

Solving large-scale linear systems

- Brief revision: Gaussian reduction
- Matrix $\mathbf{A} = \mathbf{LU}$ factorisation (decomposition)
- Elementary matrices for row operations
- LU factorisation methods:
 - Doolittle's algorithm
 - Crout's algorithm
 - Cholesky's algorithm

- Swapping two rows
- Multiplying a row by a constant
- Adding a multiple of one row to another

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- Quite often, one needs to solve a number of linear systems $\mathbf{Ax}_i = \mathbf{b}_i$ for different \mathbf{b}_i but with the same matrix \mathbf{A} .
- It would be inefficient to reduce $[\mathbf{A} \mid \mathbf{b}_i]$ to REF each time.
- This could be done using the inverted matrix \mathbf{A}^{-1} , however inversion is often numerically unstable and increases errors.
- **LU factorisation** provides a quicker method to solve the system $\mathbf{Ax}_i = \mathbf{b}_i$ for a number of vectors \mathbf{b}_i .
- If we can reduce a square matrix \mathbf{A} to echelon form without row swaps, then it can be written as the product of an upper triangular matrix \mathbf{U} and a lower triangular matrix \mathbf{L} :

$$\mathbf{A} = \mathbf{LU}$$

(slightly more complicated if we need to also use row swaps).

To solve the system $\mathbf{Ax} = \mathbf{b}$ we decompose $\mathbf{A} = \mathbf{LU}$ where

$$\mathbf{L} = \begin{bmatrix} * & 0 & 0 & 0 \\ * & * & 0 & 0 \\ * & * & * & 0 \\ * & * & * & * \end{bmatrix}, \quad \mathbf{U} = \begin{bmatrix} * & * & * & * \\ 0 & * & * & * \\ 0 & 0 & * & * \\ 0 & 0 & 0 & * \end{bmatrix},$$

so the system can be written as: $\mathbf{Ax} = (\mathbf{LU})\mathbf{x} = \mathbf{L}(\mathbf{Ux}) = \mathbf{b}$.

Letting $\mathbf{Ux} = \mathbf{y}$ we get $\mathbf{L}(\mathbf{Ux}) = \mathbf{Ly} = \mathbf{b}$.

In this way, we obtain two equations to solve instead of one:

$$\begin{cases} \mathbf{Ly} = \mathbf{b} & \text{(to find } y \text{ first)} \\ \mathbf{Ux} = \mathbf{y} & \text{(to find } x \text{ then)} \end{cases}$$

however each of these is much quicker to solve.

We solve $\mathbf{L}\mathbf{y} = \mathbf{b}$ first. This is easy because \mathbf{L} is triangular:

$$\mathbf{L}\mathbf{y} = \begin{bmatrix} * & 0 & 0 & 0 \\ * & * & 0 & 0 \\ * & * & * & 0 \\ * & * & * & * \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$$

We find the solution by forward substitution

($y_1 = b_1/*$, $y_2 = (b_2 - * \cdot y_1)/*$, and so on)

Then we can solve $\mathbf{U}\mathbf{x} = \mathbf{y}$. Also easy, because \mathbf{U} is triangular:

$$\mathbf{U}\mathbf{x} = \begin{bmatrix} * & * & * & * \\ 0 & * & * & * \\ 0 & 0 & * & * \\ 0 & 0 & 0 & * \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}$$

This is solved by backward substitution ($x_4 = y_4/*$, etc.)

Summary: To solve (numerically) a system $\mathbf{Ax} = \mathbf{b}$:

- 1 Obtain, if possible, matrices \mathbf{L} and \mathbf{U} such that $\mathbf{A} = \mathbf{LU}$, where \mathbf{L} is a lower triangular and \mathbf{U} is an upper triangular matrix. Then $\mathbf{LUx} = \mathbf{b}$.
- 2 Assuming $\mathbf{y} = \mathbf{Ux}$, solve $\mathbf{Ly} = \mathbf{b}$ for \mathbf{y} using forward substitution.
- 3 Having obtained \mathbf{y} , solve $\mathbf{Ux} = \mathbf{y}$ for \mathbf{x} using backward substitution.

Another question is, how to obtain the required LU factorisation.

NB: Not every matrix has a LU factorisation; e.g. try $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
— but upon a row swap, it becomes factorable.

Gaussian reduction of a given square matrix

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

through row operations, brings it into echelon form like

$$\mathbf{A} \sim \begin{bmatrix} * & * & * & * \\ 0 & * & * & * \\ 0 & 0 & * & * \\ 0 & 0 & 0 & * \end{bmatrix}$$

which is actually an upper-triangular matrix.

This makes a link to LU factorisation — via elementary matrices.

Consider a general matrix

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

and the following examples of **elementary** matrices:

$$\tilde{\mathbf{E}}_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & k \end{bmatrix} \quad \tilde{\mathbf{E}}_{31} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ k & 0 & 1 \end{bmatrix} \quad \mathbf{P}_{12} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

The actions of these elementary matrices over \mathbf{A} are defined by matrix multiplications from the left:

$$\tilde{\mathbf{E}}_3 \mathbf{A} = \dots; \quad \tilde{\mathbf{E}}_{13} \mathbf{A} = \dots; \quad \mathbf{P}_{12} \mathbf{A} = \dots$$

The action of the elementary matrix $\tilde{\mathbf{E}}_3$ over \mathbf{A} is as follows:

$$\begin{aligned}\tilde{\mathbf{E}}_3 \mathbf{A} &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & k \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \\ &= \begin{bmatrix} 1 \cdot a_{11} + 0 \cdot a_{21} + 0 \cdot a_{31} & 1 \cdot a_{12} + 0 \cdot a_{22} + 0 \cdot a_{32} & 1 \cdot a_{13} + 0 \cdot a_{23} + 0 \cdot a_{33} \\ 0 \cdot a_{11} + 1 \cdot a_{21} + 0 \cdot a_{31} & 0 \cdot a_{12} + 1 \cdot a_{22} + 0 \cdot a_{32} & 0 \cdot a_{13} + 1 \cdot a_{23} + 0 \cdot a_{33} \\ 0 \cdot a_{11} + 0 \cdot a_{21} + k \cdot a_{31} & 0 \cdot a_{12} + 0 \cdot a_{22} + k \cdot a_{32} & 0 \cdot a_{13} + 0 \cdot a_{23} + k \cdot a_{33} \end{bmatrix} \\ &= \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ ka_{31} & ka_{32} & ka_{33} \end{bmatrix}\end{aligned}$$

This corresponds to an elementary row operation:

$$\tilde{\mathbf{E}}_3 \mathbf{A} \Leftrightarrow R_3 \rightarrow k \cdot R_3 \quad \text{multiply row by a factor}$$

The action of the elementary matrix $\tilde{\mathbf{E}}_{13}$ over \mathbf{A} is as follows:

$$\begin{aligned}\tilde{\mathbf{E}}_{31}\mathbf{A} &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ k & 0 & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \\ &= \begin{bmatrix} 1 \cdot a_{11} + 0 \cdot a_{21} + 0 \cdot a_{31} & 1 \cdot a_{12} + 0 \cdot a_{22} + 0 \cdot a_{32} & 1 \cdot a_{13} + 0 \cdot a_{23} + 0 \cdot a_{33} \\ 0 \cdot a_{11} + 1 \cdot a_{21} + 0 \cdot a_{31} & 0 \cdot a_{12} + 1 \cdot a_{22} + 0 \cdot a_{32} & 0 \cdot a_{13} + 1 \cdot a_{23} + 0 \cdot a_{33} \\ k \cdot a_{11} + 0 \cdot a_{21} + 1 \cdot a_{31} & k \cdot a_{12} + 0 \cdot a_{22} + 1 \cdot a_{32} & k \cdot a_{13} + 0 \cdot a_{23} + 1 \cdot a_{33} \end{bmatrix} \\ &= \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} + ka_{11} & a_{32} + ka_{12} & a_{33} + ka_{13} \end{bmatrix}\end{aligned}$$

This corresponds to an elementary row operation:

$$\tilde{\mathbf{E}}_{31}\mathbf{A} \quad \Leftrightarrow \quad R_3 \rightarrow (R_3 + k \cdot R_1) \quad \text{add a multiple of a row to another}$$

The action of the elementary matrix \mathbf{P}_3 over \mathbf{A} is as follows:

$$\begin{aligned}\mathbf{P}_{12}\mathbf{A} &= \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \\ &= \begin{bmatrix} 0 \cdot a_{11} + 1 \cdot a_{21} + 0 \cdot a_{31} & 0 \cdot a_{12} + 1 \cdot a_{22} + 0 \cdot a_{32} & 0 \cdot a_{13} + 1 \cdot a_{23} + 0 \cdot a_{33} \\ 1 \cdot a_{11} + 0 \cdot a_{21} + 0 \cdot a_{31} & 1 \cdot a_{12} + 0 \cdot a_{22} + 0 \cdot a_{32} & 1 \cdot a_{13} + 0 \cdot a_{23} + 0 \cdot a_{33} \\ 0 \cdot a_{11} + 0 \cdot a_{21} + 1 \cdot a_{31} & 0 \cdot a_{12} + 0 \cdot a_{22} + 1 \cdot a_{32} & 0 \cdot a_{13} + 0 \cdot a_{23} + 1 \cdot a_{33} \end{bmatrix} \\ &= \begin{bmatrix} a_{21} & a_{22} & a_{23} \\ a_{11} & a_{12} & a_{13} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}\end{aligned}$$

This corresponds to an elementary row operation:

$$\mathbf{P}_{12}\mathbf{A} \quad \Leftrightarrow \quad R_1 \leftrightarrow R_2 \quad \text{swap two rows}$$

Other examples:

$$\tilde{\mathbf{E}}_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & k & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \tilde{\mathbf{E}}_{21} = \begin{bmatrix} 1 & 0 & 0 \\ k & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \mathbf{P}_{23} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

Generally, elementary matrices are built from \mathbf{I} by modifications:

$$e_{ii} = k \quad \Leftrightarrow \quad \mathbf{R}_i \rightarrow k \cdot \mathbf{R}_i \quad \text{multiplies row } i \text{ by } k$$

$$e_{ij} = k \quad \Leftrightarrow \quad \mathbf{R}_i \rightarrow (\mathbf{R}_i + k \cdot \mathbf{R}_j) \quad \text{adds } k \times \text{row } j \text{ to row } i$$

$$\begin{cases} e_{ij} = e_{ji} = 1 \\ e_{ii} = e_{jj} = 0 \end{cases} \quad \Leftrightarrow \quad \mathbf{R}_i \leftrightarrow \mathbf{R}_j \quad \text{swaps rows } i \text{ and } j$$

Subsequent multiplication $\tilde{\mathbf{E}}_{(\text{step } m)} \cdots \tilde{\mathbf{E}}_{(\text{step } 2)} \tilde{\mathbf{E}}_{(\text{step } 1)} \mathbf{A}$ by a chain of appropriate elementary matrices brings \mathbf{A} to REF.

Example: row-reduce a fun matrix

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

- To eliminate $a_{21} = 4$ we use $\tilde{\mathbf{E}}_{21}|_{-4}$

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

- To eliminate $a_{31} = 7$ we use $\tilde{\mathbf{E}}_{31}|_{-7}$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -7 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 \\ 0 & -3 & -6 \\ 7 & 8 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 \\ 0 & -3 & -6 \\ 0 & -6 & -12 \end{bmatrix}$$

- To eliminate $a_{32} = -6$ we use $\tilde{\mathbf{E}}_{32}|_{-2}$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -2 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 \\ 0 & -3 & -6 \\ 0 & -6 & -12 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 \\ 0 & -3 & -6 \\ 0 & 0 & 0 \end{bmatrix}$$

These subsequent multiplications reduce \mathbf{A} into echelon form

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -2 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -7 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ -4 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\text{Elementary matrices}} \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix} =$$

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

whereas the product of elementary matrices is a low triangular matrix.

Regarding the last equation as $\mathbf{L}^{-1}\mathbf{A} = \mathbf{U}$

$$\text{where } \mathbf{L}^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ -4 & 1 & 0 \\ 1 & -2 & 1 \end{bmatrix} \quad \text{and so } \mathbf{L} = \begin{bmatrix} 1 & 0 & 0 \\ 4 & 1 & 0 \\ 7 & 2 & 1 \end{bmatrix}$$

this result provides a factorisation $\mathbf{A} = \mathbf{L}\mathbf{U}$.

- The row reduction above can be expressed in matrix form as

$$\tilde{\mathbf{E}}_{32} \tilde{\mathbf{E}}_{31} \tilde{\mathbf{E}}_{21} \mathbf{A} = \mathbf{U}$$

- This is equivalent to

$$\mathbf{A} = (\tilde{\mathbf{E}}_{32} \tilde{\mathbf{E}}_{31} \tilde{\mathbf{E}}_{21})^{-1} \mathbf{U} = \tilde{\mathbf{E}}_{21}^{-1} \tilde{\mathbf{E}}_{31}^{-1} \tilde{\mathbf{E}}_{32}^{-1} \mathbf{U} = \mathbf{L} \mathbf{U}$$

- So using a row-reduction algorithm, we have obtained

$$\mathbf{L} = \tilde{\mathbf{E}}_{21}^{-1} \tilde{\mathbf{E}}_{31}^{-1} \tilde{\mathbf{E}}_{32}^{-1}$$

$$\mathbf{U} = \tilde{\mathbf{E}}_{32} \tilde{\mathbf{E}}_{31} \tilde{\mathbf{E}}_{21} \mathbf{A}$$

- The point is that inverting elementary matrices is very easy.

Inverted matrices \mathbf{E}_{ij}^{-1} are very easy to construct.

Their actions just revert the original $\tilde{\mathbf{E}}_{ij}$ operation:

$$\tilde{\mathbf{E}}_{32}|_{-2} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -2 & 1 \end{bmatrix} \quad \tilde{\mathbf{E}}_{32}^{-1}|_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 2 & 1 \end{bmatrix}$$

$$\tilde{\mathbf{E}}_{31}|_{-7} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -7 & 0 & 1 \end{bmatrix} \quad \tilde{\mathbf{E}}_{31}^{-1}|_7 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 7 & 0 & 1 \end{bmatrix}$$

$$\tilde{\mathbf{E}}_{21}|_{-4} = \begin{bmatrix} 1 & 0 & 0 \\ -4 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \tilde{\mathbf{E}}_{21}^{-1}|_4 = \begin{bmatrix} 1 & 0 & 0 \\ 4 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

It is easy to check that $\tilde{\mathbf{E}}_{ij}|_k \tilde{\mathbf{E}}_{ij}^{-1}|_{-k} = \tilde{\mathbf{E}}_{ij}^{-1}|_{-k} \tilde{\mathbf{E}}_{ij}|_k = \mathbf{I}$.

If we also use row scaling, e.g.

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1/3 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 \\ 0 & -3 & -6 \\ 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 \\ 0 & 1 & 2 \\ 0 & 0 & 0 \end{bmatrix}$$

then the corresponding inverted matrix is also straightforward:

$$\tilde{\mathbf{E}}_{ii}^{-1} \Big|_{\frac{1}{k}} = \tilde{\mathbf{E}}_{ii} \Big|_k$$

$$\tilde{\mathbf{E}}_{22} \Big|_{-\frac{1}{3}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1/3 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \tilde{\mathbf{E}}_{22}^{-1} \Big|_{-3} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -3 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

- In general, row reduction process may require row swapping. This is done by permutation matrices.
- Permutation matrix \mathbf{P}_{ij} is constructed from identity matrix by swapping rows i and j :

$$\mathbf{P}_{12} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \mathbf{P}_{23} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \quad \mathbf{P}_{31} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

- An inverted permutation matrix equals to the original one:

$$\mathbf{P}_{ij}^{-1} = \mathbf{P}_{ji} = \mathbf{P}_{ij}$$

- Any elementary row operation on \mathbf{A} is represented by left-multiplication of \mathbf{A} by a suitable elementary matrix.
- Hence row reduction is a sequence of left-multiplications.
- Apart from row swaps, elementary matrices (and their inverses) are all lower triangular.
- Thus, row reduction is equivalent to $\mathbf{A} = \mathbf{LU}$ process.
- In case row swaps \mathbf{PA} are required, these are performed first; the same is required for the right-hand side: $\mathbf{b} \rightarrow \mathbf{Pb}$.
- So, in general, $\mathbf{PA} = \mathbf{LU}$ (which is the same as $\mathbf{A} = \mathbf{PLU}$).

To solve a system $\mathbf{Ax} = \mathbf{b}$ in the most general case:

- 1 Perform row swaps first (importantly, for both \mathbf{A} and \mathbf{b}):
 $\mathbf{PAx} = \mathbf{Pb}$
- 2 Factorise $\mathbf{PA} = \mathbf{LU}$, where \mathbf{L} is a lower triangular and \mathbf{U} is an upper triangular matrix. Then $\mathbf{LUx} = \mathbf{Pb}$.
- 3 Denoting $\mathbf{y} = \mathbf{Ux}$, solve $\mathbf{Ly} = \mathbf{Pb}$ for \mathbf{y} (with forward substitution).
- 4 Having obtained \mathbf{y} , solve $\mathbf{Ux} = \mathbf{y}$ for \mathbf{x} (with backward substitution).

The general strategy for row swaps is in arranging the largest numbers along the matrix diagonal, as much as possible.

There is no unique way of factorising a matrix into a product of upper and lower triangular matrices \mathbf{L} and \mathbf{U} . To get a unique factorisation, one can impose additional conditions.

- **Doolittle's** method implies that the diagonal elements of the lower triangular matrix \mathbf{L} are equal to 1.
- **Crout's** method, by contrast, requires that the diagonal elements of the upper triangular matrix \mathbf{U} are equal to 1.

We will now have a look at these two methods in more detail.

3×3 case:

Consider \mathbf{A} as a product of \mathbf{L} (lower triangular) and \mathbf{U} (upper triangular), with the diagonal elements of \mathbf{L} equal to 1:

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

To find the u_{ij} and l_{ij} we multiply the \mathbf{L} and \mathbf{U} matrices:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ l_{21}u_{11} & l_{21}u_{12} + u_{22} & l_{21}u_{13} + u_{23} \\ l_{31}u_{11} & l_{31}u_{12} + l_{32}u_{22} & l_{31}u_{13} + l_{32}u_{23} + u_{33} \end{bmatrix}$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ l_{21}u_{11} & l_{21}u_{12} + u_{22} & l_{21}u_{13} + u_{23} \\ l_{31}u_{11} & l_{31}u_{12} + l_{32}u_{22} & l_{31}u_{13} + l_{32}u_{23} + u_{33} \end{bmatrix}$$

This provides the following equations for the entries of \mathbf{L} and \mathbf{U} :

$$u_{11} = a_{11}, \quad u_{12} = a_{12}, \quad u_{13} = a_{13}$$

$$l_{21}u_{11} = a_{21} \quad \Rightarrow \quad l_{21} = a_{21}/u_{11}$$

$$l_{21}u_{12} + u_{22} = a_{22} \quad \Rightarrow \quad u_{22} = a_{22} - l_{21}u_{12}$$

$$l_{21}u_{13} + u_{23} = a_{23} \quad \Rightarrow \quad u_{23} = a_{23} - l_{21}u_{13}$$

$$l_{31}u_{11} = a_{31} \quad \Rightarrow \quad l_{31} = a_{31}/u_{11}$$

$$l_{31}u_{12} + l_{32}u_{22} = a_{32} \quad \Rightarrow \quad l_{32} = (a_{32} - l_{31}u_{12})/u_{22}$$

$$l_{31}u_{13} + l_{32}u_{23} + u_{33} = a_{33} \quad \Rightarrow \quad u_{33} = a_{33} - l_{31}u_{13} - l_{32}u_{23}$$

The extension of this method to $n \times n$ is straightforward:

Algorithm: For $k = 1, 2, \dots, n$:

- Diagonal elements of \mathbf{L} :

$$l_{kk} = 1$$

- k -th row of \mathbf{U} :

$$u_{kj} = a_{kj} - \sum_{m=1}^{k-1} l_{km} u_{mj}, \quad k \leq j \leq n$$

- k -th column of \mathbf{L} :

$$l_{ik} = \frac{1}{u_{kk}} \left(a_{ik} - \sum_{m=1}^{k-1} l_{im} u_{mk} \right), \quad k \leq i \leq n$$

Use Doolittle's **LU** factorisation to find the solution for system

$$\begin{array}{rcl} x_1 - 2x_2 + x_3 & = & 0 \\ 2x_2 - 8x_3 & = & 8 \\ -4x_1 + 5x_2 + 9x_3 & = & -9 \end{array} \quad \begin{bmatrix} 1 & -2 & 1 \\ 0 & 2 & -8 \\ -4 & 5 & 9 \end{bmatrix} \mathbf{x} = \begin{bmatrix} 0 \\ 8 \\ -9 \end{bmatrix}$$

$$u_{11} = a_{11} = 1, \quad u_{12} = a_{12} = -2, \quad u_{13} = a_{13} = 1,$$

$$l_{21} = a_{21}/u_{11} = 0, \quad l_{31} = a_{31}/u_{11} = -4,$$

$$u_{22} = a_{22} - l_{21}u_{12} = 2, \quad u_{23} = a_{23} - l_{21}u_{13} = -8,$$

$$l_{32} = (a_{32} - l_{31}u_{12})/u_{22} = -3/2,$$

$$u_{33} = a_{33} - l_{31}u_{13} - l_{32}u_{23} = 1$$

$$\mathbf{L} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -4 & -\frac{3}{2} & 1 \end{bmatrix} \quad \mathbf{U} = \begin{bmatrix} 1 & -2 & 1 \\ 0 & 2 & -8 \\ 0 & 0 & 1 \end{bmatrix}$$

So $\mathbf{A} = \mathbf{LU}$ with

$$\mathbf{L} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -4 & -\frac{3}{2} & 1 \end{bmatrix} \quad \mathbf{U} = \begin{bmatrix} 1 & -2 & 1 \\ 0 & 2 & -8 \\ 0 & 0 & 1 \end{bmatrix}$$

Now we can split $\mathbf{Ax} = \mathbf{b}$ into solving $\mathbf{Ly} = \mathbf{b}$ and then $\mathbf{Ux} = \mathbf{y}$.

The $\mathbf{Ly} = \mathbf{b}$ equation is

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -4 & -\frac{3}{2} & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 8 \\ -9 \end{bmatrix}$$

With forward substitution we obtain $y_1 = 0$, $y_2 = 8$, $y_3 = 3$

Now we use $\mathbf{U}\mathbf{x} = \mathbf{y}$ to find \mathbf{x} :

$$\begin{bmatrix} 1 & -2 & 1 \\ 0 & 2 & -8 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 8 \\ 3 \end{bmatrix}$$

With backward substitution we get $x_3 = 3$, $x_2 = 16$, $x_1 = 29$.

So the final solution is

$$\mathbf{x} = \begin{bmatrix} 29 \\ 16 \\ 3 \end{bmatrix}$$

3×3 case:

Consider \mathbf{A} as a product of \mathbf{L} (lower triangular) and \mathbf{U} (upper triangular) where the diagonal elements of \mathbf{U} are equal to 1:

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

To find the u_{ij} and l_{ij} we multiply the \mathbf{L} and \mathbf{U} matrices:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} l_{11} & l_{11}u_{12} & l_{11}u_{13} \\ l_{21} & l_{21}u_{12} + l_{22} & l_{21}u_{13} + l_{22}u_{23} \\ l_{31} & l_{31}u_{12} + l_{32} & l_{31}u_{13} + l_{32}u_{23} + l_{33} \end{bmatrix}$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} l_{11} & l_{11}u_{12} & l_{11}u_{13} \\ l_{21} & l_{21}u_{12} + l_{22} & l_{21}u_{13} + l_{22}u_{23} \\ l_{31} & l_{31}u_{12} + l_{32} & l_{31}u_{13} + l_{32}u_{23} + l_{33} \end{bmatrix}$$

This provides the following equations for the entries of \mathbf{L} and \mathbf{U} :

$$l_{11} = a_{11}, \quad l_{21} = a_{21}, \quad l_{31} = a_{31}$$

$$l_{11}u_{12} = a_{12} \quad \Rightarrow \quad u_{12} = a_{12}/l_{11}$$

$$l_{21}u_{12} + l_{22} = a_{22} \quad \Rightarrow \quad l_{22} = a_{22} - l_{21}u_{12}$$

$$l_{31}u_{12} + l_{32} = a_{32} \quad \Rightarrow \quad l_{32} = a_{32} - l_{31}u_{12}$$

$$l_{11}u_{13} = a_{13} \quad \Rightarrow \quad u_{13} = a_{13}/l_{11}$$

$$l_{21}u_{13} + l_{22}u_{23} = a_{23} \quad \Rightarrow \quad u_{23} = (a_{23} - l_{21}u_{13})/l_{22}$$

$$l_{31}u_{13} + l_{32}u_{23} + l_{33} = a_{33} \quad \Rightarrow \quad l_{33} = a_{33} - l_{31}u_{13} - l_{32}u_{23}$$

The extension of this method to an $n \times n$ is also straightforward:

Algorithm: Calculate the \mathbf{L} and \mathbf{U} matrix elements as

$$u_{ii} = 1 \qquad i = 1, 2, \dots, n$$

$$u_{ij} = \frac{1}{l_{ii}} \left(a_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj} \right) \qquad i < j = 2, 3, \dots, n.$$

$$l_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik} u_{kj} \qquad i \geq j = 1, 2, \dots, n$$

Decompose the following matrix using Crout's method:

$$\mathbf{A} = \begin{bmatrix} 2 & -1 & 1 \\ 4 & 3 & -1 \\ 3 & 2 & 2 \end{bmatrix}$$

$$l_{11} = a_{11} = 2, \quad l_{21} = a_{21} = 4, \quad l_{31} = a_{31} = 3$$

$$u_{12} = a_{12}/l_{11} = -\frac{1}{2} \quad u_{13} = a_{13}/l_{11} = \frac{1}{2}$$

$$l_{22} = a_{22} - l_{21}u_{12} = 5 \quad l_{32} = a_{32} - l_{31}u_{12} = \frac{7}{2}$$

$$u_{23} = \frac{a_{23} - l_{21}u_{13}}{l_{22}} = -\frac{3}{5} \quad l_{33} = a_{33} - l_{31}u_{13} - l_{32}u_{23} = \frac{13}{5}$$

$$\mathbf{A} = \begin{bmatrix} 2 & -1 & 1 \\ 4 & 3 & -1 \\ 3 & 2 & 2 \end{bmatrix} = \begin{bmatrix} 2 & 0 & 0 \\ 4 & 5 & 0 \\ 3 & 7/2 & 13/5 \end{bmatrix} \begin{bmatrix} 1 & -1/2 & 1/2 \\ 0 & 1 & -3/5 \\ 0 & 0 & 1 \end{bmatrix} = \mathbf{L}\mathbf{U}$$

Doolittle's and Crout's algorithms are reliable and easy to code.

However, for certain matrices, these algorithms still fail.

In such cases, it is necessary to swap some rows of the matrix and attempt an LU factorisation of the permuted matrix:

$$\mathbf{PA} = \mathbf{LU}$$

Reminder: once \mathbf{P} is established, the same row swap should be performed over (every) right-hand side: $\mathbf{b}_i \rightarrow \mathbf{P}\mathbf{b}_i$.

The general strategy for row swaps is in arranging the largest numbers along the matrix diagonal, as much as possible.

If \mathbf{A} is a square matrix which can be reduced to row echelon form without row swaps, then \mathbf{A} can be factorised uniquely as $\mathbf{A} = \mathbf{LDU}$, where \mathbf{L} is lower triangular, \mathbf{U} upper triangular, and \mathbf{D} is a strictly diagonal matrix.

This is called an LDU-factorisation of matrix \mathbf{A} :

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \begin{bmatrix} d_1 & 0 & 0 \\ 0 & d_2 & 0 \\ 0 & 0 & d_3 \end{bmatrix} \begin{bmatrix} 1 & u_{12} & u_{13} \\ 0 & 1 & u_{23} \\ 0 & 0 & 1 \end{bmatrix}$$

Multiplying the right two matrices gives the Doolittle's method; multiplying the left two matrices gives the Crout's method.

With swaps, the most general factorisation is: $\mathbf{A} = \mathbf{PLDU}$.

Quite often, a matrix is **symmetric**: $a_{ij} = a_{ji}$:

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{12} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \dots & \vdots \\ a_{1n} & a_{2n} & \dots & a_{nn} \end{bmatrix}$$

Symmetric matrices are equal to their own transpose: $\mathbf{A}^T = \mathbf{A}$.

So if there is an LU factorisation $\mathbf{A} = \mathbf{L}\mathbf{U}$ for a symmetric matrix, then $\mathbf{L}\mathbf{U} = (\mathbf{L}\mathbf{U})^T = \mathbf{U}^T\mathbf{L}^T$. Thus we have $\mathbf{L} = \mathbf{U}^T$.

Then we can decompose a symmetric matrix \mathbf{A} into the form $\mathbf{A} = \mathbf{U}^T\mathbf{U}$ where \mathbf{U} is an upper triangular matrix.

An efficient method for finding the LU factorisation of a symmetric *positive definite* matrix is due to Choleski.

Definition: A square matrix \mathbf{A} is **positive definite** if

$$\mathbf{x}^T \mathbf{A} \mathbf{x} > 0 \quad \forall \mathbf{x} \neq \mathbf{0}$$

Remark: A symmetric matrix is positive definite if and only if all its eigenvalues are positive.

Definition: A square $n \times n$ matrix \mathbf{A} is **diagonally dominant** if

$$|a_{ii}| > \sum_{j=1, j \neq i}^n |a_{ij}| \quad \forall i = 1, 2, \dots, n$$

Theorem: If \mathbf{A} is a diagonally dominant symmetric matrix, and if $a_{ii} > 0 \quad \forall i = 1, 2, \dots, n$, then \mathbf{A} is positive definite.

Note: This is a *sufficient*, but not *necessary* condition.

Obtaining Cholesky factorisation $\mathbf{A} = \mathbf{U}^T \mathbf{U}$ is straightforward:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{bmatrix} = \mathbf{U}^T \mathbf{U} = \begin{bmatrix} u_{11} & 0 & 0 \\ u_{12} & u_{22} & 0 \\ u_{13} & u_{23} & u_{33} \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$
$$= \begin{bmatrix} u_{11}^2 & u_{11}u_{12} & u_{11}u_{13} \\ u_{11}u_{12} & u_{12}^2 + u_{22}^2 & u_{12}u_{13} + u_{22}u_{23} \\ u_{11}u_{13} & u_{12}u_{13} + u_{22}u_{23} & u_{13}^2 + u_{23}^2 + u_{33}^2 \end{bmatrix}$$

From here, we easily find the elements of the \mathbf{U} matrix:

$$u_{11} = \sqrt{a_{11}}, \quad u_{12} = a_{12}/u_{11}, \quad u_{13} = a_{13}/u_{11},$$

$$u_{22} = \sqrt{a_{22} - u_{12}^2}, \quad u_{23} = \frac{a_{23} - u_{12}u_{13}}{u_{22}},$$

$$u_{33} = \sqrt{a_{33} - u_{13}^2 - u_{23}^2}.$$

The extension of $\mathbf{A} = \mathbf{U}^T \mathbf{U}$ factorisation to $n \times n$ is as follows:

$$u_{11} = \sqrt{a_{11}}$$

$$\text{For } j = 2, 3, \dots, n : \quad u_{1j} = \frac{a_{1j}}{u_{11}}$$

$$\text{For } i = 2, 3, \dots, n : \quad u_{ii} = \sqrt{a_{ii} - \sum_{k=1}^{i-1} u_{ki}^2}$$

$$\left\{ \begin{array}{l} \text{For } i = 2, 3, \dots, n \\ j = i + 1, i + 2, \dots, n \end{array} : \quad u_{ij} = \frac{1}{u_{ii}} \left(a_{ij} - \sum_{k=1}^{i-1} u_{ki} u_{kj} \right) \right.$$

$$\text{For } i > j : \quad u_{ij} = 0$$

Let us consider an example with symmetric $a_{ij} = a_{ji}$ matrix:

$$\begin{bmatrix} 1 & 2 & 3 \\ 2 & 5 & 10 \\ 3 & 10 & 26 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 10 \\ 26 \\ 55 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2 & 3 \\ 2 & 5 & 10 \\ 3 & 10 & 26 \end{bmatrix} = \mathbf{U}^T \mathbf{U} = \begin{bmatrix} u_{11}^2 & u_{11}u_{12} & u_{11}u_{13} \\ u_{11}u_{12} & u_{12}^2 + u_{22}^2 & u_{12}u_{13} + u_{22}u_{23} \\ u_{11}u_{13} & u_{12}u_{13} + u_{22}u_{23} & u_{13}^2 + u_{23}^2 + u_{33}^2 \end{bmatrix}$$

$$u_{11} = \sqrt{1} = 1, \quad u_{12} = 2/u_{11} = 2, \quad u_{13} = 3/u_{11} = 3,$$

$$u_{22} = \sqrt{5 - u_{12}^2} = 1, \quad u_{23} = (10 - u_{12}u_{13})/u_{22} = 4,$$

$$u_{33} = \sqrt{26 - u_{13}^2 - u_{23}^2} = 1.$$

The decomposed form $\mathbf{Ax} = \mathbf{U}^T \mathbf{Ux} = \mathbf{b}$ then reads

$$\begin{bmatrix} 1 & 2 & 3 \\ 2 & 5 & 10 \\ 3 & 10 & 26 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 3 & 4 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 \\ 0 & 1 & 4 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 10 \\ 26 \\ 55 \end{bmatrix}$$

We can then solve it as $\mathbf{Ux} = \mathbf{y}$ and $\mathbf{U}^T \mathbf{y} = \mathbf{b}$

$$\begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 3 & 4 & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 10 \\ 26 \\ 55 \end{bmatrix}$$

Thus $y_1 = 10$, $y_2 = 26 - 2y_1 = 6$, $y_3 = 55 - 3y_1 - 4y_2 = 1$:

$$\mathbf{y} = \begin{bmatrix} 10 \\ 6 \\ 1 \end{bmatrix}$$

Now we can solve $\mathbf{U}\mathbf{x} = \mathbf{y}$:

$$\begin{bmatrix} 1 & 2 & 3 \\ 0 & 1 & 4 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 10 \\ 6 \\ 1 \end{bmatrix}$$

Then $x_3 = 1$, $x_2 = 6 - 4x_3 = 2$, $x_1 = 10 - 3x_3 - 2x_2 = 3$ so

$$\mathbf{x} = \begin{bmatrix} 3 \\ 2 \\ 1 \end{bmatrix}$$

Check:

$$\mathbf{Ax} = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 5 & 10 \\ 3 & 10 & 26 \end{bmatrix} \begin{bmatrix} 3 \\ 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 10 \\ 26 \\ 55 \end{bmatrix} = \mathbf{b}$$

$\mathbf{A} = \mathbf{LU}$ with lower triangular \mathbf{L} and upper triangular \mathbf{U} matrices

This permits to solve $\mathbf{Ly} = \mathbf{b}$ then $\mathbf{Ux} = \mathbf{y}$ instead of $\mathbf{Ax} = \mathbf{b}$

- Row operations can be represented via elementary matrices
- Row reduction to EF is equivalent to LU factorisation
- There are efficient programming algorithms for LU:
 - *Doolittle*: diagonal elements of \mathbf{L} are all equal to 1
 - *Crout*: diagonal elements of \mathbf{U} are all equal to 1

(when these algorithms fail, retrying upon row swaps may help)

- *Cholesky*: symmetric positive definite matrix $\mathbf{A} = \mathbf{U}^T \mathbf{U}$
- Most generally, $\mathbf{A} = \mathbf{PLDU}$ (do not forget $\mathbf{b} \rightarrow \mathbf{Pb}$)

Mid-term class test (2 hours)

at the tutorials this week

covers the topics of the first five weeks