St. Xavier’s College (Autonomous), Kolkata

MSc in Data Science

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Linear Algebra

LU Decomposition

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- Expressing a Square matrix as the product of a lower and an upper triangular matrix.
- The LU decomposition is a modified form of the Gaussian elimination method.

Case1: when no row exchanges are involved.

In that case every inverse matrix $E^{-1}$is lower triangular.

$$E_p E_{p-1} \dots . E_1 A = U \Rightarrow A = E_1{}^{-1} E_{p-1}{}^{-1} \dots . E_p{}^{-1} U = LU$$

$$\boxed{\Rightarrow A = LU}$$

Note: The product of lower triangular matrices is a lower triangular matrix, and the inverse of a lower triangular matrix is also lower triangular.

Use of LU Factorization

1. **Solving a System of Linear Equations**
   Consider the system Ax = b
   with LU factorization A = LU.
   2-step solution procedure:
   1. Solve the lower triangular system Ly = b for y by forward substitution.
   2. Solve the upper triangular system Ux = y for x by back substitution.

2. **Solving Many systems of Linear Equations**
   Now consider the problem AX = B
   (i.e., many different right-hand sides that are associated with the same system matrix).

In this case we need to compute the factorization A = LU only once, and then AX = B

$\Longleftrightarrow$ LUX = B,

and we proceed as before:

1. Solve LY = B by many forward substitutions (in parallel).
2. Solve UX = Y by many back substitutions (in parallel).

3. **Inverting a Matrix**

Now consider the problem AX = B
(i.e., many different right-hand sides that are associated with the same system matrix).
Now suppose that B is the identity matrix of size n
We can use the same algorithm presented earlier to solve for each column of matrix X.
The resulting X will be inverse of A.

4. **Computing the determinant**
Given the LUP decomposition of a square matrix A, A = $P^{-1}LU$
the determinant of A can be computed straightforwardly as:

$$\det(A) = \det(P^{-1})\det(L)\det(U) = (-1)^S\left(\prod_{i=1}^{n} l_{ii}\right)\left(\prod_{i=1}^{n} u_{ii}\right)$$

The determinant of a triangular matrix is the product of its diagonal entries, and that the determinant of a permutation matrix is equal to $(-1)^S$ where S is the number of row exchanges in the decomposition.
The same method readily applies to LU decomposition by setting P equal to the identity matrix.

Existence
Not every nonsingular (invertible) n × n matrix A has an LU Decomposition.
For example, if a_{11} = 0, then the multipliers m_{i1} = a_{i1}/a_{11}, for i = 2, 3, . . . , n, are not defined

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

Note that a_{11}=$l_{11}u_{11}$

If a_{11}=0, then at least one of l_{11}or $u_{11}$and has to be zero, which implies either L or U is singular.
This is impossible if A is nonsingular (invertible).
Can be removed by simply reordering the rows of A.
Example:

$$\underset{A}{\begin{bmatrix} 0 & 1 & 1 \\ 1 & 2 & 1 \\ 2 & 7 & 9 \end{bmatrix}} \rightarrow \underset{PA}{\begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 1 \\ 2 & 7 & 9 \end{bmatrix}} \rightarrow \underset{E_{31}(-3)}{\begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 1 \\ 0 & 3 & 7 \end{bmatrix}} \rightarrow \begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 4 \end{bmatrix}$$

$$P = \begin{bmatrix} 0 & \mathbf{1} & 0 \\ \mathbf{1} & 0 & 0 \\ 0 & 0 & \mathbf{1} \end{bmatrix} \qquad PA = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 2 & 3 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 4 \end{bmatrix} = LU.$$

During Gaussian Elimination, it is necessary to interchange rows of the augmented matrix whenever the diagonal entry of the column currently being processed, known as the pivot element, is equal to zero.

The main step in Gaussian Elimination, $a_{ik}{}^{(j+1)} = a_{ik}{}^{(j)} - m_{ij} a_{jk}{}^{(j)}$, we can see that any roundoff error in the computation of $a_{ik}{}^{(j+1)}$ is amplified by m_{ij}.

$m_{ij} = a_{ij}/a_{jj}$

As the multipliers can be arbitrarily large, it follows that the error in the computed solution can be arbitrarily large, meaning that Gaussian Elimination is an unstable algorithm.

Therefore, it is helpful if it can be ensured that the multipliers are small. This can be accomplished by performing row interchanges, or pivoting, even when it is not absolutely necessary to do so for elimination to proceed.

Sometimes row exchanges are needed to produce pivots.

Every row exchange is carried out by a Permutation matrix P_{ij}.
Then A = (E^{-1} ... P^{-1} ... E^{-1} ... P^{-1})U.

A permutation matrix P has the rows of the identity matrix I in any order. We now compress those row exchanges into a single permutation matrix P.

Case2: when only row exchanges are involved.

LU factorization with Partial Pivoting

The LU factorization with Partial Pivoting (LUP) refers often to the LU factorization with row permutations only.

A proper permutation in rows (or columns) is sufficient for the LU factorization.

PA = LU

where L and U are lower and upper triangular matrices,

and P is a permutation matrix which, when left-multiplied to A, reorders the rows of A.

All square matrices can be factorized in this form.

Once the LU Decomposition P A = LU has been computed,

We have Ax = b ---(1)

$\Rightarrow$ PAx = Pb

$\Rightarrow$ LUx = Pb ---(2) [As PA = LU]

Putting Ux=y in (2),

Ly = Pb → solve for y by forward substitution

Solve Ux = y by back substitution.

Case3: Both row and column exchanges.

LU factorization with full pivoting

An LU factorization with full pivoting involves both row and column permutations.

PAQ = LU

Q is a permutation matrix that reorders the columns of A.

LDU decomposition

An LDU decomposition is a decomposition of the form A = LDU, where D is a diagonal matrix and L and U are unit triangular matrices, meaning that all the entries on the diagonals of L and U are one.

LU decomposition can be generalized to rectangular matrices as well. In that case, L and D are square matrices both of which have the same number of rows as A, and U has exactly the same dimensions as A. Upper triangular should be interpreted as having only zero entries below the main diagonal, which starts at the upper left corner