Matrix Factorization.

For any nonsingular matrix A, the linear system $Ax = b$ can be solved by Gaussian elimination, with the possibility of row interchanges.

If we knew the row interchanges that were required to solve the system by Gaussian elimination, we could arrange the original equations in an order that would ensure that no row interchanges are needed.

$\Rightarrow$ There is a rearrangement of the equations that permits Gaussian elimination to proceed without row interchanges.

This motivates the idea of a permutation matrix.

Def. An $n \times n$ permutation matrix P is obtained by rearranging the rows of the identity matrix. This gives a matrix with precisely one nonzero entry in each row & in each column. The nonzero entries are all 1's.

Ex. $P = P_{23} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$

is a 3×3 permutation matrix. Matrix multiplication from the left will exchange the second and third rows of a matrix:

$$PA = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

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

On the other hand, multiplying A on the right by P will exchange the second and third columns of A.

We will be using the following two properties of permutation matrices:

① If $k_1, \ldots, k_n$ is a permutation of the integers $1, \ldots, n$ and the permutation matrix $P = [p_{ij}]$ is defined by

$$p_{ij} = \begin{cases} 1 & \text{if } j = k_i \\ 0 & \text{otherwise} \end{cases}$$

then PA permutes the rows of A according to

$$PA = \begin{bmatrix} a_{k_1,1} & a_{k_1,2} & \cdots & a_{k_1,n} \\ a_{k_2,1} & a_{k_2,2} & \cdots & a_{k_2,n} \\ \vdots & \vdots & & \vdots \\ a_{k_n,1} & a_{k_n,2} & \cdots & a_{k_n,n} \end{bmatrix}$$

② If P is a permutation matrix, then P^{-1} exists and $P^{-1} = P^t$.

Now our approach will be to left multiply the system

$$Ax = b$$

by the appropriate permutation matrix P, so that the system

$$(PA)\,x = Pb$$

can be solved without row exchanges. Then PA can be factored into

$$PA = LU.$$

lower triangular upper triangular

This tells us that

$$P^{-1}LUx = b$$

$$LUx = Pb$$

which can be solved rapidly for x.

Ex Find the permutation matrix so that PA can be factored into the product LU

lower triangular

upper triangular

where

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

Ans We proceed according to Gaussian elimination with row interchanges

Use $E_1 \leftrightarrow E_2$

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

$E_3 - E_1 \to E_3$, $E_4 - E_1 \to E_4$ gives

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

Notice that the entries below the pivot are all zero. We can use these entries to store the matrix L as we construct it!

multiplier from $E_3 - E_1 \to E_3$

$$\left[\begin{array}{c:ccc} 1 & 1 & -1 & 2 \\ 0 & 0 & -1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \end{array}\right]$$

multiplier from $E_4 - E_1 \to E_4$

Now everything below the dashed line is used to store the entries of L, as we determine them!

$E_2 \leftrightarrow E_4$ gives

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

Notice that the multipliers are also subject to the row exchange!

We update our dashed line. No new multipliers are stored during this step

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

$E_4 + E_3 \rightarrow E_4$ gives

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

After storing the multiplier...

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

This gives $U = \begin{bmatrix} 1 & 1 & -1 & 2 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 2 \end{bmatrix}$

The lower triangular matrix is given by the matrix below the dashed line, with ones on the main diagonal

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & -1 & 1 \end{bmatrix}$$

As before, P is the composition of row exchanges:

$$P = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

exchange rows 2 & 4 (second interchange)

exchange rows 1 & 2 (first interchange)

Check:

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

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

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

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

Special Types of Matrices.

It is important to be aware of cases where Gaussian Elimination can be performed without row exchanges.

Consider first the following:

Def. An $n \times n$ matrix A is strictly diagonally dominant if

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

for each $i = 1, \ldots, n$.

eg

$$\begin{bmatrix} 3h & h & -h \\ 4 & 10 & 4 \\ 1 & 1 & -3 \end{bmatrix}$$

is strictly diagonally dominant

while

$$\begin{bmatrix} 5 & 1 & 2 & 3 \\ 1 & 4 & 1 & 1 \\ 2 & 2 & 20 & 3 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

is not.

Thm. A strictly diagonally dominant matrix A is nonsingular.

Pf. Suppose there is a nonzero solution to the system

$$A \underset{\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}}{\underset{\parallel}{x}} = 0$$

Then $\max_{1 \le j \le n} |x_j| > 0$. Let

x_k be a component for which

$$|x_k| = \max_{1 \le j \le n} |x_j|$$

Now $\sum_{j=1}^{n} a_{ij} x_j = 0 \qquad i = 1, 2, \ldots, n$

$$\Rightarrow \quad a_{kk} x_k = -\sum_{\substack{j=1 \\ j \ne k}}^{n} a_{kj} x_j$$

$$\Rightarrow \quad |a_{kk}||x_k| \le \sum_{\substack{j=1 \\ j \ne k}}^{n} |a_{kj}|\,|x_j|$$

$$\Rightarrow \quad |a_{kk}| \le \sum_{\substack{j=1 \\ j\ne k}}^{n} |a_{kj}| \frac{|x_j|}{|x_k|} \le \sum_{\substack{j=1 \\ j\ne k}}^{n} |a_{kj}|$$

But this contradicts the strict diagonal dominance of A.

Thus the only solution to $Ax = 0$ is $x = 0$

$\Rightarrow$ A is nonsingular.

Thm. Let A be a strictly diagonally dominant matrix.

Then Gaussian elimination can be performed on any linear system of the form $Ax = b$ to obtain its unique solution without ~~[illegible]~~ row or column interchanges, and the computations are stable to the growth of roundoff errors.

Pf. Since A is strictly diagonally dominant $a_{11} \neq 0$ & the operations

$$E_j - \frac{a_{ij}}{a_{11}} E_1 \to E_j \qquad 2 \leq j \leq n$$

generate a new matrix $A^{(2)}$ with

$$a_{ij}^{(2)} = a_{ij} - \frac{a_{ij}}{a_{11}} a_{i1} \qquad 2 \leq j \leq n.$$

$$\Rightarrow \sum_{\substack{j=2 \\ j\neq i}}^{n} |a_{ij}^{(2)}| = \sum_{\substack{j=2 \\ j\neq i}}^{n} \left| a_{ij} - \frac{a_{1j} a_{i1}}{a_{11}} \right|$$

$$\leq \sum_{\substack{j=2 \\ j\neq i}}^{n} |a_{ij}| + \sum_{\substack{j=2 \\ j\neq i}}^{n} \left| \frac{a_{1j} a_{i1}}{a_{11}} \right|$$

$$< |a_{ii}| - |a_{i1}| + \frac{|a_{i1}|}{|a_{11}|} \sum_{\substack{j=2 \\ j\neq i}}^{n} |a_{1j}|$$

$$< |a_{ii}| - |a_{i1}| + \frac{|a_{i1}|}{|a_{11}|} \left(|a_{11}| - |a_{1i}| \right)$$

$$= |a_{ii}| - |a_{i1}| \, |a_{1i}| / |a_{11}|$$

$$\leq |a_{ii} - a_{i1} a_{1i} / a_{11}|$$

$$= |a_{ii}^{(2)}|$$

37.12

Thus $A^{(2)}$ is strictly diagonally dominant.

Gaussian Elimination is continued until the upper triangular and strictly diagonally dominant matrix $A^{(n)}$ is obtained.

$\Rightarrow$ all the diagonal elements are nonzero

$\Rightarrow$ Gaussian elimination can be performed without row exchanges.

A reference to the stability result is provided in the text.

$\blacksquare$

The next type of matrices that we will consider are symmetric, positive definite matrices.

Def. A matrix A is positive definite if

$$x^t A x > 0$$

for every nonzero n-dimensional column vector x.

Ex Find all values of α for which

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

is positive definite.

Ans. $$x^t A x = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & 1 \\ -1 & 1 & \alpha \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$= x_1^2 - 2x_1x_3 + x_2^2 + 2x_2x_3 + \alpha x_3^2$$

$$= (x_1 - x_3)^2 + (x_2 + x_3)^2 + (\alpha - 2)x_3^2$$

A positive definite $\Leftrightarrow$ $\alpha > 2$.

Some necessary conditions for an $n \times n$ matrix to be positive definite include.

a/ A is nonsingular.

b/ $a_{ii} > 0$ for each $i = 1, 2, \dots, n$

c/ $\max\limits_{1 \le k, j \le n} |a_{kj}| \le \max\limits_{1 \le i \le n} |a_{ii}|$

d/ $(a_{ij})^2 < a_{ii} a_{jj}$ for each $i \ne j$.

These are not sufficient conditions for positive definiteness however.

We would like necessary & sufficient conditions for a matrix to be positive definite.

We will first need the following definition:

<u>A leading principal submatrix</u> of a matrix A is a matrix of the form

$$A_k = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1k} \\ a_{21} & a_{22} & \cdots & a_{2k} \\ \vdots & & & \\ a_{k1} & a_{k2} & \cdots & a_{kk} \end{bmatrix}$$

for some $1 \le k \le n$.

Based on this definition, we have the following theorem:

<u>Thm</u>: A symmetric matrix A is positive definite if and only if each of its leading principal submatrices has a positive determinant.

<u>Ex</u>. Find α so that

$$A = \begin{bmatrix} 2 & \alpha & -1 \\ \alpha & 2 & 1 \\ -1 & 1 & 4 \end{bmatrix}$$

is positive definite.

<u>Soln</u>. The matrix A is positive definite if and only if

$$\det \begin{bmatrix} 2 & \alpha \\ \alpha & 2 \end{bmatrix} = 4 - \alpha^2 > 0$$

<u>and</u> $$\det \begin{bmatrix} 2 & \alpha & -1 \\ \alpha & 2 & 1 \\ -1 & 1 & 4 \end{bmatrix}$$

$$= 2(8-1) - \alpha(4\alpha+1) - (\alpha+2) > 0$$

we need $\quad 4 - \alpha^2 > 0 \quad \& \quad 12 - 2\alpha - 4\alpha^2 > 0$

$$\alpha^2 < 4 \quad \& \quad -(\alpha - 3/2)(\alpha+2) > 0.$$

$$-2 < \alpha < 2 \quad \& \quad -2 < \alpha < 3/2$$

$$\Rightarrow \quad -2 < \alpha < 3/2$$

$\therefore$ The matrix is positive definite for $-2 < \alpha < 3/2$.

As it turns out we don't need to carry out row exchanges when Gaussian Elimination is used on a symmetric, positive definite matrix:

Thm. A symmetric matrix A is positive definite if and only if Gaussian elimination without row exchanges can be performed on the linear system $Ax = b$ with all the pivot elements positive.

Moreover, in this case, the computations are stable with respect to the growth of roundoff errors.

Some related results:

Corollary. The matrix A is symmetric positive definite if and only if A can be factored in the form LDL^t, where L is lower triangular with 1's on its diagonal and D is a diagonal matrix with positive diagonal entries.

A modification of the LU factorization can be made to factor a symmetric positive definite matrix into the form

$$LDL^t$$

Lower triangular

diagonal

This LDL^t Factorization only requires $n^3/6 + n^2 - 7n/6$ multiplications/divisions and $n^3/6 - n/6$ additions/subtractions.

This is only half the number of operations as LU factorization.

A version of this algorithm can also be constructed for matrices that are symmetric but not positive definite.

Another related result:

<u>Corollary</u>: The symmetric matrix A is positive definite if and only if A can be factored in the form LL^t where L is lower triangular with nonzero diagonal entries.

Once again, a modification of the LU factorization can be made. This method (Choleski's Algorithm) factors a symmetric positive definite matrix into the form

$$\underbrace{L}_{\text{lower triangular}}L^t$$

Choleski's Algorithm only requires

$n^3/6 + n^2/2 - 2n/3$ multiplications/divisions

and $n^3/6 - n/6$ additions/subtractions

which is even less than LDL^t factorization.

(However for small n, Choleski's Algorithm may be slower because it requires n square roots to be computed)

Another important class of matrices that arise in a wide variety of applications are <u>band matrices</u>.

These are matrices that concentrate all their nonzero entries about the diagonal.

<u>Def</u> An $n \times n$ matrix is called a band matrix if integers p and q, with $1 \le p, q \le n$, exist having the property that $a_{ij} = 0$ whenever $i + p \le j$ or $j + q \le i$.

The band width of a band matrix is defined as $w = p + q - 1$.

<u>ex</u>

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{bmatrix} \qquad \begin{bmatrix} 1 & 2 & 0 \\ 3 & 4 & 5 \\ 0 & 6 & 7 \end{bmatrix}$$

$p = 1,\ q = 1,\ w = 1 \qquad p = 2,\ q = 2,\ w = 3$

$$\begin{bmatrix} 1 & 2 & 3 & 0 \\ 0 & 4 & 5 & 6 \\ 0 & 0 & 7 & 8 \\ 0 & 0 & 0 & 9 \end{bmatrix}$$

$p = 3,\ q = 1,\ w = 3$

We will focus on the important case of tridiagonal matrices. Ie, matrices of the form

$$A = \begin{bmatrix} a_{11} & a_{12} & 0 & \cdots & 0 \\ a_{21} & a_{22} & a_{23} & \ddots & \vdots \\ 0 & a_{23} & a_{33} & \ddots & \\ \vdots & \ddots & \ddots & \ddots & 0 \\ & & \ddots & \ddots & a_{n-1n} \\ 0 & \cdots & 0 & a_{nn-1} & a_{nn} \end{bmatrix}$$

Now suppose A can be factored into the triangular matrices L and U. Suppose that the matrices can be found in the form

$$L = \begin{bmatrix} l_{11} & 0 & \cdots & & 0 \\ l_{21} & l_{22} & \ddots & & \vdots \\ 0 & \ddots & \ddots & & 0 \\ \vdots & \ddots & \ddots & \ddots & \\ 0 & \cdots & 0 & l_{nn-1} & l_{nn} \end{bmatrix} \quad \& \quad U = \begin{bmatrix} 1 & u_{12} & 0 & \cdots & 0 \\ 0 & 1 & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & u_{n-1n} \\ 0 & \cdots & & 0 & 1 \end{bmatrix}$$

The zero entries of A are automatically generated by LU.

Multiplying $A = LU$ we also find the following conditions:

$$(*)\ \begin{cases} a_{11} = l_{11} & \\ a_{i,i-1} = l_{i,i-1} & i = 2, 3, \dots, n \end{cases}$$

$$(**)\quad a_{ii} = l_{i,i-1}\, u_{i-1,i} + l_{ii} \qquad i = 2, 3, \dots, n$$

$$(***)\quad a_{i,i+1} = l_{ii}\, u_{i,i+1} \qquad i = 1, 2, \dots, n-1.$$

This system is straightforward to solve: $(*)$ gives us l_{11} and the off-diagonal entries of L

$(**)$ and $(***)$ are used alternately to obtain the remaining entries of L and U.

This solution technique is often referred to as Crout factorization

If we count up the number of of operations we find

$(5n - 4)$ multiplications / divisions

& $(3n - 3)$ additions / subtractions

Crout factorization can be applied to a matrix that is positive definite or one that is strictly diagonally dominant. See the text for another general case where it can be applied.