Solving Linear System of Equations

The “Undo” button for Linear Operations

Matrix-vector multiplication: given the data $\boldsymbol{x}$ and the operator $\boldsymbol{A}$, we can find $\boldsymbol{y}$ such that

$$\boldsymbol{y} = \boldsymbol{A}\,\boldsymbol{x}$$

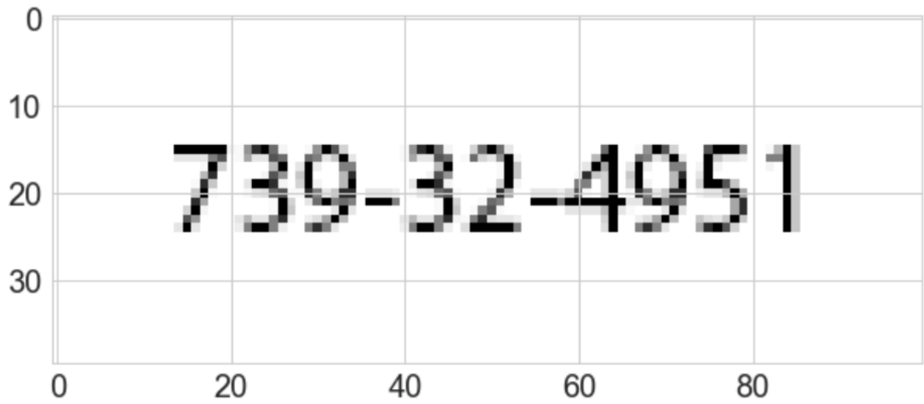
$$\boldsymbol{x} \xrightarrow[\text{transformation}]{\boldsymbol{A}} \boldsymbol{y}$$

What if we know $\boldsymbol{y}$ but not $\boldsymbol{x}$? How can we “undo” the transformation?

$$\boldsymbol{y} \xrightarrow[?]{\boldsymbol{A}^{-1}} \boldsymbol{x}$$

Solve $\boldsymbol{A}\,\boldsymbol{x} = \boldsymbol{y}$ for $\boldsymbol{x}$

Image Blurring Example



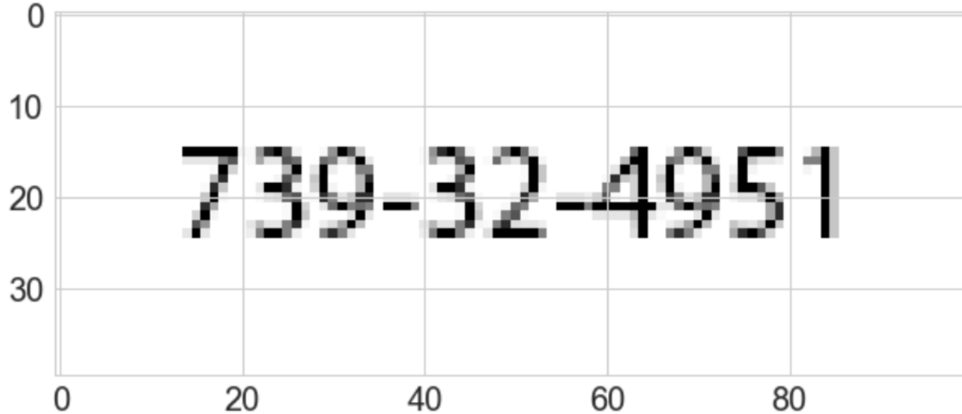
- Image is stored as a 2D array of real numbers between 0 and 1 (0 represents a white pixel, 1 represents a black pixel)
- $\boldsymbol{xmat}$ has 40 rows of pixels and 100 columns of pixels
- Flatten the 2D array as a 1D array
- $\boldsymbol{x}$ contains the 1D data with dimension 4000,
- Apply blurring operation to data $\boldsymbol{x}$, i.e.

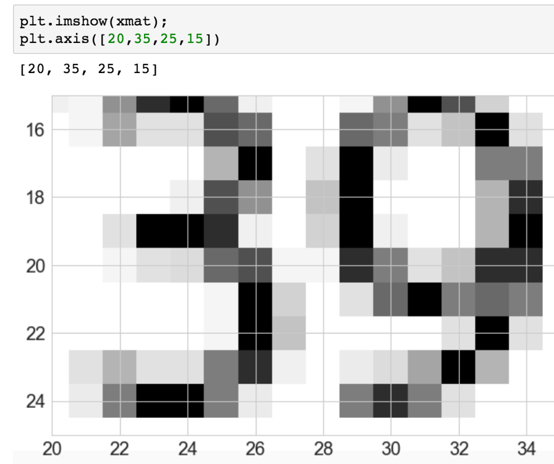
$$\boldsymbol{y} = \boldsymbol{A}\,\boldsymbol{x}$$

where $\boldsymbol{A}$ is the blur operator and $\boldsymbol{y}$ is the blurred image

Blur operator

$\boldsymbol{x}$





$\boldsymbol{A}$ Blur operator

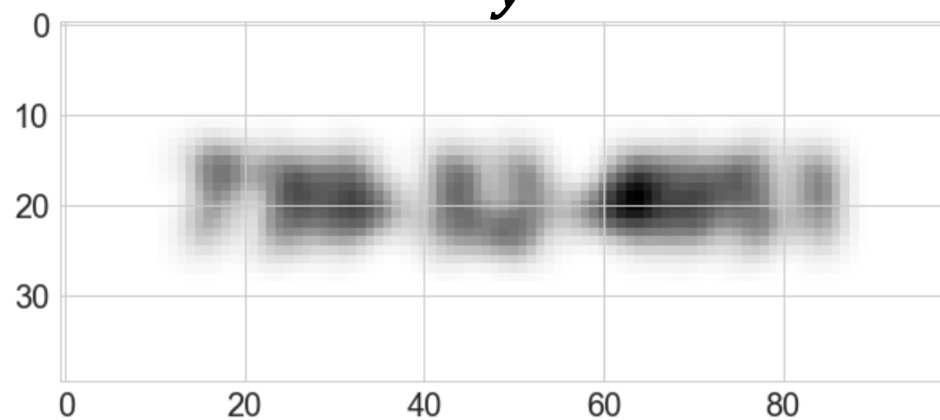
blurred image (4000,)

Blur operator (4000,4000)

"original" image (4000,)

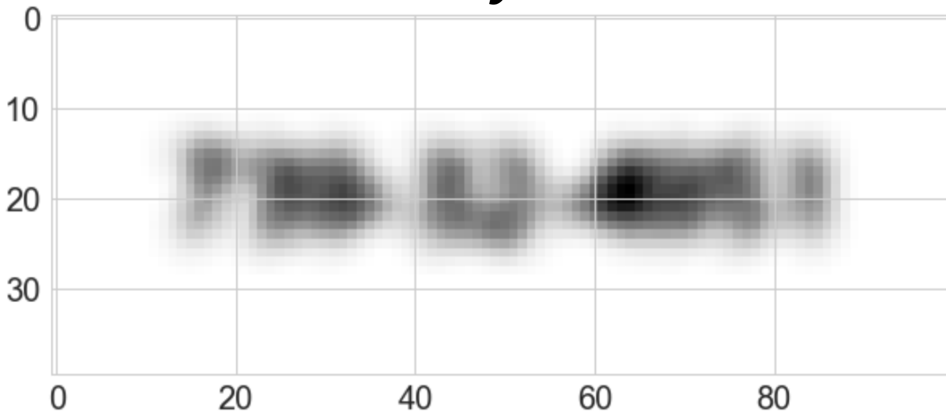
$$\boldsymbol{y} = \boldsymbol{A}\,\boldsymbol{x}$$

$\boldsymbol{y}$



"Undo" Blur to recover original image

$\boldsymbol{y}$

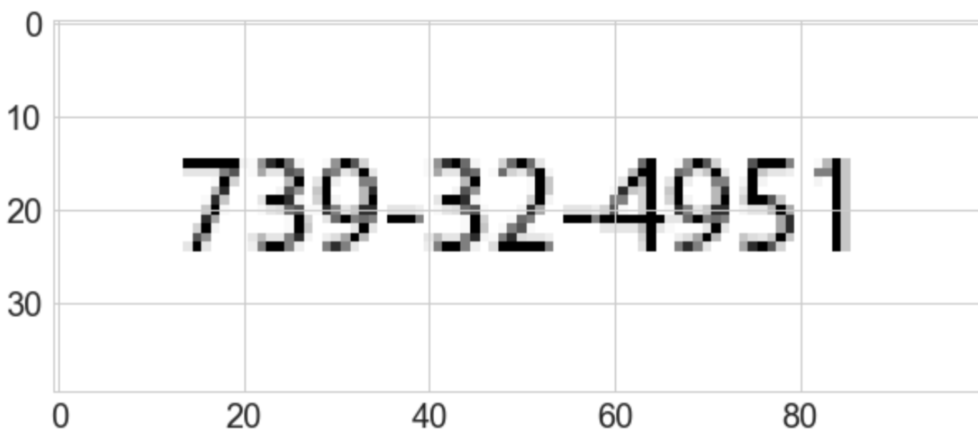


Solve

$\boldsymbol{A}\,\boldsymbol{x} = \boldsymbol{y}$

for $\boldsymbol{x}$

$\boldsymbol{x}$



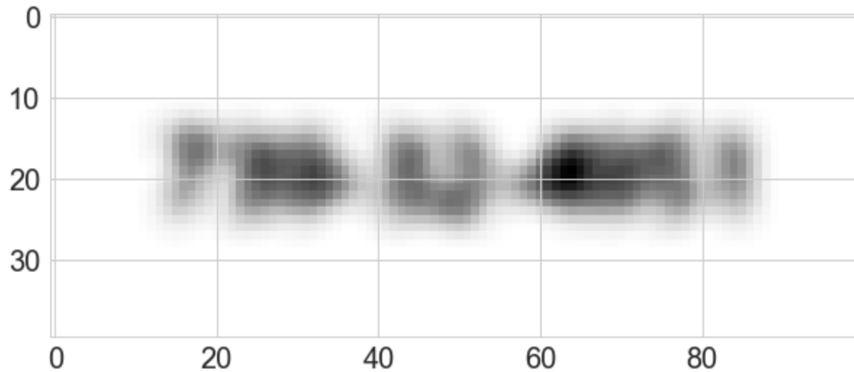
Assumptions:

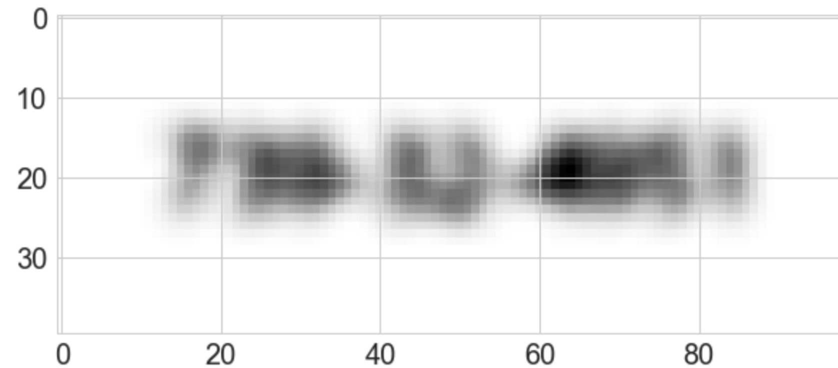
1. we know the blur operator $\boldsymbol{A}$
2. the data set $\boldsymbol{y}$ does not have any noise ("clean data"

"Undo" Blur to recover original image

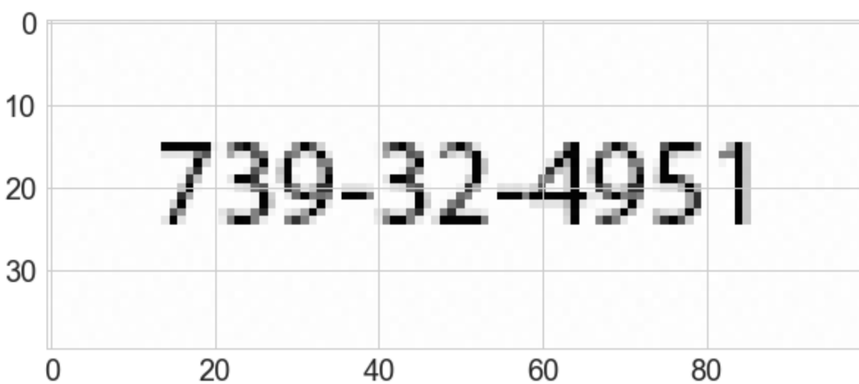
$\boldsymbol{y} + a * 10^{-6}\ (a \in (0,1))$

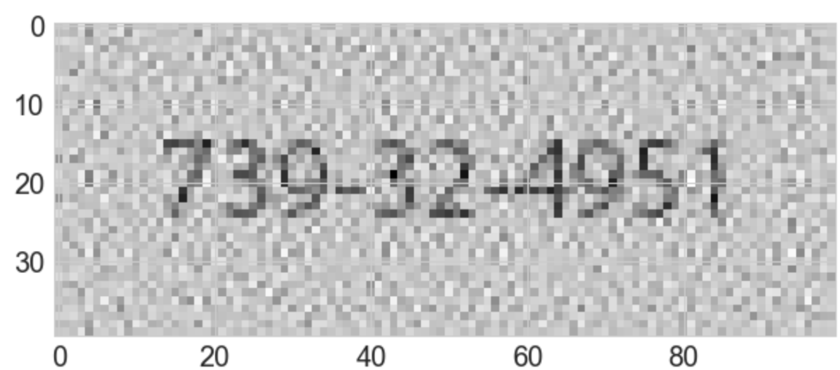
$\boldsymbol{y} + a * 10^{-4}\ (a \in (0,1))$





Solve $\boldsymbol{A}\,\boldsymbol{x} = \boldsymbol{y}$ for $\boldsymbol{x}$





How much noise can we add and still be able to recover meaningful information from the original image? At which point this inverse transformation fails?

We will talk about sensitivity of the "undo" operation later.

Linear System of Equations

How do we actually solve $\boldsymbol{A}\,\boldsymbol{x} = \boldsymbol{b}$?

We can start with an "easier" system of equations…

Let's consider triangular matrices (lower and upper):

$$\begin{pmatrix} L_{11} & 0 & \dots & 0 \\ L_{21} & L_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ L_{n1} & L_{n2} & \dots & L_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

$$\begin{pmatrix} U_{11} & U_{12} & \dots & U_{1n} \\ 0 & U_{22} & \dots & U_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & U_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

Example: Forward-substitution for lower triangular systems

$$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 3 & 2 & 0 & 0 \\ 1 & 2 & 6 & 0 \\ 1 & 3 & 4 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 2 \\ 2 \\ 6 \\ 4 \end{pmatrix}$$

$$2\,x_1 = 2 \rightarrow x_1 = 1$$

$$3\,x_1 + 2\,x_2 = 2 \rightarrow x_2 = \frac{2-3}{2} = -0.5$$

$$1\,x_1 + 2\,x_2 + 6\,x_3 = 6 \rightarrow x_3 = \frac{6-1+1}{6} = 1.0$$

$$1\,x_1 + 3\,x_2 + 4\,x_3 + 2\,x_4 = 4 \rightarrow x_3 = \frac{4-1+1.5-4}{2} = 0.25$$

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 1 \\ -0.5 \\ 1.0 \\ 0.25 \end{pmatrix}$$

Triangular Matrices

$$\begin{pmatrix} U_{11} & U_{12} & \dots & U_{1n} \\ 0 & U_{22} & \dots & U_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & U_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

Recall that we can also write $\boldsymbol{U}\,\boldsymbol{x} = \boldsymbol{b}$ as a linear combination of the columns of $\boldsymbol{U}$

$$x_1\,\mathbf{U}[:,1] + \; x_2\,\mathbf{U}[:,2] + \cdots + \; x_n\,\mathbf{U}[:,n] = \boldsymbol{b}$$

Hence we can write the solution as

$U_{nn}\; x_n = b_n$

$x_1\,\mathbf{U}[:,1] + \cdots + \; x_{n-1}\,\mathbf{U}[:,n-1] = \boldsymbol{b} - x_n\,\mathbf{U}[:,n] \rightarrow U_{n-1,n-1}\; x_{n-1} = b_{n-1} - U_{n-1,n}\,x_n$

$x_1\,\mathbf{U}[:,1] + \cdots + \; x_{n-2}\,\mathbf{U}[:,n-2] = \boldsymbol{b} - x_n\,\mathbf{U}[:,n] - \; x_{n-1}\,\mathbf{U}[:,n-1]$

Or in general (backward-substitution for upper triangular systems):

$$x_n = b_n/U_{nn} \qquad x_i = \frac{b_i - \sum_{j=i+1}^{n} U_{ij} x_j}{U_{ii}}, \qquad i = n-1, n-2, \dots, 1$$

Triangular Matrices

Forward-substitution for lower-triangular systems:

$$\begin{pmatrix} L_{11} & 0 & \dots & 0 \\ L_{21} & L_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ L_{n1} & L_{n2} & \dots & L_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

$$x_1 = b_1 / L_{11} \qquad x_i = \frac{b_i - \sum_{j=1}^{i-1} L_{ij} x_j}{L_{ii}}, \qquad i = 2, 3, \dots, n$$

Cost of solving triangular systems

$$x_n = b_n / U_{nn} \qquad x_i = \frac{b_i - \sum_{j=i+1}^{n} U_{ij} x_j}{U_{ii}}, \qquad i = n-1, n-2, \dots, 1$$

n divisions
$n(n-1)/2$ subtractions/additions
$n(n-1)/2$ multiplications

$\Rightarrow$ Computational complexity is $O(n^2)$

$$x_1 = b_1 / L_{11} \qquad x_i = \frac{b_i - \sum_{j=1}^{i-1} L_{ij} x_j}{L_{ii}}, \qquad i = 2,3, \dots, n$$

n divisions
$n(n-1)/2$ subtractions/additions
$n(n-1)/2$ multiplications

$\Rightarrow$ Computational complexity is $O(n^2)$

Linear System of Equations

How do we solve $\boldsymbol{A}\,\boldsymbol{x} = \boldsymbol{b}$ when $\boldsymbol{A}$ is a non-triangular matrix?

We can perform LU factorization: given a $n \times n$ matrix $\boldsymbol{A}$, obtain lower triangular matrix $\boldsymbol{L}$ and upper triangular matrix $\boldsymbol{U}$ such that

$$\boldsymbol{A} = \boldsymbol{L}\boldsymbol{U}$$

where we set the diagonal entries of $\boldsymbol{L}$ to be equal to 1.

$$\begin{pmatrix} 1 & 0 & \dots & 0 \\ L_{21} & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ L_{n1} & L_{n2} & \dots & 1 \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} & \dots & U_{1n} \\ 0 & U_{22} & \dots & U_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & U_{nn} \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \dots & A_{nn} \end{pmatrix}$$

LU Factorization

$$\begin{pmatrix} 1 & 0 & \dots & 0 \\ L_{21} & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ L_{n1} & L_{n2} & \dots & 1 \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} & \dots & U_{1n} \\ 0 & U_{22} & \dots & U_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & U_{nn} \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \dots & A_{nn} \end{pmatrix}$$

Assuming the LU factorization is know, we can solve the general system

$$\boldsymbol{LU\,x = b}$$

By solving two triangular systems:

$$\boldsymbol{L\,y = b} \xrightarrow{\text{Solve for } \boldsymbol{y}} \text{Forward-substitution with complexity } O(n^2)$$

$$\boldsymbol{U\,x = y} \xrightarrow{\text{Solve for } \boldsymbol{x}} \text{Backward-substitution with complexity } O(n^2)$$

But what is the cost of the LU factorization? Is it beneficial?

2x2 LU Factorization (simple example)

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ L_{21} & 1 \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} \\ 0 & U_{22} \end{pmatrix}$$

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} U_{11} & U_{12} \\ L_{21}U_{11} & L_{21}U_{12} + U_{22} \end{pmatrix}$$

$$U_{11} = A_{21}/U_{11}$$

2) $L_{21} = A_{21}/U_{11}$

3) $U_{22} = A_{22} - L_{21}U_{12}$

Seems quite simple! Can we generalize this for a $n \times n$ matrix $\boldsymbol{A}$?

Computing the Lower-Triangular Factor in LU

1 point

Consider the matrix

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

and its corresponding LU factorization ($A = LU$), where the lower and upper triangular matrices given respectively by

$$L = \begin{bmatrix} 1 & 0 \\ l_{21} & 1 \end{bmatrix} \quad \text{and} \quad U = \begin{bmatrix} u_{11} & u_{12} \\ 0 & u_{22} \end{bmatrix}.$$

l_{21} =

u_{11} =

u_{12} =

u_{22} =

LU Factorization

a_{11}: scalar

$\boldsymbol{a}_{12}$: row vector $(1\times(n-1))$

$\boldsymbol{a}_{21}$: column vector $((n-1)\times 1)$

$\boldsymbol{A}_{22}$: matrix $((n-1)\times(n-1))$

a_{11} $\quad$ $\boldsymbol{a}_{12}$

$$\begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \cdots & A_{nn} \end{pmatrix}$$

$\boldsymbol{a}_{21}$ $\quad$ $\boldsymbol{A}_{22}$

1) First row of $\boldsymbol{U}$ is the first row of $\boldsymbol{A}$

$$\begin{pmatrix} a_{11} & \boldsymbol{a}_{12} \\ \boldsymbol{a}_{21} & \boldsymbol{A}_{22} \end{pmatrix} = \begin{pmatrix} u_{11} & \boldsymbol{u}_{12} \\ u_{11}\,\boldsymbol{l}_{21} & \boldsymbol{l}_{21}\boldsymbol{u}_{12} + \boldsymbol{L}_{22}\boldsymbol{U}_{22} \end{pmatrix}$$

$$\boldsymbol{l}_{21} = \frac{1}{u_{11}}\boldsymbol{a}_{21}$$

$$\boldsymbol{A}_{22} = \boldsymbol{l}_{21}\boldsymbol{u}_{12} + \boldsymbol{L}_{22}\boldsymbol{U}_{22}$$

2) First column of $\boldsymbol{L}$ is the first column of $\boldsymbol{A}/\ u_{11}$

3) $\boldsymbol{L}_{22}\boldsymbol{U}_{22} = \overbrace{\boldsymbol{A}_{22} - \boldsymbol{l}_{21}\boldsymbol{u}_{12}}^{\text{Known!}}$

Need another factorization!

LU Factorization

a_{11}: scalar
$\boldsymbol{a}_{12}$: row vector $(1\times(n-1))$
$\boldsymbol{a}_{21}$: column vector $((n-1)\times 1)$
$\boldsymbol{A}_{22}$: matrix $((n-1)\times(n-1))$

a_{11} $\quad$ $\boldsymbol{a}_{12}$

$$\begin{pmatrix} \boxed{A_{11}} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \cdots & A_{nn} \end{pmatrix} = \begin{pmatrix} a_{11} & \boldsymbol{a}_{12} \\ \boldsymbol{a}_{21} & \boldsymbol{A}_{22} \end{pmatrix} = \begin{pmatrix} 1 & \boldsymbol{0} \\ \boldsymbol{l}_{21} & \boldsymbol{L}_{22} \end{pmatrix} \begin{pmatrix} u_{11} & \boldsymbol{u}_{12} \\ \boldsymbol{0} & \boldsymbol{U}_{22} \end{pmatrix}$$

$\boldsymbol{a}_{21}$ $\quad$ $\boldsymbol{A}_{22}$

$$\begin{pmatrix} a_{11} & \boldsymbol{a}_{12} \\ \boldsymbol{a}_{21} & \boldsymbol{A}_{22} \end{pmatrix} = \begin{pmatrix} u_{11} & \boldsymbol{u}_{12} \\ u_{11}\,\boldsymbol{l}_{21} & \boldsymbol{l}_{21}\boldsymbol{u}_{12} + \boldsymbol{L}_{22}\boldsymbol{U}_{22} \end{pmatrix}$$

1) First row of $\boldsymbol{U}$ is the first row of $\boldsymbol{A}$

2) $\boldsymbol{l}_{21} = \frac{1}{u_{11}}\boldsymbol{a}_{21}$

First column of $\boldsymbol{L}$ is the first column of $\boldsymbol{A}/\ u_{11}$

3) $\boldsymbol{M} = \boldsymbol{L}_{22}\boldsymbol{U}_{22} = \overbrace{\boldsymbol{A}_{22} - \boldsymbol{l}_{21}\boldsymbol{u}_{12}}^{\text{Known!}}$

Need another factorization!

Example

$$\boldsymbol{M} = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 1 & 2 & 3 & 3 \\ 1 & 2 & 6 & 2 \\ 1 & 3 & 4 & 2 \end{pmatrix}$$

1) First row of $\boldsymbol{U}$ is the first row of $\boldsymbol{A}$

2) First column of $\boldsymbol{L}$ is the first column of $\boldsymbol{A}/\ u_{11}$

3) $\boldsymbol{L}_{22}\boldsymbol{U}_{22} = \boldsymbol{A}_{22} - \boldsymbol{l}_{21}\boldsymbol{u}_{12}$

Example

$$M = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 1 & 2 & 3 & 3 \\ 1 & 2 & 6 & 2 \\ 1 & 3 & 4 & 2 \end{pmatrix} \quad L = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0 \end{pmatrix} \quad U = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$M = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 1 & -2 & 1 & 2.5 \\ 1 & -2 & 4 & 1.5 \\ 1 & -1 & 2 & 1.5 \end{pmatrix} \quad L = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0.5 & 1 & 0 & 0 \\ 0.5 & 1 & 0 & 0 \\ 0.5 & 0.5 & 0 & 0 \end{pmatrix} \quad U = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 0 & -2 & 1 & 2.5 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$M = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 1 & -2 & 1 & 2.5 \\ 1 & -2 & 3 & -1 \\ 1 & -1 & 1.5 & 0.25 \end{pmatrix} \quad L = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0.5 & 1 & 0 & 0 \\ 0.5 & 1 & 1 & 0 \\ 0.5 & 0.5 & 0.5 & 0 \end{pmatrix} \quad U = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 0 & -2 & 1 & 2.5 \\ 0 & 0 & 3 & -1 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$M = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 1 & -2 & 1 & 2.5 \\ 1 & -2 & 3 & -1 \\ 1 & -1 & 1.5 & 0.75 \end{pmatrix} \quad L = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0.5 & 1 & 0 & 0 \\ 0.5 & 1 & 1 & 0 \\ 0.5 & 0.5 & 0.5 & 1 \end{pmatrix} \quad U = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 0 & -2 & 1 & 2.5 \\ 0 & 0 & 3 & -1 \\ 0 & 0 & 0 & 0.75 \end{pmatrix}$$

Algorithm: LU Factorization of matrix A

```python
## Algorithm 1
## Factorization using the block-format,
## creating new matrices L and U
## and not modifying A
print("LU factorization using Algorithm 1")
L = np.zeros((n,n))
U = np.zeros((n,n))
M = A.copy()
for i in range(n):
    U[i,i:] = M[i,i:]
    L[i:,i] = M[i:,i]/U[i,i]
    M[i+1:,i+1:] -= np.outer(L[i+1:,i],U[i,i+1:])
```

Cost of LU factorization

```
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    M[i+1:,i+1:] -= np.outer(L[i+1:,i],U[i,i+1:])
```

Side note:

$$\sum_{i=1}^{m} i = \frac{1}{2}m(m+1)$$

$$\sum_{i=1}^{m} i^2 = \frac{1}{6}m(m+1)(2m+1)$$

Cost of LU factorization

Side note:

$$\sum_{i=1}^{m} i = \frac{1}{2}m(m+1)$$

$$\sum_{i=1}^{m} i^2 = \frac{1}{6}m(m+1)(2m+1)$$

```
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    M[i+1:,i+1:] -= np.outer(L[i+1:,i],U[i,i+1:])
```

Number of divisions: $(n-1)+(n-2)+\cdots+1 = n(n-1)/2$

Number of multiplications $(n-1)^2+(n-2)^2+\ldots+(1)^2 = \frac{n^3}{3} - \frac{n^2}{2} + \frac{n}{6}$

Number of subtractions: $(n-1)^2+(n-2)^2+\ldots+(1)^2 = \frac{n^3}{3} - \frac{n^2}{2} + \frac{n}{6}$

Computational complexity is $O(n^3)$

Demo "Complexity of Mat-Mat multiplication and LU"

Solving linear systems

In general, we can solve a linear system of equations following the steps:

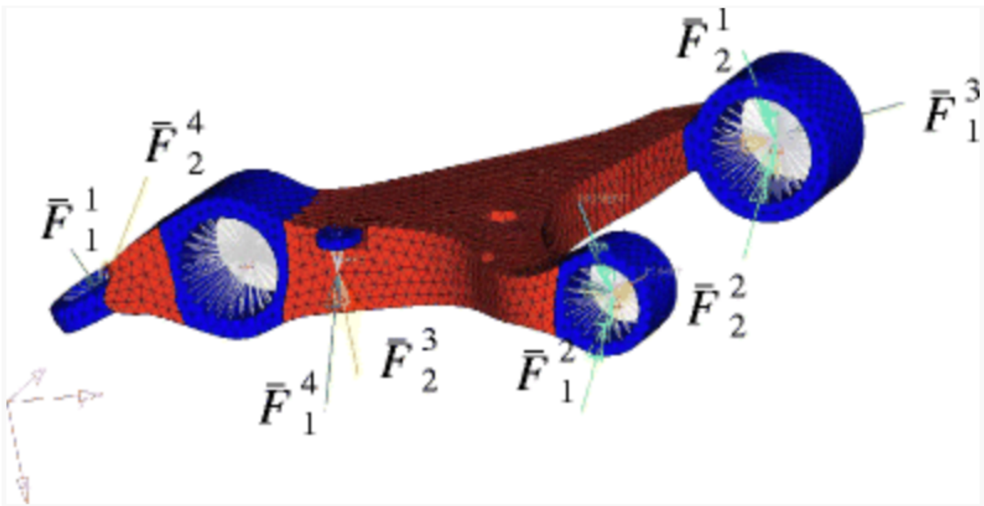
1) Factorize the matrix $\boldsymbol{A}$: $\boldsymbol{A} = \boldsymbol{LU}$ (complexity $O(n^3)$)

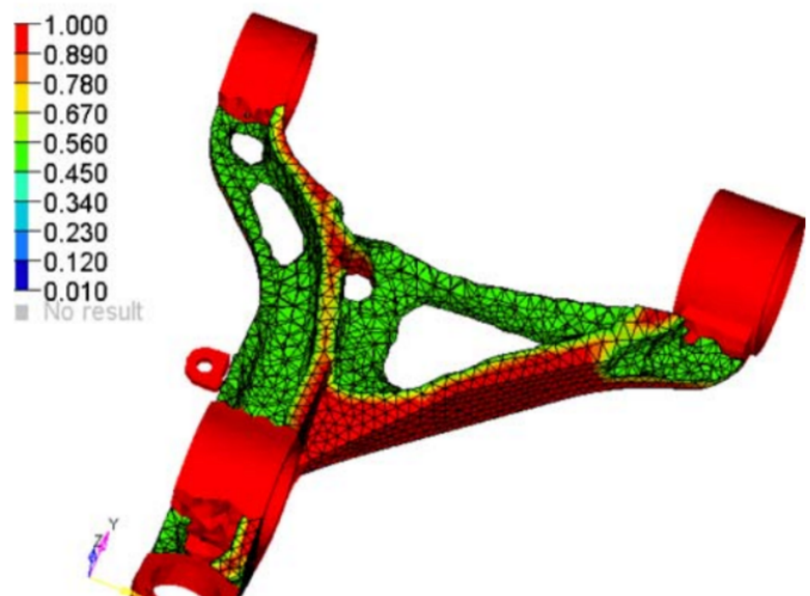
2) Solve $\boldsymbol{L}\,\boldsymbol{y} = \boldsymbol{b}$ (complexity $O(n^2)$)

3) Solve $\boldsymbol{U}\,\boldsymbol{x} = \boldsymbol{y}$ (complexity $O(n^2)$)

But why should we decouple the factorization from the actual solve? (Remember from Linear Algebra, Gaussian Elimination does not decouple these two steps…)

Example: Optimization of automotive control arm





(b)

Find the distribution of material inside the design space $(\boldsymbol{d})$ that maximizes the stiffness, i.e.,

$\min \boldsymbol{U}^T\boldsymbol{F}$ where $\boldsymbol{K}(\boldsymbol{d})\,\boldsymbol{U} = \boldsymbol{F}$ ($\boldsymbol{U}$: displacement vector, $\boldsymbol{F}$: load vector, $\boldsymbol{K}$: stiffness matrix)

Solve the linear system of equations

$$\boldsymbol{K}\,\boldsymbol{U} = \boldsymbol{F}$$

for the load vector $\boldsymbol{F}$. What if we have many different loading conditions (pothole, hitting a curb, breaking, etc)?

Iclicker question

Let's assume that when solving the system of equations $\boldsymbol{K}\,\boldsymbol{U} = \boldsymbol{F}$, we observe the following:

- When the stiffness matrix has dimensions (100,100), computing the LU factorization takes about 1 second and each solve (forward + backward substitution) takes about 0.01 seconds.

Estimate the total time it will take to find the displacement response corresponding to 10 different load vectors $\boldsymbol{F}$ when the stiffness matrix has dimensions (1000,1000)?

$A)\ \sim 10\ seconds$
$B)\ \sim 10^2\ seconds$
$C)\ \sim 10^3\ seconds$
$D)\ \sim 10^4\ seconds$
$E)\ \sim 10^5\ seconds$

What can go wrong with the previous algorithm?

```
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    L[i:,i] = M[i:,i]/U[i,i]
    M[i+1:,i+1:] -= np.outer(L[i+1:,i],U[i,i+1:])
```

If division by zero occurs, LU factorization fails.

What can we do to get something like an LU factorization?

What can go wrong with the previous algorithm?

Demo "Little c"

$$\boldsymbol{M} = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 1 & \color{red}{\mathbf{4}} & 3 & 3 \\ 1 & 2 & 6 & 2 \\ 1 & 3 & 4 & 2 \end{pmatrix} \qquad \boldsymbol{L} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0 \end{pmatrix} \qquad \boldsymbol{U} = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\boldsymbol{l}_{21}\boldsymbol{u}_{12} = \begin{pmatrix} 4 & 2 & 0.5 \\ 4 & 2 & 0.5 \\ 4 & 2 & 0.5 \end{pmatrix} \qquad \boldsymbol{M} - \boldsymbol{l}_{21}\boldsymbol{u}_{12} = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 1 & \color{red}{\mathbf{0}} & 1 & 2.5 \\ 1 & -2 & 4 & 1.5 \\ 1 & -1 & 2 & 1.5 \end{pmatrix}$$

The next update for the lower triangular matrix will result in a division by zero! LU factorization fails.

What can we do to get something like an LU factorization?

Pivoting

Approach:

1. Swap rows if there is a zero entry in the diagonal
2. Even better idea: Find the largest entry (by absolute value) and swap it to the top row.

The entry we divide by is called the pivot.

Swapping rows to get a bigger pivot is called (partial) pivoting.

$$\begin{pmatrix} a_{11} & \boldsymbol{a}_{12} \\ \boxed{\boldsymbol{a}_{21}} & \boldsymbol{A}_{22} \end{pmatrix} = \begin{pmatrix} u_{11} & \boldsymbol{u}_{12} \\ u_{11}\,\boldsymbol{l}_{21} & \boldsymbol{l}_{21}\boldsymbol{u}_{12} + \boldsymbol{L}_{22}\boldsymbol{U}_{22} \end{pmatrix}$$

Find the largest entry (in magnitude)

LU Factorization with Partial Pivoting

- LU factorization with partial pivoting can be completed for any matrix A

Suppose you are at stage k and there is no non-zero entry on or below the diagonal in column k. At this point, there is nothing else you can do, so the algorithm leaves a zero in the diagonal entry of U. Note that the matrix U is singular, and so is the matrix A. Subsequent backward substitutions using U will fail, but the LU factorization itself is still completed.

LU Factorization with Partial Pivoting

$$\boldsymbol{A} = \boldsymbol{PLU}$$

where $\boldsymbol{P}$ is a permutation matrix

$$\boldsymbol{A}\,\boldsymbol{x} = \boldsymbol{b} \;\rightarrow \boldsymbol{PLU}\,\boldsymbol{x} = \boldsymbol{b} \rightarrow \boldsymbol{LU}\,\boldsymbol{x} = \boldsymbol{P}^T\boldsymbol{b}$$

Then solve two triangular systems:

$$\boldsymbol{L}\,\boldsymbol{y} = \boldsymbol{P}^T\boldsymbol{b} \quad \text{(Solve for } \boldsymbol{y}\text{)}$$

$$\boldsymbol{U}\,\boldsymbol{x} = \boldsymbol{y} \quad \text{(Solve for } \boldsymbol{x}\text{)}$$

Example

$$\boldsymbol{A} = \boldsymbol{M} = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 1 & 2 & 3 & 3 \\ 1 & 2 & 3 & 2 \\ 1 & 3 & 4 & 2 \end{pmatrix} \quad \boldsymbol{L} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0 \end{pmatrix} \quad \boldsymbol{U} = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\boldsymbol{M} = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 1 & -2 & 1 & 2.5 \\ 1 & -2 & 1 & 1.5 \\ 1 & -1 & 2 & 1.5 \end{pmatrix} \quad \boldsymbol{L} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0.5 & 1 & 0 & 0 \\ 0.5 & 1 & 0 & 0 \\ 0.5 & 0.5 & 0 & 0 \end{pmatrix} \quad \boldsymbol{U} = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 0 & -2 & 1 & 2.5 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\boldsymbol{M} = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 1 & -2 & 1 & 2.5 \\ 1 & -2 & 0 & -1 \\ 1 & -1 & 1.5 & 0.25 \end{pmatrix} \quad \boldsymbol{L} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0.5 & 1 & 0 & 0 \\ 0.5 & 0.5 & 0 & 0 \\ 0.5 & 1.0 & 0 & 0 \end{pmatrix} \quad \boldsymbol{U} = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 0 & -2 & 1 & 2.5 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\boldsymbol{M} = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 1 & -2 & 1 & 2.5 \\ 1 & -1 & 1.5 & 0.25 \\ 1 & -2 & 0 & -1 \end{pmatrix} \quad \boldsymbol{L} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0.5 & 1 & 0 & 0 \\ 0.5 & 0.5 & 1.0 & 0 \\ 0.5 & 1.0 & 0 & 1.0 \end{pmatrix} \quad \boldsymbol{U} = \begin{pmatrix} 2 & 8 & 4 & 1 \\ 0 & -2 & 1 & 2.5 \\ 0 & 0 & 1.5 & 0.25 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Demo "Pivoting example"

$$\boldsymbol{A} = \begin{pmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{pmatrix}$$

$$\overline{\boldsymbol{A}} = \boldsymbol{PA} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{pmatrix} = \begin{pmatrix} 8 & 7 & 9 & 5 \\ 4 & 3 & 3 & 1 \\ 2 & 1 & 1 & 0 \\ 6 & 7 & 9 & 8 \end{pmatrix}$$

$$\boldsymbol{L} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0 \\ 0.25 & 0 & 0 & 0 \\ 0.75 & 0 & 0 & 0 \end{pmatrix} \qquad \boldsymbol{U} = \begin{pmatrix} 8 & 7 & 9 & 5 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad \boldsymbol{l}_{21}\boldsymbol{u}_{12} = \begin{pmatrix} 3.5 & 4.5 & 2.5 \\ 1.75 & 2.25 & 1.25 \\ 5.25 & 6.75 & 3.75 \end{pmatrix}$$

$$\overline{\boldsymbol{A}} - \boldsymbol{l}_{21}\boldsymbol{u}_{12} = \begin{pmatrix} 8 & 7 & 9 & 5 \\ 4 & -0.5 & -1.5 & -1.5 \\ 2 & -0.75 & -1.25 & -1.25 \\ 6 & 1.75 & 2.25 & 4.25 \end{pmatrix}$$

Demo "Pivoting example"

$$\overline{\boldsymbol{A}} = \overline{\boldsymbol{A}} - \boldsymbol{l}_{21}\boldsymbol{u}_{12} = \begin{pmatrix} 8 & 7 & 9 & 5 \\ 4 & -0.5 & -1.5 & -1.5 \\ 2 & -0.75 & -1.25 & -1.25 \\ 6 & 1.75 & 2.25 & 4.25 \end{pmatrix}$$

$$\overline{\boldsymbol{A}} = \boldsymbol{P}\overline{\boldsymbol{A}} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 8 & 7 & 9 & 5 \\ 6 & 1.75 & 2.25 & 4.25 \\ 2 & -0.75 & -1.25 & -1.25 \\ 4 & -0.5 & -1.5 & -1.5 \end{pmatrix} = \begin{pmatrix} 8 & 7 & 9 & 5 \\ 6 & 1.75 & 2.25 & 4.25 \\ 2 & -0.75 & -1.25 & -1.25 \\ 4 & -0.5 & -1.5 & -1.5 \end{pmatrix}$$

$$\boldsymbol{L} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0.75 & 1 & 0 & 0 \\ 0.25 & -0.428 & 0 & 0 \\ 0.5 & -0.285 & 0 & 0 \end{pmatrix} \quad \boldsymbol{U} = \begin{pmatrix} 8 & 7 & 9 & 5 \\ 0 & 1.75 & 2.25 & 4.25 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \boldsymbol{l}_{21}\boldsymbol{u}_{12} = \begin{pmatrix} -0.963 & -1.819 \\ -0.6412 & -1.2112 \end{pmatrix}$$

$$\overline{\boldsymbol{A}} = \overline{\boldsymbol{A}} - \boldsymbol{l}_{21}\boldsymbol{u}_{12} = \begin{pmatrix} 8 & 7 & 9 & 5 \\ 6 & 1.75 & 2.25 & 4.25 \\ 2 & -0.75 & -0.287 & 0.569 \\ 4 & -0.5 & -0.8587 & -0.2887 \end{pmatrix}$$

Demo "Pivoting example"

$$\bar{\boldsymbol{A}} = \bar{\boldsymbol{A}} - \boldsymbol{l}_{21}\boldsymbol{u}_{12} = \begin{pmatrix} 8 & 7 & 9 & 5 \\ 6 & 1.75 & 2.25 & 4.25 \\ 2 & -0.75 & \boxed{-0.287} & 0.569 \\ 4 & -0.5 & \boxed{-0.8587} & -0.2887 \end{pmatrix}$$

$$\bar{\boldsymbol{A}} = \boldsymbol{P}\bar{\boldsymbol{A}} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 8 & 7 & 9 & 5 \\ 6 & 1.75 & 2.25 & 4.25 \\ 2 & -0.75 & -0.287 & 0.569 \\ 4 & -0.5 & -0.8587 & -0.2887 \end{pmatrix} = \begin{pmatrix} 8 & 7 & 9 & 5 \\ 6 & 1.75 & 2.25 & 4.25 \\ 4 & -0.5 & \boxed{-0.8587} & -0.2887 \\ 2 & -0.75 & \boxed{-0.287} & 0.569 \end{pmatrix}$$

$$\boldsymbol{L} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0.75 & 1 & 0 & 0 \\ {\color{red}0.5} & {\color{red}-0.285} & 1 & 0 \\ {\color{red}0.25} & {\color{red}-0.428} & \boxed{0.334} & 0 \end{pmatrix} \qquad \boldsymbol{U} = \begin{pmatrix} 8 & 7 & 9 & 5 \\ 0 & 1.75 & 2.25 & 4.25 \\ 0 & 0 & -0.86 & \boxed{-0.29} \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\boldsymbol{L} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0.75 & 1 & 0 & 0 \\ 0.5 & -0.285 & 1 & 0 \\ 0.25 & -0.428 & 0.334 & 1 \end{pmatrix} \qquad \boldsymbol{U} = \begin{pmatrix} 8 & 7 & 9 & 5 \\ 0 & 1.75 & 2.25 & 4.25 \\ 0 & 0 & -0.86 & -0.29 \\ 0 & 0 & 0 & 0.67 \end{pmatrix}$$

$$\boldsymbol{P} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$