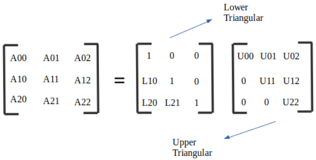
Algorithms and Data Structures

Matrix Decomposition
Gaussian Elimination (LU Decomposition)



Learning goals

- Gaussian elimination (LU decomposition)
- Properties of LU decomposition

GAUSSIAN ELIMINATION (LU DECOMPOSITION)

Aim: Solve LES of the form $\mathbf{Ax} = \boldsymbol{b}$

with $\mathbf{A} \in \mathbb{R}^{n \times n}$ **regular** (invertible), $\mathbf{x} \in \mathbb{R}^n$ and $\boldsymbol{b} \in \mathbb{R}^n$.

1. Calculate $\mathbf{A} = \mathbf{LU}$ (or $\mathbf{PA} = \mathbf{LU}$), where $\mathbf{L}$ is a normalized lower triangular matrix, $\mathbf{U}$ is an upper triangular matrix, and $\mathbf{P}$ is a permutation matrix.

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ l_{21} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ l_{n1} & \cdots & l_{n(n-1)} & 1 \end{pmatrix} \cdot \begin{pmatrix} u_{11} & \cdots & \cdots & u_{1n} \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & u_{nn} \end{pmatrix}$$

2. Solve $\mathbf{Ly} (= \mathbf{L}(\mathbf{Ux}) = \mathbf{Ax}) = \mathbf{b}$.
3. Solve $\mathbf{Ux} = \mathbf{y}$.

GAUSSIAN ELIMINATION (LU DECOMPOSITION) / 2

Let $\mathbf{Ax} = \boldsymbol{b}$ be a LES

$$\begin{pmatrix} 2 & 8 & 1 \\ 4 & 4 & -1 \\ -1 & 2 & 12 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 32 \\ 16 \\ 52 \end{pmatrix}$$

1. $\mathbf{A} = \mathbf{LU}$
   To convert **A** into an upper triangular matrix, we need 3 elementary transformations of type III:

$$\begin{pmatrix} 2 & 8 & 1 \\ 4 & 4 & -1 \\ -1 & 2 & 12 \end{pmatrix} \begin{matrix} \\ Z_2 - 2Z_1 \\ Z_3 + \frac{1}{2}Z_1 \end{matrix} \quad \rightarrow \quad \begin{pmatrix} 2 & 8 & 1 \\ 0 & -12 & -3 \\ 0 & 6 & \frac{25}{2} \end{pmatrix} \begin{matrix} \\ \\ Z_3 + \frac{1}{2}Z_2 \end{matrix}$$

$$\rightarrow \begin{pmatrix} 2 & 8 & 1 \\ 0 & -12 & -3 \\ 0 & 0 & 11 \end{pmatrix} = \mathbf{U}.$$

GAUSSIAN ELIMINATION (LU DECOMPOSITION) / 3

If we write these transformations in matrix notation, we obtain

$$\mathbf{T}_3\mathbf{T}_2\mathbf{T}_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & \frac{1}{2} & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \frac{1}{2} & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ -\frac{1}{2} & \frac{1}{2} & 1 \end{pmatrix}$$

Hence,

$$\mathbf{T}_3\mathbf{T}_2\mathbf{T}_1\mathbf{A} = \begin{pmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ -\frac{1}{2} & \frac{1}{2} & 1 \end{pmatrix} \begin{pmatrix} 2 & 8 & 1 \\ 4 & 4 & -1 \\ -1 & 2 & 12 \end{pmatrix} = \begin{pmatrix} 2 & 8 & 1 \\ 0 & -12 & -3 \\ 0 & 0 & 11 \end{pmatrix} = \mathbf{U}$$

and

$$\mathbf{A} = \mathbf{T}_1^{-1}\mathbf{T}_2^{-1}\mathbf{T}_3^{-1}\mathbf{U} = \mathbf{L}\mathbf{U}$$

with

$$\mathbf{L} = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -\frac{1}{2} & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -\frac{1}{2} & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -\frac{1}{2} & -\frac{1}{2} & 1 \end{pmatrix}.$$

GAUSSIAN ELIMINATION (LU DECOMPOSITION) / 4

General Theory:

The so-called *Frobenius matrix*

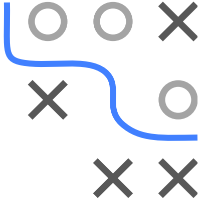
$$\mathbf{T}_k = \mathbf{I} - \mathbf{c}_k \mathbf{e}_k^\top$$

with

$$\mathbf{c}_k = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ \mu_{k+1} \\ \vdots \\ \mu_n \end{pmatrix}, \quad \mathbf{e}_k = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad \mathbf{T}_k = \begin{pmatrix} 1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & -\mu_{k+1} & 1 & \cdots & 0 \\ \vdots & \vdots & & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & -\mu_n & 0 & \cdots & 1 \end{pmatrix},$$

and $\mathbf{T}_k^{-1} = \mathbf{I} + \mathbf{c}_k \mathbf{e}_k^\top$.

GAUSSIAN ELIMINATION (LU DECOMPOSITION) / 5



Any type III row transformation that is required to eliminate the elements below the k-th pivot can be performed by multiplication with $\mathbf{T}_k$.

$$\mathbf{T}_k \mathbf{A}_{k-1} = (\mathbf{I} - \mathbf{c}_k \mathbf{e}_k^\top) \mathbf{A}_{k-1} = \mathbf{A}_{k-1} - \mathbf{c}_k \mathbf{e}_k^\top \mathbf{A}_{k-1}$$

We obtain the decomposition by

$$\mathbf{U} = \mathbf{T}_n \cdot \mathbf{T}_{n-1} \cdot \ldots \cdot \mathbf{T}_1 \cdot \mathbf{A}$$

and

$$\mathbf{L} = \mathbf{T}_1^{-1} \cdot \mathbf{T}_2^{-1} \cdot \ldots \cdot \mathbf{T}_n^{-1}$$

GAUSSIAN ELIMINATION (LU DECOMPOSITION) / 6

Example:

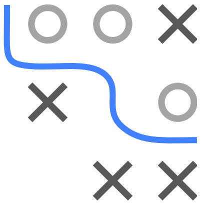
$$n = 4, \quad \mathbf{Ax} = \mathbf{b}, \quad \mathbf{A} = \begin{pmatrix} a_{11} & \cdots & a_{14} \\ \vdots & \ddots & \vdots \\ a_{41} & \cdots & a_{44} \end{pmatrix} = \mathbf{A}_0$$

Note: Multiplying by $\mathbf{T}_i$ changes the entries of the $(n-i)$ lower right block. To keep the notation readable we write a_{ij} even if the entry was modified by the multiplication. The entries that change in the respective step are highlighted in color.

Step 1:

$$\mathbf{T}_1\mathbf{A}_0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -a_{21}/a_{11} & 1 & 0 & 0 \\ -a_{31}/a_{11} & 0 & 1 & 0 \\ -a_{41}/a_{11} & 0 & 0 & 1 \end{pmatrix} \mathbf{A}_0 = \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ 0 & \color{red}{a_{22}} & \color{red}{a_{23}} & \color{red}{a_{24}} \\ 0 & \color{red}{a_{32}} & \color{red}{a_{33}} & \color{red}{a_{34}} \\ 0 & \color{red}{a_{42}} & \color{red}{a_{43}} & \color{red}{a_{44}} \end{pmatrix} = \mathbf{A}_1$$

GAUSSIAN ELIMINATION (LU DECOMPOSITION) / 7



Step 2:

$$\mathbf{T}_2\mathbf{A}_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -a_{32}/a_{22} & 1 & 0 \\ 0 & -a_{42}/a_{22} & 0 & 1 \end{pmatrix} \mathbf{A}_1 = \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ 0 & a_{22} & a_{23} & a_{24} \\ 0 & 0 & a_{33} & a_{34} \\ 0 & 0 & a_{43} & a_{44} \end{pmatrix} = \mathbf{A}_2$$

Step 3:

$$\mathbf{T}_3\mathbf{A}_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -a_{43}/a_{33} & 1 \end{pmatrix} \mathbf{A}_2 = \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ 0 & a_{22} & a_{23} & a_{24} \\ 0 & 0 & a_{33} & a_{34} \\ 0 & 0 & 0 & a_{44} \end{pmatrix} = \mathbf{U}$$

GAUSSIAN ELIMINATION (LU DECOMPOSITION) / 8

Effort in step k (in multiplications):

- $(n-k)^2$ multiplications for calculation of $\mathbf{T}_k \mathbf{A}_{k-1}$
- $(n-k)$ multiplications for $\mathbf{T}_k^{-1} \cdot \underbrace{\mathbf{T}_{k-1}^{-1} \cdot \ldots \cdot \mathbf{T}_1^{-1}}_{\text{already calculated}}$

The total effort is therefore

$$
\begin{aligned}
& \sum_{k=1}^{n} (n-k)^2 + (n-k) = \sum_{k=1}^{n} n^2 - 2nk + k^2 + n - k \\
= \quad & n^3 - 2n\frac{(n+1)n}{2} + \frac{n(n+1)(2n+1)}{6} + n^2 - \frac{n(n+1)}{2} \\
= \quad & n \cdot \left(n^2 - n^2 - n + \frac{1}{3}n^2 + \frac{1}{2}n + \frac{1}{6} + n - \frac{1}{2}n - \frac{1}{2} \right) \\
\approx \quad & \frac{1}{3}n^3 + \mathcal{O}(n).
\end{aligned}
$$

GAUSSIAN ELIMINATION (LU DECOMPOSITION) / 9

Problem: This only works if all $a_{kk} \neq 0$!

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

$\mathbf{P}$ is a permutation matrix which contains the required line switching transformations of the algorithm.

Switching lines to obtain a more stable algorithm.

Example:

$$\mathbf{A}_1 = \begin{pmatrix} 1 & 2 & -1 & 0 \\ 0 & 0 & 1/2 & 1 \\ 0 & 2 & -1/2 & 3/2 \\ 0 & -3 & 5/2 & 0 \end{pmatrix} \quad \mathbf{P}_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

$$\mathbf{P}_2\mathbf{A}_1 = \begin{pmatrix} 1 & 2 & -1 & 0 \\ 0 & -3 & 5/2 & 0 \\ 0 & 2 & -1/2 & 3/2 \\ 0 & 0 & 1/2 & 1 \end{pmatrix},$$

then $\mathbf{T}_2\mathbf{P}_2\mathbf{A}_1$ etc.

GAUSSIAN ELIMINATION (LU DECOMPOSITION) / 10

Calculation in general

$$\mathbf{A}_k = \mathbf{T}_k \mathbf{P}_k \mathbf{A}_{k-1}$$

It can be shown

$$\mathbf{T}_{k-1}\mathbf{P}_{k-1} \cdot \ldots \cdot \mathbf{T}_1\mathbf{P}_1 = \underbrace{\mathbf{T}_{k-1} \cdot \ldots \cdot \mathbf{T}_1}_{\mathbf{T}} \cdot \underbrace{\mathbf{P}_{k-1} \cdot \ldots \cdot \mathbf{P}_1}_{\mathbf{P}}$$

and thus

$$\mathbf{TPA} = \mathbf{U} \quad \text{and} \quad \mathbf{T}^{-1} = \mathbf{L}.$$

Note: When solving the linear system $\mathbf{Ax} = \mathbf{b}$ the vector $\mathbf{b}$ must also be permuted by $\mathbf{P}$.

GAUSSIAN ELIMINATION (LU DECOMPOSITION)

/ 11

2. Solve $\mathbf{L}\mathbf{y} = \mathbf{L}(\mathbf{U}\mathbf{x}) = \mathbf{A}\mathbf{x} = \mathbf{b}$

$$\begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ l_{21} & 1 & 0 & \cdots & 0 \\ l_{31} & l_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & l_{n3} & \cdots & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{pmatrix}$$

by using **forward substitution**

$$y_1 = b_1 \quad \text{and} \quad y_k = b_k - \sum_{i=1}^{k-1} l_{ki} y_i \quad \text{for} \quad k = 2, \ldots, n.$$

for our example the result is

$$\begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -\frac{1}{2} & -\frac{1}{2} & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} 32 \\ 16 \\ 52 \end{pmatrix} \Rightarrow \mathbf{y} = \begin{pmatrix} 32 \\ -48 \\ 44 \end{pmatrix}$$

GAUSSIAN ELIMINATION (LU DECOMPOSITION)

3. Solve $\mathbf{U}\mathbf{x} = \mathbf{y}$

Since **y** is now known from step 2

$$\begin{pmatrix} u_{11} & \cdots & \cdots & u_{1n} \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & u_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{pmatrix}$$

we can calculate **x** using **back substitution**:

$$x_i = \frac{1}{u_{ii}} \left(y_i - \sum_{k=i+1}^{n} u_{ik} x_k \right) \quad \text{for} \quad i = n-1, n-2, \ldots, 1.$$

For our example the solution to the LES is:

$$\begin{pmatrix} 2 & 8 & 1 \\ 0 & -12 & -3 \\ 0 & 0 & 11 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 32 \\ -48 \\ 44 \end{pmatrix} \Rightarrow \mathbf{x} = \begin{pmatrix} 2 \\ 3 \\ 4 \end{pmatrix}$$

GAUSSIAN ELIMINATION (LU DECOMPOSITION) / 13

Effort of **forward substitution**:

In step k, $k-1$ multiplications are performed. If only multiplications are taken into consideration, the resulting effort is

$$\sum_{k=2}^{n}(k-1) = \sum_{k=1}^{n-1} k = \frac{(n-1)n}{2} = \frac{1}{2}n^2 - \frac{n}{2}$$

Effort of **back substitution**:

Similar to forward substitution, the required effort is

$$\frac{1}{2}n^2 + \frac{n}{2}$$

PROPERTIES OF LU DECOMPOSITION

- "Interpretation" of the Gaussian elimination as matrix decomposition
- Numerically stable during pivoting
- **Existence:** For each **regular** matrix **A** there is a permutation matrix **P**, a normalized lower triangle matrix $\mathbf{L} \in \mathbb{R}^{n \times n}$ and a normalized upper triangular matrix $\mathbf{U} \in \mathbb{R}^{n \times n}$ such that

$$\mathbf{P} \cdot \mathbf{A} = \mathbf{L} \cdot \mathbf{U}$$

- Runtime behavior:
  - Decomposition of the matrix: $\frac{n^3}{3} + \mathcal{O}(n)$ multiplications.
  - Forward and back substitution: n^2