

Direct Methods for Solving Systems of Linear Equations

NTNU

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Solve linear systems of equations

$$\left\{ \begin{array}{l} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1 \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = b_2 \\ \vdots \\ a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = b_n \end{array} \right.$$

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Rewrite in the matrix form

$$Ax = b, \tag{1}$$

where

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

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➡ Provided that all $a_{ii} \neq 0$, then

$$x = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix}^T = \begin{bmatrix} b_1/a_{11} & b_2/a_{22} & \cdots & b_n/a_{nn} \end{bmatrix}^T .$$

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➡ If $a_{ii} = 0$ and $b_i = 0$ for some index i , then x_i can be any real number.

➡ If $a_{ii} = 0$ but $b_i \neq 0$, no solution of the system exists.

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When a linear system $Lx = b$ is **lower triangular** of the form

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Hence the forward substitution algorithm is an $O(n^2)$ algorithm.

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$$\begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ 0 & u_{22} & \cdots & u_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & u_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

provided that all $u_{ii} \neq 0$. The solution x_i are computed in a reversed order by

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Back substitution requires $n^2 + O(n)$ flops.

2 – Gaussian Elimination and LU Factorization

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The solution to the original problem $Ax = LUx = b$ is then found by a two-step triangular solve process:

$$Ly = b, \quad Ux = y. \quad (2)$$

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3. Add to an equation a multiple of some other equation (add to a row a multiple of some other row):

$$\mathcal{E}_i \leftarrow \mathcal{E}_i + \lambda \mathcal{E}_j.$$

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The matrix $A^{(k)}$ has the following form:

$$A^{(k)} = \left[\begin{array}{ccc|ccc} a_{11}^{(k)} & \cdots & a_{1,k-1}^{(k)} & a_{1k}^{(k)} & \cdots & a_{1j}^{(k)} & \cdots & a_{1n}^{(k)} \\ \vdots & \ddots & \vdots & \vdots & & \vdots & & \vdots \\ 0 & \cdots & a_{k-1,k-1}^{(k)} & a_{k-1,k}^{(k)} & \cdots & a_{k-1,j}^{(k)} & \cdots & a_{k-1,n}^{(k)} \\ \hline 0 & \cdots & 0 & a_{kk}^{(k)} & \cdots & a_{kj}^{(k)} & \cdots & a_{kn}^{(k)} \\ \hline \vdots & & \vdots & \vdots & & \vdots & & \vdots \\ 0 & \cdots & 0 & a_{ik}^{(k)} & \cdots & a_{ij}^{(k)} & \cdots & a_{in}^{(k)} \\ \vdots & & \vdots & \vdots & & \vdots & & \vdots \\ 0 & \cdots & 0 & a_{nk}^{(k)} & \cdots & a_{nj}^{(k)} & \cdots & a_{nn}^{(k)} \end{array} \right]$$

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Let $L = [l_{ik}]$ with

$$l_{ik} = \begin{cases} 0, & \text{if } i < k; \\ 1, & \text{if } i = k; \\ \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}}, & \text{if } i > k, \end{cases} \quad (5)$$

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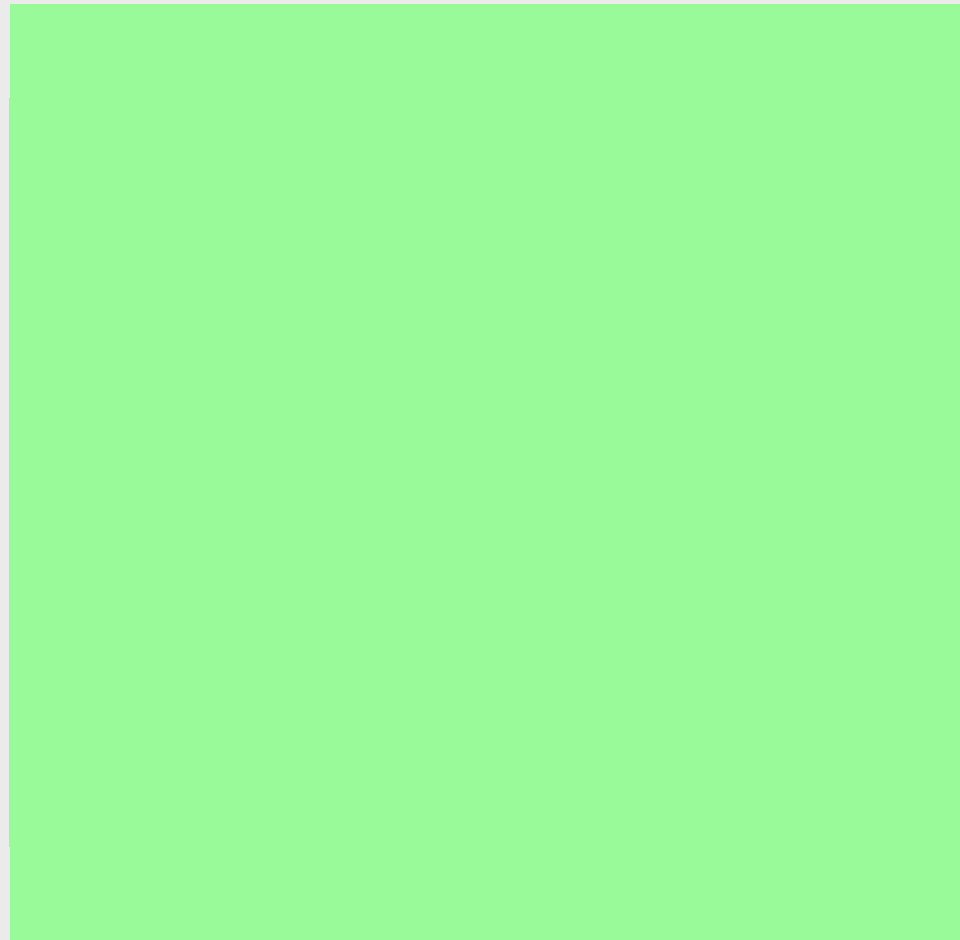
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and $U = A^{(n)}$, then L is **unit lower triangular**, U is **upper triangular**, and later we shall show that $A = LU$.



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Example 1 *Solve system of linear equations.*

$$\begin{bmatrix} 6 & -2 & 2 & 4 \\ 12 & -8 & 6 & 10 \\ 3 & -13 & 9 & 3 \\ -6 & 4 & 1 & -18 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 12 \\ 34 \\ 27 \\ -38 \end{bmatrix}$$

Solution:

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Solution:

1st step Use 6 as pivot element, the first row as pivot row, and multipliers 2, $\frac{1}{2}$, -1 are produced to reduce the system to

$$\begin{bmatrix} 6 & -2 & 2 & 4 \\ 0 & -4 & 2 & 2 \\ 0 & -12 & 8 & 1 \\ 0 & 2 & 3 & -14 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 12 \\ 10 \\ 21 \\ -26 \end{bmatrix}$$

2^{nd} **step** Use -4 as pivot element, the second row as pivot row, and multipliers 3 , $-\frac{1}{2}$ are computed to reduce the system to

$$\begin{bmatrix} 6 & -2 & 2 & 4 \\ 0 & -4 & 2 & 2 \\ 0 & 0 & 2 & -5 \\ 0 & 0 & 4 & -13 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 12 \\ 10 \\ -9 \\ -21 \end{bmatrix}$$

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3^{rd} **step** Use 2 as pivot element, the third row as pivot row, and multipliers 2 is found to reduce the system to

$$\begin{bmatrix} 6 & -2 & 2 & 4 \\ 0 & -4 & 2 & 2 \\ 0 & 0 & 2 & -5 \\ 0 & 0 & 0 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 12 \\ 10 \\ -9 \\ -3 \end{bmatrix}$$

Collect all the multipliers and let

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ \frac{1}{2} & 3 & 1 & 0 \\ -1 & -\frac{1}{2} & 2 & 1 \end{bmatrix} \quad \text{and} \quad U = \begin{bmatrix} 6 & -2 & 2 & 4 \\ 0 & -4 & 2 & 2 \\ 0 & 0 & 2 & -5 \\ 0 & 0 & 0 & -3 \end{bmatrix},$$

then one can verify that $LU = A$. ■

2.2 – Gaussian Transformation and LU Factorization

For a given vector $v \in \mathbb{R}^n$ with $v_k \neq 0$ for some $1 \leq k \leq n$, let

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and

$$M_k = I - l_k e_k^T = \begin{bmatrix} 1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & & \vdots \\ 0 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & \cdots & -l_{k+1,k} & 1 & \cdots & 0 \\ \vdots & & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & -l_{n,k} & 0 & \cdots & 1 \end{bmatrix}.$$

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$$M_k^{-1} = (I - l_k e_k^T)^{-1} = I + l_k e_k^T = \begin{bmatrix} 1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & \cdots & l_{k+1,k} & 1 & \cdots & 0 \\ \vdots & & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & l_{n,k} & 0 & \cdots & 1 \end{bmatrix}.$$

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$$a_{ij}^{(2)} = \begin{cases} a_{ij}^{(1)}, & \text{for } i = 1 \text{ and } j = 1, \dots, n; \\ a_{ij}^{(1)} - l_{i1} \times a_{1j}^{(1)}, & \text{for } i = 2, \dots, n \text{ and } j = 2, \dots, n. \end{cases}$$

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 \vdots & \vdots & \ddots & \vdots & \vdots & & \vdots \\
 0 & 0 & \cdots & a_{k-1,k-1}^{(k)} & a_{k-1,k}^{(k)} & \cdots & a_{k-1,n}^{(k)} \\
 \hline
 0 & 0 & \cdots & 0 & a_{kk}^{(k)} & \cdots & a_{kn}^{(k)} \\
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If the pivot $a_{kk}^{(k)} \neq 0$, then the multipliers

$$\ell_{ik} = \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}}, \quad i = k + 1, \dots, n,$$

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$$M_k = I - l_k e_k^T, \quad \text{where } l_k = \begin{bmatrix} 0 & \cdots & 0 & l_{k+1,k} & \cdots & l_{nk} \end{bmatrix},$$

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in which

$$a_{ij}^{(k+1)} = \begin{cases} a_{ij}^{(k)}, & \text{for } i = 1, \dots, k, j = 1, \dots, n; \\ 0, & \text{for } i = k + 1, \dots, n, j = k; \\ a_{ij}^{(k)} - \ell_{ik} a_{kj}^{(k)}, & \text{for } i = k + 1, \dots, n, j = k + 1, \dots, n. \end{cases}$$

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Upon the completion,

$$U \equiv A^{(n)} = M_{n-1} \cdots M_2 M_1 A$$

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$$\begin{aligned} L \equiv M_1^{-1} M_2^{-1} \cdots M_{n-1}^{-1} &= (I - l_1 e_1^T)^{-1} (I - l_2 e_2^T)^{-1} \cdots (I - l_{n-1} e_{n-1}^T)^{-1} \\ &= (I + l_1 e_1^T) (I + l_2 e_2^T) \cdots (I + l_{n-1} e_{n-1}^T) \\ &= I + l_1 e_1^T + l_2 e_2^T + \cdots + l_{n-1} e_{n-1}^T \\ &= \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ l_{21} & 1 & 0 & \cdots & 0 \\ l_{31} & l_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & l_{n3} & \cdots & 1 \end{bmatrix} \end{aligned}$$

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is **unit lower triangular**. This matrix factorization is called the ***LU*-factorization** of A .

Algorithm 4 (*LU* Factorization) Given a *nonsingular square* matrix $A \in \mathbb{R}^{n \times n}$, this algorithm computes a *unit lower triangular* matrix L and an *upper triangular* matrix U such that $A = LU$. The matrix A is overwritten by L and U .



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This algorithm requires

$$\sum_{k=1}^{n-1} \sum_{i=k+1}^n 2(n-k) = \frac{2}{3}n^3 - \frac{1}{2}n^2 + \frac{1}{3}n \text{ flops.}$$

2.3 – Existence and Uniqueness of LU Factorization

Definition 1 (Leading principal minor) Let A be an $n \times n$ matrix. The *upper left* $k \times k$ submatrix, denoted as

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

is called the *leading* $k \times k$ *principal submatrix*, and the determinant of A_k , $\det(A_k)$, is called the *leading principal minor*.

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- (ii) Assume that the leading principal submatrices A_1, \dots, A_k are nonsingular and A_k has an LU-factorization $A_k = L_k U_k$, where L_k is unit lower triangular and U_k is upper triangular.
- (iii) Show that there exist an unit lower triangular matrix L_{k+1} and an upper triangular matrix U_{k+1} such that $A_{k+1} = L_{k+1} U_{k+1}$.

Write

$$A_{k+1} = \begin{bmatrix} A_k & v_k \\ w_k^T & a_{k+1,k+1} \end{bmatrix},$$

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$$L_{k+1} = \begin{bmatrix} L_k & 0 \\ z_k^T & 1 \end{bmatrix} \quad \text{and} \quad U_{k+1} = \begin{bmatrix} U_k & y_k \\ 0 & a_{k+1,k+1} - z_k^T y_k \end{bmatrix}.$$

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 L_{k+1}U_{k+1} &= \begin{bmatrix} L_k U_k & L_k y_k \\ z_k^T U_k & z_k^T y_k + a_{k+1,k+1} - z_k^T y_k \end{bmatrix} \\
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This proves the theorem. ■

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3 – Pivoting

3.1 – The Need for Pivoting

Example. The algorithm would fail at the first step on

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

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since the first pivot element is zero. But if we interchange the rows, the system

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

becomes trivial to solve.

Example. The simple Gaussian elimination algorithm would produce relatively large error on the system

$$\begin{bmatrix} \varepsilon & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix},$$

where $\varepsilon < \varepsilon_M$.

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since in the computer, if ε is small enough, $1 - \frac{1}{\varepsilon}$ and $2 - \frac{1}{\varepsilon}$ will be computed to be the same as $-\frac{1}{\varepsilon}$.

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$$\begin{bmatrix} \varepsilon & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \neq \begin{bmatrix} 1 \\ 2 \end{bmatrix}.$$

But actually $x_1 = x_2 = 1$ would be a much better solution since

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The strategy of interchange rows/columns as described above is called “[pivoting](#)”.

3.2 – Partial Pivoting and Complete Pivoting

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Roundoff introduced in computing

$$a_{ij}^{(k+1)} = a_{ij}^{(k)} - l_{ik}a_{kj}^{(k)}, \quad i = k + 1, \dots, n, \quad j = k + 1, \dots, n,$$

will be **large**.

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To ensure that no large entries appear in the computed triangular factors, one can choose a pivot element to be the **largest** entry among $|a_{kk}^{(k)}|, \dots, |a_{nk}^{(k)}|$.

Let P_1, \dots, P_{k-1} be the **permutations** chosen and M_1, \dots, M_{k-1} denote the **Gaussian transformations** performed in the first $k - 1$ steps.

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$$|(P_k M_{k-1} \cdots M_1 P_1 A)_{kk}| = \max_{k \leq i \leq n} |(M_{k-1} \cdots M_1 P_1 A)_{ik}|.$$

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therefore,

$$P_{n-1} \cdots P_1 A = (M_{n-1} P_{n-1} \cdots M_2 P_2 M_1 P_2 \cdots P_{n-1})^{-1} U.$$

In summary, Gaussian elimination with partial pivoting leads to the LU factorization

$$PA = LU, \quad (7)$$

where

$$P = P_{n-1} \cdots P_1$$

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$$\begin{aligned} L &\equiv (M_{n-1}P_{n-1} \cdots M_2P_2M_1P_2 \cdots P_{n-1})^{-1} \\ &= P_{n-1} \cdots P_2M_1^{-1}P_2M_2^{-1} \cdots P_{n-1}M_{n-1}^{-1}. \end{aligned}$$

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Since, for $i < j$,

$$\begin{aligned} e_i^T P_j &= e_i^T, \quad e_i^T l_j = 0, \\ P_j l_i &= \begin{bmatrix} 0 & \cdots & 0 & \tilde{l}_{i+1,i} & \cdots & \tilde{l}_{n,i} \end{bmatrix}^T \equiv \tilde{l}_i, \end{aligned}$$

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$$P_2M_1^{-1}P_2 = P_2(I + l_1e_1^T)P_2 = I + \tilde{l}_1e_1^T$$

⇒

$$P_2 M_1^{-1} P_2 M_2^{-1} = (I + \tilde{\ell}_1 e_1^T)(I + \ell_2 e_2^T) = I + \tilde{\ell}_1 e_1^T + \ell_2 e_2^T,$$

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$$P_3 (P_2 M_1^{-1} P_2 M_2^{-1}) P_3 = I + \hat{\ell}_1 e_1^T + \tilde{\ell}_2 e_2^T$$

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Therefore, L is unit lower triangular.

⇒

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Algorithm 5 [*LU-factorization with Partial Pivoting*] Given a nonsingular square matrix $A \in \mathbb{R}^{n \times n}$, this algorithm finds an appropriate permutation matrix P ,

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Algorithm 5 [*LU-factorization with Partial Pivoting*] Given a nonsingular square matrix $A \in \mathbb{R}^{n \times n}$, this algorithm finds an appropriate permutation matrix P , and computes a unit lower triangular matrix L

\Rightarrow

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Algorithm 5 [*LU-factorization with Partial Pivoting*] Given a nonsingular square matrix $A \in \mathbb{R}^{n \times n}$, this algorithm finds an appropriate permutation matrix P , and computes a unit lower triangular matrix L and an upper triangular matrix U

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Algorithm 5 [*LU-factorization with Partial Pivoting*] Given a nonsingular square matrix $A \in \mathbb{R}^{n \times n}$, this algorithm finds an appropriate permutation matrix P , and computes a unit lower triangular matrix L and an upper triangular matrix U such that $PA = LU$. The matrix A is overwritten by L and U ,

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For $k = 1, \dots, n - 1$

End For

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Since the **Gaussian elimination with partial pivoting** produces the factorization (7), the linear system problem should comply accordingly

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where P, Q are **permutation** matrices, L is **unit lower triangular**, and U is **upper triangular**.

4 – Some Special Linear Systems

4.1 – Symmetric Positive Definite System and Cholesky Factorization

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Lemma 1 If $A \in \mathbb{R}^{n \times n}$ is **positive definite**, then A is **nonsingular** and $a_{ii} > 0$ for $i = 1, \dots, n$.

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Proof: Suppose A is singular.

$\Rightarrow \exists x \in \mathbb{R}^n$ and $x \neq 0$ such that $Ax = 0$.

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Lemma 1 If $A \in \mathbb{R}^{n \times n}$ is **positive definite**, then A is **nonsingular** and $a_{ii} > 0$ for $i = 1, \dots, n$.

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$$a_{kk} = \sum_{j=1}^k g_{kj}^2,$$

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hence the k -th column of G can be computed by

$$g_{ik} = \left(a_{ik} - \sum_{j=1}^{k-1} g_{ij}g_{kj} \right) / g_{kk}, \quad i = k + 1, \dots, n. \quad (11)$$

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In addition to n square root operations, there are approximately

$$\sum_{k=1}^n [2k - 1 + 2k(n - k)] = \frac{1}{3}n^3 + n^2 - \frac{1}{3}n$$

floating-point arithmetic required by the algorithm.

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$$\sum_{j=1}^n a_{kj} x_j = 0 \implies a_{kk} x_k = - \sum_{j=1, j \neq k}^n a_{kj} x_j \implies |a_{kk}| |x_k| \leq \sum_{j=1, j \neq k}^n |a_{kj}| |x_j|,$$

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

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Thus $A^{(2)}$ is still diagonally dominant. Since the subsequent steps of Gaussian elimination mimic the first, except for being applied to submatrices of smaller size, it suffices to conclude that Gaussian elimination without pivoting preserves the diagonal dominance of a matrix. ■

4.3 – Tridiagonal System

A square matrix $A = [a_{ij}]$ is said to be **tridiagonal** if

$$A = \begin{bmatrix} a_{11} & a_{12} & & & \\ a_{21} & a_{22} & \ddots & & \\ & \ddots & \ddots & & \\ & & & a_{n-1,n} & \\ & & a_{n,n-1} & a_{n,n} & \end{bmatrix} .$$

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If Gaussian elimination can be applied safely without pivoting. Then L and U factors would have the form

$$L = \begin{bmatrix} 1 & & & & \\ l_{21} & 1 & & & \\ & \ddots & \ddots & & \\ & & & l_{n,n-1} & 1 \end{bmatrix} \quad \text{and} \quad U = \begin{bmatrix} u_{11} & u_{12} & & & \\ & u_{22} & \ddots & & \\ & & \ddots & & \\ & & & u_{n-1,n} & \\ & & & & u_{nn} \end{bmatrix},$$

and the entries are computed by the simple algorithm which only costs $3n$ flops.

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End For

A tridiagonal linear system arises in many applications, such as finite difference discretization to second order linear boundary-value problem and the cubic spline approximations.

4.4 – General Banded Systems

In many applications that involve linear systems, the coefficient matrix is banded. Formally, we say that $A = [a_{ij}]$ has upper bandwidth q if $a_{ij} = 0$ whenever $j > i + q$ and lower bandwidth p if $a_{ij} = 0$ whenever $i > j + p$. Substantial economies can be realized when solving banded systems because the triangular factors in the LU factorization are also banded.

5 – Perturbation Analysis

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Definition 3 Let \hat{x} be the **computed** solution to the linear system of equations $Ax = b$. Then the vector

$$r = b - A\hat{x}$$

is called the **residual vector**.

Then we can derive the residual equation

$$Ae = Ax - A\hat{x} = b - A\hat{x} = r \quad (12)$$

between the error vector and the residual vector.

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Notice that \hat{x} is the exact solution of the linear system

$$A\hat{x} = \hat{b},$$

which has a perturbed right-hand side

$$\hat{b} = b - r.$$

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Theorem 5

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Lemma 4 Suppose that x and \tilde{x} satisfy

$$Ax = b \quad \text{and} \quad (A + \Delta A)\tilde{x} = b + \Delta b,$$

where $A \in \mathbb{R}^{n \times n}$, $\Delta A \in \mathbb{R}^{n \times n}$, $0 \neq b \in \mathbb{R}^n$, and $\Delta b \in \mathbb{R}^n$, with

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Lemma 4 Suppose that x and \tilde{x} satisfy

$$Ax = b \quad \text{and} \quad (A + \Delta A)\tilde{x} = b + \Delta b,$$

where $A \in \mathbb{R}^{n \times n}$, $\Delta A \in \mathbb{R}^{n \times n}$, $0 \neq b \in \mathbb{R}^n$, and $\Delta b \in \mathbb{R}^n$, with

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If $\kappa(A) \cdot \delta < 1$, then $A + \Delta A$ is nonsingular and

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