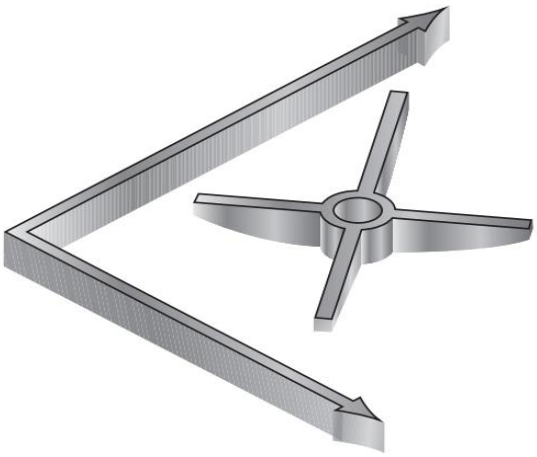


1. Linear Algebraic Equations and Matrices

Suppose that we have 3 equations and 3 unknowns as follows

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 &= b_1 \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 &= b_2 \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 &= b_3 \quad (1.1) \end{aligned}$$

This is a called a *linear system of equations* and is one of the most widely studied and used technique in science and engineering. The systems can be written compactly as the following

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}, x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}, b = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

$$Ax = b$$

The general solution to the system involves inverting the matrix

$$x = A^{-1}b$$

Which is a very costly operation for large matrix.

1.1. Solvability of Linear Systems

We can write any linear system as

$$Ax = b$$

Where $A \in \mathbb{R}^{m \times n}$, $x \in \mathbb{R}^n$ and $b \in \mathbb{R}^m$. The solvability of such as system will fall into one of the three following categories

a) The system may not admit any solution
b) The system may have a single unique solution
c) The system may have infinitely many solution

To get an insight into the solvability of a system, we shall take a geometric perspective. We know that the matrix vector product $Ax = b$ can be viewed as a linear combination of the columns of A

with weights from x. Thus $Ax = b$ is only solvable when $b \in col\ A$. In a broad perspective, the shape of the matrix A bears considerable information about the solvability of $Ax = b$.

- First let us consider the case when the matrix A is wide, i.e., $n > m$. Each column in a vector in $\mathbb{R}^m$. Since $n > m$, the n columns of A must be linearly dependent which implies that there exist some weights $x_0 \neq 0$ which satisfies $Ax_0 = 0$. If we can solve $Ax = b$ for some x then $A(x + \alpha x_0) = Ax + \alpha Ax_0 = b + 0 = b$ for any $\alpha \in \mathbb{R}$. In summary, *no wide system admits a unique solution.*
- When A is tall, i.e., $m > n$, then its n columns can not possibly span the larger dimensional $\mathbb{R}^m$. For this reason, there could be some $b_0 \notin col\ A$ so by definition $Ax = b_0$ cannot be solved exactly for any x. In summary, *for every tall matrix A, there exists a b_0 such that $Ax = b_0$ is not solvable.*

In this lecture we shall consider the linear systems which are square and thus admits only one unique solution (if it exists). We shall assume that the matrix A is not singular i.e., A^{-1} exists which implies $\det A \neq 0$. For the other cases, we need to use a technique known as *least squares* or *pseudoinverse* A^+ which we shall cover in another lecture.

2. Gaussian Elimination (Naïve)

This method is to solve an $n \times n$ system of linear equations

2.1. Forward Elimination of Unknowns

he first phase is designed to reduce the set of equations to an upper triangular system.

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n = b_1 \quad (1.2)$$
$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \cdots + a_{2n}x_n = b_2 \quad (1.3)$$
$$a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \cdots + a_{nn}x_n = b_n \quad (1.4)$$

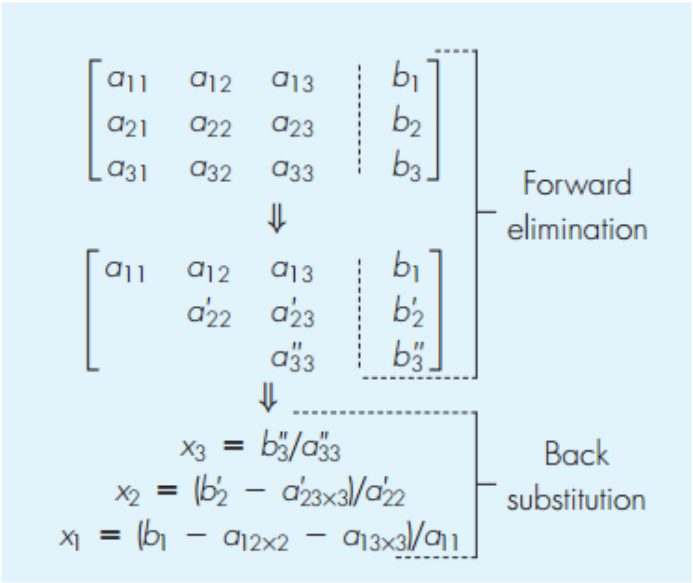


FIGURE 9.3
The two phases of Gauss elimination: forward elimination and back substitution. The primes indicate the number of times that the coefficients and constants have been modified.

The initial step will be to eliminate the first unknown, x_1, from the second through the n-th equations. To do this multiply eq 1.2 by a_{21}/a_{11} to give

$$a_{21}x_1 + \frac{a_{21}}{a_{11}}a_{12}x_2 + \cdots + \frac{a_{21}}{a_{11}}a_{1n}x_n = \frac{a_{21}}{a_{11}}b_1 \quad (1.5)$$

Now this equation can be subtracted from eq 1.3 to give

$$\left(a_{22} - \frac{a_{21}}{a_{11}}a_{12}\right)x_2 + \cdots + \left(a_{2n} - \frac{a_{21}}{a_{11}}a_{1n}\right)x_n = b_2 - \frac{a_{21}}{a_{11}}b_1 \quad (1.6)$$

Or,

$$a'_{22}x_2 + \cdots + a'_{2n}x_n = b'_2$$

The procedure is then repeated for the remaining equations. The new system is then

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n &= b_1 \quad (1.7)\\ a'_{22}x_2 + a'_{23}x_3 + \cdots + a'_{2n}x_n &= b'_2 \quad (1.8)\\ a'_{32}x_2 + a'_{33}x_3 + \cdots + a'_{3n}x_n &= b'_3 \quad (1.9)\\ a'_{n2}x_2 + a'_{n3}x_3 + \cdots + a'_{nn}x_n &= b'_n \quad (1.10) \end{aligned}$$

For the foregoing steps, Eq. 1.2 is called the pivot equation and a_{11} is called the *pivot* coefficient or element. Now repeat the above to eliminate the second unknown from eq 1.9 through eq 1.10

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n &= b_1\\ a'_{22}x_2 + a'_{23}x_3 + \cdots + a'_{2n}x_n &= b'_2\\ a''_{33}x_3 + \cdots + a''_{3n}x_n &= b''_3\\ a''_{n3}x_3 + \cdots + a''_{nn}x_n &= b''_n \end{aligned}$$

The procedure can be continued using the remaining pivot equations. The final manipulation in the sequence is to use the $n-1$ th equation to eliminate the x_{n-1} term from the nth equation. At this point, the system will have been transformed to an upper triangular system

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n &= b_1 \quad (1.11)\\ a'_{22}x_2 + a'_{23}x_3 + \cdots + a'_{2n}x_n &= b'_2 \quad (1.12)\\ a''_{33}x_3 + \cdots + a''_{3n}x_n &= b''_3 \quad (1.13)\\ a_{nn}^{n-1}x_n &= b_n^{n-1} \quad (1.14) \end{aligned}$$

2.2. Backward Substitution

Equation 1.14 can now be solved for $x_n = \frac{b_n^{(n-1)}}{a_{nm}^{(n-1)}}$

This result can then be back substituted into the $(n-1)$ th equation for solve for x_{n-1}. The procedure which is repeated to evaluate the remaining x's can be represented as the following formula

$$x_i = \frac{b_i^{i-1} - \sum_{j=i+1}^{n} a_{ij}^{(i-1)}x_j}{a_{ii}^{(i-1)}} \quad for\ i = n-1, n-2, \ldots, 1 \quad (1.15)$$

2.3. Pivoting

The primary reason that the foregoing technique is called "naive" is that during both the elimination and the back-substitution phases, it is possible that a division by zero can occur. The same problem may also occur if the pivot element is very close to zero. Therefore, before each row is normalized, it is advantageous to determine the coefficient with the largest absolute value in the column below the

pivot element. The rows can then be switched so that the largest element is the pivot element. This is called *partial pivoting*

2.4. Computing the Determinant

After the elimination process is done, the determinant of the matrix A is as follows

$$\det A = \prod_{i=1}^{n-1} a_{ii}^{(i-1)}$$

If the pivoting is used then

$$\det A = (-1)^p \prod_{i=1}^{n-1} a_{ii}^{(i-1)}$$

Where p represents the number of times that rows are pivoted.

3. LU Decomposition/Factorization

Although the Gaussian elimination is a sound was to the solve the system

$$Ax = b$$

But it becomes inefficient when solving equations with same A but different b. LU factorization methods separate the time-consuming elimination of the matrix A from the manipulations of the right-hand side b. Thus, once A has been "factored" or "decomposed," multiple right-hand-side vectors can be evaluated in an efficient manner.

3.1. Overview of the LU Factorization

Just as was the case with Gauss elimination, LU factorization requires pivoting to avoid division by zero. However, to simplify the following description, we will omit pivoting. In addition, the following explanation is limited to a set of three simultaneous equations. The results can be directly extended to n-dimensional systems. The equation $Ax = b$ can be rearranged to give

$$Ax - b = 0 \ (1.16)$$

Suppose that 1.16 can be represented as an upper triangular system as

$$\begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \end{bmatrix} \quad (1.17)$$

Recognize that this is similar to the manipulation that occurs in the first step of Gauss elimination. That is, elimination is used to reduce the system to upper triangular form. Equation 1.17 can also be expressed as

$$Ux - d = 0 \ \ (1.18)$$

Now assume that there is a lower diagonal matrix with 1's on the diagonal,

$$L = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \quad (1.18)$$

Which has the property that

$$LUx - Ld = Ax - b \quad (1.19)$$

$$LU = A \quad (1.20)$$

$$Ld = b \quad (1.21)$$

A two-step strategy can be summarized as follows

1. LU Factorization step: A is factored into lower and upper triangular matrices
2. Substitution step: L and U are used to determine a solution x for a right-hand side b. This step itself consists of two steps. First, Eq. 1.21 is used to generate an intermediate vector d by forward substitution. Then, the result is substituted into Eq. 1.17 which can be solved by back substitution for x.

Just as partial pivoting was necessary for Gaussian elimination, LU decomposition may also require partial pivoting. This is done with the help of the *permutation matrix* P. The permutation matrix is an identity matrix I_n where we interchange the i-th row and j-th column and left multiplying a matrix A by P will switch the corresponding the row and right multiplying will switch the corresponding columns.

1. The elimination is represented as
$$PA = LU$$
2. Solving for d is then
$$Ld = Pb$$
3. The solution for x is simply
$$Ux = d$$

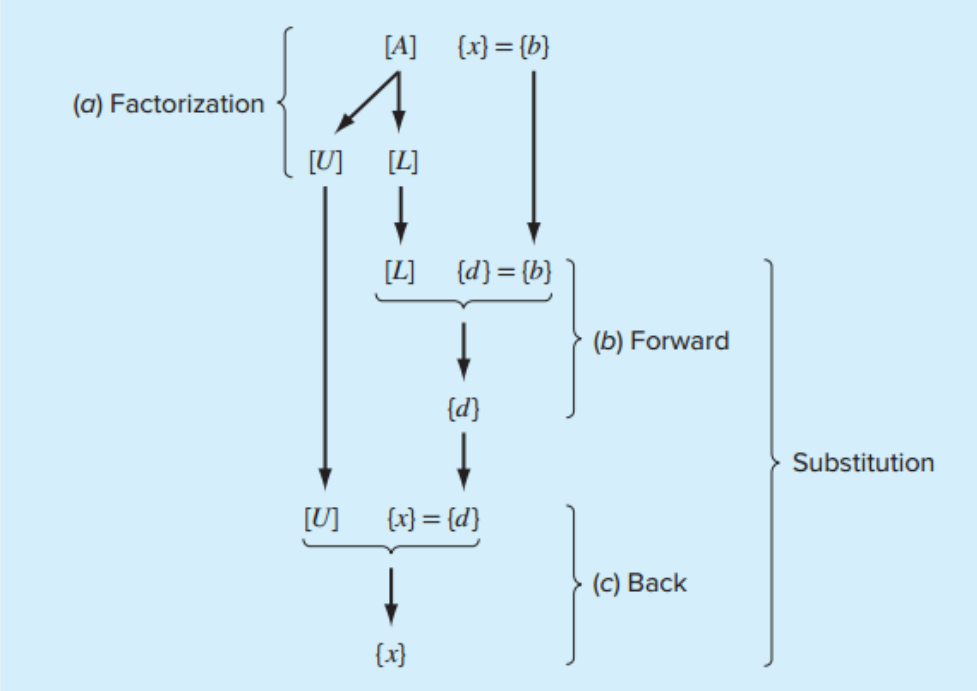


FIGURE 10.1
The steps in *LU* factorization.

Now we shall see how the Gaussian elimination can be used to compute the LU factorization

3.2. Gaussian Elimination for LU Factorization

Although it might appear at face value to be unrelated to LU factorization, Gauss elimination can be used to decompose A into L and U. This can be easily seen for U, which is a direct product of the forward elimination. Recall that the forward-elimination step is intended to reduce the original coefficient matrix A to the form

$$U = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a'_{22} & a'_{23} \\ 0 & 0 & a''_{33} \end{bmatrix} \quad (1.22)$$

which is in the desired upper triangular format.

Though it might not be as apparent, the matrix L is also produced during the step. This can be readily illustrated for a three-equation system,

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \quad (1.23)$$

The first step in Gauss elimination is to multiply row 1 by the factor

$$f_{21} = \frac{a_{21}}{a_{11}}$$

and subtract the result from the second row to eliminate a_{21}. Similarly, row 1 is multiplied by

$$f_{31} = \frac{a_{31}}{a_{11}}$$

and the result subtracted from the third row to eliminate a_{31}. The final step is to multiply the modified second row by

$$f_{32} = \frac{a'_{32}}{a'_{22}}$$

and subtract the result from the third row to eliminate a'_{32}

Now we have

$$A \to LU$$

where

$$U = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a'_{22} & a'_{23} \\ 0 & 0 & a''_{33} \end{bmatrix}$$

and

$$L = \begin{bmatrix} 1 & 0 & 0 \\ f_{21} & 1 & 0 \\ f_{31} & f_{32} & 1 \end{bmatrix}$$

4. Matrix Inverse

The inverse of a matrix A is defined as

$$AA^{-1} = A^{-1}A = I_n$$

One of the most important applications of the LU decomposition is computing the inverse of a matrix A and this can be done in a column-by-column fashion, i.e., we solve the system

$$Ax = b$$

Using the LU decomposition once for

$$b = \begin{bmatrix} 1 \\ \vdots \\ 0 \end{bmatrix}$$

Then for

$$b = \begin{bmatrix} 0 \\ 1 \\ \vdots \end{bmatrix}$$

4.1. Error Analysis and System Condition

Aside from its engineering and scientific applications, the inverse also provides a means to discern whether systems are ill-conditioned. Three direct methods can be devised for this purpose:

1. Multiply the inverse by the original coefficient matrix and assess whether the result is close to the identity matrix. If not, it indicates ill-conditioning.
2. Invert the inverted matrix and assess whether the result is sufficiently close to the original coefficient matrix. If not, it again indicates that the system is ill-conditioned.

5. The Gauss-Seidel Iterative Method

Iterative methods are an iterative way to approximate the solution to the linear system of equations. The Gauss-Seidel method is the most commonly used iterative method for solving linear algebraic equations. Assume that we are given a set of n equations:

$$Ax = b$$

Where $A \in \mathbb{R}^{n\times n}$ and $x, b \in \mathbb{R}^n$. Suppose that for the ease of illustration we limit ourselves to 3×3 systems. Then the variables x_1, x_2, x_3 are solved as

$$x_1^{(j)} = \frac{b_1 - a_{12}x_2^{(j-1)} - a_{13}x_3^{(j-1)}}{a_{11}} \quad (1.24)$$

$$x_2^{(j)} = \frac{b_2 - a_{21}x_1^{(j)} - a_{23}x_3^{(j-1)}}{a_{22}} \quad (1.25)$$

$$x_3^{(j)} = \frac{b_3 - a_{31}x_1^{(j)} - a_{32}}{a_{33}} \quad (1.26)$$

where j and $j-1$ are the present and previous iterations. Where $x_1^{(0)}, x_2^{(0)}, x_3^{(0)}$ are initialized randomly. Convergence can be checked as

$$\varepsilon_{a,i} = \left|\frac{x_i^{(j)} - x_i^{(j-1)}}{x_i^{(j)}}\right| 100\% \leq \varepsilon_s \quad (1.27)$$

For the general case, and computational convenience, we can represent the whole process using a matrix-vector based approach which is usually the preferred way. Let the matrix A be written in the following form

$$A = L + U$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix} = \begin{bmatrix} a_{11} & 0 & \dots & 0 \\ a_{21} & a_{22} & \dots & 0 \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} + \begin{bmatrix} 0 & a_{12} & \dots & a_{1n} \\ 0 & 0 & \dots & a_{2n} \\ 0 & 0 & \dots & 0 \end{bmatrix}$$

The system $Ax = b$ can now be written as

$$\begin{aligned} Ax &= b \\ (L+U)x &= b \\ Lx + Ux &= b \\ Lx &= b - Ux \end{aligned}$$

Then for $x^{(0)}$ initialized

$$x^{(k+1)} = L^{-1}\left(b - Ux^{(k)}\right)\ k = 0, 1, 2 \ldots$$

There could be many possibilities to the stopping criteria (check for convergence) such as

- $\left\|x^{(k+1)} - x^{k}\right\| < \varepsilon$
- $Ax^{(k+1)} - b < \varepsilon$

5.1. Convergence and Diagonal Dominance

The Gauss-Seidel will converge if the matrix is *diagonally dominant* or the matrix is positive definite. The definition of a positive definite matrix is

$$xA^{T}x \geq 0$$

For any vector $x \in \mathbb{R}^{n} - \{0\}$. The convergence criteria for the diagonal dominance can be derived as following:

Suppose that we have two equations represented by two functions $u(x, y)$ and $v(x, y)$. Gauss-Seidel will converge if

$$\left|\frac{\partial u}{\partial x}\right| + \left|\frac{\partial u}{\partial y}\right| < 1 \quad (1.28)$$

$$\left|\frac{\partial v}{\partial x}\right| + \left|\frac{\partial v}{\partial y}\right| < 1 \quad (1.29)$$

Equations 1.24-1.26 can be expressed as following for the case of two unknowns

$$u(x_1, x_2) = \frac{b_1}{a_{11}} - \frac{a_{12}}{a_{11}}x_2 \quad (1.30)$$

$$v(x_1, x_2) = \frac{b_2}{a_{22}} - \frac{a_{21}}{a_{22}}x_1 \quad (1.31)$$

The partial derivatives of these two functions are

$$\frac{\partial u}{\partial x_1} = 0, \frac{\partial u}{\partial x_2} = -\frac{a_{12}}{a_{11}}$$

$$\frac{\partial v}{\partial x_1} = -\frac{a_{21}}{a_{22}}, \frac{\partial v}{\partial x_2} = 0$$

Which can be substituted into eq 1.28 and 1.29 to get

$$\left|\frac{a_{12}}{a_{11}}\right| < 1 \quad (1.32)$$

$$\left|\frac{a_{21}}{a_{22}}\right| < 1 \quad (1.33)$$

Rearranging yields,

$$|a_{11}| > |a_{12}|$$

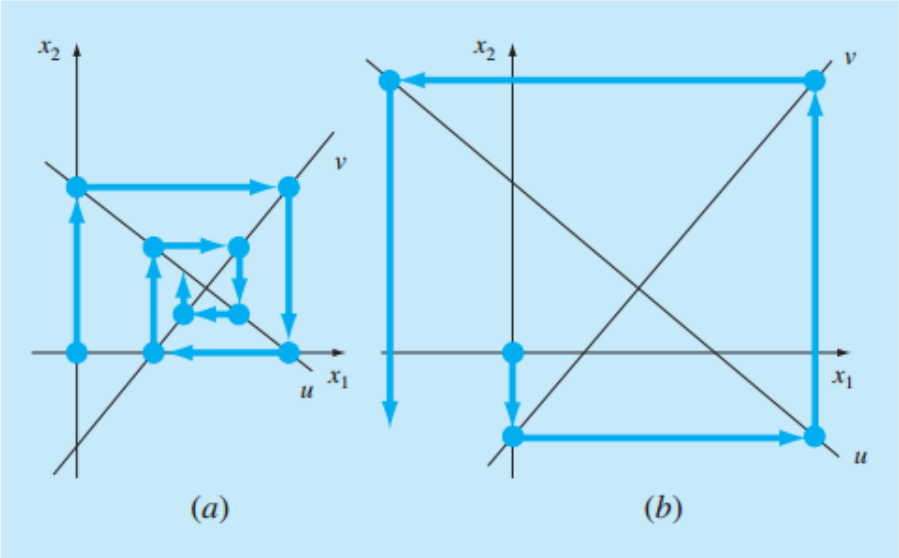
And

$$|a_{22}| > |a_{21}|$$

That says that the diagonal elements must be greater than the off-diagonal elements. This condition can be easily extended for the case of n equations and n unknowns.

$$|a_{ii}| > \sum_{\substack{j=1 \\ j \neq i}}^{n} |a_{ij}|$$

FIGURE 11.5
Iteration cobwebs illustrating (*a*) convergence and (*b*) divergence of the Gauss-Seidel method. Notice that the same functions are plotted in both cases (*u*: $11x_1 + 13x_2 = 286$; *v*: $11x_1 - 9x_2 = 99$). Thus, the order in which the equations are implemented (as depicted by the direction of the first arrow from the origin) dictates whether the computation converges.



6. The Matrix Eigen Analysis Problem

The following equation describes the problem that we are trying to solve

$$Av = \lambda v \ (1.35)$$

Where v is called the eigenvector of A and λ is the associated eigenvalue and in general $\lambda \in \mathbb{C}$. For an $n \times n$ matrix there are exactly n eigenvectors and n eigenvalues. Any square matrix A can be *diagonalized* as following

$$A = Q\Lambda Q^{-1}$$

Where Q contains all the eigenvectors as its columns and $\Lambda = diag\{\lambda_1, \lambda_2, \dots \lambda_n\}$. This decomposition gives a nice way to compute A^p as

$$A^p = Q\Lambda^p Q^{-1}$$

Where $\Lambda^p \stackrel{\text{def}}{=} diag\{\lambda_1^p, \lambda_2^p, \dots, \lambda_n^p\}$

Previously we dealt with the system of the following form:

$$Av = b$$

Which are called *nonhomogeneous systems* because of the arbitrary vector b. On the other hand, the following system is called a *homogeneous system*

$$Av = 0, v \neq 0$$

The engineering problems associated with eigen analysis is of the form

$$(A - \lambda I)v = 0, v \neq 0 \quad (1.36)$$

For nontrivial solutions to be possible, the determinant of the matrix must equal zero:

$$|A - \lambda I| = 0 \quad (1.37)$$

Expanding the determinant yields a polynomial in λ which is called the *characteristic polynomial* of A. The roots of this polynomial are the eigenvalues. Let us understand this for the case of two equations

$$(a_{11} - \lambda)v_1 + a_{12}v_2 = 0$$
$$a_{21}v_1 + (a_{22} - \lambda)v_2 = 0$$

Expanding for the determinant of the coefficient matrix gives

$$\begin{vmatrix} a_{11} - \lambda & a_{12} \\ a_{21} & a_{22} - \lambda \end{vmatrix} = \lambda^2 - (a_{11} + a_{22})\lambda - a_{12}a_{21}$$

Which is the characteristic polynomial and the quadratic formula can then be used to solve for the two eigenvalues λ_1 and λ_2

$$\begin{matrix} \lambda_1 \\ \lambda_2 \end{matrix} = \frac{(a_{11} - a_{22}) \pm \sqrt{(a_{11} - a_{22})^2 - 4a_{12}a_{21}}}{2}$$

Now substituting λ_1 into eq 1.36 shall give us the first eigen vector v_1 and for λ_2 it will give us the second eigen vector v_2.

6.1. QR Decomposition and the Iteration

Given a square $n \times n$ real symmetric matrix A, we can compute all the eigenvalues of A (which are real) by decomposing

$$A = QR$$

Where Q is an orthonormal matrix and R is an upper triangular matrix. We shall discuss the decomposition without any proof. The *projection* of a vector a on u is defined as

$$Proj_u a = \frac{\langle u, a \rangle}{\langle u, u \rangle} u$$

Where $\langle x, y\rangle = x^T y$ is the dot product of x and y. Then we can compute an orthonormal basis from the columns of A as following (a_k are the columns of the matrix A):

$$u_1 = a_1$$

$$u_k = a_k - \sum_{j=1}^{k-1} Proj_{u_j} a_k, \;\; \hat{u}_k = \frac{u_k}{\|u_k\|}, \qquad k = 2,3, \ldots$$

We can now express the columns of A over our newly computed orthonormal basis as

$$A = QR$$

where,

$$Q = [\hat{u}_1, \hat{u}_2, \ldots, \hat{u}_n]$$

And,

$$R = \begin{bmatrix} \langle \hat{u}_1, a_1 \rangle & \langle \hat{u}_1, a_2 \rangle & \ldots & \langle \hat{u}_1, a_n \rangle \\ 0 & \langle \hat{u}_2, a_2 \rangle & \ldots & \langle \hat{u}_2, a_n \rangle \\ 0 & 0 & \ldots & \langle \hat{u}_3, a_n \rangle \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \langle \hat{u}_n, a_n \rangle \end{bmatrix}$$

Now the eigenvalues and eigenvectors of an SPD matrix A can be computed according to the following iterative criteria called the QR iteration algorithm:

1. Begin with the initial matrix $A_0 = A$ and $V_0 = I$
2. Repeat for $k = 0, 1, 2 \ldots$ until A_k becomes an upper triangular matrix
3. Factorize $A_k = Q_k R_k$
4. Compute $A_{k+1} = R_k Q_k$
5. $V_{k+1} = V_k Q_k$

After the algorithm converges, the eigenvalues are on the diagonal of A and the eigenvectors are the columns of V.

6.2. The Singular Value Decomposition (SVD)

The singular value decomposition (SVD) of a matrix is a central matrix decomposition method in linear algebra. It has been referred to as the "fundamental theorem of linear algebra" because it can be applied to all matrices, not only to square matrices, and it always exists.

Let $A \in \mathbb{R}^{m \times n}$ with rank $0 \leq r \leq \min(m, n)$. The rank r of a matrix A is defined as the number of linearly independent columns of A. A set of vectors $x_1, x_2, \ldots x_n$ are linearly independent if

$$\sum_j \alpha_j x_j \neq 0, \;\; \alpha_j \in \mathbb{R}$$

$$X\alpha \neq 0$$

For example, if $x_1 = [4, 5, 2]^T, x_2 = [-2, 3, 1]^T$ then for $\alpha_1 = 2, \alpha_2 = -1$

$$x_3 = \alpha_1 x_1 - x_2$$
$$= [10, 7, 3]^T$$

Thus x_3 is linearly dependent of x_1 and x_2 satisfying the equation

$$x_3 - \alpha_1 x_1 + x_2 = 0$$

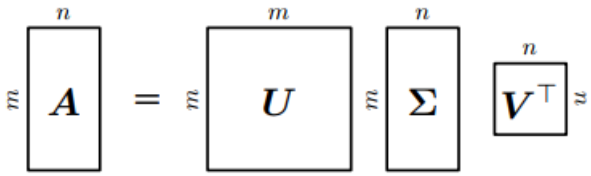
When a set of vectors are linearly independent, $b \in span\{x_1, x_2, \dots x_n\}$ for any b. Geometrically this means that any vector b can be written as

$$b = \sum_j \alpha_j x_j$$

This has a great impact on the solvability of a general linear system.

The *SVD (Singular Value Decomposition)* of a rectangular matrix A is a decomposition of the form

$$A = U\Sigma V^T$$



Where U and V with columns u_i and v_i are orthonormal. Σ is a matrix with $\Sigma_{ii} = \sigma_i \geq 0$ and $\Sigma_{ij} = 0$ if $i \neq j$.

The diagonal elements $\sigma_i, i = 1,2, \dots, r$ are called the *singular values*, u_i and v_i are called left and right singular vectors respectively. By convention $\sigma_1 \geq \sigma_2 \geq \cdots \sigma_r \geq 0$. If $m > n$ then the matrix has diagonal structure up to row n and then consists of 0^T row vectors from $n + 1$ to m. If $m < n$, then the matrix has diagonal structure up to column m and columns that consist of 0 from $m + 1$ to n

6.2.1. The Construction of Singular Value Decomposition (SVD)

We know that any symmetric positive definite matrix A can be decomposed as

$$A = Q\Lambda Q^T$$

To compute the SVD, we make use of the following two facts:

Let $A \in \mathbb{R}^{m \times m}$ be a square matrix, then the following two results are true:

- If v is a unit length eigenvector of $A^T A$ with non-zero eigenvalue λ, then Av is an eigenvector of AA^T with same eigenvalue λ. Furthermore, the norm of Av is $\sqrt{\lambda}$.
- If u is a unit length eigenvector of AA^T with non-zero eigenvalue λ, then $A^T u$ is an eigenvector of $A^T A$ with the same eigenvalue λ. Furthermore, the norm of $A^T u$ is $\sqrt{\lambda}$.

From the above two results, it can be stated that the matrices $A^T A$ and AA^T have the same eigenvalues $\lambda_1, \lambda_2, \dots \lambda_m$. If the m orthonormal eigenvectors of $A^T A$ are $v_1, v_2, \dots v_m$ and the m orthonormal

eigenvectors of AA^T are $u_1, u_2, \dots u_m$ each having same eigenvalues $\lambda_1, \lambda_2, \dots \lambda_m$ then the following identity holds

$$Av_i = \sqrt{\lambda} u_i, i = 1, 2, \dots m$$

Theorem (Existence of SVD): Let the columns of the $m \times m$ matrix V contain all the m orthonormal eigenvectors of $A^T A$ and let Σ be an $m \times m$ diagonal matrix with diagonal entries containing the square roots of the corresponding eigenvalues. By convention, the columns of V and Σ are ordered so that the singular values are in nonincreasing order. Then it is possible to find an $m \times m$ orthonormal matrix U containing all the orthonormal eigenvectors of AA^T, such that the following holds

$$A = U\Sigma V^T$$

SVD of a Rectangular Matrix: Consider an $m \times n$ matrix A with real entries. Such as matrix can always be factorized as following

$$A = U\Sigma V^T$$

Where U is an $m \times m$ matrix with orthonormal columns containing the left singular vectors, Σ is an $m \times n$ rectangular "diagonal" matrix with diagonal entries containing the nonnegative singular values in decreasing order and V is a $n \times n$ matrix with orthonormal columns containing the right singular vectors.

The following are some important properties of the right and left singular vectors:

1. The m columns of U are referred to as the left singular vectors corresponding to m eigenvectors of the $m \times m$ matrix AA^T
2. The n columns of V which are the right singular vectors, corresponds to the n eigenvectors of the $n \times n$ matrix $A^T A$.
3. The diagonal entries of the $m \times n$ matrix Σ contain the singular values, which are the square roots of the $\min(m, n)$ largest eigenvalues of $A^T A$ or AA^T.
4. By convention, the columns of U, V and Σ are ordered by decreasing singular values.

Computing SVD of a Rectangular Matrix: The columns of V are the eigenvectors of $A^T A$, so they can be computed using algorithms like for example the QR iteration. Rewriting $A = U\Sigma V^T$ as $AV = U\Sigma$, the columns of U corresponding to non-zero singular values in Σ are the normalized columns of AV (here the normalization factor is $\frac{1}{\sqrt{\lambda_i}}$). The remaining columns of U satisfies $AA^T u_i = 0$ which can be computed using methods like the LU decomposition. The diagonal entries of the matrix Σ are computed as following

$$\Sigma_{ij} = \begin{cases} \sqrt{\lambda_i}, & i = j \\ 0, & otherwise \end{cases}$$

Readings for this Chapter

- Chapter 3, section 3.1 of the book Numerical Algorithms.
- Chapter 9, 10 and 11 of the book Numerical Methods for Engineers.
- For section 6 of this lecture note, see chapter 4-6 of the book Numerical Algorithms.