

Solving linear systems on an industrial scale

- Matrix inversion \mathbf{A}^{-1}
- Brief revision: Gaussian reduction
- Matrix $\mathbf{A} = \mathbf{LU}$ decomposition (factorisation)
- General decomposition $\mathbf{PA} = \mathbf{LU}$
- Connection between Gaussian reduction and \mathbf{LU} factorisation
 - Crout's method
 - Doolittle's method
 - Cholesky's method
- \mathbf{LDU} decomposition

Matrix inversion method

- A system of n equations with n unknowns

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n = b_1, \\ a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n = b_2, \\ \vdots \quad \quad \quad \vdots \quad \quad \quad \dots \quad \quad \quad \vdots \quad \quad \quad \vdots \\ a_{n1}x_1 + a_{n2}x_2 + \dots + a_{nn}x_n = b_n. \end{cases}$$

can be written in a matrix form

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \dots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}.$$

- So $\mathbf{Ax} = \mathbf{b}$ and therefore $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$ (if \mathbf{A} is invertible)
- Inversion is very slow for large matrices ($2n^3$ operations)

Revision: Gaussian reduction / elimination

Row operations that can be used:

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

With these operations, matrix is first reduced to echelon form (EF):

- All non-zero rows are above any rows of all zeroes.
- Each leading entry (first non-zero entry) of a row is in a column to the right of the leading entry of the row above it.
- All entries in a column below a leading entry are zeroes.

$$\begin{bmatrix} \blacksquare & * & * & * \\ 0 & \blacksquare & * & * \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} 0 & \blacksquare & * & * & * & * & * & * & * & * \\ 0 & 0 & 0 & \blacksquare & * & * & * & * & * & * \\ 0 & 0 & 0 & 0 & \blacksquare & * & * & * & * & * \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \blacksquare & * \end{bmatrix}$$

Revision: Gaussian reduction / elimination

The next step is to obtain a reduced echelon form (REF):

$$\begin{bmatrix} 1 & 0 & * & * \\ 0 & 1 & * & * \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} 0 & 1 & * & 0 & 0 & 0 & * & * & 0 & * \\ 0 & 0 & 0 & 1 & 0 & 0 & * & * & 0 & * \\ 0 & 0 & 0 & 0 & 1 & 0 & * & * & 0 & * \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & * \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & * \end{bmatrix}$$

REF matrix, in addition to EF form, has the properties

- The leading entry in each non-zero row is 1
- The leading 1 is the only non-zero entry in its column

An echelon form is not unique, however reduced echelon form is:

Theorem: Any matrix is row-equivalent to one and only one matrix in reduced echelon form.

Revision: Gaussian reduction / elimination

Reduction into EF and then REF is achieved via standard steps:

- 1 Select the leftmost non-zero entry for the first pivot.
If necessary, swap rows to move the first pivot to the first row.
- 2 Set the leftmost non-zero entry (in the upper row) as a pivot.
- 3 Add multiples of the pivot row to the rows below, to create zeros in all positions below the pivot.
- 4 Cover the row containing the pivot (and any rows above it).
Apply the same steps 2–4 to the remaining sub-matrix.
Repeat until there are no more non-zero rows to modify.
- 5 Beginning with the rightmost pivot and working upward and to the left, create zeroes above each pivot.
- 6 If a pivot is not 1, make it 1 by a row scaling operation.

Generally, it needs $2n^3/3$ operations (3 times faster than inversion).

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:

$$\mathbf{E}_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & k \end{bmatrix} \quad \mathbf{E}_2 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \mathbf{E}_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ k & 0 & 1 \end{bmatrix}$$

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

$$\mathbf{E}_1\mathbf{A} \quad \mathbf{E}_2\mathbf{A} \quad \mathbf{E}_3\mathbf{A}$$

Elementary matrices

The action of the elementary matrix \mathbf{E}_1 over \mathbf{A} is as follows:

$$\begin{aligned}\mathbf{E}_1 \mathbf{A} &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & k \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \\&= \begin{bmatrix} 1 \cdot a_{11} + 0 \cdot a_{21} + 0 \cdot a_{31} & 1 \cdot a_{12} + 0 \cdot a_{22} + 0 \cdot a_{32} & 1 \cdot a_{13} + 0 \cdot a_{23} + 0 \cdot a_{33} \\ 0 \cdot a_{11} + 1 \cdot a_{21} + 0 \cdot a_{31} & 0 \cdot a_{12} + 1 \cdot a_{22} + 0 \cdot a_{32} & 0 \cdot a_{13} + 1 \cdot a_{23} + 0 \cdot a_{33} \\ 0 \cdot a_{11} + 0 \cdot a_{21} + k \cdot a_{31} & 0 \cdot a_{12} + 0 \cdot a_{22} + k \cdot a_{32} & 0 \cdot a_{13} + 0 \cdot a_{23} + k \cdot a_{33} \end{bmatrix} \\&= \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ ka_{31} & ka_{32} & ka_{33} \end{bmatrix}\end{aligned}$$

This corresponds to an elementary row operation:

$$\mathbf{E}_1 \mathbf{A} \Leftrightarrow R_3 \rightarrow kR_3 \quad \text{multiply row by a factor}$$

Elementary matrices

The action of the elementary matrix \mathbf{E}_2 over \mathbf{A} is as follows:

$$\begin{aligned}\mathbf{E}_2\mathbf{A} &= \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \\ &= \begin{bmatrix} 0 \cdot a_{11} + 1 \cdot a_{21} + 0 \cdot a_{31} & 0 \cdot a_{12} + 1 \cdot a_{22} + 0 \cdot a_{32} & 0 \cdot a_{13} + 1 \cdot a_{23} + 0 \cdot a_{33} \\ 1 \cdot a_{11} + 0 \cdot a_{21} + 0 \cdot a_{31} & 1 \cdot a_{12} + 0 \cdot a_{22} + 0 \cdot a_{32} & 1 \cdot a_{13} + 0 \cdot a_{23} + 0 \cdot a_{33} \\ 0 \cdot a_{11} + 0 \cdot a_{21} + 1 \cdot a_{31} & 0 \cdot a_{12} + 0 \cdot a_{22} + 1 \cdot a_{32} & 0 \cdot a_{13} + 0 \cdot a_{23} + 1 \cdot a_{33} \end{bmatrix} \\ &= \begin{bmatrix} a_{21} & a_{22} & a_{23} \\ a_{11} & a_{12} & a_{13} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}\end{aligned}$$

This corresponds to an elementary row operation:

$$\mathbf{E}_2\mathbf{A} \Leftrightarrow R_1 \leftrightarrow R_2 \quad \text{swap two rows}$$

Elementary matrices

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

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

This corresponds to an elementary row operation:

$$\mathbf{E}_3\mathbf{A} \quad \Leftrightarrow \quad R_3 \rightarrow (R_3 + kR_1) \quad \text{add a multiple of a row to another}$$

Elementary matrices

Other examples:

$$\mathbf{E}_4 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & k & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \mathbf{E}_5 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \quad \mathbf{E}_6 = \begin{bmatrix} 1 & 0 & 0 \\ k & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

So, generally,

$$\begin{aligned} e_{ii} = k & \Leftrightarrow R_i \rightarrow kR_i && \text{multiplies row } i \text{ by } k \\ \begin{cases} e_{ij} = e_{ji} = 1 \\ e_{ii} = e_{jj} = 0 \end{cases} & \Leftrightarrow R_i \leftrightarrow R_j && \text{swaps rows } i \text{ and } j \\ e_{ij} = k & \Leftrightarrow R_i \rightarrow (R_i + kR_j) && \text{adds } k \text{ times row } j \text{ to row } i \end{aligned}$$

Subsequent multiplication (from the left) $\mathbf{E}_m \dots \mathbf{E}_2 \mathbf{E}_1 \mathbf{A}$ by a chain of appropriate elementary matrices eventually reduces \mathbf{A} into REF.

LU factorisation (decomposition)

- 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 $\mathbf{Ax}_i = \mathbf{b}_i$ to REF each time.
- **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).

LU factorisation

To solve the system $\mathbf{Ax} = \mathbf{b}$ we express $\mathbf{A} = \mathbf{LU}$ 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:

$$\begin{cases} \mathbf{Ly} = \mathbf{b} \\ \mathbf{Ux} = \mathbf{y} \end{cases}$$

however each of these is much quicker to solve.

LU factorisation

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

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

We find the solution by forward substitution.

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

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

We solve this system by backward substitution.

LU factorisation

Summary: To solve the 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 matrix 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.

The question now is, how to obtain the required LU factorisation.

Gaussian reduction and LU factorisation

Example: row-reduce a fun matrix $\mathbf{A} = \{1, 2, 3; 4, 5, 6; 7, 8, 9\}$

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

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

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

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

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

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

Gaussian reduction and LU factorisation

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

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

- Multiplication of such elementary matrices produces a low triangular matrix. Regarding the last equation as $\mathbf{L}^{-1}\mathbf{A} = \mathbf{U}$

$$\text{where } \mathbf{L}^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ -4 & 1 & 0 \\ -7 & -2 & 1 \end{bmatrix} \quad \text{and so } \mathbf{L} = \begin{bmatrix} 1 & 0 & 0 \\ 4 & 1 & 0 \\ 15 & 2 & 1 \end{bmatrix}$$

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

Gaussian reduction and LU factorisation

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

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

- This is equivalent to

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

- So with a single row-reduction algorithm, we have obtained

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

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

- The inverted elementary matrices however are very easy.

Gaussian reduction and LU factorisation

- Inverted matrices \mathbf{E}_{ij}^{-1} are very easy to construct.
Their actions just revert the original \mathbf{E}_{ij} operation:

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

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

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

- It's easy to see that $\mathbf{E}_{ij}|_k \mathbf{E}_{ij}^{-1}|_{-k} = \mathbf{E}_{ij}^{-1}|_{-k} \mathbf{E}_{ij}|_k = \mathbf{I}$ where \mathbf{I} is an identity matrix.

Gaussian reduction and LU factorisation

- 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:

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

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

Permutation (row swapping)

- In general, Gaussian 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 ; and of course $\mathbf{P}_{ij} = \mathbf{P}_{ji}$:

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

- Quite naturally, an inverted permutation matrix equals to the original matrix,

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

Gaussian reduction and LU factorisation

- Any elementary row operation on \mathbf{A} is represented by pre-multiplication of \mathbf{A} by a suitable elementary matrix.
- Hence Gaussian reduction is a sequence of pre-multiplications.
- Apart from row swaps, elementary matrices (and their inverses) are all lower triangular.
- Thus, Gaussian reduction is equivalent to $\mathbf{A} = \mathbf{LU}$ process.
- In case row swaps \mathbf{PA} are required, these are performed first.
- So in the most general case, $\mathbf{PA} = \mathbf{LU}$

LU factorisation methods

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

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

Crout's method

For Crout's method, we have the following theorem on the existence of the decomposition:

Theorem

If, for an $n \times n$ matrix \mathbf{A} , all the n sub-matrices

$$\Delta_k = \begin{pmatrix} a_{11} & \cdots & a_{1k} \\ \vdots & & \vdots \\ a_{k1} & \cdots & a_{kk} \end{pmatrix}, \quad 1 \leq k \leq n, \quad \text{are invertible,}$$

then there exists a lower triangular matrix $\mathbf{L} = \{l_{ij}\}$ and an upper triangular matrix $\mathbf{U} = \{u_{ij}\}$ with $u_{ii} = 1 \quad \forall i$, such that

$$\mathbf{A} = \mathbf{L}\mathbf{U}.$$

Moreover, this factorisation is unique.

Crout's method

3×3 case: We want to obtain **A** as a product of **L** (lower triangular) and **U** (upper triangular) where the diagonal elements of **U** are equal to 1:

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

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

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

Crout's method

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

This provides the following equations for the entries of **L** and **U**:

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

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

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

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

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

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

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

Crout's method

The extension of this method to an $n \times n$ matrix is straightforward.

Algorithm:

For $\mathbf{A} = \mathbf{LU}$ decomposition, matrix elements are determined by

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

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

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

Crout's method (example)

Decompose the following matrix using Crout's method:

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

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

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

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

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

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

Doolittle's method

3×3 case: We want to obtain **A** as a product of **L** (lower triangular) and **U** (upper triangular), now with the diagonal elements of **L** equal to 1:

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

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

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

Doolittle's method

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

This provides the following equations for the entries of **L** and **U**:

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

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

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

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

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

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

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

Doolittle's method

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

Algorithm: For $\mathbf{A} = \mathbf{LU}$ decomposition, matrix elements are

- For $i = 1, 2, \dots, n$: $l_{ii} = 1$ (diagonal of \mathbf{L});
- For $k = 1, 2, \dots, n$:
 - Diagonal elements of \mathbf{U} :

$$u_{kk} = a_{kk} - \sum_{m=1}^{k-1} l_{km} u_{mk}$$

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

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

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

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

Doolittle's method (example)

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

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

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

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

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

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

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

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

Doolittle's method (example)

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 $y_1 = 0$, $y_2 = 8$, $y_3 = 3$

Doolittle's method (example)

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

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

LU factorisation

- Both the Doolittle's and Crout's methods are easy to code and are quite reliable.
- However, for certain matrices, these algorithms can fail.
- In such cases, one can usually swap suitable rows of the matrix and obtain an **LU** decomposition of the permuted matrix:

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

(swapping rows is an elementary row operation, so this does not change the solution).

An easy criterion for **LU** decomposition

Definition: A square $(n \times n)$ matrix **A** is **diagonally dominant** if for each $i = 1, 2, \dots, n$

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

Theorem: If an $n \times n$ matrix **A** is diagonally dominant, then:

- **A** is non-singular (and therefore, is invertible);
- There exist $n \times n$ matrices **L** and **U** which are lower- and upper-triangular matrices respectively, satisfying **A** = **LU**.

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

Check these examples:

$$\begin{pmatrix} -5 & 3 & 1 \\ 2 & -9 & 4 \\ 3 & 2 & 6 \end{pmatrix} \quad \begin{pmatrix} 6 & 2 & -2 \\ 9 & 4 & -5 \\ 3 & 3 & -7 \end{pmatrix}$$

Choleski method (pre-requisites)

In many applications of linear algebra, matrices have certain special properties that help solving the associated problems.

For example, **sparse matrices**, in which most of the elements are equal to zero, can be treated by special methods.

Another common type of matrix is a **symmetric** matrix: $a_{ij} = a_{ji}$.

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

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

Choleski method (pre-requisites)

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

Definition: A square $(n \times n)$ matrix **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.

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

For a symmetric matrix, $\mathbf{A}^T = \mathbf{A}$, thus $\mathbf{LU} = (\mathbf{LU})^T = \mathbf{U}^T \mathbf{L}^T$.

This suggests that we can decompose **A** uniquely in the form $\mathbf{A} = \mathbf{U}^T \mathbf{U}$ where **U** is an upper triangular matrix.

Choleski method

Obtaining Cholesky decomposition is straightforward:

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

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

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

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

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

Choleski method

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

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

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

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

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

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

Choleski method (example)

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

$$\begin{bmatrix} 1 & 2 & 3 \\ 2 & 5 & 10 \\ 3 & 10 & 26 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 10 \\ 26 \\ 55 \end{bmatrix}$$

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

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

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

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

Choleski method (example)

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 $\mathbf{U}^T \mathbf{y} = \mathbf{b}$

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

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

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

Choleski method (example)

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: $x_3 = 1$, $x_2 = 6 - 4x_3 = 2$, $x_1 = 10 - 3x_3 - 2x_2 = 3$ and

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

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

LDU decomposition

- 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-decomposition 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 last two matrices leads to Doolittle's method; multiplying the first two matrices leads to Crout's method.

Next lecture

Friday 6 April

9:00

CB 06.03.022

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