Fast Solution for the Diagonal Elements of the Inverse of a Tridiagonal Matrix *

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Let T be an $N \times N$ tridiagonal matrix and let its inverse be $\lambda \equiv T^{-1}$. We shall show here how the entire set of diagonal elements λ_{ii}, $1 \leq i \leq N$, can be found in order N operations.

The equation for the inverse can be written $T\lambda = 1$, or, in component form,

$$-A_i \lambda_{i-1,j} + B_i \lambda_{ij} - C_i \lambda_{i+1,j} = \delta_{ij}. \tag{B1}$$

For any fixed value of j this equation can be solved by one of two forms of Gaussian elimination. In the usual implementation the elimination proceeds from $i = 1$ to $i = N$, followed by backsubstitution from $i = N$ to $i = 1$,

$$D_i = (B_i - A_i D_{i-1})^{-1} C_i, \qquad D_0 \equiv 0, \tag{B2}$$

$$Z_{ij} = (B_i - A_i D_{i-1})^{-1}(\delta_{ij} + A_i Z_{i-1,j}), \qquad Z_{0j} \equiv 0, \tag{B3}$$

$$\lambda_{ij} = D_i \lambda_{i+1,j} + Z_{ij}, \qquad \lambda_{N+1,j} \equiv 0. \tag{B4}$$

It is also possible to implement the method using the reverse order,

$$E_i = (B_i - C_i E_{i+1})^{-1} A_i, \qquad E_{N+1} \equiv 0, \tag{B5}$$

$$W_{ij} = (B_i - C_i E_{i+1})^{-1}(\delta_{ij} + C_i W_{i+1,j}), \qquad W_{N+1,j} \equiv 0, \tag{B6}$$

$$\lambda_{ij} = E_i \lambda_{i-1,j} + W_{ij}, \qquad \lambda_{0j} \equiv 0. \tag{B7}$$

The crucial idea of the present method is to use parts of *both* of these implementations to find the diagonal elements λ_{ii}.

Since $\delta_{ij} = 0$ for $i \neq j$, it follows from equations (B3) and (B6) that

$$Z_{ij} = 0, \qquad \text{for } i < j, \tag{B8}$$

$$W_{ij} = 0, \qquad \text{for } i > j. \tag{B9}$$

Thus, from equations (B3) and (B4) we obtain, for special choices of i and j,

$$Z_{ii} = (B_i - A_i D_{i-1})^{-1}, \tag{B10}$$

$$\lambda_{ii} = D_i \lambda_{i+1,i} + Z_{ii}, \tag{B11}$$

$$\lambda_{i-1,i} = D_{i-1} \lambda_{ii}, \tag{B12}$$

Similarly, from equations (B6) and (B7),

$$W_{ii} = (B_i - C_i E_{i+1})^{-1}, \tag{B13}$$

$$\lambda_{ii} = E_i \lambda_{i-1,i} + W_{ii}, \tag{B14}$$

$$\lambda_{i+1,i} = E_{i+1} \lambda_{ii}. \tag{B15}$$

From equations (B10), (B11), and (B15) we eliminate Z_{ii} and $\lambda_{i+1,i}$ to obtain

$$\lambda_{ii} = (1 - D_i E_{i+1})^{-1}(B_i - A_i D_{i-1})^{-1}. \tag{B16}$$

The right hand side now depends only on the single-index quantities A_i and B_i, which are given, and D_i and E_i, which can be found by two passes through the depth grid, using the recursion relations (B2) and (B5). Thus all λ_{ii} can be found in order N operations.

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If one is already performing a formal solution of the transfer equation based on the matrix T, there is very little extra work involved in determining the diagonal elements λ_{ii}, since the quantities A_i, B_i, C_i, and D_i are common to both problems. One needs only to include the recursion relation (B5) as part of the backsubstitution to find the E_i. The quantities $(B_i - A_i D_{i-1})^{-1}$ are required for the recursion relations (B2) and (B3), so they are most conveniently stored, rather than recomputed, for use in equation (B16).

An alternate set of equations for obtaining λ_{ii} can be found by using equations (B12), (B13), and (B14), eliminating W_{ii} and $\lambda_{i-1,i}$ to obtain

$$\lambda_{ii} = (1 - E_i D_{i-1})^{-1} (B_i - C_i E_{i+1})^{-1}. \tag{B17}$$

This form is more convenient if the associated formal solution of the transfer equation is being done in reverse order, starting with recursions from $i = N$ to $i = 1$.

Once the diagonal elements λ_{ii} have been found, off-diagonal elements can be found from the recursion relations,

$$\lambda_{ij} = D_i \lambda_{i+1,j}, \qquad \text{for } i < j, \tag{B18}$$

$$\lambda_{ij} = E_i \lambda_{i-1,j}, \qquad \text{for } i > j, \tag{B19}$$

which follow from equations (B4) and (B8), and from equations (B7) and (B9), respectively. Thus a band of width M about the diagonal can be found in order MN operations. The entire inverse could in principle be constructed in this way in order N^2 operations; however, this is not an obvious improvement over the usual method, which also requires of order N^2 operations.

We have implicitly assumed that the elements of the tridiagonal matrix T and its inverse λ are scalars, and thus so are all the various auxilliary quantities introduced here. However, it should be noted that all formulas of this appendix have been written in forms that will apply as well to block tridiagonal matrices. In that case the term "operations" must be interpreted to mean "block matrix operations," so that the method would require of order NF^3 scalar operations for blocks of size $F \times F$.

The method of this appendix can also be formulated in terms of the improved Feautrier solution of appendix A, thus giving it the advantage of better numerical conditioning. Such a formulation has been incorporated into a FORTRAN subroutine, which simultaneously solves the formal solution and solves for a band of the inverse operator. This routine has been extensively used in the code MALI-L and has proven itself to be reliable and accurate.