\}_{ij}$. The eigenvalues of $\{\mathsf{A}^{-1}\}_{ij}$ can be conveniently expressed by a matrix form, the diagonal matrix $\mathbf{\Delta}_{ij}$, the mth element of which can be directly obtained as

$$\Delta_{ij}(m) = -\frac{\cosh(k+1-|i-j|)\lambda_m - \cosh(k+1-i-j)\lambda_m}{2\sinh\lambda_m \sinh(k+1)\lambda_m} \qquad \text{for } m = 1, 2, \ldots, N \tag{8}$$

where λ_m is given by (7). In addition, the corresponding orthogonal eigenfunctions are the $\{x_m^{(n)}\}$ given by (6). We note that from (7) and (8) one can show that for fixed $\{N, k, , i, j\}$ and D, the absolute value of $\Delta_{ij}(m)$ is a decreasing function of m.

We are now in a position to evaluate analytically each of the $N \times N$ elements contained in the submatrix $\{\mathsf{A}^{-1}\}_{ij}$ by the Schur decomposition scheme, which states that any well-defined symmetric matrix can be decomposed into a product of its diagonal matrix sandwiched by its corresponding unitary matrix [8]. In other words, we can write

$$\{\mathsf{A}^{-1}\}_{ij} = \boldsymbol{U}\boldsymbol{\Delta}_{ij}\boldsymbol{U}^{\mathrm{T}} \tag{9}$$

where $\boldsymbol{U}$ is the unitary matrix of $\{\mathsf{A}^{-1}\}_{ij}$, and the (m, n)th element of $\boldsymbol{U}$ is $x_m^{(n)}$. Applying (6) and (8) to (9), we obtain the (l, m)th element of submatrix $\{\mathsf{A}^{-1}\}_{ij}$ as

$$\{\mathsf{A}^{-1}\}_{ij}^{(lm)} = \sum_{n=1}^{N} x_n^{(l)} \Delta_{ij}(n) x_n^{(m)} = \sum_{n=1}^{N} \alpha_{lm}(n)\Delta_{ij}(n) \tag{10}$$

where

$$\alpha_{lm}(n) = x_n^{(l)} x_n^{(m)} = \frac{2}{N+1} \sin\frac{nl\pi}{N+1} \sin\frac{nm\pi}{N+1} \tag{11}$$

and $\Delta_{ij}(n)$ is given by (8).

Equation (10) is the key result of our paper. It provides the analytical solution for the generalized DPE of (1). Some comments are as follows. First, for the simplest case of $N = 1$, there is only one term in (10), and its corresponds to that of the one-dimensional (1D) generalized DPE [5]. Second, in general each matrix element in A^{-1} as expressed by (10) has very similar structures. It is a linear superposition of the diagonal term $\Delta_{ij}(n)$ (which has the form (8) similar to that of the inverse matrix elements to the corresponding one-dimensional problem), modulated by the sinusoidal coefficient $\alpha_{lm}(n)$. In this way, if we look at the rectangle for the generalized DPE, each additional row contributes one more term to the sum in (10) and it will modify the magnitude of $\alpha_{lm}(n)$ and $\Delta_{ij}(n)$. Furthermore, (10) is very useful for those systems where the number of rows is much less than that of the columns. In particular, it can be applied to study the single charge tunnelling in the 2D arrays of tunnel junctions [4] with equal junction capacitances and equal stray capacitances. Here we apply (10) first to the two coupled 1D arrays (a 2D system with $N = 2$) of junctions, where analytical results are known [9], and then to derive analytical expressions for the three-rows ($N = 3$) 2D system.

For the 2D system with $N = 2$, there are only two terms on the right-hand side of (10). In this case, (8) can be written as

$$R_{lm}^{\pm} \equiv \Delta_{lm} = \frac{\cosh(k+1-l-m)\lambda^{\pm} - \cosh(k+1-|l-m|)\lambda^{\pm}}{2\sinh\lambda^{\pm}\sinh(k+1)\lambda^{\pm}} \tag{12}$$

where the plus sign is for $n = 1$ and minus sign is for $n = 2$, with

$$-2\cosh\lambda^{\pm} = D \pm 1. \tag{13}$$

Also, from (11) one has $\alpha_{11}(1) = \alpha_{22}(1) = \alpha_{11}(2) = \alpha_{22}(2) = \alpha_{12}(1) = \alpha_{21}(1) = 1/2$, and $\alpha_{12}(2) = \alpha_{21}(2) = -1/2$. Thus, (10) reduces to only two kinds of expressions

$$G_{lm} \equiv \{\mathsf{A}^{-1}\}_{11,lm} = \{\mathsf{A}^{-1}\}_{22,lm} = \tfrac{1}{2}(R_{lm}^{+} + R_{lm}^{-}) \tag{14}$$

$$B_{lm} \equiv \{\mathsf{A}^{-1}\}_{12,lm} = \{\mathsf{A}^{-1}\}_{21,lm} = \tfrac{1}{2}(R_{lm}^{+} - R_{lm}^{-}). \tag{15}$$

We note that (12)–(15) give the analytical inverse matrix elements for the matrix appearing in the electrostatic problem of a particular configuration of two coupled 1D arrays, where the values of the coupling capacitances are the same as those of the junction capacitances. In fact, (12)–(15) corresponds to equations (8)–(11) of [9] for the case where the coupling capacitance C_c equals the junction capacitance C.

Our next example is the three-rows ($N = 3$) system, where there are three terms on the right-hand side of (10). In this case, (8) can be written as

$$-2\cosh\lambda_1 = D + \sqrt{2} \qquad -2\cosh\lambda_2 = D \qquad -2\cosh\lambda_3 = D - \sqrt{2}. \tag{16}$$

By means of (10), one finds for the case of the $N = 3$ system, it is convenient to write the block inverse matrix of (2) as a 3×3 block matrix

$$\mathbf{A}^{-1} = \begin{pmatrix} \frac{1}{2}(\mathbf{G}_k + \mathbf{M}_k^{-1}) & \frac{1}{\sqrt{2}}\mathbf{B}_k & \frac{1}{2}(\mathbf{G}_k - \mathbf{M}_k^{-1}) \\ \frac{1}{\sqrt{2}}\mathbf{B}_k & \mathbf{G}_k & \frac{1}{2}\mathbf{B}_k \\ \frac{1}{2}(\mathbf{G}_k - \mathbf{M}_k^{-1}) & \frac{1}{\sqrt{2}}\mathbf{B}_k & \frac{1}{2}(\mathbf{G}_k + \mathbf{M}_k^{-1}) \end{pmatrix} \tag{17}$$

where $\mathbf{M}_k^{-1}$, $\mathbf{G}_k$, and $\mathbf{B}_k$ are $k \times k$ matrices, and the elements of $\mathbf{M}_k^{-1}$ are given by

$$R_{lm} = \frac{\cosh(k+1-l-m)\lambda - \cosh(k+1-|l-m|)\lambda}{2\sinh\lambda\,\sinh(k+1)\lambda} \tag{18}$$

with

$$-2\cosh\lambda = D. \tag{19}$$

In addition, the elements of $\mathbf{G}_k$ and $\mathbf{B}_k$ in (17) are given by (14) and (15), respectively, except that $\lambda^{\pm}$ now has a new definition as

$$-2\cosh\lambda^{\pm} = D \pm \sqrt{2}. \tag{20}$$

In summary, in this paper, we have solved the generalized discrete Poisson equation (1) analytically deriving the formula (10) for the inversion of the tridiagonal matrix with fringes, equation (2). Our results are very useful for a variety of problems in mathematics and physics, which require the numerical solution of the Poisson equation. As examples, the formula has been applied to 2D junction arrays with two and three rows, where very simple forms for the inverse matrix are presented.

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