Determinants, Cholesky, and Linear Systems of Equations

For a two-by-two matrix, the inverse is

$$\mathbf{A} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \quad \Leftrightarrow \quad \mathbf{A}^{-1} = \frac{1}{\det(\mathbf{A})} \cdot \begin{bmatrix} A_{22} & -A_{12} \\ -A_{21} & A_{11} \end{bmatrix} \tag{1}$$

where the determinant, which clearly cannot be zero, is

$$\det(\mathbf{A}) = A_{11}A_{22} - A_{12}A_{21} \tag{2}$$

For higher-dimension matrices the determinant, which is often written $|\mathbf{A}|$, is obtained by adding and subtracting products of diagonals, as shown in Figure 1. For higher-dimension matrices the topic of matrix inversion is better dealt with in the context of the problem of solving systems of equations.

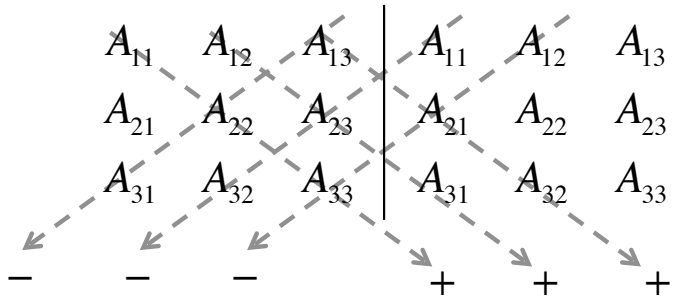

Figure 1: Calculation of matrix determinant.

Systems of Equations and Eigenvalue Problems

A system of linear equations, used as an example above, is generically written

$$\mathbf{Ax} = \mathbf{b} \tag{3}$$

where $\mathbf{A}$ is the coefficient matrix of known constants, $\mathbf{x}$ is the vector of sought unknowns, and $\mathbf{b}$ is a vector of known constants. Symbolically, the solution to the system of equations is

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{b} \tag{4}$$

In words, the inverse of the coefficient matrix features prominently, at least as a concept, in the solution of a linear system of equations. The inverse of a matrix only exists when the determinant of the coefficient matrix is zero. In fact, the system of linear equations in Eq. (3) has a unique non-trivial solution only if $\det(\mathbf{A})\neq 0$. Conversely, if this determinant is zero then the system has no solution or infinitely many solutions. A special version of Eq. (3) is when $\mathbf{b}=\mathbf{0}$. Then the system of equations is said to be homogeneous. A homogeneous system always has the trivial solution $\mathbf{x}=\mathbf{0}$. In fact, if $\det(\mathbf{A})\neq 0$ then the system only has the trivial solution. Conversely, if $\det(\mathbf{A})=0$ non-trivial solutions exist. A special version of Eq. (3) of homogeneous systems is

$$\mathbf{Ax} = \lambda\mathbf{x} \quad \Leftrightarrow \quad (\mathbf{A} - \lambda\mathbf{I})\mathbf{x} = \mathbf{0} \tag{5}$$

which is called an eigenvalue problem that is written more generally as

$$(\mathbf{A} - \lambda\mathbf{B})\mathbf{x} = \mathbf{0} \tag{6}$$

Like other homogeneous systems, non-trivial solutions exist only when the determinant of the coefficient matrix is zero, i.e., when

$$\det(\mathbf{A} - \lambda\mathbf{B}) = 0 \tag{7}$$

The roots λ_i of Eq. (7) are called eigenvalues. Each eigenvalue has one eigenvector, or eigen-mode, associated with it. The eigenvectors are not unique; they are determined by setting one of the elements of **x** in Eq. (6) equal to unity and solving for the others. This is repeated for each eigenvalue to obtain all eigenvectors. Any scaled version of an eigenvector is also an eigenvector because the choice of unity of one element is arbitrary. Upon computing the eigenvalues of a square matrix **A** it is possible to diagonalize it into a matrix **D** that has the eigenvalues on the diagonal:

$$\mathbf{D} = \mathbf{X}^{-1}\mathbf{AX} \tag{8}$$

where **X** is a matrix with the eigenvectors of **A** as diagonals. Within the numerical methods for linear algebra there are several methods for solving linear systems of equations.

Decomposition and Substitution

One approach is LU-factorization, in which the coefficient matrix is decomposed into a lower and an upper triangular matrix:

$$\mathbf{A} = \mathbf{LU} \tag{9}$$

where **L** is a lower-tringular matrix and **U** is an upper-triangular matrix, both having diagonal elements that are typically different from zero and unity. Using this decomposition, Eq. (3) reads

$$\mathbf{L}\underbrace{\mathbf{Ux}}_{\mathbf{y}} = \mathbf{Ly} = \mathbf{b} \tag{10}$$

where the auxiliary vector

$$\mathbf{y} = \mathbf{Ux} \tag{11}$$

has been defined. Assuming **L** and **U** have already been determined, the vector **y** is determined by solving Eq. (10), i.e., by the forward substitution algorithm

$$y_i = \frac{b_i - \sum_{j=1}^{i-1}\left(L_{ij}y_j\right)}{L_{ii}} \qquad \text{for} \quad i = 1, \ \ldots \ , n \tag{12}$$

where n is the number of equations. Once **y** is determined, **x** is determined by solving Eq. (11), i.e., by the backward substitution algorithm

$$x_i = \frac{y_i - \sum_{j=i+1}^{n} \left(U_{ij} x_j \right)}{U_{ii}} \qquad \text{for} \quad i = n, \ \ldots \ ,1 \tag{13}$$

If the Cholesky decomposition is used (see below) then $\mathbf{U}=\mathbf{L}^T$ and Eq. (13) is readily modified to accommodate that situation by setting $U_{ij}=L_{ji}$ (notice the switch of indices) and $U_{ii}=L_{ii}$. If the system of equations needs to be solved repeated with the same **A**-matrix but different right-hand-sides **b** then the decomposition is done once while the forward/backward substitution is repeated for each **b**-vector.

Cholesky Decomposition

Cholesky decomposition is one of the methods to decompose the coefficient matrix. It is based on selecting $\mathbf{U}=\mathbf{L}^T$ so that

$$\mathbf{A} = \mathbf{L}\mathbf{L}^T \tag{14}$$

The Cholesky decomposition, which is named after Andre-Louis Cholesky (1857-1918) and takes a symmetric and positive definite matrix as input, has broader use than solving systems of equations. For example, it appears in reliability analysis when random variables are transformed into the standard normal variable space. Several algorithms exist for obtaining **L** and its inverse (Kreyszig 1988). One calculates the components of the matrix row-by-row from left to right:

$$L_{ij} = \begin{cases} \sqrt{A_{ij} - \sum_{k=0}^{i-1} L_{ik}^2} & \text{for } i = j \\ \dfrac{A_{ij} - \sum_{k=0}^{j-1} \left(L_{ik} L_{jk} \right)}{L_{jj}} & \text{for } i > j \\ 0 & \text{for } i < j \end{cases} \tag{15}$$

followed by the calculation of $\mathbf{L}^{-1}$ row-by-row from right to left:

$$invL_{ij} = \begin{cases} \dfrac{1}{L_{ii}} & \text{for } i = j \\ -\dfrac{\sum_{k=j}^{i-1} \left(L_{ik} \cdot invL_{kj} \right)}{L_{jj}} & \text{for } i > j \\ 0 & \text{for } i < j \end{cases} \tag{16}$$

For applications in reliability analysis, notice that the lower-triangular Cholesky decomposition of a correlation matrix that reads

$$\mathbf{R} = \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix} \tag{17}$$

is simply

$$\mathbf{L} = \begin{bmatrix} 1 & 0 \\ \rho & \sqrt{1-\rho^2} \end{bmatrix} \tag{18}$$

Determinant and Matrix Inversion

Here we return to the objective of solving Eq. (3), now using Cramer's rule and determinants. This approach is inefficient compared with decomposition and iterative algorithms and it essentially establishes the inverse of the coefficient matrix **A** to obtain the solution as

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{b} \tag{19}$$

The approach is often referred to as Cramer's rule after Gabriel Cramer (1704–1752). Interestingly, it can be used to solve for individual values x_i leaving the other values of **x** unknown. One way to write Cramer's rule is

$$x_i = \frac{\det(\mathbf{A}_i)}{\det(\mathbf{A})} \tag{20}$$

where det($\mathbf{A}_i$) is the determinant of $\mathbf{A}_i$, which is the matrix obtained by replacing column number i in **A** by **b**. Another way to write Cramer's rule is

$$\mathbf{A}^{-1} = \frac{\text{adj}(\mathbf{A}_i)}{\det(\mathbf{A})} \tag{21}$$

where adj(**A**) is the adjoint matrix of **A**, i.e., the transposed matrix of cofactors. For a square matrix **A** the cofactor of a component is

$$C_{ij} = (-1)^{i+j} \cdot M_{ij} \tag{22}$$

where M_{ij} is the minor

$$M_{ij} = \det(\mathbf{A}_{\text{reduced}}) \tag{23}$$

where $\mathbf{A}_{\text{reduced}}$ is the reduced version of **A** with row i and column j removed. This leads to a recursive formula when the determinant is calculated as the sum over an arbitrary row or column:

$$\det(\mathbf{A}) = \sum \left(A_{ij} \cdot C_{ij} \right) \tag{24}$$

In the C++ implementation the sum is always taken over the first row, and the iteration takes place when the determinant-algorithm calls the cofactor-algorithm. Once the algorithms to calculate cofactors and determinant are in place the solution to **Ax**=**b** is calculated using Eq. (20). It can also be solved by establishing the inverse and calculating $\mathbf{x}=\mathbf{A}^{-1}\mathbf{b}$.

Other Algorithms and Applications for the Determinant

The algorithm above is only one of several to calculate the determinant. Liebniz and Laplace had their respective algorithms, and using LU decomposition is another approach. The determinant is defined for square matrices and was originally named by Gauss (Lagrange had earlier called it resultant) because of its ability to predict whether a solution to **Ax**=**b** exists. Chinese scholars had understood similar concepts several hundred years BC and people like Cardano and Leibniz had also used such tests. In

passing, it is noted that for an inhomogeneous system of equations, i.e., when **b** is nonzero, a zero-valued determinant indicates there exist either infinite or no solutions, i.e., the determinant must be non-zero to obtain a unique solution. Conversely, for homogeneous systems (**b**=**0**) a zero determinant is the only way to get nontrivial solutions, which there will be an infinite number of. Also, a matrix **A** is said to be positive definite if the scalar $\mathbf{z}^T\mathbf{A}\mathbf{z}$ is positive for every non-zero column vector **z**. The determinant of a positive definite matrix is always positive; hence, a positive definite matrix is always nonsingular. A matrix is singular if its determinant is zero, i.e., a matrix with nonzero determinant is non-singular. In practice the determinant is rarely calculated to check if **Ax**=**b** is solvable but it does indeed appear in Cramer's approach for solving that system of linear equations, as seen above.