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UPDATING THE INVERSE OF A MATRIX*

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Abstract. The Sherman–Morrison–Woodbury formulas relate the inverse of a matrix after a small-rank perturbation to the inverse of the original matrix. The history of these fomulas is presented and various applications to statistics, networks, structural analysis, asymptotic analysis, optimization, and partial differential equations are discussed. The Sherman–Morrison–Woodbury formulas express the inverse of a matrix after a small rank perturbation in terms of the inverse of the original matrix. This paper surveys the history of these formulas and we examine some applications where these formulas are helpful.

Key words. Sherman–Morrison, Woodbury, matrix updates, matrix perturbations

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1. History. This paper is in response to Gene Golub's suggestion that an expository paper be prepared concerning various applications of the Sherman–Morrison and Woodbury formulas. We focus on the following result. If both $\mathbf{A}$ and $\mathbf{I}-\mathbf{V}\mathbf{A}^{-1}\mathbf{U}$ are invertible, then $\mathbf{A}-\mathbf{U}\mathbf{V}$ is invertible and

$$[\mathbf{A}-\mathbf{U}\mathbf{V}]^{-1}=\mathbf{A}^{-1}+\mathbf{A}^{-1}\mathbf{U}(\mathbf{I}-\mathbf{V}\mathbf{A}^{-1}\mathbf{U})^{-1}\mathbf{V}\mathbf{A}^{-1}. \tag{1}$$

The matrix $\mathbf{I}-\mathbf{V}\mathbf{A}^{-1}\mathbf{U}$ is often called the *capacitance matrix*. Suppose that $\mathbf{U}$ is $n\times m$ with columns $\mathbf{u}_1,\mathbf{u}_2,\cdots,\mathbf{u}_m$ and $\mathbf{V}$ is $m\times n$ with rows $\mathbf{v}_1,\mathbf{v}_2,\cdots,\mathbf{v}_m$. From the identity

$$\mathbf{U}\mathbf{V}=\sum_{i=1}^{m}\mathbf{u}_i\mathbf{v}_i,$$

we see that (1) provides a formula for the inverse of a matrix after it is modified by m rank 1 corrections. Observe that the matrix $\mathbf{I}-\mathbf{V}\mathbf{A}^{-1}\mathbf{U}$ is $m\times m$. Formula (1) is useful in situations where m is much smaller than n and the structure of $\mathbf{A}$ is "nice" so that the effort involved in evaluating the correction $\mathbf{A}^{-1}\mathbf{U}(\mathbf{I}-\mathbf{V}\mathbf{A}^{-1}\mathbf{U})^{-1}\mathbf{V}\mathbf{A}^{-1}$ is small relative to the effort involved in inverting a general $n\times n$ matrix.

In the special case where $\mathbf{U}$ is a column vector $\mathbf{u}$ and $\mathbf{V}$ is a row vector $\mathbf{v}$,[1] (1) simplifies to

$$[\mathbf{A}-\mathbf{u}\mathbf{v}]^{-1}=\mathbf{A}^{-1}+\alpha\mathbf{A}^{-1}\mathbf{u}\mathbf{v}\mathbf{A}^{-1}\quad\text{where }\alpha=1/(1-\mathbf{v}\mathbf{A}^{-1}\mathbf{u}). \tag{2}$$

Frequently, (2) is called the Sherman–Morrison formula while (1) is called the Woodbury formula. However, a study of the literature reveals that (1) appeared in several papers before Woodbury's report [52] while (2) is actually a formula given by Bartlett [6]. In this section, we give a brief history of the Inverse Matrix Modification Formula.

The Modification Formula emanates from studies of partitioned matrices. Let us generalize (1) by replacing $\mathbf{V}$ with $\mathbf{D}^{-1}\mathbf{V}$, giving us the relation

$$\mathbf{B}^{-1}=\mathbf{A}^{-1}+\mathbf{A}^{-1}\mathbf{U}(\mathbf{D}-\mathbf{V}\mathbf{A}^{-1}\mathbf{U})^{-1}\mathbf{V}\mathbf{A}^{-1} \tag{3}$$

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[1] Our convention is that all vectors are column vectors except for $\mathbf{v}$, which is a row vector.

where $\mathbf{B} = \mathbf{A} - \mathbf{U}\mathbf{D}^{-1}\mathbf{V}$. A matrix with the form of $\mathbf{B}$ is called a *Schur complement*. Hence, the Modification Formula provides an expression for the inverse of a Schur complement. An excellent review of Schur complements and their applications is given by Cottle in [12].

Letting $\mathbf{x}$ denote the solution to $\mathbf{B}\mathbf{x} = \mathbf{b}$ and defining the vector

$$\mathbf{y} = -(\mathbf{D} - \mathbf{V}\mathbf{A}^{-1}\mathbf{U})^{-1}\mathbf{V}\mathbf{A}^{-1}\mathbf{b},$$

we have from (3) that the pair $(\mathbf{x}, \mathbf{y})$ satisfies the block-partitioned equation

$$\begin{bmatrix} \mathbf{A} & \mathbf{U} \\ \mathbf{V} & \mathbf{D} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix}. \tag{4}$$

Duncan's 1944 paper [16] gives two different representations for the inverse of the coefficient matrix in (4). In particular, if $\mathbf{M}$ denotes the coefficient matrix given by

$$\mathbf{M} = \begin{bmatrix} \mathbf{A} & \mathbf{U} \\ \mathbf{V} & \mathbf{D} \end{bmatrix},$$

then

$$\mathbf{M}^{-1} = \begin{bmatrix} \mathbf{A}^{-1} + \mathbf{A}^{-1}\mathbf{U}\mathbf{C}^{-1}\mathbf{V}\mathbf{A}^{-1} & -\mathbf{A}^{-1}\mathbf{U}\mathbf{C}^{-1} \\ -\mathbf{C}^{-1}\mathbf{V}\mathbf{A}^{-1} & \mathbf{C}^{-1} \end{bmatrix} \tag{5a}$$

where $\mathbf{C} = \mathbf{D} - \mathbf{V}\mathbf{A}^{-1}\mathbf{U}$ and

$$\mathbf{M}^{-1} = \begin{bmatrix} \mathbf{B}^{-1} & -\mathbf{B}^{-1}\mathbf{U}\mathbf{D}^{-1} \\ -\mathbf{D}^{-1}\mathbf{V}\mathbf{B}^{-1} & \mathbf{D}^{-1} + \mathbf{D}^{-1}\mathbf{V}\mathbf{B}^{-1}\mathbf{U}\mathbf{D}^{-1} \end{bmatrix}. \tag{5b}$$

Observe that (5b) is obtained from (5a) by interchanging rows and columns and relabeling the coefficients. Equating the (1, 1) elements of (5a) and (5b) and setting $\mathbf{D} = \mathbf{I}$, we obtain (1) (see [16, eq. (4.10)]).

Assuming that both $\mathbf{A}$ and $\mathbf{C} = \mathbf{D} - \mathbf{V}\mathbf{A}^{-1}\mathbf{U}$ are invertible, the identity (5a) is obtained using block Jordan elimination, starting in the upper left corner. Assuming that both $\mathbf{D}$ and $\mathbf{B} = \mathbf{A} - \mathbf{U}\mathbf{D}^{-1}\mathbf{V}$ are invertible, the identity (5b) is obtained using block Jordan elimination, starting in the lower right corner. These assumptions overlap in the sense that if $\mathbf{A}$, $\mathbf{D}$, and $\mathbf{C}$ are invertible, then $\mathbf{B}$ is invertible. To prove this, we multiply the first block of rows from $\mathbf{M}$ by $\mathbf{V}\mathbf{A}^{-1}$ and subtract from the second block of rows to obtain

$$\begin{bmatrix} \mathbf{I} & \mathbf{0} \\ -\mathbf{V}\mathbf{A}^{-1} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{A} & \mathbf{U} \\ \mathbf{V} & \mathbf{D} \end{bmatrix} = \begin{bmatrix} \mathbf{A} & \mathbf{U} \\ \mathbf{0} & \mathbf{D} - \mathbf{V}\mathbf{A}^{-1}\mathbf{U} \end{bmatrix} = \begin{bmatrix} \mathbf{A} & \mathbf{U} \\ \mathbf{0} & \mathbf{C} \end{bmatrix}, \tag{6a}$$

and we multiply the second block of rows from $\mathbf{M}$ by $\mathbf{U}\mathbf{D}^{-1}$ and subtract from the first block of rows to obtain

$$\begin{bmatrix} \mathbf{I} & -\mathbf{U}\mathbf{D}^{-1} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{A} & \mathbf{U} \\ \mathbf{V} & \mathbf{D} \end{bmatrix} = \begin{bmatrix} \mathbf{A} - \mathbf{U}\mathbf{D}^{-1}\mathbf{V} & \mathbf{0} \\ \mathbf{V} & \mathbf{D} \end{bmatrix} = \begin{bmatrix} \mathbf{B} & \mathbf{0} \\ \mathbf{V} & \mathbf{D} \end{bmatrix}. \tag{6b}$$

Taking the determinant of (6a) and (6b) gives us the relations

$$\det \mathbf{M} = \det \mathbf{A} \det \mathbf{C} = \det \mathbf{D} \det \mathbf{B}.$$

Thus if $\mathbf{A}$ is invertible, then $\mathbf{M}$ is invertible if and only if $\mathbf{C}$ is invertible. And if $\mathbf{D}$ is invertible, then $\mathbf{M}$ is invertible if and only if $\mathbf{B}$ is invertible. Moreover, if $\mathbf{A}$ and $\mathbf{D}$ are invertible, then $\mathbf{B}$ is invertible if and only if $\mathbf{C}$ is invertible.

The Modification Formula also appears in Guttman's 1946 paper [24] dealing with enlargement methods for computing the inverse of a matrix. In highlighting

some of the features of this method. Guttman remarks that "The first-order procedure outlined in the next section has been learned by statistical clerks in about ten minutes. People who calculate inverses only occasionally and forget the process between times should find the method as economical as those who must constantly compute inverses." In the enlargement method for inverting a matrix, we successively compute the inverses of the leading principal submatrices using (5a) to express the inverse of a $(k+1)\times(k+1)$ submatrix in terms of the inverse of a previously computed $k\times k$ submatrix. At the end of his paper, Guttman exhibits some matrix identities such as (1) relevant to (5a). He also notes that the special case where **A** is a diagonal matrix is treated in his earlier work [25] and [26].

The formula (1) in the work of Duncan and Guttman did not attract much attention since the formula was presented as an interesting identity arising in the study of partitioned matrices, somewhat unconnected with applications. Then in 1949 Sherman and Morrison considered the seemingly unrelated problem of computing an inverse of a matrix after making a change in the elements in a single column. Their one-third-page statistical abstract [45] (also see [46]) contains the following result. If **A** is an $n\times n$ square invertible matrix and **B** is identical to **A** except for the elements in some column, say column k, then the elements b_{ij}^{-1} of $\mathbf{B}^{-1}$ can be expressed in terms of the elements a_{ij}^{-1} of $\mathbf{A}^{-1}$:

$$b_{kj}^{-1}=\frac{a_{kj}^{-1}}{\sum_{i=1}^{n} a_{ki}^{-1}b_{ik}} \quad \text{for } j=1,2,\cdots,n, \tag{7}$$

$$b_{ij}^{-1}=a_{ij}^{-1}-b_{kj}^{-1}\sum_{l=1}^{n} a_{il}^{-1}b_{lk} \quad \text{for } i\neq k \quad \text{and} \quad j=1,2,\cdots,n. \tag{8}$$

The formulas above correct some typographic errors appearing in [45]. For example, the minus sign appearing in the formula for b_{ij}^{-1} is omitted in [45] so that a_{ij}^{-1} is multiplied by b_{kj}^{-1}. Observe that (7) and (8) can be deduced from (2) with the choice $u_i=a_{ik}-b_{ik}$ for $i=1$ to n and $v_i=0$ for $i\neq k$ while $v_k=1$. As the subsequent literature indicates, this tiny abstract caught people's attention—the problem of determining the change in the inverse matrix after a change in a column had many applications. Later in [6], Bartlett generalized the result of Sherman and Morrison to obtain (2) while Woodbury completed the generalization in his 1950 report [52], obtaining the identity (1) already contained in the papers of Duncan and Guttman. Also, in a completely independent paper [41], published in 1950, (1) is derived by Plackett when he considers the problem of updating a least-squares estimate after obtaining new data.

An important formula is not easily laid to rest. In later years, the Modification Formula is repeatedly rediscovered. Some of these rediscoveries may be due to insufficient communication between researchers in various fields. Barnett in his study [4] of stability in linear programming examines how a change in one column of the constraint matrix affects the solution to a linear program, essentially obtaining (2) during his analysis. In this review, we will highlight various features and applications of the Inverse Matrix Modification Formula.

2. The big picture. Although there are many different ways to utilize the Modification Formula, the most common applications have the following structure. We are given a linear system $\mathbf{Bx}=\mathbf{b}$, where **B** deviates slightly from a "nice" matrix **A** and the difference $\mathbf{A}-\mathbf{B}$ can be expressed in the form **UV**, where **U** and **V** have relatively small rank. For example, **A** may be a tridiagonal matrix, an orthogonal

matrix, a sparse matrix (one with many zeros), or a matrix that has been factored previously into a convenient form. Typically, the solution $\mathbf{x}$ to the equation $\mathbf{Bx} = \mathbf{b}$ (where $\mathbf{B} = \mathbf{A} - \mathbf{UV}$) is computed in the following way:

(1) Solve $\mathbf{Ay} = \mathbf{b}$ for the unknown $\mathbf{y}$.
(2) Compute the matrix $\mathbf{W} = \mathbf{A}^{-1}\mathbf{U}$ by solving the linear systems $\mathbf{Aw}_i = \mathbf{u}_i$, where $\mathbf{w}_i$ and $\mathbf{u}_i$ denote the ith column of $\mathbf{W}$ and $\mathbf{U}$, respectively.
(3) Form the matrix $\mathbf{C} = \mathbf{I} - \mathbf{VW}$, form the vector $\mathbf{Vy}$, and solve the linear system $\mathbf{Cz} = \mathbf{Vy}$ for the unknown $\mathbf{z}$.
(4) Finally, $\mathbf{x} = \mathbf{y} + \mathbf{Wz}$.

If the $\mathbf{A}$ matrix has a convenient structure, then the linear systems associated with $\mathbf{A}$ in steps (1) and (2) are solved quickly. If $\mathbf{V}$ is $m \times n$, where m is much smaller than n, then the rank of the modification $\mathbf{UV}$ is small relative to the dimension n of $\mathbf{A}$ and the system of m linear equations $\mathbf{Cz} = \mathbf{Vy}$ is solved quickly. In many applications, $m = 1$ and $\mathbf{z}$ is the scalar $\mathbf{Vy}/\mathbf{C}$. In summary, the Modification Formula can be useful whenever the coefficient matrix for a linear system can be expressed as the sum of a "nice" matrix and a small rank perturbation.

When applying the Modification Formula, $\mathbf{U}$ and $\mathbf{V}$ must be chosen carefully—there are many different ways to express the difference $\mathbf{A} - \mathbf{B}$ in the form $\mathbf{UV}$, and some of these choices lead to an ill-conditioned matrix $\mathbf{C} = \mathbf{I} - \mathbf{VA}^{-1}\mathbf{U}$ for which the numerical errors associated with step (3) make the computed solution worthless. The condition number κ of a matrix $\mathbf{M}$ is given by

$$\kappa(\mathbf{M}) = \|\mathbf{M}\|\,\|\mathbf{M}^{-1}\|.$$

Potentially, the computed solution to a linear system has no correct digits whenever the condition number is larger than the reciprocal of the machine epsilon (see [30]). In [53] Yip shows that if either $\mathbf{U}$ or $\mathbf{V}$ is formed from the columns of the identity matrix, then for the standard norms,

$$\kappa(\mathbf{C}) \leqq \kappa(\mathbf{A})\kappa(\mathbf{B}). \tag{9}$$

Moreover, in the 2-norm, the inequality $\kappa_2(\mathbf{C}) \leqq \kappa_2(\mathbf{A})\kappa_2(\mathbf{B})$ is valid if either $\mathbf{U}$ or $\mathbf{V}$ is formed from the columns of an orthogonal matrix. When (9) holds, the condition number of $\mathbf{C}$ is bounded in terms of the condition numbers of $\mathbf{A}$ and $\mathbf{B}$, and if both $\mathbf{A}$ and $\mathbf{B}$ are well conditioned, then so is $\mathbf{C}$. In applications where $\mathbf{B}$ is the same as $\mathbf{A}$ except for elements in a few columns, it is natural to take $\mathbf{U} = \bar{\mathbf{A}} - \bar{\mathbf{B}}$, where $\bar{\mathbf{A}}$ and $\bar{\mathbf{B}}$ denote the submatrices of $\mathbf{A}$ and $\mathbf{B}$ corresponding to the columns that differ while $\mathbf{V}$ is composed of the rows of the identity matrix corresponding to the columns where $\mathbf{A}$ and $\mathbf{B}$ differ. For this choice of $\mathbf{U}$ and $\mathbf{V}$, (9) holds.

3. Least squares. An application of the Modification Formula to statistics arises in the following context. We are trying to estimate some parameters in a linear model. As new data is received, the least-squares estimate for the parameters is updated to reflect the new data. Some references include Anderson [2] and [3], Plackett [41], and Riddell [44]. To illustrate this application, let us consider an overdetermined linear system $\mathbf{Ax} = \mathbf{b}$, where $\mathbf{A}$ is $l \times n$ with $l > n$. When we assume that the columns of $\mathbf{A}$ are linearly independent, the $\mathbf{x}$ that minimizes the Euclidean norm of the residual $\mathbf{b} - \mathbf{Ax}$ is given by

$$\mathbf{x} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{b}. \tag{10}$$

Now, suppose we receive new data that gives us the relation $\mathbf{vx} = c$. The new $\mathbf{A}$ matrix corresponding to the additional data is

$$\mathbf{A}^{\text{new}} = \begin{bmatrix} \mathbf{A} \\ \mathbf{v} \end{bmatrix}.$$

If $\mathbf{B}$ denotes the product $\mathbf{A}^T\mathbf{A}$ that is inverted in (10), then the new $\mathbf{B}$ corresponding to the new $\mathbf{A}$ can be expressed as

$$\mathbf{B}^{\text{new}} = \mathbf{B}^{\text{old}} + \mathbf{uv}$$

where $\mathbf{u} = \mathbf{v}^T$. By the Inverse Matrix Modification Formula we have

$$[\mathbf{B}^{\text{new}}]^{-1} = [\mathbf{B} + \mathbf{uv}]^{-1} = \mathbf{B}^{-1} - \alpha\mathbf{B}^{-1}\mathbf{uv}\mathbf{B}^{-1} \quad \text{where } \alpha = 1/(1 + \mathbf{vB}^{-1}\mathbf{u}).$$

In other words, if the old inverse of $\mathbf{B}$ is available, then the new inverse of $\mathbf{B}$ is found by adding a rank 1 correction to the old inverse. With this substitution for the new $\mathbf{B}^{-1}$, the new least squares estimate for $\mathbf{x}$ can be expressed as

$$\mathbf{x}^{\text{new}} = \mathbf{x} + \mathbf{k}[c - \mathbf{vx}] \quad \text{where } \mathbf{k} = \frac{\mathbf{B}^{-1}\mathbf{u}}{1 + \mathbf{vB}^{-1}\mathbf{u}}.$$

In a similar fashion, the adjustment to the inverse of $\mathbf{B}$ associated with m new equations can be obtained from (1). If the new equations are expressed $\mathbf{Vx} = \mathbf{c}$, then the new least-squares estimate is

$$\mathbf{x}^{\text{new}} = \mathbf{x} + \mathbf{K}[\mathbf{c} - \mathbf{Vx}] \quad \text{where } \mathbf{K} = \mathbf{B}^{-1}\mathbf{U}[\mathbf{I} + \mathbf{VB}^{-1}\mathbf{U}]^{-1}$$

where $\mathbf{U} = \mathbf{V}^T$ while the new inverse of $\mathbf{B}$ is

$$[\mathbf{B}^{\text{new}}]^{-1} = \mathbf{B}^{-1} - \mathbf{B}^{-1}\mathbf{U}[\mathbf{I} + \mathbf{VB}^{-1}\mathbf{U}]^{-1}\mathbf{VB}^{-1}.$$

4. Networks and structures. In network problems, nodes are connected together by various electrical devices. After a "base-case" solution is obtained, the network may be modified and a new solution computed. Some references include [1], [32], and [33]. As a simple illustration of an electrical network, let us consider a collection of $n + 1$ nodes labeled $0, 1, \cdots, n$ connected by resistors. Let V_i denote the potential of node i and assume that node zero is the ground: $V_0 = 0$. The current along the branch-connecting nodes i and j is the voltage difference $V_j - V_i$ divided by the resistance R_{ij}. By Kirchhoff's first law, the sum of the currents entering each node is zero. Summing over the branches connected to node i, we have

$$\sum_{j=0}^{n} \frac{V_j - V_i}{R_{ij}} = I_i, \qquad i = 1, 2, \cdots, n \tag{11}$$

where I_i is an external current injected into node i. Since $R_{ij} = R_{ji}$, the resulting linear system is symmetric. Equation (11) has the form $\mathbf{Ax} = \mathbf{b}$, where $x_i = V_i$, $b_i = I_i$,

$$a_{ij} = \frac{1}{R_{ij}} \quad \text{for } i \neq j, \qquad a_{ii} = -\sum_{\substack{j=0 \\ j \neq i}}^{n} \frac{1}{R_{ij}}.$$

Suppose that after we factor the coefficient matrix $\mathbf{A}$ and solve the linear system $\mathbf{Ax} = \mathbf{b}$, the network is altered. To be specific, suppose that the resistance between nodes 1 and 3 is changed to S_{13}. This change in the resistance produces a change in

the coefficient matrix that can be expressed as

$$\mathbf{A}^{\text{new}} = \mathbf{A} - d\mathbf{u}\mathbf{u}^T$$

where

$$d = \frac{1}{S_{13}} - \frac{1}{R_{13}} \quad \text{and} \quad \mathbf{u} = \begin{bmatrix} 1 \\ 0 \\ -1 \\ 0 \\ 0 \\ \vdots \\ \vdots \end{bmatrix}. \tag{12}$$

Thus the voltages corresponding to the altered resistance can be computed using the Modification Formula.

The illustration given above is called *branch-oriented modification* (see [1]) since a correction term is added to the coefficient matrix corresponding to the altered branch. If m branches in the circuit are altered, then the correction term has the form $\mathbf{UDU}^T$, where $\mathbf{U}$ is a matrix for which all elements in each column are zero except for a + 1 entry and a − 1 entry, and $\mathbf{D}$ is a diagonal matrix. An alternative viewpoint is *node-oriented modification*. If there are m nodes associated with modified branches, then the correction term again has the form $\mathbf{UDU}^T$. However, $\mathbf{U}$ now consists of the columns of the identity matrix corresponding to the altered nodes, and $\mathbf{D}$ is zero except for the elements corresponding to altered branches. The node-oriented modification corresponding to changing the resistance R_{13} to S_{13} is given by

$$\mathbf{UDU}^T = \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 1 \\ 0 & 0 \\ \vdots & \vdots \\ \vdots & \vdots \end{bmatrix} \begin{bmatrix} d & -d \\ -d & d \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 1 & 0 & \cdots \end{bmatrix}$$

where d is defined in (12). In this example, branch-oriented modification leads to a simpler correction term than node-oriented modification. When fewer nodes than branches are modified, node-oriented modification may be preferable.

The technique described above for relating the solution of the modified network to the solution of the original network using the modification formula is often called the *compensation method*. These same techniques are also used in structural analysis to compute the change in stress and strain due to an alteration in part of the structure. In the structural mechanics literature, the relevant terminology is *static reanalysis* (see [37]).

In some applications, the modifications to the coefficient matrix are performed in an incremental fashion. For example, with an electric network, the *base-case* solution is computed first. Then we successively modify one branch after another, recomputing the solution after each modification. A specific illustration of this appears in [31], where lightning is modeled—as a lightning flash propagates in a thundercloud, a sequence of corrections are added to the coefficient matrix. After each modification of the coefficient matrix, the potential field in the thundercloud is reevaluated; depending on the value of the potential, the flash either continues or it is extinguished. When applying the Modification Formula (1) in this incremental context, it is inefficient to refactor the capacitance matrix $\mathbf{C}$ after each incremental change in the

coefficient matrix. In §10, we explain how to incrementally update a factorization of **C**.

5. Asymptotic analysis. In some applications, the perturbation to the coefficient matrix in a linear system involves a parameter, and we are interested in the limiting solution as the parameter tends to infinity. The Modification Formula often facilitates the analysis of the limit. We illustrate this application using three examples: (a) electrical breakdown in a network; (b) a constrained quadratic program; and (c) preconditioning for penalty and multiplier methods in constrained optimization.

Consider a large electric network such as a thunderstorm (this example is taken from [31]). The electric field along a line segment connecting two nodes in the network is approximated by the voltage difference divided by the distance between the nodes. When the electric field between two nodes reaches the "breakdown threshold," the resistance between these nodes tends to zero and there is an arc. The voltages throughout the network after the discharge can be evaluated using the Modification Formula. As we saw in §4, the new coefficient matrix corresponding to the altered resistance can be expressed $\mathbf{A}^{\text{new}} = \mathbf{A} - d\mathbf{u}\mathbf{u}^T$, where d tends to infinity as the branch resistance tends to zero and $\mathbf{u}$ is a vector with every component equal to zero except for one component which is $+1$ and another component which is -1. By (2) the limit of the inverse of the new $\mathbf{A}$ is given by

$$[\mathbf{A}^{\text{new}}]^{-1} = \mathbf{A}^{-1} + \lim_{d\to\infty} \frac{d\mathbf{A}^{-1}\mathbf{u}\mathbf{u}^T\mathbf{A}^{-1}}{1 - d\mathbf{u}^T\mathbf{A}^{-1}\mathbf{u}} = \mathbf{A}^{-1} - \frac{\mathbf{A}^{-1}\mathbf{u}\mathbf{u}^T\mathbf{A}^{-1}}{\mathbf{u}^T\mathbf{A}^{-1}\mathbf{u}}.$$

In the limit as d tends to infinity, there is cancellation and the d's disappear.

Note that if the limiting inverse of $\mathbf{A}^{\text{new}}$ is premultiplied by $\mathbf{u}^T$, we obtain the relation $\mathbf{u}^T[\mathbf{A}^{\text{new}}]^{-1} = \mathbf{0}$. Since every component of $\mathbf{u}$ is zero except for the $+1$ and -1 components, it follows that the discharge process equilibrates the potential at the two nodes associated with the electrical breakdown. In general, if there are m branches along which electrical breakdown occurs, the Modification Formula leads us to the following expression for the limiting inverse of the new $\mathbf{A}$:

$$[\mathbf{A}^{\text{new}}]^{-1} = \mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{U}[\mathbf{U}^T\mathbf{A}^{-1}\mathbf{U}]^{-1}\mathbf{U}^T\mathbf{A}^{-1}.$$

Here $\mathbf{U}$ is a matrix with all elements in each column zero, except for a $+1$ entry and a -1 entry that correspond to a pair of adjacent nodes where the electric field exceeds the breakdown threshold. After the discharge, the potential is equal at all nodes associated with the electrical breakdown.

For our second example, let us consider a constrained least-squares problem:

$$\underset{\mathbf{x}}{\text{minimize}} \{\|\mathbf{Q}\mathbf{x} - \mathbf{q}\|_2^2 : \mathbf{V}\mathbf{x} = \mathbf{c}\}. \tag{13}$$

In other words, minimize over $\mathbf{x}$ the 2-norm of the residual $\mathbf{Q}\mathbf{x} - \mathbf{q}$ subject to the constraint $\mathbf{V}\mathbf{x} = \mathbf{c}$, where $\mathbf{V}$ is a given matrix and $\mathbf{c}$ is a given vector in the range space of $\mathbf{V}$. By [27, Thm. 2.4], (13) has a unique solution if

$$\mathbf{Q}\mathbf{x} \neq \mathbf{0} \quad \text{whenever } \mathbf{V}\mathbf{x} = \mathbf{0} \quad \text{and} \quad \mathbf{x} \neq \mathbf{0}. \tag{14}$$

To compute the solution to (13) when the rows of $\mathbf{V}$ are linearly independent and (14) holds, we form the penalized problem, apply the Modification Formula, and let the penalty tend to infinity. The penalty approximation is the unconstrained problem:

$$\text{minimize } \{\|\mathbf{Q}\mathbf{x} - \mathbf{q}\|_2^2 + r\|\mathbf{V}\mathbf{x} - \mathbf{c}\|_2^2\} \tag{15}$$

where r is the penalty parameter. As r tends to infinity, the solution to this unconstrained optimization problem approaches the solution to (13). Setting the derivative to zero, we see that the solution to (15) satisfies the following equation:

$$(\mathbf{A}+r\mathbf{V}^T\mathbf{V})\mathbf{x}=\mathbf{Q}^T\mathbf{q}+r\mathbf{V}^T\mathbf{c} \tag{16}$$

where $\mathbf{A}=\mathbf{Q}^T\mathbf{Q}$.

Although the coefficient matrix in (16) has the same structure as the coefficient matrix in the electrical breakdown example, the parameter r in (16) now appears on the right side of the equation as well as the left side. Due to this extra r, the expansion must be extended one term further. By the Modification Formula,

$$(\mathbf{A}+r\mathbf{V}^T\mathbf{V})^{-1}=\mathbf{A}^{-1}-r\mathbf{A}^{-1}\mathbf{V}^T[\mathbf{I}+r\mathbf{V}\mathbf{A}^{-1}\mathbf{V}^T]^{-1}\mathbf{V}\mathbf{A}^{-1}. \tag{17}$$

Using the expansion

$$[\mathbf{I}+\mathbf{P}]^{-1}=\mathbf{P}^{-1}-\mathbf{P}^{-2}+\mathbf{P}^{-3}-\cdots,$$

which is valid when the spectral radius of $\mathbf{P}$ is less than 1, we can write the bracketed expression in (17) as

$$[\mathbf{I}+r\mathbf{V}\mathbf{A}^{-1}\mathbf{V}^T]^{-1}=r^{-1}(\mathbf{V}\mathbf{A}^{-1}\mathbf{V}^T)^{-1}-r^{-2}(\mathbf{V}\mathbf{A}^{-1}\mathbf{V}^T)^{-2}+O(r^{-3}). \tag{18}$$

Inserting this expansion into (17) and taking the limit as r tends to infinity, we see that the solution to (16) approaches

$$\mathbf{x}=\mathbf{A}^{-1}\mathbf{V}^T(\mathbf{V}\mathbf{A}^{-1}\mathbf{V}^T)^{-1}\mathbf{c}+\mathbf{A}^{-1}\mathbf{Q}^T\mathbf{q}-\mathbf{A}^{-1}\mathbf{V}^T(\mathbf{V}\mathbf{A}^{-1}\mathbf{V}^T)^{-1}\mathbf{V}\mathbf{A}^{-1}\mathbf{Q}^T\mathbf{q},$$

which is the solution to (13).

For our final example in this section, we present a preconditioning result related to penalty and multiplier methods for solving constrained optimization problems. These results are stated in the context of a constrained quadratic program, although they apply to general optimization problems (see [28]). As in (13), let us consider the quadratic program

$$\text{minimize } \{\mathbf{x}^T\mathbf{A}\mathbf{x}-2\mathbf{q}^T\mathbf{x}:\mathbf{V}\mathbf{x}=\mathbf{0}\}. \tag{19}$$

Again, the penalty approximation is

$$\text{minimize } \{\mathbf{x}^T(\mathbf{A}+r\mathbf{V}^T\mathbf{V})\mathbf{x}-2\mathbf{q}^T\mathbf{x}\}. \tag{20}$$

Although the solution to (20) approaches the solution to (19) as r tends to infinity, the convergence rate of gradient methods for solving (20) is arbitrarily slow as r increases. The convergence rate is governed by the ratio λ_n/λ_1 between the largest eigenvalue λ_n and the smallest eigenvalue λ_1 of $\mathbf{A}+r\mathbf{V}^T\mathbf{V}$. As r tends to infinity, the ratio λ_n/λ_1 tends to infinity, making the convergence slow. In contrast, for preconditioned gradient techniques, the convergence rate is governed by the ratio between the largest and smallest eigenvalues of the matrix $(\mathbf{A}+r\mathbf{V}^T\mathbf{V})\mathbf{P}^{-1}$, where $\mathbf{P}$ denotes the preconditioner. To solve the penalized problem quickly using a preconditioned gradient method, we must choose $\mathbf{P}$ so that the eigenvalues of the product $(\mathbf{A}+r\mathbf{V}^T\mathbf{V})\mathbf{P}^{-1}$ are well conditioned.

As we will see, a preconditioner of the form $\mathbf{P}=\mathbf{S}+r\mathbf{V}^T\mathbf{V}$, where $\mathbf{S}$ is any symmetric positive definite matrix, yields well-conditioned eigenvalues; that is, under fairly standard assumptions, the eigenvalue ratio associated with the preconditioned problem is bounded by a constant independent of r. To establish this result, let us use

(17) and the expansion (18) to evaluate the product $(\mathbf{A} + r\mathbf{V}^T\mathbf{V})(\mathbf{S}+r\mathbf{V}^T\mathbf{V})^{-1}$. Omitting the algebra, we have

$$(\mathbf{A}+r\mathbf{V}^T\mathbf{V})(\mathbf{S}+r\mathbf{V}^T\mathbf{V})^{-1}=\mathbf{Z}+O(r^{-1})$$

where

$$\mathbf{Z}=\mathbf{A}\mathbf{S}^{-1}+(\mathbf{I}-\mathbf{A}\mathbf{S}^{-1})\mathbf{V}^T(\mathbf{V}\mathbf{S}^{-1}\mathbf{V}^T)^{-1}\mathbf{V}\mathbf{S}^{-1}.$$

Thus the preconditioner has "canceled" the larger eigenvalues of $\mathbf{A} + r\mathbf{V}^T\mathbf{V}$. In addition, we must check to see that the preconditioner has not introduced new small eigenvalues. If $\mathbf{Z}$ is singular, then a new $O(r^{-1})$ eigenvalue will be introduced. In [28] it is proved that if the rows of $\mathbf{V}$ are linearly independent, then $\mathbf{Z}$ is nonsingular if and only if

$$\underset{\substack{\mathbf{V}\mathbf{y}=\mathbf{0}\\ \|\mathbf{y}\|=1}}{\text{minimum}}\ \underset{\substack{\mathbf{V}\mathbf{x}=\mathbf{0}\\ \|\mathbf{x}\|=1}}{\text{maximum}}\ \mathbf{x}^T\mathbf{A}\mathbf{y}>0. \tag{21}$$

This condition is weaker than the usual second-order sufficient condition associated with (19)—for further discussion of inf-sup conditions such as in (21), see the survey article [29]. Note that the following block matrix is nonsingular if and only if the rows of $\mathbf{V}$ are linearly independent and (21) holds:

$$\begin{bmatrix}\mathbf{A} & \mathbf{V}^T\\ \mathbf{V} & \mathbf{0}\end{bmatrix}.$$

If $\mathbf{S} = \mathbf{I}$ and the rows of $\mathbf{V}$ are linearly independent, then the Modification Formula reveals that the preconditioner $(\mathbf{I} + r\mathbf{V}^T\mathbf{V})^{-1}$ is nearly a projection:

$$\lim_{r\to\infty}[\mathbf{I}+r\mathbf{V}^T\mathbf{V}]^{-1}=\mathbf{I}-\mathbf{V}^T(\mathbf{V}\mathbf{V}^T)^{-1}\mathbf{V}. \tag{22}$$

Since the right side of (22) projects a vector into the null space of $\mathbf{V}$, we conclude that $(\mathbf{I} + r\mathbf{V}^T\mathbf{V})^{-1}$ nearly projects a vector into the null space of $\mathbf{V}$ when r is large.

6. Sensitivity in linear programming. A standard format for linear programming problems is the following:

$$\text{minimize}\quad \mathbf{c}^T\mathbf{x}\quad \text{subject to}\quad \mathbf{M}\mathbf{x}=\mathbf{b},\quad \mathbf{x}\geqq\mathbf{0} \tag{23}$$

where $\mathbf{c}$, $\mathbf{b}$, and $\mathbf{M}$ are given data and $\mathbf{M}$ is $m \times n$ with n larger than m. A fundamental theorem in linear programming states that if (23) has a solution and the rows of $\mathbf{M}$ are linearly independent, then (23) has a *basic optimal solution* (see [36]). By a basic optimal solution, we mean that the components of the optimal solution can be partitioned to form two vectors denoted $\mathbf{x}_\mathbf{B}$ and $\mathbf{x}_\mathbf{N}$, where $\mathbf{x}_\mathbf{N} = \mathbf{0}$ and $\mathbf{x}_\mathbf{B}$ is an m-component vector for which the corresponding columns of $\mathbf{M}$ are linearly independent. Let $\mathbf{B}$ and $\mathbf{N}$ denote the submatrices of $\mathbf{M}$ corresponding to $\mathbf{x}_\mathbf{B}$ and $\mathbf{x}_\mathbf{N}$, respectively. The equation $\mathbf{M}\mathbf{x} = \mathbf{b}$ and the condition $\mathbf{x}_\mathbf{N} = \mathbf{0}$ imply that $\mathbf{x}_\mathbf{B} = \mathbf{B}^{-1}\mathbf{b}$.

Typically, in real-life linear programming problems, the data defining the problem is uncertain. In sensitivity analysis, we investigate how the solution to the linear program and the optimal cost depend on the data. Let $\mathbf{c}_\mathbf{B}$ denote the vector formed by those components of $\mathbf{c}$ corresponding to the components of $\mathbf{x}_\mathbf{B}$ and let $\mathbf{c}_\mathbf{N}$ denote the vector formed by the remaining components of $\mathbf{c}$. To simplify the analysis, we assume that each component of both $\mathbf{x}_\mathbf{B}$ and the relative-cost vector

$$\mathbf{r}_\mathbf{N}^T=\mathbf{c}_\mathbf{N}^T-\mathbf{c}_\mathbf{B}^T\mathbf{B}^{-1}\mathbf{N}$$

are positive. When the data are altered, the solution to (23) is given by $\mathbf{x_B} = \mathbf{B}^{-1}\mathbf{b}$ and $\mathbf{x_N} = \mathbf{0}$ as long as $\mathbf{B}^{-1}\mathbf{b} \geqq 0$ and the corresponding relative-cost vector remains nonnegative. Hence, for small changes in $\mathbf{c}$, $\mathbf{b}$, or $\mathbf{M}$, the solution to (23) is $\mathbf{x_B} = \mathbf{B}^{-1}\mathbf{b}$ and $\mathbf{x_N} = \mathbf{0}$. When we let $C = \mathbf{c}_\mathbf{B}^T\mathbf{B}^{-1}\mathbf{b}$ denote the optimal cost associated with (23), it follows that

$$\frac{\partial C}{\partial b_i} = \lambda_i \quad \text{and} \quad \frac{\partial C}{\partial c_i} = \begin{cases} 0 & \text{if } c_i \text{ is a component of } \mathbf{c_N}, \\ x_i & \text{if } c_i \text{ is a component of } \mathbf{c_B} \end{cases}$$

where $\lambda = \mathbf{B}^{-T}\mathbf{c_B}$ is the dual solution.

When investigating how the cost depends on the coefficient matrix $\mathbf{M}$, we often consider a perturbation of the form

$$\mathbf{B} = \mathbf{A} - \sigma \mathbf{u}\mathbf{v}$$

where σ is related to the uncertainty associated with elements of the coefficient matrix. Applying the Modification Formula and differentiating with respect to σ, we find that

$$\frac{\partial C}{\partial \sigma} = \frac{(\mathbf{c}_\mathbf{B}^T\mathbf{A}^{-1}\mathbf{u})(\mathbf{v}\mathbf{A}^{-1}\mathbf{b})}{(1 - \sigma \mathbf{v}\mathbf{A}^{-1}\mathbf{u})^2}.$$

Hence, at $\sigma = 0$, we have

$$\left.\frac{\partial C}{\partial \sigma}\right|_{\sigma=0} = \lambda_\Lambda \mathbf{u}\mathbf{v}\mathbf{x}_\Lambda$$

where $\mathbf{x}_\Lambda = \mathbf{A}^{-1}\mathbf{b}$ is the optimal solution and $\lambda_\Lambda = \mathbf{c}_\mathbf{B}^T\mathbf{A}^{-1}$ is the dual solution corresponding to $\sigma = 0$.

Another important sensitivity question is to determine the first value of σ where there is a change in the optimal basis. Equivalently, determine the largest interval $[\sigma_1, \sigma_2]$ containing zero with the property that both $\mathbf{x_B} = \mathbf{B}^{-1}\mathbf{b}$ and the relative cost are nonnegative whenever $\sigma_1 \leqq \sigma \leqq \sigma_2$. By the Modification Formula, the values of σ that do not change the optimal basis satisfy the following inequalities:

$$\mathbf{x}_\Lambda + \sigma\left[\frac{\mathbf{v}\mathbf{A}^{-1}\mathbf{b}}{1 - \sigma \mathbf{v}\mathbf{A}^{-1}\mathbf{u}}\right]\mathbf{A}^{-1}\mathbf{u} \geqq \mathbf{0}, \tag{24}$$

$$\mathbf{r}_\Lambda^T - \sigma\left[\frac{\mathbf{c}_\mathbf{B}^T\mathbf{A}^{-1}\mathbf{u}}{1 - \sigma \mathbf{v}\mathbf{A}^{-1}\mathbf{u}}\right]\mathbf{v}\mathbf{A}^{-1}\mathbf{N} \geqq \mathbf{0} \tag{25}$$

where $\mathbf{r}_\Lambda$ is the relative cost corresponding to $\sigma = 0$:

$$\mathbf{r}_\Lambda^T = \mathbf{c}_\mathbf{N}^T - \mathbf{c}_\mathbf{B}^T\mathbf{A}^{-1}\mathbf{N}.$$

Assuming that either the σ term in (24) or the σ term in (25) does not vanish, we conclude that $1 \geqq \sigma \mathbf{v}\mathbf{A}^{-1}\mathbf{u}$ for σ in the desired interval $[\sigma_1, \sigma_2]$. That is, as σ passes through the pole $\sigma = 1/\mathbf{v}\mathbf{A}^{-1}\mathbf{u}$, one of (24) or (25) is violated; hence, we restrict σ to the side of the pole corresponding to $\sigma = 0$. Multiplying through by the denominator $1 - \mathbf{v}\mathbf{A}^{-1}\mathbf{u}$ in (24) and (25), we obtain the following pair of inequalities:

$$\mathbf{x}_\Lambda \geqq \sigma \mathbf{y} \quad \text{and} \quad \mathbf{r}_\Lambda \geqq \sigma \mathbf{z} \tag{26}$$

where

$$\mathbf{y} = (\mathbf{v}\mathbf{A}^{-1}\mathbf{u})\mathbf{x}_\Lambda - (\mathbf{v}\mathbf{A}^{-1}\mathbf{b})\mathbf{A}^{-1}\mathbf{u} \quad \text{and} \quad \mathbf{z}^T = (\mathbf{v}\mathbf{A}^{-1}\mathbf{u})\mathbf{r}_\Lambda^T + (\mathbf{c}_\mathbf{B}^T\mathbf{A}^{-1}\mathbf{u})\mathbf{v}\mathbf{A}^{-1}\mathbf{N}.$$

The endpoints σ_1 and σ_2 of the interval corresponding to those σ's that satisfy (26) are given by

$$\sigma_1 = \underset{i,j}{\text{maximum}} \left\{ \frac{(\mathbf{r}_A)_i}{z_i}, \frac{(\mathbf{x}_A)_j}{y_j} : z_i < 0, y_j < 0 \right\},$$

$$\sigma_2 = \underset{i,j}{\text{minimum}} \left\{ \frac{(\mathbf{r}_A)_i}{z_i}, \frac{(\mathbf{x}_A)_j}{y_j} : z_i > 0, y_j > 0 \right\}.$$

Papers that examine stability of the optimal basis in linear programming include [4] by Barnett and [18] by Flavell and Salkin. The book [17] by Fiacco is a comprehensive reference for sensitivity analysis in nonlinear programming.

7. Partial differential equations. After obtaining a numerical approximation to the solution of a partial differential equation using one boundary condition, we may be asked to solve the equation again using a slightly different boundary condition. Often the Modification Formula can be used to take advantage of the previously computed solution. To illustrate how boundary conditions enter the coefficient matrix of an approximating finite difference system, we consider the equation

$$-x''(t) = f(t), \qquad 0 \leqq t \leqq 1. \tag{27}$$

Partitioning the interval [0, 1] into N subintervals of equal width $\Delta t = 1/N$, the standard centered difference approximation to (27) is

$$-x_{i-1} + 2x_i - x_{i+1} = (\Delta t)^2 f_i, \qquad i = 1, 2, \cdots, N-1 \tag{28}$$

where f_i is the value of f at $t = i/N$ and x_i approximates $x(i/N)$. For a Dirichlet boundary condition $x(0) = x(1) = 0$, we have the relation $x_0 = x_N = 0$ so that the finite difference system (28) reduces to

$$\begin{bmatrix} 2 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & & & \\ & & & \ddots & & \\ & & & & 2 & -1 \\ & & & & -1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{N-1} \end{bmatrix} = \begin{bmatrix} (\Delta t)^2 f_1 \\ (\Delta t)^2 f_2 \\ \vdots \\ (\Delta t)^2 f_{N-1} \end{bmatrix}. \tag{29}$$

Now let us replace the Dirichlet condition $x(1) = 0$ with the Neumann condition $x'(1) = 0$. The usual finite difference approximation to the Neumann condition is $x_N = x_{N-1}$. Combining this discrete Neumann condition with (28), we obtain the following linear system:

$$\begin{bmatrix} 2 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & & & \\ & & & \ddots & & \\ & & & & 2 & -1 \\ & & & & -1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{N-1} \end{bmatrix} = \begin{bmatrix} (\Delta t)^2 f_1 \\ (\Delta t)^2 f_2 \\ \vdots \\ (\Delta t)^2 f_{N-1} \end{bmatrix}. \tag{30}$$

In going from (29) to (30), the only difference is that the last coefficient in row $N-1$ is changed from 2 to 1.

Finally, let us replace the Neumann boundary condition by the periodic boundary condition $x'(0) = x'(1)$. The usual finite difference approximation to this periodic

condition is

$$x_1 - x_0 = x_N - x_{N-1},$$

which implies that $x_N = x_{N-1} + x_1 - x_0$. Combining this with (28), we have the following linear system:

$$\begin{bmatrix} 2 & -1 & & & & 0 \\ -1 & 2 & -1 & & & \\ & -1 & 2 & \ddots & & \\ & & & \ddots & & \\ & & & & 2 & -1 \\ -1 & & & & -1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ \\ x_{N-1} \end{bmatrix} = \begin{bmatrix} (\Delta t)^2 f_1 \\ (\Delta t)^2 f_2 \\ \vdots \\ \\ (\Delta t)^2 f_{N-1} \end{bmatrix}. \tag{31}$$

Observe that any of the coefficient matrices in (29), (30), or (31) can be obtained from any of the other ones by a rank 1 perturbation. Hence, the Modification Formula can be used to compute the change in the solution due to a change in the boundary condition. For boundary-value problems in more than one space dimension, the rank of the perturbation matrix associated with the boundary conditions depends on the number of meshpoints on the boundary of the domain.

The Modification Formula is also closely connected with both the capacitance matrix method and domain decomposition techniques. In the capacitance matrix method (see [43]), fast solution techniques such as the Fast Fourier Transform or cyclic reduction (see [10], [14], [34], [35], [50], or [51]), which are tailored to a regular mesh and a rectangular domain, are applied to an equation defined on a domain with a curved boundary. The basic strategy is to extend the equation from the given domain to a circumscribing box. The finite difference equations corresponding to the meshpoints on the boundary of the original domain destroy the regular structure of the coefficient matrix associated with the box. However, adding a small-rank perturbation to the coefficient matrix restores the regular structure. Consequently, the Modification Formula can be used to recover the solution on the original domain from the solution on the box corresponding to the regular coefficient matrix.

We illustrate these ideas using (27), the finite difference system (28), and the boundary condition $x(0) = x'(1) = 0$. Let us extend the domain to the interval $0 \leqq t \leqq 2$, setting f to zero on the interval $1 \leqq t \leqq 2$, and impose the Dirichlet boundary condition $x(2) = 0$ (the conditions on the boundary of the extended domain are chosen to be convenient; for example, periodic boundary conditions are convenient if Fast Fourier Transforms are used to solve the extended problem). The matrix representation of the finite difference approximation to the extended problem is the following:

$$\begin{bmatrix} 2 & -1 & & & & & & & & \\ -1 & 2 & -1 & & & & & & & \\ & -1 & 2 & \ddots & & & & & & \\ & & & \ddots & & & & & & \\ & & & & 2 & -1 & & & & \\ & & & & -1 & 1 & 0 & & & \\ & & & & & -1 & 2 & -1 & & \\ & & & & & & -1 & \ddots & & \\ & & & & & & & \ddots & 2 & -1 \\ & & & & & & & & -1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ \\ x_{N-1} \\ x_N \\ \vdots \\ \\ x_{2N-1} \end{bmatrix} = \begin{bmatrix} (\Delta t)^2 f_1 \\ (\Delta t)^2 f_2 \\ \vdots \\ \\ (\Delta t)^2 f_{N-1} \\ 0 \\ \vdots \\ \\ 0 \end{bmatrix}. \tag{32}$$

Observe that the first $N-1$ equations correspond to (30) while the last N equations correspond to the new region $1 \leqq t \leqq 2$. By adding a rank 1 correction to the coefficient matrix in (32), the elements in row $N-1$ can be changed to produce the symmetric tridiagonal matrix with every diagonal element equal to 2 and with every subdiagonal and superdiagonal element equal to -1. In general, when there are m meshpoints on the boundary of the curved domain, a regular structure for the coefficient matrix is achieved using a rank m perturbation. The extended finite difference system is solved using a fast solver while the solution to the original equation is recovered using the Modification Formula.

In domain decomposition techniques, the domain associated with a partial differential equation is partitioned into subdomains and the discrete equations are partitioned into two sets: the equations associated with variables corresponding to the interior of each subdomain and the equations relating variables in different subdomains. If the interior equations are grouped together in one set and the connection equations are grouped together in another set, then we obtain a 2×2 block partitioned system, similar to the 2×2 system of §1. Some references for domain decomposition techniques include [8a–c] and [11].

Finally, we point out an application of the Modification Formula to the boundary element method for linear elasticity. In [19] Ghosh and Mukherjee obtain a system $\mathbf{Bx} = \mathbf{b}$, where every third row of $\mathbf{B}$ is dense (contains few zeros) while the intervening rows are zero except for a few nonzeros near the diagonal. The dense rows correspond to boundary integrals while the sparse rows correspond to compatibility conditions. They apply the Modification Formula in the following way. Let $\mathbf{A}$ be the matrix that is identical to $\mathbf{B}$ for the sparse rows and is the corresponding row of the identity matrix for the dense rows. The columns of $\mathbf{U}$ are the negatives of the rows of the identity matrix inserted in $\mathbf{A}$. The rows of $\mathbf{V}$ are the dense rows of $\mathbf{B}$ except that 1 is subtracted from each diagonal element. With these definitions, $\mathbf{B} = \mathbf{A} - \mathbf{UV}$, where $\mathbf{A}$ is an invertible band matrix. Since $\mathbf{A}$ is a band matrix, the time needed to solve $\mathbf{Bx} = \mathbf{b}$ using the algorithm of §2 is essentially the time needed to factor the dense capacitance matrix $\mathbf{C}$. An operation count reveals that if there are N dense equations, then factoring the $N \times N$ matrix $\mathbf{C}$ is about 27 times faster than Gaussian elimination applied to the original $3N \times 3N$ system.

8. Tearing and mending. The basic idea in tearing is to use the Modification Formula to annihilate elements that complicate the structure of the coefficient matrix for a linear system. For example, suppose that the coefficient matrix of $\mathbf{Bx} = \mathbf{b}$ can be expressed as $\mathbf{B} = \mathbf{L} - \mathbf{P}$, where $\mathbf{L}$ is lower triangular and all the columns of the perturbation $\mathbf{P}$ are completely zero except for m columns. If the nonzeros in $\mathbf{P}$ are annihilated, then we are left with a lower triangular system that can be solved by forward substitution. The Modification Formula essentially gives us a way to annihilate these nonzero elements. Letting $\mathbf{U}$ denote the submatrix of $\mathbf{P}$ consisting of the nonzero columns and letting $\mathbf{V}$ denote the corresponding rows of the identity matrix, we have $\mathbf{P} = \mathbf{UV}$. Since $\mathbf{B} = \mathbf{L} - \mathbf{UV}$, the algorithm of §2 can be used to solve $\mathbf{Bx} = \mathbf{b}$. The pioneering work on tearing was performed by Kron (see [38]–[40]). A brief but informative survey of tearing is contained in the paper [15] by Duff. Other references include [9], [47], and [48]. One difficulty with tearing is that in a complicated problem, an efficient tearing may not be obvious.

The Modification Formula can be used both to tear the coefficient matrix, annihilating undesired nonzero elements, and to mend the coefficient matrix, changing the value of an undesired zero element. In the usual Gaussian elimination algorithm, multiples of one row are subtracted from the rows beneath it to annihilate the

coefficients beneath the diagonal. In the kth elimination step, multiples of row k are subtracted from the rows beneath it to annihilate the coefficients in column k beneath the diagonal. But if the kth diagonal coefficient is zero, then the elimination step breaks down; if the kth diagonal coefficient is small relative to the other coefficients in the column, then numerical errors can overwhelm the computations. Usually, Gaussian elimination is stabilized by performing a pivot before each elimination step. In row pivoting, we interchange row k with the one beneath it that has the largest absolute entry in column k beneath the diagonal. On the other hand, in solving a large sparse linear system, pivoting may ruin the storage structure.

In [49] Stewart stabilizes the elimination process by adding or subtracting a perturbation of the form $\mathbf{u}_k\mathbf{u}_k^T$, where every component of $\mathbf{u}_k$ is zero except for component k. By an appropriate choice of $\mathbf{u}_k$, it can be arranged so that the kth diagonal coefficient of the perturbed matrix is larger in magnitude than the other coefficients in column k beneath the diagonal. In this way, the pivot operation is avoided. The solution to the original equation is recovered from the solution of the perturbed equation using the Modification Formula. Of course, each time that we modify the coefficient matrix, the dimension of the capacitance matrix increases by 1. If we modify the coefficient matrix before each Gaussian elimination step, then the cost of solving the linear system associated with the capacitance matrix is greater than the cost of solving the original linear system. Hence, this modification technique is practical only when it is performed infrequently.

9. Quasi-Newton methods. The Modification Formula is often employed in quasi-Newton methods for finding a root of a function or for performing an unconstrained minimization. Given a function $\mathbf{f}$ mapping R^n to R^n, Newton's method for approximating a root to $\mathbf{f}(\mathbf{x}) = \mathbf{0}$ is given by the iteration

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{J}(\mathbf{x}_k)^{-1}\mathbf{f}(\mathbf{x}_k)$$

where $\mathbf{J}$ denotes the Jacobian of $\mathbf{f}$. In one type of quasi-Newton method, we attempt to approximate the Jacobian using rank 1 corrections. The $(k+1)$st approximation $\mathbf{A}_{k+1}$ is obtained from the kth approximation $\mathbf{A}_k$ by the rule

$$\mathbf{A}_{k+1} = \mathbf{A}_k - \mathbf{u}_k\mathbf{v}_k \tag{33}$$

where $\mathbf{u}_k$ and $\mathbf{v}_k$ are chosen so that $\mathbf{A}_{k+1}$ approximates the Jacobian at $\mathbf{x}_{k+1}$ "better" than $\mathbf{A}_k$ approximates the Jacobian at $\mathbf{x}_k$. Typically, $\mathbf{u}_k$ and $\mathbf{v}_k$ are chosen so that

$$\mathbf{A}_{k+1}(\mathbf{x}_{k+1} - \mathbf{x}_k) = \mathbf{f}_{k+1} - \mathbf{f}_k \tag{34}$$

where $\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{A}_k^{-1}\mathbf{f}_k$ and $\mathbf{f}_k = \mathbf{f}(\mathbf{x}_k)$. Using (34) to solve for $\mathbf{u}_k$ and $\mathbf{v}_k$, we obtain

$$\mathbf{v}_k^T = \mathbf{x}_{k+1} - \mathbf{x}_k \quad \text{and} \quad \mathbf{u}_k = \frac{\mathbf{A}_k\mathbf{v}_k^T - \mathbf{g}_k}{\mathbf{v}_k\mathbf{v}_k^T} \tag{35}$$

where $\mathbf{g}_k = \mathbf{f}_{k+1} - \mathbf{f}_k$. (It can be shown that the perturbation $\mathbf{P}_k$ with the smallest 2-norm that satisfies the equation

$$(\mathbf{A}_k - \mathbf{P}_k)(\mathbf{x}_{k+1} - \mathbf{x}_k) = \mathbf{f}_{k+1} - \mathbf{f}_k$$

is a rank 1 matrix; see review exercise 3–11 in [30].)

To implement the quasi-Newton iteration $\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{A}_k^{-1}\mathbf{f}_k$, we need the inverse of $\mathbf{A}_k$. Applying the Modification Formula to (33), substituting from (35), and simplifying yields the following recurrence for the inverse of $\mathbf{A}_k$:

$$\mathbf{A}_{k+1}^{-1} = \mathbf{A}_k^{-1} + \frac{(\mathbf{v}_k^T - \mathbf{A}_k^{-1}\mathbf{g}_k)\mathbf{v}_k\mathbf{A}_k^{-1}}{\mathbf{v}_k\mathbf{A}_k^{-1}\mathbf{g}_k}. \tag{36}$$

Powell observes in [42] that there is some suppression of rounding errors if the inverse matrix is updated using (36) rather than the formula

$$\mathbf{A}_{k+1}^{-1} = \mathbf{A}_k^{-1} + \frac{\mathbf{A}^{-1}\mathbf{u}_k\mathbf{v}_k\mathbf{A}_k^{-1}}{1 - \mathbf{v}_k\mathbf{A}_k^{-1}\mathbf{u}_k}$$

obtained directly from (2). Quasi-Newton methods and their properties are surveyed in [13].

10. Updating a factorization. As mentioned in §4, some applications involve making a series of rank 1 changes to the coefficient matrix and solving a linear system after each change. After m rank 1 changes, the capacitance matrix $\mathbf{C}$ is $m \times m$. If m is large, then the algorithm of §2 can be costly due to the same time spent solving the linear system associated with the capacitance matrix. Moreover, in some applications, such as the simplex method in linear programming, m can be larger than n. In situations where m is large but n is not too large, it may be more efficient to store the inverse of the coefficient matrix and to successively update the inverse after each rank 1 change using (2). The quasi-Newton recurrence (36) is an example of these successive updates. As an alternative to successively updating the inverse matrix, we can store the original matrix in factored form and update the factors. One method for updating a triangular factorization is presented by Bennett [7] while the series of papers by Bartels, Gill, Golub, Murray, and Saunders ([5], [20]–[22]) provides a comprehensive study of *many* different ways to update the standard factorizations after a rank 1 change in the coefficient matrix.

Updating a factorization is not only an alternative to the Modification Formula, but also a useful tool in its implementation. In this section we discuss how to update a factorization of $\mathbf{C} = \mathbf{I} - \mathbf{V}\mathbf{A}^{-1}\mathbf{U}$ either after adding a column to $\mathbf{U}$ and a row to $\mathbf{V}$, or after deleting a column from $\mathbf{U}$ and a row from $\mathbf{V}$. We focus on triangular factorizations although orthogonal factorizations can be updated using a similar technique. Suppose that $\mathbf{C}$ is an $(m-1) \times (m-1)$ matrix factored into the product $\mathbf{LR}$ between a unit lower triangular matrix $\mathbf{L}$ and an upper triangular matrix $\mathbf{R}$. If a new column is added to the right side of $\mathbf{U}$ and a new row is added to the bottom of $\mathbf{V}$, then the new $\mathbf{C}$ is identical to the old $\mathbf{C}$ except for the elements in row m and column m. To complete the factorization using the standard Gaussian elimination algorithm, multiples of the rows of $\mathbf{R}$ are subtracted from the bottom row of $\mathbf{C}$, annihilating all coefficients but the diagonal coefficient. When we initialize $r_{mi} = c_{mi}$ and $r_{im} = c_{im}$ for i between 1 and m, the updated coefficients in row m of $\mathbf{L}$ and in column m of $\mathbf{R}$ are evaluated by the following algorithm:

$j = 1$ to $m-1$

  $r_{im} \leftarrow r_{im} - l_{ij}r_{jm}$ for $i = j+1$ to $m-1$

next j

$i = 1$ to $m-1$

  $l_{mi} \leftarrow r_{mi}/r_{ii}$

  $r_{mj} \leftarrow r_{mj} - r_{ij}l_{mi}$ for $j = i$ to m

next i

For a general matrix, this algorithm is unstable since pivoting is not performed. On the other hand, Gaussian elimination with pivoting cannot be implemented in this incremental fashion, where one row and column are added at a time. Hence, the

factorization given above should only be used when pivoting is not required. It is well known that pivoting is not needed when a symmetric positive definite matrix is factored. Consequently, the algorithm given above can be applied when $\mathbf{V} = \mathbf{U}^T$ and $\mathbf{A}$ is symmetric and negative definite, since $\mathbf{C} = \mathbf{I} - \mathbf{V}\mathbf{A}^{-1}\mathbf{U}$ is positive definite. Moreover, in this case $\mathbf{C}$ can be written in a Cholesky product $\mathbf{L}\mathbf{L}^T$, where $\mathbf{L}$ is lower triangular with positive diagonal elements. The standard formulas for the new coefficients in a Cholesky factorization associated with adding a new row and column to $\mathbf{C}$ are

$$l_{mj} = \frac{c_{mj} - \sum_{k=1}^{j-1} l_{jk} l_{mk}}{l_{jj}}$$

for $j = 1$ to $m - 1$, and

$$l_{mm} = \sqrt{c_{mm} - \sum_{k=1}^{m-1} l_{mk}^2}.$$

When a new row and column are added to the border of $\mathbf{C}$, we compute the new row and column of the updated factorization without altering the previously computed factorization. On the other hand, when a column from $\mathbf{U}$ and a row from $\mathbf{V}$ are deleted, the entire factorization may change unless the deleted elements lie on the border of the matrix. Suppose that column k from $\mathbf{U}$ is deleted, $\mathbf{V} = \mathbf{U}^T$, and $\mathbf{C}$ is stored in the Cholesky factorization $\mathbf{L}\mathbf{L}^T$. Following Gill and Murray in [21], the new $\mathbf{C}$ obtained by deleting column k from $\mathbf{U}$ can be expressed $\mathbf{C}^{\text{new}} = \bar{\mathbf{L}}\bar{\mathbf{L}}^T + \mathbf{u}\mathbf{u}^T$, where $\bar{\mathbf{L}}$ is obtained from $\mathbf{L}$ by deleting both row and column k and $\mathbf{u}$ is column k from $\mathbf{L}$ with element k deleted. Since the new $\mathbf{C}$ is expressed as the sum of a Cholesky factored matrix and a rank 1 correction, any of the algorithms developed in [20], [21], or [22] can be used to update the factorization.

For completeness, we now give a direct procedure to update the Cholesky factorization of the new $\mathbf{C}$. First, augment the matrix $\bar{\mathbf{L}}$ by inserting $\mathbf{u}$ between column $k - 1$ and column k. The augmented matrix $\mathbf{M}$ is the same as $\mathbf{L}$ but with row k deleted. The structure of $\mathbf{M}$ is indicated in Fig. 1—the top part of the matrix is zero while the bottom part is generally nonzero. The new $\mathbf{C}$ can be expressed as $\mathbf{C}^{\text{new}} = \mathbf{M}\mathbf{M}^T$. To generate the Cholesky factorization, we annihilate the "superdiagonal" bulge of $\mathbf{M}$ using a sequence of Givens rotations (see [23] or [30]). These rotations have the following structure:

$$\begin{bmatrix} 1 & & & & & & & \\ & \ddots & & & & & & \\ & & 1 & & & & & \\ & & & c & -s & & & \\ & & & s & c & & & \\ & & & & & 1 & & \\ & & & & & & \ddots & \\ & & & & & & & 1 \end{bmatrix}$$

where $c^2 + s^2 = 1$. Observe that if

$$c = \frac{x_1}{\sqrt{x_1^2 + x_2^2}} \quad \text{and} \quad s = \frac{x_2}{\sqrt{x_1^2 + x_2^2}},$$

then $c^2 + s^2 = 1$ and

$$[x_1, x_2] \begin{bmatrix} c & -s \\ s & c \end{bmatrix} = [\sqrt{x_1^2 + x_2^2}, 0].$$

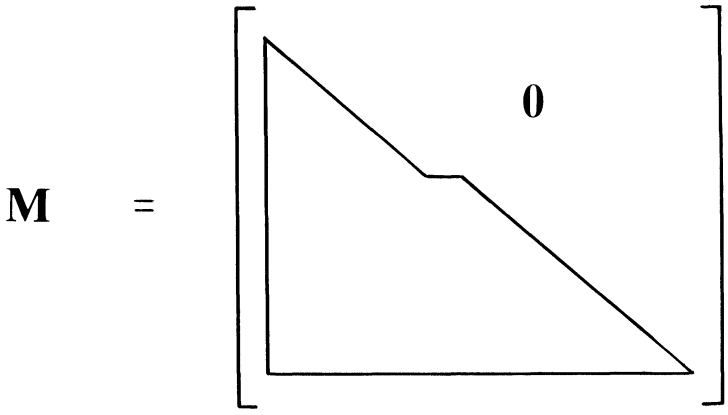

FIG. 1. *The augmented matrix* **M**.

In other words, the second component of **x** is annihilated and the first component is replaced by the length of **x**. Letting **G** denote the product of the Givens rotations that annihilate the nonzero superdiagonal elements depicted in Fig. 1, we have

$$\mathbf{C}^{\text{new}} = (\mathbf{MG})(\mathbf{G}^T\mathbf{M}).$$

Deleting the last column of **MG**, which is zero, we obtain the lower triangular Cholesky factor of the new **C**. In detail, if **C** is $m \times m$, then the updated Cholesky factor **L** associated with the deletion of column k and row k from **C** is obtained by the following procedure:

$j = k$ to $m-1$

$p \leftarrow j+1$

if $l_{jp} = 0$ goto next j

$t \leftarrow [l_{jp}^2 + l_{jj}^2]^{1/2}$

$c \leftarrow l_{jj}/t$ and $s \leftarrow l_{jp}/t$

$i = j$ to $m-1$

$t \leftarrow l_{ip}$

$l_{ip} \leftarrow tc - sl_{ij}$

$l_{ij} \leftarrow l_{ij}c + st$

next i

next j

Note that the product **MG** can also be computed using a "fast Givens" procedure, which eliminates about half the multiplications—see [23] or [30].

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