5. Matrix Inversion. Matrix Eigenvalues.

NUMERICAL ANALYSIS. Prof. Y. Nishidate (323-B, nisidate@u-aizu.ac.jp)
http://web-int.u-aizu.ac.jp/∼nisidate/na/

Determinant of a Matrix

A square matrix has a determinant which is given by the following recursive formula:

$$|\mathbf{A}| = a_{11}M_{11} - a_{12}M_{12} + a_{13}M_{13} - ... - (-1)^n a_{1n}M_{1n}$$

where M_{ij} is the determinant of the matrix with row i and column j missing, and the determinant of 1×1 matrix is just equal to the particular element.

Hence,

$$\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}a_{22} - a_{12}a_{21}$$

and

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = a_{11}(a_{22}a_{33} - a_{23}a_{32}) - a_{12}(a_{21}a_{33} - a_{23}a_{31}) + a_{13}(a_{21}a_{32} - a_{22}a_{31})$$

By rearranging the terms in a different order it is possible to expand the determinant, not by the first row, but by any other row or column. Thus it follows that the determinant is zero if any row or column of a matrix is null. It can also be shown that the determinant is zero if either rows or columns exhibit a linear relationship.

For large matrices the direct calculation of the determinant is very time consuming. Fortunately, the determinant of a matrix can be computed from its **LU** decomposition. This follows from these determinant properties:

1) The determinant of a product of two matrices is equal to the product of their determinants;

2) The determinant of a triangular matrix is the product of its diagonal elements.

If matrix **A** has the **LU** decomposition

$$A = \begin{bmatrix} m_{11} & 0 & 0 & 0 \\ m_{21} & m_{22} & 0 & 0 \\ m_{31} & m_{32} & m_{33} & 0 \\ m_{41} & m_{42} & m_{43} & m_{44} \end{bmatrix} \begin{bmatrix} 1 & u_{12} & u_{13} & u_{14} \\ 0 & 1 & u_{23} & u_{24} \\ 0 & 0 & 1 & u_{34} \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

the determinant can be computed as follows

$$|\mathbf{A}| = m_{11}m_{22}\cdots m_{nn}$$

Matrix Inverse

The inverse of a square matrix **A** is denoted as $\mathbf{A}^{-1}$ and is defined as

$$\mathbf{A}\mathbf{A}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$$

where **I** is the identity matrix.

To determine the coefficients of the inverse matrix, it is possible to use the equation

$$\mathbf{A}\mathbf{A}^{-1} = \mathbf{I}$$

Then the inverse matrix can be found by solving n times the equation

$$\mathbf{A}\mathbf{x}_i = \mathbf{e}_i$$

Here $\mathbf{e}_i$ is the ith column of the identity matrix **I**. After n solutions the inverse matrix can be composed of n columns $\mathbf{x}_i$.

The matrix inverse should be mostly thought of as a useful algebraic concept rather than as an aid to numerical computations. The matrix inversion is a computationally expensive operation. Therefore, in practical computing it is usually used just for matrices of very small dimensions (2-4). In other cases the equation solution is employed.

Gaussian Elimination for calculating matrix inverse

The Gaussian Elimination can be applied not only for finding solution of the equation system. As mentioned in previous section, the inverse of matrices can be found by solving the following equation system for $i = 1, 2, \cdots, n$

$$\mathbf{A}\mathbf{x}_i = \mathbf{e}_i$$

where $\mathbf{x}_i$ corresponds to ith column elements of $\mathbf{A}^{-1}$. That means, it requires solution of equation system n times. However, it is possible to arrange the matrix **A** and $\mathbf{e}_i$ into the tabular like the Gaussian Elimination procedure with n right hand sides. Thus the equation system for $i = 1, 2, \cdots, n$ can be solved simultaneously.

$$\left[\begin{array}{cccc|cccc} a_{11} & a_{12} & \cdots & a_{1n} & 1 & 0 & \cdots & 0 \\ a_{21} & a_{22} & \cdots & a_{2n} & 0 & 1 & \cdots & 0 \\ & & \ddots & & & & \ddots & \\ a_{n1} & a_{n2} & \cdots & a_{nn} & 0 & 0 & \cdots & 1 \end{array}\right]$$

Then apply the Gaussian Elimination procedure. After the forward elimination procedure for the 1st column, appearance of the tabular may be as follows

$$\left[\begin{array}{cccc|cccc} a_{11} & a_{12} & \cdots & a_{1n} & 1 & 0 & \cdots & 0 \\ 0 & a_{22}^{(1)} & \cdots & a_{2n}^{(1)} & -a_{21}/a_{11} & 1 & \cdots & 0 \\ & & \ddots & & & & \ddots & \\ 0 & a_{n2}^{(1)} & \cdots & a_{nn}^{(1)} & -a_{n1}/a_{11} & 0 & \cdots & 1 \end{array}\right]$$

The remaining coefficients should be eliminated step by step, as usually done in the Gaussian Elimination procedure, until the left side of the tabular becomes the identity matrix **I**.

$$\left[\begin{array}{cccc|cccc} 1 & 0 & \cdots & 0 & c_{11} & c_{12} & \cdots & c_{1n} \\ 0 & 1 & \cdots & 0 & c_{21} & c_{22} & \cdots & c_{2n} \\ & & \ddots & & & & \ddots & \\ 0 & 0 & \cdots & 1 & c_{n1} & c_{n2} & \cdots & c_{nn} \end{array}\right]$$

Finally, the elements in right side of the tabular c_{ij} should be the elements of $\mathbf{A}^{-1}$.

Eigenvalues of a Matrix

An eigenvalue and corresponding eigenvector of a matrix satisfy the property that the eigenvector multiplied by the matrix yields a vector proportional to itself. The algebraic equation for the eigenvalue λ and corresponding eigenvector **q** of a matrix **A** is given by

$$\mathbf{A}\mathbf{q} = \lambda\mathbf{q}$$

For this equation **A** must be square. Hence only square matrices have eigenvalues. The above equation can be rewritten in the form

$$(\lambda\mathbf{I} - \mathbf{A})\mathbf{q} = 0$$

any non-trivial solution of which must satisfy the characteristic equation

$$\begin{vmatrix} \lambda - a_{11} & -a_{12} & ... & -a_{1n} \\ -a_{21} & \lambda - a_{22} & ... & -a_{2n} \\ ... & ... & ... & ... \\ -a_{n1} & -a_{n2} & ... & \lambda - a_{nn} \end{vmatrix} = 0$$

The characteristic equation has the following general form

$$\lambda^n + c_{n-1}\lambda^{n-1} + ... + c_1\lambda + c_0 = 0$$

Solving the characteristic equation gives eigenvalues of the matrix.

Example. The matrix $\mathbf{A}$ shown below

$$\mathbf{A} = \begin{bmatrix} 2 & -1 & 0 \\ -2 & 2 & 1 \\ 0 & -1 & 2 \end{bmatrix}$$

exhibits the property

$$\begin{bmatrix} 2 & -1 & 0 \\ -2 & 2 & 1 \\ 0 & -1 & 2 \end{bmatrix} \begin{Bmatrix} 1 \\ -1 \\ 1 \end{Bmatrix} = 3 \begin{Bmatrix} 1 \\ -1 \\ 1 \end{Bmatrix}$$

showing that it has an eigenvalue equal to 3 with a corresponding eigenvector $\begin{Bmatrix} 1 & -1 & 1 \end{Bmatrix}$. The characteristic equation

$$\begin{vmatrix} \lambda - 2 & 1 & 0 \\ 2 & \lambda - 2 & -1 \\ 0 & 1 & \lambda - 2 \end{vmatrix} = 0$$

can be written as the following nonlinear equation

$$\lambda^3 - 6\lambda^2 + 11\lambda - 6 = 0$$

This equation can be factorized into

$$(\lambda - 1)(\lambda - 2)(\lambda - 3) = 0$$

Thus eigenvalues of the considered matrix are $\lambda_1 = 1$, $\lambda_2 = 2$ and $\lambda_3 = 3$.

The characteristic equation method is not a good procedure for the numerical determination of the matrix eigenvalues. For a large fully populated matrix, the number of multiplications required to obtain the coefficients of the characteristic equation is proportional to n^4. Thus other methods should be used.

Eigenvalues and Eigenvectors of a Symmetrical Matrix

Finding the eigenvalues of a symmetrical matrix is easier since all eigenvalues are real. A transformation method transforms the matrix under investigation into another matrix with the same eigenvalues. Usually such transformations are carried out until the matrix is in a form which can be easily analyzed by alternative procedures. The most general transformation which preserves the eigenvalues of a matrix is a *similarity transformation*

$$\bar{\mathbf{A}} = \mathbf{N}^{-1}\mathbf{A}\mathbf{N}$$

where $\mathbf{N}$ may be any non-singular matrix of the same order. If $\mathbf{N}$ is orthogonal then $\mathbf{N}^{-1} = \mathbf{N}^T$ and the similarity transformation becomes

$$\bar{\mathbf{A}} = \mathbf{N}^T\mathbf{A}\mathbf{N}$$

If $\mathbf{A}$ is symmetric then $\bar{\mathbf{A}}$ will also be symmetric. The use of orthogonal transformation ensures that matrix symmetry is preserved.

If a symmetric matrix $\mathbf{A}$ has an eigenvalue λ_i and corresponding eigenvector $\mathbf{q}_i$ such that $\mathbf{A}\mathbf{q}_i = \lambda_i\mathbf{q}_i$ then

$$\begin{aligned} \mathbf{N}\bar{\mathbf{A}}\mathbf{N}^T\mathbf{q}_i &= \lambda_i\mathbf{q}_i \\ \bar{\mathbf{A}}(\mathbf{N}^T\mathbf{q}_i) &= \lambda_i(\mathbf{N}^T\mathbf{q}_i) \end{aligned}$$

Thus the eigenvalues of $\bar{\mathbf{A}}$ are the same as eigenvalues of $\mathbf{A}$ with its eigenvectors $\bar{\mathbf{A}}$

$$\bar{\mathbf{q}}_i = \mathbf{N}^T\mathbf{q}_i$$

For convenience in later sections, $\bar{\mathbf{q}}_i$ is arranged into matrix like $\bar{\mathbf{Q}} = [\bar{\mathbf{q}}_1, \bar{\mathbf{q}}_2, \cdots, \bar{\mathbf{q}}_n]$, and $\mathbf{q}_i$ is arranged into another matrix like $\mathbf{Q} = [\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_n]$. Then they are related as follows

$$\bar{\mathbf{Q}} = \mathbf{N}^T\mathbf{Q}$$

If a symmetric matrix $\mathbf{A}$ can be transformed until all its off-diagonal elements become zero through iterative similarity transformations, the set of eigenvalues appears on the diagonal elements.

Jacobi diagonalization. Each Jacobi transformation eliminates one pair of off-diagonal elements in a symmetric matrix. In order to eliminate pair of equal elements a_{pq} and a_{qp} an orthogonal transformation matrix $\mathbf{N}$ with the following components is used

$$\begin{aligned} &n_{pp} = n_{qq} = \cos\alpha \\ &n_{pq} = -\sin\alpha \\ &n_{qp} = \sin\alpha \\ &n_{ii} = 1 \qquad i \neq p,\ q \\ &n_{ij} = 0 \qquad i \neq j \qquad i,\ j \neq p,\ q \end{aligned}$$

The choise of α must be such that after transformation $\bar{\mathbf{A}} = \mathbf{N}^T\mathbf{A}\mathbf{N}$ the elements $\bar{a}_{pq} = \bar{a}_{qp} = 0$. This gives the equation for α

$$\bar{a}_{pq} = (-a_{pp} + a_{qq})\cos\alpha\sin\alpha + a_{pq}(\cos^2\alpha - \sin^2\alpha) = 0$$

Hence

$$\tan 2\alpha = \frac{2a_{pq}}{a_{pp} - a_{qq}}$$

The Jacobi transformation only affects rows p and q and columns p and q. The two diagonal elements modified by the transformation become

$$\begin{aligned} \bar{a}_{pp} &= a_{pp}\cos^2\alpha + a_{qq}\sin^2\alpha + 2a_{pq}\sin\alpha\cos\alpha \\ \bar{a}_{qq} &= a_{pp}\sin^2\alpha + a_{qq}\cos^2\alpha - 2a_{pq}\sin\alpha\cos\alpha \end{aligned}$$

The other elements affected by the transformation are modified according to the relations

$$\begin{aligned} \bar{a}_{ip} &= \bar{a}_{pi} = a_{ip}\cos\alpha + a_{iq}\sin\alpha \\ \bar{a}_{iq} &= \bar{a}_{qi} = -a_{ip}\sin\alpha + a_{iq}\cos\alpha \end{aligned}$$

The computational procedure performs a series of Jacobi transformations, with each transformation eliminating the off-diagonal element of the largest absolute value. Unfortunately, elements which have been eliminated do not necessarily stay zero, and hence the Jacobi method is iterative in character.

If the matrix after $k-1$ transformations is denoted as $\mathbf{A}^{(k)}$ then the kth transformation can be written as

$$\mathbf{A}^{(k+1)} = \mathbf{N}_k^T\mathbf{A}^{(k)}\mathbf{N}_k$$

and the eigenvector matrices of $\mathbf{A}^{(k)}$ and $\mathbf{A}^{(k+1)}$ are related by the equation

$$\mathbf{Q}^{(k+1)} = \mathbf{N}_k^T\mathbf{Q}^{(k)}$$

If s transformations are necessary to diagonalize the matrix $\mathbf{A}$ then the eigenvectors of the original matrix appears as columns of the matrix

$$\mathbf{Q} = \mathbf{N}_1\mathbf{N}_2\cdots\mathbf{N}_s$$

The eigenvalues of the original matrix are the diagonal elements of the matrix $\mathbf{A}^{(s+1)}$ obtained after s transformations. In computational practice the series of transformations is terminated when the largest off-diagonal element of the matrix $\mathbf{A}^{(k)}$ becomes less than the desired error tolerance.

Jacobi's algorithm. The algorithm of Jacobi diagonalization can be implemented in following steps:

1. Set the matrix $\mathbf{A}$ to the matrix whose eigenvalues are sought.
2. Set the matrix $\mathbf{Q}$ to an identity matrix $\mathbf{I}$.
3. Find the largest off-diagonal element, a_{pq}, of the matrix $\mathbf{A}$.
4. Build the transformation $\mathbf{N}$ eliminating the element a_{pq}.
5. Transform the matrix $\bar{\mathbf{A}} = \mathbf{N}^T\mathbf{A}\mathbf{N}$.
6. Transform the matrix $\mathbf{Q}' = \mathbf{Q}\mathbf{N}$.
7. Set $\mathbf{A} = \bar{\mathbf{A}}$ and $\mathbf{Q} = \mathbf{Q}'$.
8. If $|a_{pq}| < \varepsilon$ then go to step 9; go to step 3 otherwise.
9. The eigenvalues are the diagonal elements of the matrix $\mathbf{A}$, and the eigenvectors are the columns of the matrix $\mathbf{Q}$.