- **Systems of Linear Equations**

  Systems of linear equations occur in solving problems in a wide variety of disciplines, including mathematics, statistics, engineering, biological science, social sciences, business, and *physical science.*

  Examples: QM problem (Heisenberg, matrix mechanics), Least squares fit (more later), Electric circuit:

Fig_Circuit

$$
\begin{array}{rcrcrcr}
R_1 I_1 & + & R_2 I_2 & & & = & V_1 \\
 & - & R_2 I_2 & + & R_3 I_3 & = & V_2 \\
I_1 & - & I_2 & - & I_3 & = & 0
\end{array}
\tag{1}
$$

Rewrite the equation in terms of matrices,

$$\mathbf{R}\mathbf{I} = \mathbf{V}$$

where

$$\mathbf{R} \equiv \begin{pmatrix} R_1 & R_2 & 0 \\ 0 & -R_2 & R_3 \\ 1 & -1 & -1 \end{pmatrix}$$

and

$$\mathbf{I} \equiv \begin{pmatrix} I_1 \\ I_2 \\ I_3 \end{pmatrix} \qquad \mathbf{V} \equiv \begin{pmatrix} V_1 \\ V_2 \\ 0 \end{pmatrix}$$

<u>General Form</u>: for a system of n linear equations in the n unknowns $x_1, x_2, \cdots, x_n$, one has

$$\sum_{j=1}^{n} a_{ij} x_j = b_i \ . \tag{2}$$

In matrix notation,

$$\mathbf{A}\mathbf{X} = \mathbf{b} \ , \tag{3}$$

with

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \quad \mathbf{X} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \quad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

- **Matrix Arithmetic**

1. A matrix is a rectangular array of numbers.

   It is said to have order $m \times n$, where m is the number of rows and n is the number of columns. Square matrices, $m = n$.

2. The *transpose* of a matrix is an $n \times m$ matrix

$$A^T = \begin{pmatrix} a_{11} & a_{21} & \cdots & a_{n1} \\ a_{12} & a_{22} & \cdots & a_{n2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{1n} & a_{2n} & \cdots & a_{nn} \end{pmatrix} \qquad (a^T)_{ij} = a_{ji}$$

3. Multiple by a constant, cA.

4. Addition: (same order)

$$A + B \Rightarrow [A + B]_{ij} = a_{ij} + b_{ij}, A + B = B + A$$

5. Matrix multiplication: let A have order $m \times n$ and B have order $n \times p$, then $C = AB$ is a matrix of order $m \times p$ and its element c_{ij} is defined by

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}, \qquad 1 \leq i \leq m, \qquad 1 \leq j \leq p\ .$$

   (See previous example.)

6. Properties of various types of matrices.

   (see the attached table)

7. The *Determinant*: for a square matrix A of order n, its determinant is given by

$$det(A) = \sum_{i,j,k,\cdots} \epsilon_{i,j,k,\cdots} a_{1i} a_{2j} a_{3k} \cdots \ .$$

Here, $\epsilon_{i,j,k,\cdots}$ is the Levi-Civita symbol, equals to $1, -1$ and 0.

Examples:

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \qquad det(A) = a_{11}a_{22} - a_{12}a_{21} \ .$$

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

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

Properties of a determinant:

(a) Addition for single column/row.

(b) Multiplication by a constant.

(c) $det(A^T) = det(A)$.

(d) $det(AB) = det(A)det(B)$.

8. <u>Theorem</u> about the solution of linear equations:

   (a) $det(A) \neq 0$.

   (b) For each right side b, Eq. (3) has exactly one solution x.

   (c) For each right side b, Eq. (3) has at least one solution x.

   (d) The *homogeneous* form of Eq. (3) has exactly one solution $x_1 = x_2 = \cdots = x_n = 0$.

   Examples:

$$\begin{pmatrix} 3 & 2 \\ 6 & 4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

9. The Identity matrix:

$$I_{n\times n}, \qquad I_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$$

$$AI_n = A, \qquad I_m A = A, \qquad IA = AI = A.$$

10. Matrix inversion, A^{-1} is called the *inverse* of A, if

$$AA^{-1} = A^{-1}A = I \ .$$

   If A has an inverse, then it has exactly one inverse.

Examples:

$$\begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{pmatrix}, \qquad \frac{1}{4}\begin{pmatrix} 3 & -2 & 1 \\ -2 & 4 & -2 \\ 1 & -2 & 3 \end{pmatrix}.$$

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}, \qquad \frac{1}{ad-bc}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix},$$

if $ad - bc = det(A) \neq 0$.

<u>Theorem</u>: A square matrix A has an inverse if and only if $det(A) \neq 0$ $(nonsingular)$.

If A^{-1} exists, then Eq. (3) can be solved

$$A^{-1}(Ax) = A^{-1}b \Rightarrow x = A^{-1}b \; .$$

- **Library Routines**

  Math library, Mathematica, IMSL, Linpack, Eispack, Nag, Numerical Receipts, etc.

  1. Matrix manipulations: MATMUL, TRANSPOSE, etc.
  2. Linear systems: LUsolve, LINSYS, IMSL routines;
  3. Inverse and Determinant: use Gaussian elimination routines.

- **Gaussian Elimination**

  Example:

$$
\begin{array}{rcrcrcl}
x_1 & + & 2x_2 & + & x_3 & = & 0 \qquad E(1) \\
2x_1 & + & 2x_2 & + & 3x_3 & = & 3 \qquad E(2) \\
-x_1 & - & 3x_2 & - & & = & 2 \qquad E(3)
\end{array}
\tag{4}
$$

Step 1: Eliminate x_1 from $E(2)$ and $E(3)$ to get

$$
\begin{array}{rcrcrcl}
x_1 & + & 2x_2 & + & x_3 & = & 0 \qquad E(1) \\
 & - & 2x_2 & + & x_3 & = & 3 \qquad E(2) \\
 & - & x_2 & + & x_3 & = & 2 \qquad E(3)
\end{array}
\tag{5}
$$

Step 2: Eliminate x_2 from $E(3)$ to get

$$
\begin{array}{rcrcrcl}
x_1 & + & 2x_2 & + & x_3 & = & 0 \qquad E(1) \\
 & - & 2x_2 & + & x_3 & = & 3 \qquad E(2) \\
 & & & & \frac{1}{2}x_3 & = & \frac{1}{2} \qquad E(3)
\end{array}
\tag{6}
$$

Step 3: In succession, solve for x_3, x_2, and x_1,

$$
\begin{aligned}
x_3 &= 1 \\
-2x_2 + 1 &= 3 \quad \Rightarrow \quad x_2 = -1 \\
x_1 + 2(-1) + 1 &= 0 \quad \Rightarrow \quad x_1 = 1
\end{aligned}
$$

Step 1 and 2 are the *elimination* steps, resulting in Eq. (6), which is called an *upper triangular system* of linear equation. Step 3 is called solution by *back substitution*. The entire process is called *Gaussian elimination*.

For general nonsingular system of n linear equations,

$$a_{11}^{(1)}x_1 + \cdots + a_{1n}^{(1)}x_n = b_1^{(1)} \qquad E(1)$$

$$\vdots \qquad\qquad \vdots$$

$$a_{n1}^{(1)}x_1 + \cdots + a_{nn}^{(1)}x_n = b_n^{(1)} \qquad E(n)$$

Step k: Eliminate x_k from $E(k+1)$ through $E(n)$. Assume $a_{kk}^{(k)} \neq 0$, and define the multipliers

$$m_{ik} = a_{ik}^{(k)}/a_{kk}^{(k)}, \qquad i = k+1, \cdots, n$$

For equations $i = k+1, \cdots, n$, subtract m_{ik} times $E(k)$ from $E(i)$, eliminating x_k from $E(i)$. The new coefficients in $E(k+1)$ through $E(n)$ are defined by

$$\begin{aligned} a_{ij}^{(k+1)} &= a_{ij}^{(k)} - m_{ik}a_{kj}^{(k)}, \qquad i,j = k+1, \cdots, n \\ b_i^{(k+1)} &= b_i^{(k)} - m_{ik}b_k^{(k)}, \qquad i = k+1, \cdots, n \end{aligned} \tag{7}$$

When step $n-1$ is completed, the linear system will be in upper triangular form,

$$\begin{aligned} u_{11}x_1 + \cdots + u_{1n}x_n &= g_1 \\ &\vdots \\ u_{nn}x_n &= g_n \end{aligned} \tag{8}$$

where $u_{ij} = a_{ij}^{(i)}, \qquad g_i = b_i^{(i)}.$

Step n: Solve Eq. (8) using back substitution.

$$x_n = \frac{g_n}{u_{nn}}$$

$$x_i = \frac{g_i - \Sigma_{j=i+1}^{n} u_{ij} x_j}{u_{ii}}, \qquad i = n-1, \cdots, 1$$

Moreover

$$det(A) = u_{11} u_{22} \cdots u_{nn}.$$

Partial Pivoting: to remove the assumption of $a_{kk}^{(k)} \neq 0$ *and* for numerical accuracy. (examples)

At step k, calculate $c = max|a_{ik}^{(k)}|, k \leq i \leq n$. If the element $|a_{kk}^{(k)}| < c$, then interchange $E(k)$ with one of the following equations, to obtain a new equation $E(k)$ in which $|a_{kk}^{(k)}| = c$. The element $a_{kk}^{(k)}$ is called the *pivot element* for step k of the elimination. This process is called *partial pivoting*. There are other forms of pivoting.

Note that $|m_{ik}| < 1, 1 \leq k < i \leq n$, helps to reduce loss-of-significance errors.

Operations Count: important for choosing algorithms.

1. The elimination step.

Table I. Operations Count for $A \to U$:

Step	Additions	Multiplications	Divisions
1	$(n-1)^2$	$(n-1)^2$	$(n-1)$
2	$(n-2)^2$	$(n-2)^2$	$(n-2)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$n-1$	1	1	1
Total	$\frac{n(n-1)(2n-1)}{6}$	$\frac{n(n-1)(2n-1)}{6}$	$\frac{n(n-1)}{2}$

$$
\begin{aligned}
AS(A \to U) &= \frac{n(n-1)(2n-1)}{6} \\
MD(A \to U) &= \frac{n(n-1)(2n-1)}{6} + \frac{n(n-1)}{2} = \frac{n(n^2-1)}{3}
\end{aligned}
$$

AS denotes additions/subtractions and MD denotes multiplications/divisions.

- Modification of the right side b to g.

$$
\begin{aligned}
AS(b \to g) &= (n-1) + (n-2) + \cdots + 1 = \frac{n(n-1)}{2} \\
MD(b \to g) &= (n-1) + (n-2) + \cdots + 1 = \frac{n(n-1)}{2}
\end{aligned}
$$

- The back substitution step, find x from Eq. (8).

$$
\begin{aligned}
AS(g \to x) &= 0 + 1 + \cdots + (n-1) = \frac{n(n-1)}{2} \\
MD(g \to x) &= 1 + 2 + \cdots + n = \frac{n(n+1)}{2}
\end{aligned}
$$

- **The LU Factorization**

Let A be a nonsingular matrix, refer to Gaussian elimination procedure, we define

$$U = \begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ 0 & u_{22} & & u_{2n} \\ \vdots & & \ddots & \cdots \\ 0 & \cdots & 0 & u_{nn} \end{pmatrix} \tag{9}$$

(*upper triangular*) where $u_{ij} = a_{ij}^{(i)}$, and

$$L = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ m_{21} & & & \\ \vdots & \ddots & & \vdots \\ m_{n1} & \cdots & m_{n,n-1} & 1 \end{pmatrix}. \tag{10}$$

(*lower triangular*) then we have

<u>Theorem:</u> if U is produced without pivoting, then

$$LU = A$$

This is called the *LU factorization* of A.

Solving $Ax = b$ is equivalent to solving $LUx = b$. And this is equivalent to solving the two systems

$$Lg = b, \qquad by\ forward\ substitution \tag{11}$$

$$Ux = g, \qquad by\ backward\ substitution. \tag{12}$$

Direct calculation of L and U (*Doolittle's method*)

Step 1: compare the first row and column of both sides of $A = LU$ yields

$$a_{11} = u_{11} \quad a_{12} = u_{12} \quad \cdots \quad a_{1n} = u_{1n}$$

$$a_{21} = u_{11}m_{21} \quad a_{31} = u_{11}m_{31} \quad \cdots$$

Step 2: compare the second row and column of both sides of $A = LU$ to obtain $u_{2k}, k = 2, 3, \cdots$ and then $m_{l2}, l = 3, 4, \cdots$.

By alternating between the columns and rows, we can solve for all the elements of L and U.

We assumed $u_{ii} \neq 0$. If not, pivoting is needed.

The Gaussian elimination and Doolittle's methods are mathematically equivalent and have equal operation counts. But Doolittle's method can be used to greatly reduce the number of rounding errors, with only a minimal increase in cost.

Tridiagonal Systems

$$A = \begin{pmatrix} d_1 & c_1 & 0 & 0 & \cdots & \cdots & 0 \\ a_2 & d_2 & c_2 & 0 & & & 0 \\ 0 & a_3 & d_3 & c_3 & & & 0 \\ \vdots & & \ddots & & & & \vdots \\ 0 & & \cdots & & a_{n-1} & d_{n-1} & c_{n-1} \\ 0 & & \cdots & & 0 & a_n & d_n \end{pmatrix} \tag{13}$$

The LU factorization have the following general form

$$LU = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ \alpha_2 & 1 & 0 & \cdots & 0 \\ 0 & \alpha_3 & 1 & \cdots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \alpha_n & 1 \end{pmatrix} \cdot \begin{pmatrix} \beta_1 & c_1 & 0 & \cdots & 0 \\ 0 & \beta_2 & c_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ 0 & 0 & 0 & \beta_{n-1} & c_{n-1} \\ 0 & 0 & \cdots & 0 & \beta_n \end{pmatrix} \tag{14}$$

$$\begin{aligned} \beta_1 &= d_1 : \text{row 1 of LU} \\ \alpha_2\beta_1 = a_2, \qquad \alpha_2 c_1 + \beta_2 &= d_2 : \text{row 2 of LU} \\ \alpha_j\beta_{j-1} = a_j, \quad \alpha_j c_{j-1} + \beta_j &= d_j : \text{row } j \geq 3 \text{ of LU.} \end{aligned} \tag{15}$$

Thus

$$\begin{aligned} \beta_1 &= d_1 \\ \alpha_j &= a_j/\beta_{j-1}, \quad \beta_j = d_j - \alpha_j c_{j-1}, \quad j = 2, \cdots, n \end{aligned} \tag{16}$$

Again, to solve the system $Ax = b$, simply solve

$$Lg = b, \qquad Ux = g \ .$$

Forward substitution in $Lg = b$ gives

$$\begin{aligned} g_1 &= b_1 \\ g_j &= b_j - \alpha_j g_{j-1}, \qquad j = 2, 3, \cdots, n \end{aligned} \tag{17}$$

and *back substitution in* $Ux = g$ gives

$$\begin{aligned} x_n &= g_n/\beta_n \\ x_j &= (g_j - c_j x_{j+1})/\beta_j, \qquad j = n-1, \cdots, 1 \end{aligned} \tag{18}$$

Operations count: *linearly* proportional to n!

Storage: $3n$.

Pivoting? Not necessary if

$$\begin{aligned} |d_1| &> |c_1| \\ |d_j| &\geq |a_j| + |c_j|, j = 2, 3, \cdots, n-1 \\ |d_n| &> |a_n| \end{aligned} \tag{19}$$

- **The Eigenvalue Problem**

For a *square* matrix, the number λ is called an *eigenvalue* of A and the column matrix v the corresponding *eigenvector* if

$$Av = \lambda v, \qquad v \neq 0 \ . \tag{21}$$

Example: normal modes.

<u>The Characteristic Polynomial</u>

Rewrite Eq. (21) as

$$(\lambda I - A)v = 0, \qquad v \neq 0 \ .$$

This is a homogeneous system of linear equations for *nonzero* solution v, thus one must have

$$0 = det(\lambda I - A) \equiv f(\lambda).$$

$f(\lambda)$ is called the *characteristic polynomial* of A, and its roots are the eigenvalues of A.

In general $f(\lambda)$ is a polynomial of degree n

$$f(\lambda) = \lambda^n + \alpha_{n-1}\lambda^{n-1} + \cdots + \alpha_1\lambda + \alpha_0.$$

Example: $n = 2$,

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

Note that

$$Tr(A) = a_{11} + a_{22} = \lambda_1 + \lambda_2 (= \alpha_{n-1})$$

$$det(A) = a_{11}a_{22} - a_{21}a_{12} = \lambda_1\lambda_2 (= \alpha_0)$$

Corresponding eigenvectors can be obtained by solving a homogeneous linear equation, $Av_i = \lambda_i v_i$.

<u>Matrix Diagonalization</u>

To find a transformation matrix U such that

$$U^{-1}AU = D \equiv diag(\lambda_1, \lambda_2, \cdots, \lambda_n) \tag{22}$$

Example:

$$A = \begin{pmatrix} 1.25 & 0.75 \\ 0.75 & 1.25 \end{pmatrix}, \qquad \lambda_1 = 0.5, \quad , \lambda_2 = 2.$$

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \qquad U^T AU = \begin{pmatrix} 2 & 0 \\ 0 & 0.5 \end{pmatrix}$$

Symmetric Matrices

$$A^T = A; \qquad a_{ij} = a_{ji}.$$

Many physical systems $\Leftrightarrow$ to symmetric matrices.

Examples: Mechanics: coupled oscillators

$$U(\mathbf{x}) = \sum a_{ij} x_i x_j = \mathbf{x}^T A \mathbf{x} \ .$$

Solid state physics: tight-binding model

$$H = \sum t_{ij} c_i^\dagger c_j = \mathbf{c}^\dagger T \mathbf{c} \ .$$

Theorem:

1. all eigenvalues are real numbers;
2. $U^T = U^{-1}$, i.e., $U^T A U = Diag(\lambda)$;
3. eigenvectors are mutually orthogonal (proof?).

QR and QL Transformation

Any symmetric matrix A can always be reduced to a product of two matrices

$$A = QR, \qquad Q^{-1} = Q^\dagger$$

and R is an upper triangular matrix.

We could have a recursion relation

$$
\begin{aligned}
A(1) &\equiv A = QR = Q(1)R(1) \\
A(2) &= Q(1)^{\dagger}A(1)Q(1) = Q(1)^{\dagger}Q(1)R(1)Q(1) \\
&= R(1)Q(1) \longrightarrow Q(2)R(2) \\
A(k+1) &= Q^{\dagger}(k)A(k)Q(k) \longrightarrow D.
\end{aligned}
$$

A set of similarity (canonical) transformations.

Similarly, $A = QL$ with L being a lower triangular matrix.

<u>Library Eigenvalue Routines</u>

<u>Iteration Method</u>

For finding largest(smallest) eigenvalue.

1. Power method
2. Lanczös tridiagonalization
3. others

- **Singular Value Decomposition (SVD)**

A matrix is singular if one of its eigenvalues is zero.

It is ill-conditioned if its ratio of the largest eigenvalue to the smallest eigenvalue is too large (10^6 or 10^{12}).

How to deal with ill-conditioned matrix? **SVD**

Any $m \times n$ matrix A ($m > n$) can be written as

$$A = U \cdot Diag(\lambda_1, \lambda_2, \cdots, \lambda_n) \cdot V^T \tag{23}$$

Matrix U is column-orthogonal

$$\sum_{i=1}^{m} U_{ik} U_{il} \;=\; \delta_{kl} \qquad 1 \le k, l \le n$$

Matrix V is column- and row-orthonormal,

$$\begin{aligned} \sum_{j=1}^{n} V_{jk} V_{jl} \;&=\; \delta_{kl} \qquad 1 \le k, l \le n \\ \sum_{j=1}^{n} V_{kj} V_{lj} \;&=\; \delta_{kl} \qquad 1 \le k, l \le n \end{aligned}$$