Example Let $A = \begin{bmatrix} 2 & 4 & 2 & 3 \\ -2 & -5 & -3 & -2 \\ 4 & 7 & 6 & 8 \\ 6 & 10 & 1 & 12 \end{bmatrix}$ and $b = \begin{bmatrix} -3 \\ 3 \\ -1 \\ -16 \end{bmatrix}$ We will calculate L and U such that $A = LU$ by two different methods.

Gaussian Elimination by row operations (outer product formulation)

step 1

$$\begin{bmatrix} 2 & 4 & 2 & 3 \\ -1 & -1 & -1 & 1 \\ 2 & -1 & 2 & 2 \\ 3 & -2 & -5 & 3 \end{bmatrix}$$

$m_{i1} = \frac{a_{i1}}{a_{11}}$

$\frac{-2}{2} = -1$

Row i $-$ m_{i1} (Row1)

$4 - (-1)(-5)$

step 2

$$\begin{bmatrix} 2 & 4 & 2 & 3 \\ -1 & -1 & -1 & 1 \\ 2 & 1 & 3 & 1 \\ 3 & 2 & -3 & 1 \end{bmatrix}$$

$m_{i2} = \frac{a_{i2}}{a_{22}}$

Row$i$ $- m_{i2}$ (Row 2)

$2 - (1)(-1)$

$-5 - 2(-1)$

step 3

$$\begin{bmatrix} 2 & 4 & 2 & 3 \\ -1 & -1 & -1 & 1 \\ 2 & 1 & 3 & 1 \\ 3 & 2 & -1 & 2 \end{bmatrix}$$

$m_{i3} = \frac{a_{i3}}{a_{33}} = \frac{-3}{3}$

Row i $- m_{i3}$ (Row3)

$1 - (-1)(1)$

we found $L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 2 & 1 & 1 & 0 \\ 3 & 2 & -1 & 1 \end{bmatrix}$

$U = \begin{bmatrix} 2 & 4 & 2 & 3 \\ 0 & -1 & -1 & 1 \\ 0 & 0 & 3 & 1 \\ 0 & 0 & 0 & 2 \end{bmatrix}$

Inner Product Formulation

$A = \begin{bmatrix} 2 & 4 & 2 & 3 \\ -2 & -5 & -3 & -2 \\ 4 & 7 & 6 & 8 \\ 6 & 10 & 1 & 12 \end{bmatrix}$

- $u_{1j} = a_{1j}$
- $l_{i1} = \frac{a_{i1}}{u_{11}}$
- $u_{kj} = a_{kj} - \sum_{m=1}^{k-1} l_{km} u_{mj}$
- $l_{ik} = u_{kk}^{-1}\left(a_{ik} - \sum_{m=1}^{k-1} l_{im} u_{mk}\right)$

step1

$$\begin{bmatrix} 2 & 4 & 2 & 3 \\ -1 & -5 & -3 & -2 \\ 2 & 7 & 6 & 8 \\ 3 & 10 & 1 & 12 \end{bmatrix}$$

step 2

$$\begin{bmatrix} 2 & 4 & 2 & 3 \\ -1 & -1 & -1 & 1 \\ 2 & 1 & 6 & 8 \\ 3 & 2 & 1 & 12 \end{bmatrix}$$

$u_{22} = a_{22} - \sum_{m=1}^{1} l_{2m} u_{m2}$
$= a_{22} - l_{21} u_{12}$
$= -5 - (-1)(4)$
$= -5 + 4 = -1$

$u_{23} = a_{23} - l_{21} u_{13}$
$= -3 - (-1)(2)$

$u_{24} = a_{24} - l_{21} u_{14}$
$= (-2) - (-1)(3)$

$l_{32} = u_{22}^{-1}\left(a_{32} - \sum_{m=1}^{1} l_{3m} u_{m2}\right) \rightarrow -1\left(7 - (2(4))\right)$
$-1(-1) = 1$

$l_{42} = u_{22}^{-1}\left(a_{42} - \sum_{m=1}^{1} l_{4m} u_{m2}\right) \rightarrow (-1)\left(10 - 3(4)\right)$
$-1(-2) = 2$

step 3

$$\begin{bmatrix} 2 & 4 & 2 & 3 \\ -1 & -1 & -1 & 1 \\ 2 & 1 & 3 & 1 \\ 3 & 2 & -1 & 12 \end{bmatrix}$$

* $u_{kj} = a_{kj} - \sum_{m=1}^{k-1} l_{km} u_{mj}$

* $l_{ik} = u_{kk}^{-1}\left(a_{ik} - \sum_{m=1}^{k-1} l_{im} u_{mk}\right)$

$u_{33} = a_{33} - (l_{31} u_{13} + l_{32} u_{23})$
$= 6 - (2(2) + (1)(-1))$
$= 6 - (4 - 1) = 3$

$u_{34} = a_{34} - (l_{31} u_{14} + l_{32} u_{24})$
$= 8 - (2(3) + (1)(1))$
$= 8 - (6 + 1) = 1$

$l_{43} = u_{33}^{-1}\left[a_{43} - (l_{41} u_{13} + l_{42} u_{23})\right]$
$= \left(\frac{1}{3}\right)\left[1 - (3(2) + (2)(-1))\right]$
$= \left(\frac{1}{3}\right)\left[1 - (6 - 2)\right]$
$= \frac{1}{3}[1 - 4] = \frac{1}{3}(-3) = -1$

Step 4

$$\begin{bmatrix} 2 & 4 & 2 & 3 \\ -1 & -1 & -1 & 1 \\ 2 & 1 & 3 & 1 \\ 3 & 2 & -1 & 2 \end{bmatrix}$$

$u_{44} = a_{44} - (l_{41} u_{14} + l_{42} u_{24} + l_{43} u_{34})$
$= 12 - (3(3) + 2(1) + (-1)(1))$
$= 12 - (9 + 2 - 1)$
$= 12 - 10 = 2$

$$\begin{bmatrix} 3 & 2 & -1 & 2 \end{bmatrix}$$

$$= 12 - 10 = 2$$

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 2 & 1 & 1 & 0 \\ 3 & 2 & -1 & 1 \end{bmatrix} \qquad U = \begin{bmatrix} 2 & 4 & 2 & 3 \\ 0 & -1 & -1 & 1 \\ 0 & 0 & 3 & 1 \\ 0 & 0 & 0 & 2 \end{bmatrix}$$

$$A = \begin{bmatrix} 2 & 4 & 2 & 3 \\ -2 & -5 & -3 & -2 \\ 4 & 7 & 6 & 8 \\ 6 & 10 & 1 & 12 \end{bmatrix} \qquad b = \begin{bmatrix} -3 \\ 3 \\ -1 \\ -16 \end{bmatrix}$$

we want to solve $Ax = b$ for x,

we just found L and U such that $A = LU$

$Ux = y$ $\qquad$ $Ly = b$

First find y

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 2 & 1 & 1 & 0 \\ 3 & 2 & -1 & 1 \end{bmatrix} y = \begin{bmatrix} -3 \\ 3 \\ -1 \\ -16 \end{bmatrix}$$

We find y using "forward substitution" $\qquad y = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}$

$y_1 = -3$

$-y_1 + y_2 = 3$

$y_2 = 0$

$2y_1 + y_2 + y_3 = -1$

$2(-3) + 0 + y_3 = -1$

$y_3 = 5$

$3y_1 + 2y_2 - y_3 + y_4 = -16$

$-9 + 0 - 5 + y_4 = -16$

$-14 + y_4 = -16$

$y_4 = -2$

$$y = \begin{bmatrix} -3 \\ 0 \\ 5 \\ -2 \end{bmatrix}$$

$Ux = y$

$$\begin{bmatrix} 2 & 4 & 2 & 3 \\ 0 & -1 & -1 & 1 \\ 0 & 0 & 3 & 1 \\ 0 & 0 & 0 & 2 \end{bmatrix} x = \begin{bmatrix} -3 \\ 0 \\ 5 \\ -2 \end{bmatrix} \qquad x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}$$

we find x by back substitution

$2x_4 = -2$

$x_4 = -1$

$3x_3 + x_4 = 5$

$3x_3 - 1 = 5$

$x_3 = 2$

$-x_2 - x_3 + x_4 = 0$

$-x_2 - 2 - 1 = 0$

$x_2 = -3$

$2x_1 + 4x_2 + 2x_3 + 3x_4 = -3$

$2x_1 + 4(-3) + 2(2) + 3(-1) = -3$

$2x_1 - 12 + 4 - 3 = -3$

$2x_1 = 8$

$$x = \begin{bmatrix} 4 \\ -3 \\ \ldots \end{bmatrix}$$

$$x = \begin{bmatrix} 4 \\ -3 \\ 2 \\ -1 \end{bmatrix}$$

$2x_1 - 12 + 4 - 3 = -3$

$2x_1 = 8$

$x_1 = 4$

$Ax = b$

$A^{-1}(Ax) = A^{-1}b$

$x = A^{-1}b$

We know A and we know b.
Finding the inverse matrix is not easy.

- We will return to discuss variations of LU decomposition and Gaussian elimination with pivots

Cholesky Decomposition

A special case of LU decomposition

If we have $Ax = b$
and A is positive definite matrix
Then
$A = R^T R$ where R is an upper triangular matrix.

Positive Definite Matrix:

$x^T A x > 0$ for any non zero x

Theorem (Cholesky Decomposition)
Let A be positive definite. Then A can be decomposed in exactly one way into a product

$$A = R^T R$$

such that R is upper triangular and has all main diagonal entries r_{ii} positive. R is called the Cholesky factor of A.

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ \vdots & & & & \\ a_{n1} & a_{n2} & \cdots & & a_{nn} \end{bmatrix} = \overset{R^T}{\begin{bmatrix} r_{11} & 0 & \cdots & & 0 \\ r_{12} & r_{22} & 0 & \cdots & 0 \\ r_{13} & r_{23} & r_{33} & 0 \cdots & 0 \\ \vdots & & & \ddots & \vdots \\ r_{1n} & \cdots & & & r_{nn} \end{bmatrix}} \overset{R}{\begin{bmatrix} r_{11} & r_{12} & r_{13} & \cdots & r_{1n} \\ 0 & r_{22} & r_{23} & \cdots & r_{2n} \\ 0 & 0 & r_{33} & \cdots & r_{3n} \\ \vdots & & & \ddots & \vdots \\ 0 & \cdots & & 0 & r_{nn} \end{bmatrix}}$$

first row of R^T time j^{th} column of R

first row of R^T time j^{th} column of R

First row of A

$$a_{1j} = r_{11} r_{1j} + 0 + \dots + 0 = r_{11} r_{1j}$$

In particular,

$$a_{11} = r_{11}^2$$

Thus $$r_{11} = +\sqrt{a_{11}}$$

and $$r_{1j} = a_{1j}/r_{11} = a_{1j}/\sqrt{a_{11}} \qquad j = 2, \dots n$$

Second row of A

Second row of R^T times j^{th} column of R

$$a_{2j} = r_{12} r_{1j} + r_{22} r_{2j} + 0 \dots 0$$

In particular

$$a_{22} = r_{12} r_{12} + r_{22} r_{22} = r_{12}^2 + r_{22}^2$$

we found above

$$r_{22}^2 = a_{22} - r_{12}^2$$

$$r_{22} = +\sqrt{a_{22} - r_{12}^2}$$

Thus, $$r_{2j} = \frac{a_{2j} - r_{12} r_{1j}}{r_{22}} \qquad j = 3, \dots n$$

General with i^{th} row of A

$$a_{ij} = r_{1i} r_{1j} + r_{2i} r_{2j} + \dots + r_{ii} r_{ij}$$

In particular,

$$a_{ii} = r_{1i}^2 + r_{2i}^2 + \dots r_{i-1,i}^2 + r_{ii}^2.$$

Solve for r_{ii}

$$r_{ii} = +\sqrt{a_{ii} - \sum_{k=1}^{i-1} r_{ki}^2}$$

Then $$r_{ij} = \frac{\left(a_{ij} - \sum_{k=1}^{i-1} r_{ki} r_{kj}\right)}{r_{ii}} \qquad j = i+1, \dots n$$

The above is the inner-product formulation of a Cholesky decomposition.

Exercise Let $A = \begin{bmatrix} 4 & 0 \\ 0 & 9 \end{bmatrix}$

(a) Prove that A is positive definite

(b) Calculate the Cholesky factor of A

(a) Let $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ $\qquad x^T = (x_1 \; x_2)$

$$x^T A x = \underset{1\times 2}{(x_1 \; x_2)} \underset{2\times 2}{\begin{pmatrix} 4 & 0 \\ 0 & 9 \end{pmatrix}} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

$$x^T A x = \overset{1\times 2}{(x_1 \;\; x_2)} \overset{2\times 2}{\begin{pmatrix} 4 & 0 \\ 0 & 9 \end{pmatrix}} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

$$= (4x_1 \;\; 9x_2) \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

$$= 4x_1^2 + 9x_2^2 > 0 \text{ for any nonzero vector } x.$$

(b) What is R?

$$R = \begin{bmatrix} 2 & 0 \\ 0 & 3 \end{bmatrix} \qquad R^T = \begin{bmatrix} 2 & 0 \\ 0 & 3 \end{bmatrix}$$

$$R^T R = \begin{bmatrix} 4 & 0 \\ 0 & 9 \end{bmatrix}$$

Cholesky's Algorithm (inner product form)

for $i = 1, \dots n$

 for $k = 1, \dots i-1$ (not executed when $i=1$)

  $a_{ii} \leftarrow a_{ii} - a_{ki}^2$

 if $a_{ii} \le 0$ (A is not positive definite)

  end program.

 else

  $a_{ii} \leftarrow \sqrt{a_{ii}}$ (This is r_{ii})

 for $j = i+1, \dots, n$ (do not executed if $i=n$)

  for $k = 1, \dots, i-1$ (do not execute if $i=1$)

   $a_{ij} \leftarrow a_{ij} - a_{ki} a_{kj}$

  $a_{ij} \leftarrow a_{ij} / a_{ii}$ (This is r_{ij})

The upper part of A becomes R.
lower part of A remains unchanged.

Example Let $A = \begin{pmatrix} 4 & -2 & 4 & 2 \\ -2 & 10 & -2 & -7 \\ 4 & -2 & 8 & 4 \\ 2 & -7 & 4 & 7 \end{pmatrix}$ and $b = \begin{bmatrix} 8 \\ 2 \\ 16 \\ 6 \end{bmatrix}$

Use Cholesky Method to show A is positive definite
Find R and b

$r_{11} = \sqrt{a_{11}} = 2$ $\rightarrow r_{ii} = \sqrt{a_{ii} - \sum_{k=1}^{i-1} r_{ki}^2}$

$r_{12} = a_{12}/r_{11} = \frac{-2}{2} = -1$ $\rightarrow r_{ij} = \dfrac{\left(a_{ij} - \sum_{k=1}^{i-1} r_{ki} r_{kj}\right)}{r_{ii}}$

$r_{13} = a_{13}/r_{11} = 2$

$r_{13} = a_{13}/r_{11} = 2$

$r_{14} = 1$

$$r_{ij} = \frac{\left(a_{ij} - \sum_{k=1} r_{ki} r_{kj}\right)}{r_{ii}}$$

$j = i+1, \ldots n$

$$r_{22} = \sqrt{a_{22} - \sum_{k=1} r_{k2}^2}$$

$$= \sqrt{a_{22} - r_{12}^2} = \sqrt{10 - (-1)^2} = 3$$

$$r_{23} = \frac{a_{23} - \sum_{k=1}^{1} r_{k2} r_{k3}}{r_{22}} = \frac{a_{23} - r_{12} r_{13}}{3} = \frac{-2 - (-1)(2)}{3} = 0$$

$$r_{24} = \frac{a_{24} - r_{12} r_{14}}{r_{22}} = \frac{-7 - (-1)(1)}{3} = -2$$

$$r_{33} = \sqrt{a_{33} - \sum_{k=1}^{2} r_{k3}^2} = \sqrt{8 - [2^2 + 0^2)} = \sqrt{4} = 2$$

$$r_{34} = \frac{a_{34} - (r_{13} r_{14} + r_{23} r_{24})}{r_{33}} = \frac{4 - (2(1) + 0(-2))}{2} = \frac{4-2}{2} = 1$$

$r_{44} = 1$

$$R = \begin{bmatrix} 2 & -1 & 2 & 1 \\ 0 & 3 & 0 & -2 \\ 0 & 0 & 2 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Not collected

- Use Python to write a function to calculate R using the inner product formulation.