Gauss Elimination Method: Pivoting

- First Step: $R'_i = R_i - (a_{i1}/a_{11}) \times R_1$ i=2 to n
- Second step: $R''_i = R'_i - (a'_{i2}/a'_{22}) \times R'_2$ i= 3 to n; and so on..
- The multiplying factor at each step is equal to the corresponding element of the row divided by the pivot element
- If we want round-off errors to be attenuated, this factor should be small in magnitude.
- Since order of equations is immaterial, we can interchange rows without affecting the solution
- Partial Pivoting: Scan the elements below the diagonal <u>in that particular column</u>, find the largest magnitude, and interchange rows so that the pivot element becomes the largest.

Pivoting

- Complete Pivoting: Scan the elements <u>in the entire submatrix</u>, find the largest magnitude, and interchange <u>rows and columns</u>, so that the pivot element becomes the largest.

$$
\begin{bmatrix}
a_{11} & a_{12} & a_{13} & a_{14} & \cdots & a_{1k} & a_{1k+1} & \cdots & a_{1n} \\
0 & a_{22} & a_{23} & a_{24} & \cdots & a_{2k} & a_{2k+1} & \cdots & a_{2n} \\
0 & 0 & a_{33} & a_{34} & \cdots & a_{3k} & a_{3k+1} & \cdots & a_{3n} \\
0 & 0 & 0 & a_{44} & \cdots & a_{4k} & a_{4k+1} & \cdots & a_{4n} \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & 0 & 0 & \cdots & a_{kk} & a_{kk+1} & \cdots & a_{kn} \\
0 & 0 & 0 & 0 & \cdots & a_{k+1k} & a_{k+1k+1} & \cdots & a_{k+1n} \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & 0 & 0 & \cdots & a_{nk} & a_{nk+1} & \cdots & a_{nn}
\end{bmatrix}
$$

Partial Complete

Pivoting

- Parial Pivoting does not need any additional bookkeeping. Complete pivoting, due to an exchange of columns, needs to keep track of this exchange.
- If we exchange columns *k* and *l*: after the solution, the values of x_k and x_l have to be interchanged.

Examples: Partial Pivoting:

$$\begin{bmatrix} 2 & 4 & 1 \\ 1 & 2 & 3 \\ 3 & 1 & 5 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 13 \\ 14 \\ 20 \end{Bmatrix}; \begin{bmatrix} 3 & 1 & 5 \\ 1 & 2 & 3 \\ 2 & 4 & 1 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 20 \\ 14 \\ 13 \end{Bmatrix}; \begin{bmatrix} 3 & 1 & 5 \\ 0 & 5/3 & 4/3 \\ 0 & 10/3 & -7/3 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 20 \\ 22/3 \\ -1/3 \end{Bmatrix}$$

$$\begin{bmatrix} 3 & 1 & 5 \\ 0 & 10/3 & -7/3 \\ 0 & 5/3 & 4/3 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 20 \\ -1/3 \\ 22/3 \end{Bmatrix}; \begin{bmatrix} 3 & 1 & 5 \\ 0 & 10/3 & -7/3 \\ 0 & 0 & 5/2 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 20 \\ -1/3 \\ 15/2 \end{Bmatrix};$$

Soln:
1,2,3

Example: Complete (or Full) Pivoting

$$\begin{bmatrix} 2 & 4 & 1 \\ 1 & 2 & 3 \\ 3 & 1 & 5 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 13 \\ 14 \\ 20 \end{Bmatrix}; \quad \begin{bmatrix} 3 & 1 & 5 \\ 1 & 2 & 3 \\ 2 & 4 & 1 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 20 \\ 14 \\ 13 \end{Bmatrix}; \quad \begin{bmatrix} 5 & 1 & 3 \\ 3 & 2 & 1 \\ 1 & 4 & 2 \end{bmatrix} \begin{Bmatrix} x_3 \\ x_2 \\ x_1 \end{Bmatrix} = \begin{Bmatrix} 20 \\ 14 \\ 13 \end{Bmatrix};$$

- Note the interchange, of the variables x_1 and x_3. While computing, we deal with only [A] and {b}. So we make a note of this exchange and do it after the solution is obtained.

$$\begin{bmatrix} 5 & 1 & 3 \\ 0 & 1.4 & -0.8 \\ 0 & 3.8 & 1.4 \end{bmatrix} \{x\} = \begin{Bmatrix} 20 \\ 2 \\ 9 \end{Bmatrix}; \quad \begin{bmatrix} 5 & 1 & 3 \\ 0 & 3.8 & 1.4 \\ 0 & 1.4 & -0.8 \end{bmatrix} \{x\} = \begin{Bmatrix} 20 \\ 9 \\ 2 \end{Bmatrix};$$

$$\begin{bmatrix} 5 & 1 & 3 \\ 0 & 3.8 & 1.4 \\ 0 & 0 & -25/19 \end{bmatrix} \{x\} = \begin{Bmatrix} 20 \\ 9 \\ -25/19 \end{Bmatrix}; \ \text{Solution}: 3,2,1. \ \text{Interchange}: 1,2,3$$

Other considerations

- Round-off errors are typically large if the elements of the [A] matrix are of very different magnitudes.
- **Scaling** of variable and **equilibration** of equation are used to make the coefficient matrix elements roughly of the same order
- For example, $\begin{bmatrix} 0.02 & 4 & 1 \\ 0.01 & 2 & 3 \\ 0.03 & 1 & 5 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 13 \\ 14 \\ 20 \end{Bmatrix}$ may be because x_1 is in cm and others in m
- Scaling of x_1 to $x'_1=x_1/100$ will result in $\begin{bmatrix} 2 & 4 & 1 \\ 1 & 2 & 3 \\ 3 & 1 & 5 \end{bmatrix} \begin{Bmatrix} x'_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 13 \\ 14 \\ 20 \end{Bmatrix};$
- Similarly, $\begin{bmatrix} 2 & 4 & 1 \\ 1 & 2 & 3 \\ 1/20 & 1/60 & 1/12 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 13 \\ 14 \\ 1/3 \end{Bmatrix};$ may be because the the third equation is in hr and others are in minutes
- Equilibrating by multiplying the third equation by 60.

Gauss Elimination Method, LU decomposition

- GE reduces the matrix [A] to upper triangular form
- If there are several RHS vectors, an "augmented" [A] matrix could be used to obtain the solution for all of these through the same algorithm
- Sometimes, an RHS vector depends on the solution for the previous RHS vector.
- The LU decomposition method is then more efficient, since solution of two triangular systems involves much less computational effort

$$[A] = [L][U] \Rightarrow [L]\{y\} = \{b\} \quad \text{where, } \{y\} = [U]\{x\}$$

- The effort in decomposition is needed only once (The assumption, of course, is that [A] is not changing!)

LU decomposition: Alternative ways

$$\begin{bmatrix} a_{11} & a_{12} & . & . & a_{1n} \\ a_{21} & a_{22} & . & . & a_{2n} \\ . & . & . & . & . \\ . & . & . & . & . \\ a_{n1} & a_{n2} & . & . & a_{nn} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & . & . & 0 \\ l_{21} & l_{22} & . & . & 0 \\ . & . & . & . & . \\ . & . & . & . & . \\ l_{n1} & l_{n2} & . & . & l_{nn} \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & . & . & u_{1n} \\ 0 & u_{22} & . & . & u_{2n} \\ . & . & . & . & . \\ . & . & . & . & . \\ 0 & 0 & . & . & u_{nn} \end{bmatrix}$$

- n^2 equations, n^2+n “unknowns”. The way the “floating” n values are fixed: different algorithms
- Doolittle: All diagonal elements of [L] are 1
- Crout: All diagonal elements of [U] are 1
- Cholesky (some call it Choleski): Works only for symmetric positive definite [A]: $n(n+1)/2$ eqns. $[U]=[L]^T$

LU decomposition: Doolittle

$$\begin{bmatrix} a_{11} & a_{12} & . & . & a_{1n} \\ a_{21} & a_{22} & . & . & a_{2n} \\ . & . & . & . & . \\ . & . & . & . & . \\ a_{n1} & a_{n2} & . & . & a_{nn} \end{bmatrix} = \begin{bmatrix} 1 & 0 & . & . & 0 \\ l_{21} & 1 & . & . & 0 \\ . & . & . & . & . \\ . & . & . & . & . \\ l_{n1} & l_{n2} & . & . & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & . & . & u_{1n} \\ 0 & u_{22} & . & . & u_{2n} \\ . & . & . & . & . \\ . & . & . & . & . \\ 0 & 0 & . & . & u_{nn} \end{bmatrix}$$

$$= \begin{bmatrix} u_{11} & u_{12} & . & . & u_{1n} \\ l_{21}u_{11} & l_{21}u_{12} + u_{22} & . & . & l_{21}u_{1n} + u_{2n} \\ . & . & . & . & . \\ . & . & . & . & . \\ l_{n1}u_{11} & l_{n1}u_{12} + l_{n2}u_{22} & . & . & l_{n1}u_{1n} + l_{n2}u_{2n} + \ldots + u_{nn} \end{bmatrix}$$

- n^2 equations, n^2 “unknowns”: $(n^2-n)/2$ in [L] and $(n^2+n)/2$ in [U]
- Sequential computations: $u_{11}=a_{11}$, $u_{12}=a_{12}$,…, $u_{1n}=a_{1n}$; $l_{21}=a_{21}/u_{11}$, $l_{31}=a_{31}/u_{11}$,…, $l_{n1}=a_{n1}/u_{11}$; $u_{22}=(a_{22}-l_{21} x u_{12})$, $u_{23}=(a_{23}-l_{21} x u_{13})$, …, $u_{2n}=(a_{2n}-l_{21} x u_{1n})$;$l_{32}=(a_{32}-l_{31} x u_{12})/u_{22}$,…

LU decomposition: Crout

$$\begin{bmatrix} a_{11} & a_{12} & . & . & a_{1n} \\ a_{21} & a_{22} & . & . & a_{2n} \\ . & . & . & . & . \\ . & . & . & . & . \\ a_{n1} & a_{n2} & . & . & a_{nn} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & . & . & 0 \\ l_{21} & l_{22} & . & . & 0 \\ . & . & . & . & . \\ . & . & . & . & . \\ l_{n1} & l_{n2} & . & . & l_{nn} \end{bmatrix} \begin{bmatrix} 1 & u_{12} & . & . & u_{1n} \\ 0 & 1 & . & . & u_{2n} \\ . & . & . & . & . \\ . & . & . & . & . \\ 0 & 0 & . & . & 1 \end{bmatrix}$$

$$= \begin{bmatrix} l_{11} & l_{11}u_{12} & . & . & l_{11}u_{1n} \\ l_{21} & l_{21}u_{12}+l_{22} & . & . & l_{21}u_{1n}+l_{22}u_{2n} \\ . & . & . & . & . \\ . & . & . & . & . \\ l_{n1} & l_{n1}u_{12}+l_{n2} & . & . & l_{n1}u_{1n}+l_{n2}u_{2n}+\ldots+l_{nn} \end{bmatrix}$$

- n^2 equations, n^2 "unknowns": $(n^2+n)/2$ in [L] and $(n^2-n)/2$ in [U]
- Sequential computations: $l_{11}=a_{11}$, $l_{21}=a_{21}$,…, $l_{n1}=a_{n1}$; $u_{12}=a_{12}/l_{11}$, $u_{13}=a_{13}/l_{11}$,…, $u_{1n}=a_{1n}/l_{11}$; $l_{22}=(a_{22}-l_{21}xu_{12})$, $l_{32}=(a_{32}-l_{31}xu_{12})$, …, $l_{n2}=(a_{n2}-l_{n1}xu_{12})$;$u_{23}=(a_{23}-l_{21}xu_{13})/l_{22}$,…

LU decomposition: Cholesky

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

Symmetric: $a_{ij}=a_{ji}$

$$= \begin{bmatrix} l_{11}^2 & l_{11}l_{21} & . & . & l_{11}l_{n1} \\ l_{11}l_{21} & l_{21}^2 + l_{22}^2 & . & . & l_{21}l_{n1} + l_{22}l_{n2} \\ . & . & . & . & . \\ . & . & . & . & . \\ l_{11}l_{n1} & l_{21}l_{n1} + l_{22}l_{n2} & . & . & l_{n1}^2 + l_{n2}^2 + \ldots + l_{nn}^2 \end{bmatrix}$$

- $n(n+1)/2$ equations, $n(n+1)/2$ “unknowns” in [L]
- Sequential computations: $l_{11}=\sqrt{a_{11}}$, $l_{21}=a_{21}/l_{11}$,…, $l_{n1}=a_{n1}/l_{11}$; $l_{22}=\sqrt{(a_{22}-l^2_{21})}$, $l_{32}=(a_{32}-l_{31}xl_{21})/l_{22}$, …, $l_{n2}=(a_{n2}-l_{n1}xl_{21})/l_{22}$;

LU decomposition: Examples

$$\begin{bmatrix} 9 & 3 & -2 \\ 3 & 6 & 1 \\ -2 & 1 & 9 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 10 \\ 10 \\ 8 \end{Bmatrix}$$

Doolittle:

$$\begin{bmatrix} 9 & 3 & -2 \\ 3 & 6 & 1 \\ -2 & 1 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1/3 & 1 & 0 \\ -2/9 & 1/3 & 1 \end{bmatrix} \begin{bmatrix} 9 & 3 & -2 \\ 0 & 5 & 5/3 \\ 0 & 0 & 8 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 1/3 & 1 & 0 \\ -2/9 & 1/3 & 1 \end{bmatrix} \begin{Bmatrix} y_1 \\ y_2 \\ y_3 \end{Bmatrix} = \begin{Bmatrix} 10 \\ 10 \\ 8 \end{Bmatrix}$$

$$\begin{bmatrix} 9 & 3 & -2 \\ 0 & 5 & 5/3 \\ 0 & 0 & 8 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 10 \\ 20/3 \\ 8 \end{Bmatrix}$$

LU decomposition: Examples

$$\begin{bmatrix} 9 & 3 & -2 \\ 3 & 6 & 1 \\ -2 & 1 & 9 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 10 \\ 10 \\ 8 \end{Bmatrix}$$

Crout:

$$\begin{bmatrix} 9 & 3 & -2 \\ 3 & 6 & 1 \\ -2 & 1 & 9 \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} 1 & u_{12} & u_{13} \\ 0 & 1 & u_{23} \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 9 & 0 & 0 \\ 3 & 5 & 0 \\ -2 & 5/3 & 8 \end{bmatrix} \begin{bmatrix} 1 & 1/3 & -2/9 \\ 0 & 1 & 1/3 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 9 & 0 & 0 \\ 3 & 5 & 0 \\ -2 & 5/3 & 8 \end{bmatrix} \begin{Bmatrix} y_1 \\ y_2 \\ y_3 \end{Bmatrix} = \begin{Bmatrix} 10 \\ 10 \\ 8 \end{Bmatrix}$$

$$\begin{bmatrix} 1 & 1/3 & -2/9 \\ 0 & 1 & 1/3 \\ 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 10/9 \\ 4/3 \\ 1 \end{Bmatrix}$$

LU decomposition: Examples

$$\begin{bmatrix} 9 & 3 & -2 \\ 3 & 6 & 1 \\ -2 & 1 & 9 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 10 \\ 10 \\ 8 \end{Bmatrix}$$

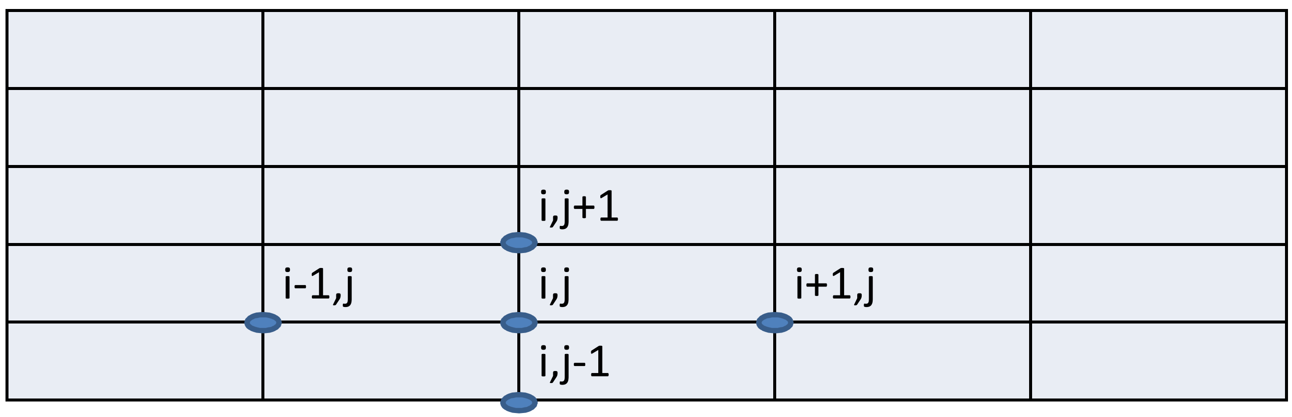
Cholesky:

$$\begin{bmatrix} 9 & 3 & -2 \\ 3 & 6 & 1 \\ -2 & 1 & 9 \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} l_{11} & l_{21} & l_{31} \\ 0 & l_{22} & l_{32} \\ 0 & 0 & l_{33} \end{bmatrix} = \begin{bmatrix} 3 & 0 & 0 \\ 1 & \sqrt{5} & 0 \\ -2/3 & \sqrt{5}/3 & \sqrt{8} \end{bmatrix} \begin{bmatrix} 3 & 1 & -2/3 \\ 0 & \sqrt{5} & \sqrt{5}/3 \\ 0 & 0 & \sqrt{8} \end{bmatrix}$$

$$\begin{bmatrix} 3 & 0 & 0 \\ 1 & \sqrt{5} & 0 \\ -2/3 & \sqrt{5}/3 & \sqrt{8} \end{bmatrix} \begin{Bmatrix} y_1 \\ y_2 \\ y_3 \end{Bmatrix} = \begin{Bmatrix} 10 \\ 10 \\ 8 \end{Bmatrix} \qquad \begin{bmatrix} 3 & 1 & -2/3 \\ 0 & \sqrt{5} & \sqrt{5}/3 \\ 0 & 0 & \sqrt{8} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 10/3 \\ 4\sqrt{5}/3 \\ \sqrt{8} \end{Bmatrix}$$

Banded and Sparse matrices

Several of the matrices in engineering applications are **sparse**, i.e., have very few non-zero elements. For example, solution of differential equations:



$$\frac{\partial T}{\partial t} = \frac{T_{i,j}^{t+\Delta t} - T_{i,j}^{t}}{\Delta t}; \frac{\partial^2 T}{\partial x^2} = \frac{\dfrac{T_{i+1,j} - T_{i,j}}{\Delta x} - \dfrac{T_{i,j} - T_{i-1,j}}{\Delta x}}{\Delta x} = \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{\Delta x^2}$$

If the non-zero elements occur within a “narrow” band around the diagonal, it is called **banded** matrix. The fact that most of the elements are zero can be used to save computational effort.

Banded Matrix

$$\begin{bmatrix} \times & \times & . & 0 & 0 \\ \times & \times & . & . & 0 \\ . & . & . & . & . \\ 0 & . & . & \times & \times \\ 0 & 0 & . & \times & \times \end{bmatrix}$$

- *Band width:* If main diagonal, adjacent r row elements, and adjacent c column elements ***maybe*** non-zero, the band-width is $r+c+1$. In GE method, since we know that elements beyond the band are already zero, we do not need to perform the computations to make them zero.
- Simplest case: Tridiagonal, $r=c=1$ (e.g., in 1-d finite diff.)
- Thomas Algorithm