1 LU

We define arrays

$$L_k := \begin{bmatrix} | & | & & | & | & | & & | \\ | & | & & | & | & | & & | \\ \mathbf{e}_1 & \mathbf{e}_2 & \cdots & \mathbf{e}_{k-1} & \mathbf{v}_k & \mathbf{e}_{k+1} & \cdots & \mathbf{e}_n \\ | & | & & | & | & | & & | \\ | & | & & | & | & | & & | \end{bmatrix} \tag{1}$$

with

$$\mathbf{v}_k := \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ -\frac{a_{k+1,k}^{(k-1)}}{a_{k,k}^{(k-1)}} \\ \cdots \\ -\frac{a_{n,k}^{(k-1)}}{a_{k,k}^{(k-1)}} \end{bmatrix} \tag{2}$$

We might as well say

$$L_k = I_n - \frac{1}{a_{k,k}^{(k-1)}} \begin{bmatrix} 0 & \cdots & 0 & 0 & \cdots & 0 \\ \cdots & \cdots & \vdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & 0 & \cdots & \cdots & \cdots \\ \cdots & \cdots & a_{k+1,k}^{(k-1)} & \cdots & \cdots & \cdots \\ \cdots & \cdots & a_{k+2,k}^{(k-1)} & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & a_{n,k}^{(k-1)} & 0 & \cdots & 0 \end{bmatrix}$$

With L_k we have that

$$\tilde{L}A = L_{n-1}L_{n-2}\cdots L_1 A = U \tag{3}$$

and so

$$A = L_1^{-1}L_2^{-1}\cdots L_{n-1}^{-1}U = LU \tag{4}$$

Now, we want to define an LU factorization in order to invert a matrix. It is pointless to ask the computer to simply invert and obtain L_k^{-1} to obtain L. But it is possible to show that due to the simple form of the L_k matrices, we can show the inverse of L_k is obtained by flipping the signs of certain elements:

$$L_k^{-1} = I_n + \frac{1}{a_{k,k}^{(k-1)}} \begin{bmatrix} 0 & \cdots & 0 & 0 & \cdots & 0 \\ \cdots & \cdots & \vdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & 0 & \cdots & \cdots & \cdots \\ \cdots & \cdots & a_{k+1,k}^{(k-1)} & \cdots & \cdots & \cdots \\ \cdots & \cdots & a_{k+2,k}^{(k-1)} & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & a_{n,k}^{(k-1)} & 0 & \cdots & 0 \end{bmatrix} \tag{5}$$

or in L_k as above, simply replace $\mathbf{v}_k$ by

$$\mathbf{v}_k^- := \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ \frac{a_{k+1,k}^{(k-1)}}{a_{k,k}^{(k-1)}} \\ \cdots \\ \frac{a_{n,k}^{(k-1)}}{a_{k,k}^{(k-1)}} \end{bmatrix} \tag{6}$$

Initializing `U=A.copy()` in Python, suppose at step k you have modified A so far $k-1$ times. By this step k, U is the so far modified A_{k-1}, i.e., in the algorithm so far we have

$$U = A_{k-1} = L_{k-1} \cdots L_1 A \tag{7}$$

and

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L_k=np.eye(n)
L_k[k+1: , k]=-U[k+1:, k]/U[k,k].
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Now, you could say you get L by applying (4). Note

$$L = L_1^{-1} \cdots L_{n-1}^{-1} \text{ has } k\text{th column equal to (6) definition of } \mathbf{v}_k^- \leftarrow !!! \tag{8}$$

In other words,

$$L = \begin{bmatrix} | & | & & | \\ \mathbf{v}_1^- & \mathbf{v}_2^- & \vdots & \mathbf{v}_n^- \\ | & | & & | \end{bmatrix} \leftarrow ! \tag{9}$$

I tried to verify by noting

$$L_1^{-1}L_2^{-1} = \begin{bmatrix} | & | & | & \cdots & | \\ \mathbf{v}_1^- & \mathbf{e}_2 & \mathbf{e}_3 & \cdots & \mathbf{e}_n \\ | & | & | & \cdots & | \end{bmatrix} \begin{bmatrix} | & | & | & \cdots & | \\ \mathbf{e}_1 & \mathbf{v}_2^- & \mathbf{e}_3 & \cdots & \mathbf{e}_n \\ | & | & | & \cdots & | \end{bmatrix} \tag{10}$$

if expanded as $\sum$ (columns $\times$ rows) we get

$$L_1^{-1}L_2^{-1} = \mathbf{v}_1^- \mathbf{e}_1^* + \mathbf{e}_2\mathbf{e}_2^* + \sum_{k=3}^{n} \mathbf{e}_k \left(\frac{a_{k,2}^{(1)}}{a_{2,2}^{(1)}} \mathbf{e}_2 + \mathbf{e}_k \right)^*$$

and note what $\mathbf{e}_k\mathbf{e}_2^*$ is: It is ALMOST the zero matrix, with all elements but TWO equal to zero, and the remaining elements in positions (row,col)$= (k,2)$, (k,k) are

$$\frac{a_{k,2}^{(1)}}{a_{2,2}^{(1)}} \left(\mathbf{e}_k\mathbf{e}_2^*\right)_{k,2} = \frac{a_{k,2}^{(1)}}{a_{2,2}^{(1)}} \qquad \text{and} \qquad (\mathbf{e}_k\mathbf{e}_k^*)_{k,k} = 1 \tag{11}$$

Thus, effectively we have the first step of the following induction, claiming that if

$$L_1^{-1}L_2^{-1}\cdots L_k^{-1} = \begin{bmatrix} | & \cdots & | & | & \cdots & | \\ \mathbf{v}_1^- & \cdots & \mathbf{v}_k^- & \mathbf{e}_{k+1} & \cdots & \mathbf{e}_n \\ | & \cdots & | & | & \cdots & | \end{bmatrix} \tag{12}$$

then

$$(L_1^{-1}L_2^{-1}\cdots L_k^{-1})L_{k+1}^{-1} = \begin{bmatrix} | & \cdots & | & | & \cdots & | \\ \mathbf{v}_1^- & \cdots & \mathbf{v}_{k+1}^- & \mathbf{e}_{k+2} & \cdots & \mathbf{e}_n \\ | & \cdots & | & | & \cdots & | \end{bmatrix}. \tag{13}$$

2 Outer Products and LU

$$LU = \begin{bmatrix} | & & | \\ \mathbf{l}_1 & \cdots & \mathbf{l}_n \\ | & & | \end{bmatrix} \begin{bmatrix} \text{——} & \mathbf{u}_1^* & \text{——} \\ & \cdots & \\ \text{——} & \mathbf{u}_n^* & \text{——} \end{bmatrix} = \mathbf{l}_1\mathbf{u}_1^* + \cdots + \mathbf{l}_n\mathbf{u}_n^* \tag{14}$$

where remember the outer product of vectors gives a matrix:

$$\mathbf{a}\mathbf{b}^* = \begin{bmatrix} a_1 \\ \vdots \\ a_m \end{bmatrix} \begin{bmatrix} b_1 & \cdots & b_m \end{bmatrix} = \begin{bmatrix} a_1b_1 & a_1b_2 & \cdots & a_1b_m \\ a_2b_1 & a_2b_2 & \cdots & a_2b_m \\ \cdots & \cdots & \cdots & \cdots \\ a_mb_1 & a_mb_2 & \cdots & a_mb_m \end{bmatrix} \tag{15}$$

We want to find factors that make (14) true while at the same time, define L as a unit lower triangular matrix and U an upper triangular matrix. *We omit permutation matrices at the moment.*

What we know about L is that

$$L = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ l_{2,1} & 1 & 0 & 0 & \cdots & 0 \\ l_{3,1} & l_{3,2} & 1 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ l_{n,1} & l_{n,2} & l_{n,3} & \cdots & l_{n,n-1} & 1 \end{bmatrix} = \begin{bmatrix} | & & | \\ \mathbf{l}_1 & \cdots & \mathbf{l}_1 \\ | & & | \end{bmatrix} \tag{16}$$

so that

$$\mathbf{l}_k = \begin{bmatrix} 0 \\ \cdots \\ 1 \\ l_{k+1,k} \\ l_{k+2,k} \\ \cdots \\ l_{n,k} \end{bmatrix} \tag{17}$$

Note that under this convention, the first row of U is the first row of A! In other words

$$\mathbf{u}_1^* = [A_{1,1} \ \ A_{12} \cdots \ \ A_{1n}] \quad (\texttt{=A[1,:]}) \tag{18}$$

3 What L_k do

Remember the L_k are the matrix operators that reduce the matrix A one row at a time. Suppose

$$A = \begin{bmatrix} 3 & 0 & -1 & 1 \\ 2 & -1 & 1 & 0 \\ -2 & 2 & 3 & 3 \\ 7 & 0 & 0 & 2 \end{bmatrix} \tag{19}$$

And then of course we choose to divide each row by $A_{1,1} = 3$. For the first column we maintain the first row as is. Note as we go down the first column, we have the second row $[2, -2, 7]^T$ must kill off its first component using the first row. We do require

$$[2, -1, 1, 0] - \frac{2}{3}[3, 0, -1, 1] = [0, -1, 5/3, -2/3] \tag{20}$$

for the next row we need

$$[-2, 2, 3, 3] - \frac{-2}{3}[3, 0, -1, 1] = [0, 2, 7/3, 11/3] \tag{21}$$

and the next row

$$[7, 0, 0, 2] - \frac{7}{3}[3, 0, -1, 1] = [0, 0, 7/3, -1/3] \tag{22}$$

Note this is like grabbing the submatrix for $i = 0$, as

$$A[i+1:, :] = \begin{bmatrix} 2 & -1 & 1 & 0 \\ -2 & 2 & 3 & 3 \\ 7 & 0 & 0 & 2 \end{bmatrix} \tag{23}$$

and then taken with $\mathbf{v}'_i = \mathbf{v}_i[i+1:] \leftarrow$[1]

$$A[i+1:, :] - \underbrace{\texttt{np.dot}(\mathbf{v}'_i, A[i])}_{\text{outer product!}} \tag{24}$$

$$= \begin{bmatrix} 2 & -1 & 1 & 0 \\ -2 & 2 & 3 & 3 \\ 7 & 0 & 0 & 2 \end{bmatrix} - \begin{bmatrix} 2/3 \\ -2/3 \\ 7/3 \end{bmatrix} [3, 0, -1, 1]$$

$$= \begin{bmatrix} 0 & -1 & 5/3 & -2/3 \\ 0 & 2 & 7/3 & 11/3 \\ 0 & 0 & 7/3 & -1/3 \end{bmatrix}$$

and note

$$L_1 A = \begin{bmatrix} 3 & 0 & -1 & 1 \\ 0 & -1 & 5/3 & -2/3 \\ 0 & 2 & 7/3 & 11/3 \\ 0 & 0 & 7/3 & -1/3 \end{bmatrix} \tag{25}$$

[1] Note NOT $\mathbf{v}_i$! We extract the part of $\mathbf{v}_i$ below the 1 on the diagonal! $\mathbf{v}_0 = [1 \;\; 2/3 \;\; -2/3 \;\; 7/3]^T$.