LU decomposition (factorization)

During the Gauss elimination process, a matrix A is transformed to a new matrix, the upper triangular matrix U (stored in the upper triangular part of A). Moreover, the multipliers l_{ik}, $i = k+1, \cdots, n$, $k = 1, \cdots, n-1$, are generated, and those can be stored in a strictly lower triangular matrix L, or in the strictly lower triangular part of A.

If we extend L setting 1s on the main diagonal, that is, produce a unit lower triangular matrix L, making L just lower triangular (and not strictly), then we can show that

$$A = L \cdot U. \tag{2.1}$$

This fundamental relation expresses the decomposition or factorization of A into its L and U factors.

In the following, after an example, we will further analyze the factors L and U and give pointers why (2.1) holds.

Imptt

LU decomposition (factorization) -- example

Let

$$A = \begin{bmatrix} 1 & -2 & 1 & 1 \\ 2 & -1 & 5 & -4 \\ -1 & 3 & -1 & 1 \\ -3 & 7 & -5 & 1 \end{bmatrix}.$$

We have applied GE to A, and, as we have seen, we obtained the matrix

$$U = A^{(3)} = \begin{bmatrix} 1 & -2 & 1 & 1 \\ 0 & 3 & 3 & -6 \\ 0 & 0 & -1 & 4 \\ 0 & 0 & 0 & -6 \end{bmatrix},$$

and used the multipliers $2, -1, -3$ (step 1), $\frac{1}{3}, \frac{1}{3}$ (step 2), and 3 (step 3). (Recall: the multipliers are given by $a_{ik} = a_{ik} / a_{kk}$, and the elimination formula $a_{ij} = a_{ij} - a_{ik} a_{kj}$ involves a minus in front of the multiplier).

Let's write the multipliers in a strictly lower triangular matrix L, proceeding column-by-column, and let's also introduce 1s on the diagonal, to make L simply lower triangular, that is,

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

If we compute the product $L \cdot U$, we will see that we obtain A.

LU decomposition (factorization) -- example -- step 1

In step 1 of GE, x_1 was eliminated from rows (equations) 2 to 4 through the row operations

$\rho_2^{(1)} \leftarrow \rho_2 - 2\rho_1$

$\rho_3^{(1)} \leftarrow \rho_3 - (-\rho_1)$

$\rho_4^{(1)} \leftarrow \rho_4 - (-3\rho_1)$

in which the multipliers $l_{21} = 2$, $l_{31} = -1$ and $l_{41} = -3$ were used.

The above row operations can be expressed by the application of the matrix

$$M^{(1)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -l_{21} & 1 & 0 & 0 \\ -l_{31} & 0 & 1 & 0 \\ -l_{41} & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 3 & 0 & 0 & 1 \end{bmatrix}$$

to A, since

$$M^{(1)} A \equiv M^{(1)} A^{(0)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 3 & 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & -2 & 1 & 1 \\ 2 & -1 & 5 & -4 \\ -1 & 3 & -1 & 1 \\ -3 & 7 & -5 & 1 \end{bmatrix} = \begin{bmatrix} 1 & -2 & 1 & 1 \\ 0 & 3 & 3 & -6 \\ 0 & 1 & 0 & 2 \\ 0 & 1 & -2 & 4 \end{bmatrix} = A^{(1)}.$$

LU decomposition (factorization) -- example -- step 2

In step 2 of GE, x_2 was eliminated from rows (equations) 3 to 4 through the row operations

$\rho_3^{(2)} \leftarrow \rho_r^{(1)} - \frac{1}{3}\rho_2^{(1)}, \quad \rho_4^{(2)} \leftarrow \rho_r^{(1)} - \frac{1}{3}\rho_2^{(1)}$

in which the multipliers $l_{32} = \frac{1}{3}$ and $l_{42} = \frac{1}{3}$ were used.

The above row operations can be expressed by the application of the matrix

$$M^{(2)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -l_{32} & 1 & 0 \\ 0 & -l_{42} & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -1/3 & 1 & 0 \\ 0 & -1/3 & 0 & 1 \end{bmatrix},$$

to $A^{(1)}$, since

$$M^{(2)} A^{(1)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -1/3 & 1 & 0 \\ 0 & -1/3 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & -2 & 1 & 1 \\ 0 & 3 & 3 & -6 \\ 0 & 1 & 0 & 2 \\ 0 & 1 & -2 & 4 \end{bmatrix} = \begin{bmatrix} 1 & -2 & 1 & 1 \\ 0 & 3 & 3 & -6 \\ 0 & 0 & -1 & 4 \\ 0 & 0 & -3 & 6 \end{bmatrix} = A^{(2)}.$$

LU decomposition (factorization) -- example -- step 3

In step 3 of GE, x_3 was eliminated from row (equation) 4 through the row operation $\rho_4^{(3)} \leftarrow \rho_4^{(2)} - 3\rho_3^{(2)}$
in which the multiplier $l_{43} = 3$ was used.
The above row operation can be expressed by the application of the matrix

$$M^{(3)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -l_{43} & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -3 & 1 \end{bmatrix},$$

to $A^{(2)}$, since

$$M^{(3)}A^{(2)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -3 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & -2 & 1 & 1 \\ 0 & 3 & 3 & -6 \\ 0 & 0 & -1 & 4 \\ 0 & 0 & -3 & 6 \end{bmatrix} = \begin{bmatrix} 1 & -2 & 1 & 1 \\ 0 & 3 & 3 & -6 \\ 0 & 0 & -1 & 4 \\ 0 & 0 & 0 & -6 \end{bmatrix} = A^{(3)} \equiv U.$$

Processing of the right-hand side vector -- example -- steps 1, 2, 3

$$M^{(1)}b \equiv M^{(1)}b^{(0)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 3 & 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 5 \\ -5 \\ 1 \\ -10 \end{bmatrix} = \begin{bmatrix} 5 \\ -15 \\ 6 \\ 5 \end{bmatrix} = b^{(1)}$$

$$M^{(2)}b^{(1)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -1/3 & 1 & 0 \\ 0 & -1/3 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 5 \\ -15 \\ 6 \\ 5 \end{bmatrix} = \begin{bmatrix} 5 \\ -15 \\ 11 \\ 10 \end{bmatrix} = b^{(2)}$$

$$M^{(3)}b^{(2)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -3 & 1 \end{bmatrix} \cdot \begin{bmatrix} 5 \\ -15 \\ 11 \\ 10 \end{bmatrix} = \begin{bmatrix} 5 \\ -15 \\ 11 \\ -23 \end{bmatrix} = b^{(3)} \equiv c$$

LU decomposition (factorization) and GE -- example -- summary of steps 1, 2, 3

Initially: $Ax = b$

Step 1: $M^{(1)}Ax = M^{(1)}b$ or $A^{(1)}x = b^{(1)}$

Step 2: $M^{(2)}M^{(1)}Ax = M^{(2)}M^{(1)}b$ or $A^{(2)}x = b^{(2)}$

Step 3: $M^{(3)}M^{(2)}M^{(1)}Ax = M^{(3)}M^{(2)}M^{(1)}b$ or $A^{(3)}x = b^{(3)}$ or $Ux = c$

Given the above, we have $M^{(3)}M^{(2)}M^{(1)}A = U$. Taking into account that $M^{(k)}$, $k = 1, 2, 3$, are unit lower triangular, therefore non-singular, we have $A = (M^{(1)})^{-1}(M^{(2)})^{-1}(M^{(3)})^{-1}U$, and $A = (M^{(3)}M^{(2)}M^{(1)})^{-1}U$,
Equivalently, if $M = M^{(3)}M^{(2)}M^{(1)}$, we have $MA = U$ and $A = M^{-1}U$.

Taking into account that

- The inverse of a unit lower triangular matrix is a unit lower triangular matrix, and
- The product of unit lower triangular matrices is a unit lower triangular matrix,

we have that $(M^{(1)})^{-1}(M^{(2)})^{-1}(M^{(3)})^{-1}$ (equivalently M^{-1}) is unit lower triangular. Let $L = (M^{(1)})^{-1}(M^{(2)})^{-1}(M^{(3)})^{-1}$. Then $A = LU$.

LU decomposition (factorization) and GE -- example -- summary of steps 1, 2, 3

Thus, during GE, the elements of matrices L and U, where L is unit lower triangular and U is upper triangular are generated, and the relation $A = LU$ holds. Moreover, L is the product of the inverses of the $M^{(k)}$ matrices. The matrices $M^{(k)}$ are called **elementary Gauss transformations**.

Properties of triangular matrices

The following can be shown:

- The product of lower (upper) triangular matrices is a lower (upper) triangular matrix.
- The product of unit lower (upper) triangular matrices is a unit lower (upper) triangular matrix.
- The inverse of a non-singular lower (upper) triangular matrix is a lower (upper) triangular matrix.
- The inverse of a unit lower (upper) triangular matrix is a unit lower (upper) triangular matrix.

Elementary Gauss transformations

An **elementary Gauss transformation** is a matrix with the following properties:

− it is unit lower triangular;

− its only non-zero elements are the 1's on the diagonal, and the elements of one column below the diagonal.

- It can be shown that the inverse of an elementary Gauss transformation is a matrix like itself, with the signs of the non-zero off-diagonal elements reversed.

$$G = \begin{bmatrix} 1 & 0 & . & 0 & 0 & 0 & . & 0 \\ 0 & 1 & . & . & . & . & . & . \\ . & 0 & . & 0 & . & . & . & . \\ . & . & . & 1 & . & . & . & . \\ . & . & . & 0 & 1 & 0 & . & . \\ . & . & . & . & g_{k+1,k} & 1 & . & . \\ . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & . & 0 \\ 0 & 0 & . & 0 & g_{n,k} & 0 & . & 1 \end{bmatrix}, \quad G^{-1} = \begin{bmatrix} 1 & 0 & . & 0 & 0 & 0 & . & 0 \\ 0 & 1 & . & . & . & . & . & . \\ . & 0 & . & 0 & . & . & . & . \\ . & . & . & 1 & . & . & . & . \\ . & . & . & 0 & 1 & 0 & . & . \\ . & . & . & . & -g_{k+1,k} & 1 & . & . \\ . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & . & 0 \\ 0 & 0 & . & 0 & -g_{n,k} & 0 & . & 1 \end{bmatrix}$$

Elementary Gauss transformations and GE

In the general $n \times n$ case, during GE, we have the elementary Gauss transformations

$$M^{(1)} = \begin{bmatrix} 1 & 0 & . & . & . & . & 0 \\ -l_{21} & 1 & 0 & . & . & . & 0 \\ -l_{31} & 0 & 1 & 0 & . & . & . \\ . & . & 0 & 1 & 0 & . & . \\ . & . & . & 0 & 1 & . & . \\ . & . & . & . & . & . & 0 \\ -l_{n1} & 0 & 0 & . & . & 0 & 1 \end{bmatrix}, \quad M^{(2)} = \begin{bmatrix} 1 & 0 & . & . & . & . & 0 \\ 0 & 1 & 0 & . & . & . & 0 \\ . & -l_{32} & 1 & 0 & . & . & . \\ . & -l_{42} & 0 & 1 & 0 & . & . \\ . & . & . & 0 & 1 & . & . \\ . & . & . & . & . & . & 0 \\ 0 & -l_{n2} & 0 & . & . & 0 & 1 \end{bmatrix}$$

$$M^{(k)} = \begin{bmatrix} 1 & 0 & . & . & . & . & 0 \\ 0 & 1 & 0 & . & . & . & 0 \\ . & 0 & 1 & 0 & . & . & . \\ . & . & 0 & 1 & 0 & . & . \\ . & . & . & -l_{k+1,k} & 1 & . & . \\ . & . & . & . & . & . & 0 \\ 0 & 0 & 0 & -l_{n,k} & . & 0 & 1 \end{bmatrix}, \quad M^{(n-1)} = \begin{bmatrix} 1 & 0 & . & . & . & . & 0 \\ 0 & 1 & 0 & . & . & . & 0 \\ . & 0 & 1 & 0 & . & . & . \\ . & . & 0 & 1 & 0 & . & . \\ . & . & . & 0 & 1 & . & . \\ . & . & . & . & . & . & 0 \\ 0 & 0 & 0 & . & . & -l_{n,n-1} & 1 \end{bmatrix}$$

LU decomposition (factorization) and GE, $A = LU$

Initially: $Ax = b$

Step 1: $M^{(1)}Ax = M^{(1)}b$ or $A^{(1)}x = b^{(1)}$

Step 2: $M^{(2)}M^{(1)}Ax = M^{(2)}M^{(1)}b$ or $A^{(2)}x = b^{(2)}$

Step k: $M^{(k)} \cdots M^{(1)}Ax = M^{(k)} \cdots M^{(1)}b$ or $A^{(k)}x = b^{(k)}$

Step $n-1$: $M^{(n-1)} \cdots M^{(1)}Ax = M^{(n-1)} \cdots M^{(1)}b$ or $A^{(n-1)}x = b^{(n-1)}$ or $Ux = c$

Also

$M^{(n-1)} \cdots M^{(1)}A = U \Rightarrow A = (M^{(1)})^{-1} \cdots (M^{(n-1)})^{-1}U \Rightarrow A = (M^{(n-1)} \cdots M^{(1)})^{-1}U$,

Equivalently, if $M = M^{(n-1)} \cdots M^{(1)}$, we have $MA = U$ and $A = M^{-1}U$.

Let $L = (M^{(1)})^{-1} \cdots (M^{(n-1)})^{-1}$. Then $A = LU$.

Thus, during GE, the elements of matrices L and U, where L is unit lower triangular and U is upper triangular are generated, and the relation $A = LU$ holds. Moreover, L is the product of the inverses of the $M^{(k)}$ matrices, i.e. $L = (M^{(1)})^{-1} \cdots (M^{(n-1)})^{-1}$.

Note: For computational purposes, the matrices $M^{(k)}$ and their inverses are never stored individually.

Solution of a general linear system using the LU factorization, related cost

Let $Ax = b$. Assume we apply the GE algorithm to A and we obtain the L and U factors of A, that is L is unit lower triangular, U is upper triangular, and $A = LU$.

Then the solution of $Ax = b$ is reduced to the solutions of $Lc = b$ and $Ux = c$, therefore, one forward and one back substitution are required.

Cost of solving a general linear system using the LU factorization and GE

Operation counts:

LU factorization / GE: $\frac{n^3}{3}$ pairs of additions and multiplications (flops), and $\frac{n^2}{2}$ divisions.

Forward substitution: $\frac{n^2}{2}$ pairs of additions and multiplications (flops). (The n divisions are not needed, since L has 1s on the main diagonal.)

Back substitution: $\frac{n^2}{2}$ pairs of additions and multiplications (flops), and n divisions.

Total: $\frac{n^3}{3} + 2 \times \frac{n^2}{2}$ pairs of additions and multiplications (flops), and $\frac{n^2}{2} + n$ divisions.

LU factorization -- Gauss elimination

We have seen two ways of solving a linear system $Ax = b$, both based on GE.

The first applies GE to A and b simultaneously, and obtains an upper triangular matrix U and a transformed vector $c = b^{(n-1)}$, such that $Ax = b$ is equivalent to $Ux = c$, then applies back substitution to $Ux = c$ to compute x. In this case, the multipliers are computed, but do not need to be stored.

The second applies GE to A, and obtains the L and U factors, thus $A = LU$, then applies f/s to $Lc = b$ to compute an intermediate vector c, and then applies b/s to $Ux = c$, to compute x. In this case, the multipliers are computed and stored in the strictly lower triangular part of A.

The two ways are mathematically equivalent and involve the same computational cost. However, when we need to solve several linear systems with the same matrix and different right-hand side vectors, we should adopt the second way, apply GE/LU once, store the L and U factors, then apply a pair of f/s and b/s for each right-hand side vector.

Cost for solving m linear systems of size $n \times n$ with the same matrix: $\frac{n^3}{3} + m(\frac{n^2}{2} + \frac{n^2}{2}) = \frac{n^3}{3} + mn^2$ flops, and $\frac{n^2}{2} + mn$ divisions.

Properties of LU factorization

- The L, U factors of the LU decomposition of a given matrix A are unique. That is, if $A = LU$ and $A = \tilde{L}\tilde{U}$, where $L, \tilde{L}$ unit lower triangular and $U, \tilde{U}$ upper triangular, then $L = \tilde{L}$ and $U = \tilde{U}$.
- The LU decomposition can also be written in the form $A = LD\hat{U}$, where D diagonal matrix, and $\hat{U}$ unit upper triangular matrix, More specifically, if $A = LU$, where L unit lower triangular and U upper triangular, then $A = LD\hat{U}$, where $d_{ii} = u_{ii}$, $i = 1, \cdots, n$ (i.e. $D = diag(u_{11}, u_{22}, \cdots, u_{n,n})$), and $\hat{u}_{ij} = \frac{u_{ij}}{u_{ii}}$, $i = 1, \cdots, n$, $j = i, \cdots, n$.
- For matrices with certain special properties, such as symmetry, symmetry and positive definiteness and bandedness, the L, U factors have also some special properties, which we discuss later.

Properties of LU factorization -- symmetric matrices

Assume A is symmetric.

- Each step of GE preserves symmetry of the submatrix $A(k+1 \cdots n, k+1 \cdots n)$, that is, step k of GE produces a symmetric $(n-k) \times (n-k)$ submatrix. This happens because the operation
$$a_{ij}^{(k)} = a_{ij}^{(k-1)} - a_{ik}^{(k-1)} \;/\; a_{kk}^{(k-1)} \cdot a_{kj}^{(k-1)}$$
and the operation
$$a_{ji}^{(k)} = a_{ji}^{(k-1)} - a_{jk}^{(k-1)} \;/\; a_{kk}^{(k-1)} \cdot a_{ki}^{(k-1)}$$
end up to be the same, since A is symmetric.
- Thus, we can obtain the LU factorization of A by doing only half of the operations (either those corresponding to the upper triangular part, or those corresponding to the lower triangular part). This reduces the work of LU factorisation of symmetric matrices to $\frac{n^3}{6}$ flops.
- The LU factorisation of a symmetric matrix takes the form $A = LDL^T$, i.e. $\hat{U} = L^T$, $U = DL^T$, where D diagonal matrix.

Properties of LU factorization -- symmetric positive definite matrices

Assume A is symmetric positive definite, i.e. $A = A^T$ and $x^T Ax > 0$, $\forall x \neq 0$.

- It can be shown that the elements of D of the factorization $A = LDL^T$ are positive, i.e. $d_{ii} > 0$, $i = 1, \cdots, n$.
  The LU factorisation of a symmetric positive definite matrix takes the form $A = CC^T$, where $C = LD^{1/2}$, and $D^{1/2}$ a matrix such that $D^{1/2} \cdot D^{1/2} = D$.
  (In this case, since D is diagonal, $D^{1/2}$ is also diagonal and we have $(D^{1/2})_{ii} = (d_{ii})^{1/2}$).
- The factorization $A = CC^T$ is called the **Choleski factorization** of A, and C is called the **Choleski factor** of A.
  The Choleski algorithm is an algorithm based on GE, which computes the entries of the Choleski factor C of a symmetric positive definite matrix A. Note that C is lower triangular (not unit lower triangular).

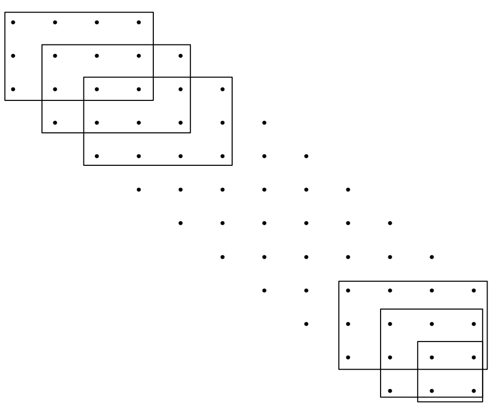
Properties of LU factorization -- banded matrices

Recall: A square matrix A is *banded* with lower bandwidth l and upper bandwidth u, i.e. (l, u)-banded, if $a_{ij} = 0$ when $i - j > l$ and $j - i > u$.
In other words, in a (l, u)-banded matrix, all entries below the lth subdiagonal and above the uth superdiagonal are 0.
Total bandwidth: $l + u + 1$.

- Each step of GE preserves bandedness of the matrix. That is, if A is (l, u)-banded, the L and U matrices arising from GE are $(l, 0)$- and $(0, u)$-banded, respectively.
  Note: L is both unit lower triangular and $(l, 0)$-banded, and U is both upper triangular and $(0, u)$-banded.
- Thus, we can obtain the LU factorization of A by doing only the operations within the band of non-zero entries. This reduces the work of LU factorisation of (l, u)-banded matrices, to $l \cdot u \cdot n$ flops, approximately.

LU factorisation by Gauss elimination (GE) for (l, u)-banded matrices

Steps of banded LU/GE



Each step of GE processes a rectangular array (submatrix) of size $(l + 1) \times (u + 1)$. In each of the last $l - 1$ or $u - 1$ (precisely max $\{l - 1, u - 1\}$) steps the size of the submatrix decreases by 1, so that it does not go out of bounds.

The algorithm requires $\approx \sum_{k=1}^{n-1} (l + 1)(u + 1) \approx \sum_{k=1}^{n} lu = (n - 1)lu \approx nlu$ flops (pairs of additions and multiplications).

LU factorisation by Gauss elimination (GE) for (l, u)-banded matrices

LU factorisation by Gauss elimination (GE) for (l, u)-banded matrices algorithm

```
for k = 1 to n-1
    for i = k+1 to min {k + l, n}
        a_ik = a_ik / a_kk /* a_kk pivot */
        for j = k+1 to min {k + u, n}
            a_ij = a_ij - a_ik a_kj  /* a_ik mult. */
        endfor
    endfor
endfor
```

The above algorithm overwrites the strictly lower triangular part of A by the strictly lower triangular part of L and the upper triangular part of A with (the upper triangular part of) U. The 1's on the diagonal of L are not stored.
There exist variations of this algorithm with different ordering of the i, j and k loops.

Forward and back substitutions for banded matrices

Forward substitution for $Ly = b$, where L is $(l, 0)$-banded

```
for i = 1 to n
    for j = max {i - l, 1} to i-1
        b_i = b_i - l_ij b_j
    endfor
    b_i = b_i / l_ii
endfor
```

Back substitution for $Ux = y$, where U is $(0, u)$-banded

```
for i = n down to 1
    for j = i+1 to min {i + u, n}
        y_i = y_i - u_ij y_j
    endfor
    y_i = y_i / u_ii
endfor
```

The forward substitution algorithm overwrites the right side b by y.
The back substitution algorithm overwrites the right side y by x.

There exist variations of these algorithms with different ordering of the i and j loops.

The forward substitution algorithm requires $\sum_{i=1}^{n} (l + 1) = n(l + 1) \approx nl$ flops.

The back substitution algorithm requires $\sum_{i=1}^{n} (u + 1) = n(u + 1) \approx nu$ flops.

Thus, the solution of an (l, u)-banded linear system by GE/LU and f/b/s requires $nlu + n(l + u)$ flops.

Computing the inverse of a matrix

Recall: Given a square matrix $A \in \mathbb{R}^{n\times n}$, if there exists a matrix $X \in \mathbb{R}^{n\times n}$ for which $A \cdot X = X \cdot A = \mathbf{I}$, then X is called inverse of A, and is denoted by A^{-1}.

How is X computed? The basic relation governing X is $A \cdot X = \mathbf{I}$.

Let X_j denote the jth column of X, and $e_j = [0, 0, \cdots, 0, 1, 0, \cdots, 0]^T$ be the unit vector with "1" in the jth row. Note that $X_j \in \mathbb{R}^{n\times 1}$ and $e_j \in \mathbb{R}^{n\times 1}$. The relation $A \cdot X = \mathbf{I}$ consists of the relations

$$A \cdot X_j = e_j, \; j = 1, \cdots, n. \tag{2.2}$$

For each j, relation $A \cdot X_j = e_j$ forms a linear system with matrix A (same for each j) and right-hand side e_j (different for each j). Thus, relation (2.2) involves n linear systems.
Therefore, to find the inverse X of A, it suffices to compute all the columns of X, X_j, $j = 1, \cdots, n$, that is, it suffices to solve all the systems in (2.2).

Computing the inverse of a matrix

Assume we have computed the LU factorization of A, and let L, U the associated factors. Then, the solution of the systems in (2.2) reduces to the solution of the triangular systems

$$L \cdot Y_j = e_j, \; j = 1, \cdots, n, \tag{2.3a}$$

$$U \cdot X_j = Y_j, \; j = 1, \cdots, n, \tag{2.3b}$$

Algorithm for computing the inverse of a matrix

Compute the L, U factors of the LU factorization of A by GE
For $j = 1, \cdots, n$
    solve $L \cdot Y_j = e_j$ using f/s
    solve $U \cdot X_j = Y_j$ using b/s
endfor
Set $A^{-1} = [X_1 | X_2 | \cdots | X_n]$.

Computing the inverse of a matrix -- Computational cost

According to the cost for solving m linear systems each of size $n \times n$, with the same matrix, in this case, with $m = n$, the cost is $\frac{n^3}{3} + n(\frac{n^2}{2} + \frac{n^2}{2}) = \frac{n^3}{3} + n^3 = \frac{4n^3}{3}$ pairs of additions and multiplications, and $\frac{n^2}{2} + n \cdot n = \frac{3n^2}{2}$ divisions.

However, it can be shown, that this cost can be reduced to n^3 pairs of additions and multiplications (and $\frac{3n^2}{2}$ divisions), if we take advantage of the particular form of the right-hand side vectors e_j. The details are left as an exercise.

Thus, *the cost of computing the inverse of a matrix is n^3 flops*.

Important note: The solution of $Ax = b$ can be obtained by $x = A^{-1}b$, i.e. by computing A^{-1}, then performing the matrix-vector product $A^{-1}b$. However, the cost of this procedure is n^3 flops, which is 3 times as much as the cost of applying LU/GE and back and forward substitutions (for one right-hand side vector). Therefore, inverses of matrices are not computed, unless they are explicitly needed.

Some properties of the inverse of a matrix

The LU factorization of a symmetric matrix involves some symmetry of the factors: $A = LDL^T$

The inverse of a symmetric matrix is a symmetric matrix.

The LU factorization of a banded matrix involves some bandedness of the factors: If A is (l, u)−banded (and no pivoting is used), then L is $(l, 0)$−banded, and U is $(0, u)$−banded.

Attention! The inverse of a banded matrix is **not** (in general) a banded matrix. It is often a dense matrix.

Properties of elementary Gauss transformations

- $M^{(k)} = \mathbf{I} - \mu_k e_k^T$ where $\mu_k = [0, \cdots, 0, l_{k+1,k}, l_{k+2,k}, \cdots l_{n,k}]^T$, $e_k = [0, \cdots, 0, 1, 0, \cdots, 0]^T$, and where the "1" is in the kth row.
  Note that

$$\mu_k e_k^T = \begin{bmatrix} 0 \\ . \\ 0 \\ l_{k+1,k} \\ l_{k+2,k} \\ . \\ l_{n,k} \end{bmatrix} [0 \cdots 0 \; 1 \; 0 \cdots 0] = \begin{bmatrix} 0 & 0 & . & . & . & . & 0 \\ 0 & 0 & 0 & . & . & . & 0 \\ . & 0 & 0 & 0 & . & . & . \\ . & . & 0 & 0 & 0 & . & . \\ . & . & . & l_{k+1,k} & 0 & . & . \\ . & . & . & . & . & . & 0 \\ 0 & 0 & 0 & l_{n,k} & . & 0 & 0 \end{bmatrix}$$

- $(M^{(k)})^{-1} = \mathbf{I} + \mu_k e_k^T$
  Note that

$$\begin{aligned}(\mathbf{I} - \mu_k e_k^T)(\mathbf{I} + \mu_k e_k^T) &= \mathbf{I} - \mu_k e_k^T + \mu_k e_k^T - \mu_k e_k^T \mu_k e_k^T \\ &= \mathbf{I} - \mu_k (e_k^T \mu_k) e_k^T = \mathbf{I} - \mu_k (0) e_k^T = \mathbf{I}\end{aligned}$$

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Properties of elementary Gauss transformations

- $$(M^{(1)})^{-1}(M^{(2)})^{-1} \cdots (M^{(k)})^{-1} = \mathbf{I} + \sum_{i=1}^{k} \mu_i e_i^T$$
  Note that

$$\begin{aligned}(\mathbf{I} + \mu_1 e_1^T)(\mathbf{I} + \mu_2 e_2^T) &= \mathbf{I} + \mu_1 e_1^T + \mu_2 e_2^T + \mu_1 e_1^T \mu_2 e_2^T \\ &= \mathbf{I} + \mu_1 e_1^T + \mu_2 e_2^T + \mu_1 (e_1^T \mu_2) e_2^T \\ &= \mathbf{I} + \mu_1 e_1^T + \mu_2 e_2^T + \mu_1 (0) e_2^T \\ &= \mathbf{I} + \mu_1 e_1^T + \mu_2 e_2^T\end{aligned}$$

  and that

$$\begin{aligned}(\mathbf{I} + \mu_1 e_1^T)(\mathbf{I} + \mu_2 e_2^T)(\mathbf{I} + \mu_3 e_3^T) &= (\mathbf{I} + \mu_1 e_1^T + \mu_2 e_2^T)(\mathbf{I} + \mu_3 e_3^T) \\ &= \mathbf{I} + \mu_1 e_1^T + \mu_2 e_2^T + \mu_3 e_3^T + \mu_1 e_1^T \mu_3 e_3^T + \mu_2 e_2^T \mu_3 e_3^T \\ &= \mathbf{I} + \mu_1 e_1^T + \mu_2 e_2^T + \mu_3 e_3^T + \mu_1 (e_1^T \mu_3) e_3^T + \mu_2 (e_2^T \mu_3) e_3^T \\ &= \mathbf{I} + \mu_1 e_1^T + \mu_2 e_2^T + \mu_3 e_3^T + \mu_1 (0) e_3^T + \mu_2 (0) e_3^T \\ &= \mathbf{I} + \mu_1 e_1^T + \mu_2 e_2^T + \mu_3 e_3^T\end{aligned}$$

- By induction, we can show

$$L = (M^{(1)})^{-1} \cdots (M^{(n-1)})^{-1} = \mathbf{I} + \sum_{i=1}^{n-1} \mu_i e_i^T$$

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