1. Gaussian elimination = LU factorization

$$A = LU.$$

where L is a unit lower triangular matrix and U a upper triangular matrix.

2. Not all matrices have the LU factorization. For example,

$$A = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 2 & 1 \\ 2 & 3 & 1 \end{bmatrix} \neq LU.$$

3. A *permutation matrix* P is an identity matrix with permuted rows.

Let P, P_1, P_2 be $n \times n$ permutation matrices, and X be an $n \times n$ matrix. Then

- $P^T P = I$, i.e., $P^{-1} = P^T$.
- $\det(P) = \pm 1$.
- $P_1 P_2$ is also a permutation matrix.
- PX is the same as X with its rows permuted.
- XP is the same as X with its columns permuted.
- $P_1 X P_2$ reorders both rows and columns of X.

4. The need of pivoting, *mathematically*

The LU factorization can fail on nonsingular matrices, see the above example. But by exchanging the first and third rows, we get

$$PA = \begin{bmatrix} 2 & 3 & 1 \\ 0 & 2 & 1 \\ 0 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & \frac{1}{2} & 1 \end{bmatrix} \begin{bmatrix} 2 & 3 & 1 \\ 0 & 2 & 1 \\ 0 & 0 & -\frac{1}{2} \end{bmatrix} := LU.$$

5. The above simple observation is the basis for LU factorization with pivoting.

Theorem. If A is nonsingular, then there exist permutations P, a unit lower triangular matrix L, and a nonsingular upper triangular matrix U such that

$$PA = LU.$$

6. Function `lutx.m`

7. Solving $Ax = b$ using the LU factorization

    1. Factorize A into $PA = LU$
    2. Permute the entries of b: $b := Pb$.
    3. Solve $L(Ux) = b$ for Ux by forward substitution:
       $Ux = L^{-1}b$.
    4. Solve $Ux = L^{-1}b$ for x by back substitution:
       $x = U^{-1}(L^{-1}b)$.

8. Function `bslashx0.m`

9. The need for pivoting, *numerically*

   Let us apply LU factorization without pivoting to

$$A = \begin{bmatrix} .0001 & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 10^{-4} & 1 \\ 1 & 1 \end{bmatrix} = LU = \begin{bmatrix} 1 & \\ l_{21} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} \\ & u_{22} \end{bmatrix}$$

   in three decimal-digit floating point arithmetic. We obtain

$$\begin{aligned} L &= \begin{bmatrix} 1 & 0 \\ \mathrm{fl}(1/10^{-4}) & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 10^4 & 1 \end{bmatrix}, \\ U &= \begin{bmatrix} 10^{-4} & 1 \\ & \mathrm{fl}(1 - 10^4 \cdot 1) \end{bmatrix} = \begin{bmatrix} 10^{-4} & 1 \\ & -10^4 \end{bmatrix}, \end{aligned}$$

   so

$$LU = \begin{bmatrix} 1 & 0 \\ 10^4 & 1 \end{bmatrix} \begin{bmatrix} 10^{-4} & 1 \\ & -10^4 \end{bmatrix} = \begin{bmatrix} 10^{-4} & 1 \\ 1 & 0 \end{bmatrix} \not\approx A,$$

   where the original a_{22} has been entirely "lost" from the computation by subtracting 10^4 from it. In fact, we would have gotten the same `LU` factors whether a_{22} had been $1, 0, -2$, or any number such that $\mathrm{fl}(a_{22} - 10^4) = -10^4$. Since the algorithm proceeds to work only with L and U, it will get the same answer for all these different a_{22}, which correspond to completely different A and so completely different $x = A^{-1}b$; there is no way to guarantee an accurate answer. This is called *numerical instability*. L and U are not the exact factors of a matrix close to A.

   Let us see what happens when we go on to solve $Ax = [1, 2]^T$ for x using this LU factorization. The correct answer is $x \approx [1, 1]^T$. Instead we get the following. Solving

$$Ly = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \quad \Rightarrow y_1 = \mathrm{fl}(1/1) = 1 \text{ and } y_2 = \mathrm{fl}(2 - 10^4 \cdot 1) = -10^4.$$

   Note that the value 2 has been "lost" by subtracting 10^4 from it. Solving

$$Ux = y = \begin{bmatrix} 1 \\ -10^4 \end{bmatrix} \quad \Rightarrow \quad \hat{x}_2 = \mathrm{fl}((-10^4)/(-10^4)) = 1 \text{ and } \hat{x}_1 = \mathrm{fl}((1-1)/10^{-4}) = 0,$$

   a completely erroneous solution.

   On the other hand, the LU factorization with partial pivoting would have reversed the order of the two equations before proceeding. You can confirm that we get

$$PA = LU,$$

   where

$$P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad L = \begin{bmatrix} 1 & 0 \\ \mathrm{fl}(.0001/1) & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ .0001 & 1 \end{bmatrix},$$

   and

$$U = \begin{bmatrix} 1 & 1 \\ & \mathrm{fl}(1 - .0001 \cdot 1) \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ & 1 \end{bmatrix}.$$

   The computed LU approximates A very accurately. As a result, the computed solution x is also perfect!