# Linear equations 1

## Linear algebra basics

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Numerical Methods (6E5X0), 2023-2024

# Today's outline

- Introduction
- Matrix inversion
- Solving a linear system
- Towards larger systems
- Summary

# Overview

**Goals**

- Different ways of looking at a system of linear equations
- Determination of the inverse, determinant and the rank of a matrix
- The existence of a solution to a set of linear equations

# Different views of linear systems

- Separate equations:

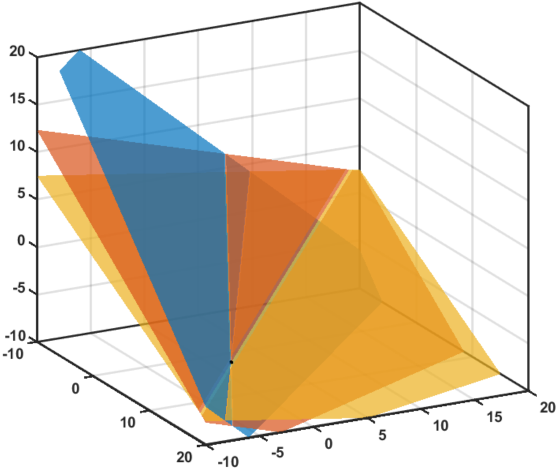
$$\begin{aligned} x+y+z&=4\\ 2x+y+3z&=7\\ 3x+y+6z&=5 \end{aligned}$$

- Matrix mapping $Mx=b$:

$$\begin{bmatrix}1&1&1\\2&1&3\\3&1&6\end{bmatrix}\begin{bmatrix}x\\y\\z\end{bmatrix}=\begin{bmatrix}4\\7\\5\end{bmatrix}$$

- Linear combination:

$$x\begin{bmatrix}1\\2\\3\end{bmatrix}+y\begin{bmatrix}1\\1\\1\end{bmatrix}+z\begin{bmatrix}1\\3\\6\end{bmatrix}=\begin{bmatrix}4\\7\\5\end{bmatrix}$$



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# Inverse of a matrix

- The inverse $M^{-1}$ is defined such that:

$$MM^{-1} = I \quad \text{and} \quad M^{-1}M = I$$

- Use the inverse to solve a set of linear equations:

$$\begin{aligned} M\boldsymbol{x} &= \boldsymbol{b} \\ M^{-1}M\boldsymbol{x} &= M^{-1}\boldsymbol{b} \\ I\boldsymbol{x} &= M^{-1}\boldsymbol{b} \\ \boldsymbol{x} &= M^{-1}\boldsymbol{b} \end{aligned}$$

# How to calculate the inverse?

- The inverse of an $N \times N$ matrix can be calculated using the co-factors of each element of the matrix:

$$M^{-1} = \frac{1}{\det\left|M\right|}\begin{bmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{bmatrix}^T$$

- $\det\left|M\right|$ is the *determinant* of matrix $M$.
- $C_{ij}$ is the *co-factor* of the $ij^{\text{th}}$ element in $M$.

# Computing the co-factors

Consider the following example matrix: $M = \begin{bmatrix} 1 & 1 & 1 \\ 2 & 1 & 3 \\ 3 & 1 & 6 \end{bmatrix}$

A co-factor (e.g. $C_{11}$) is the determinant of the elements left over when you cover up the row and column of the element in question, multiplied by $\pm 1$, depending on the position.

$$\begin{bmatrix} 1 & \times & \times \\ \times & 1 & 3 \\ \times & 1 & 6 \end{bmatrix} \qquad \begin{bmatrix} + & - & + \\ - & + & - \\ + & - & + \end{bmatrix} \qquad C_{11} = +1 \cdot \det \begin{vmatrix} 1 & 3 \\ 1 & 6 \end{vmatrix}$$

$$= 6 \times 1 - 3 \times 1 = 3$$

# Computing the co-factors

Back to our example:

$$M^{-1} = \begin{bmatrix} 1 & 1 & 1 \\ 2 & 1 & 3 \\ 3 & 1 & 6 \end{bmatrix}^{-1} = \frac{1}{\det\left|M\right|} \begin{bmatrix} 3 & -3 & -1 \\ -5 & 3 & 2 \\ 2 & -1 & -1 \end{bmatrix}^{T}$$

- The determinant is very important
- If $\det\left|M\right| = 0$, the inverse does not exist (singular matrix)

# Calculating the determinant

Compute the determinant by multiplication of each element on a row (or column) by its cofactor and adding the results:

$$\det\left(\begin{bmatrix} 1 & 1 & 1 \\ 2 & 1 & 3 \\ 3 & 1 & 6 \end{bmatrix}\right) = +\det\left(\begin{bmatrix} 1 & 3 \\ 1 & 6 \end{bmatrix}\right) - \det\left(\begin{bmatrix} 2 & 3 \\ 3 & 6 \end{bmatrix}\right) + \det\left(\begin{bmatrix} 2 & 1 \\ 3 & 1 \end{bmatrix}\right) = -1$$

$$\det\left(\begin{bmatrix} 1 & 1 & 1 \\ 2 & 1 & 3 \\ 3 & 1 & 6 \end{bmatrix}\right) = +\det\left(\begin{bmatrix} 2 & 1 \\ 3 & 1 \end{bmatrix}\right) - 3\det\left(\begin{bmatrix} 1 & 1 \\ 3 & 1 \end{bmatrix}\right) + 6\det\left(\begin{bmatrix} 1 & 1 \\ 2 & 1 \end{bmatrix}\right) = -1$$

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# Solving a linear system

- Our example:

$$\begin{bmatrix} 1 & 1 & 1 \\ 2 & 1 & 3 \\ 3 & 1 & 6 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 4 \\ 7 \\ 5 \end{bmatrix}$$

- The solution is:

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = M^{-1} b = \frac{1}{-1} \begin{bmatrix} 3 & -5 & 2 \\ -3 & 3 & -1 \\ -1 & 2 & -1 \end{bmatrix} \begin{bmatrix} 4 \\ 7 \\ 5 \end{bmatrix} = \frac{1}{-1} \begin{bmatrix} -13 \\ 4 \\ 5 \end{bmatrix} = \begin{bmatrix} 13 \\ -4 \\ -5 \end{bmatrix}$$

- The inverse exists, because $\det \left| M \right| = -1$.

# Solving a linear system in Python using the inverse

- Create the matrix:

```
>>> A = np.array([[1, 1, 1], [2, 1, 3], [3, 1, 6]])
```

- Create solution vector:

```
>>> b = np.array([4, 7, 5])
```

- Get the matrix inverse:

```
>>> Ainv = np.linalg.inv(A)
```

- Compute the solution:

```
>>> x = np.dot(Ainv, b)
```

- Python's internal direct solver:

```
>>> x = np.linalg.solve(A, b)
```

- These are black boxes! We are going over some methods later!

# Exercise: performance of inverse computation

Create a script that generates matrices with random elements of various sizes $N \times N$ (e.g. values of $N \in \{10, 20, 50, 100, 200, \ldots, 5000, 10000\}$). Compute the inverse of each matrix, and use `tic` and `toc` to see the computing time for each inversion. Plot the time as a function of the matrix size $N$.

---

Hints:

- Create an array that contains the sizes of the systems $n$
- Loop over the array elements to:
  - Create a random matrix of size $n \times n$
  - Perform the matrix inversion
  - Record the time required
- Plot the time required for inversion vs size of the system on a double-log scale

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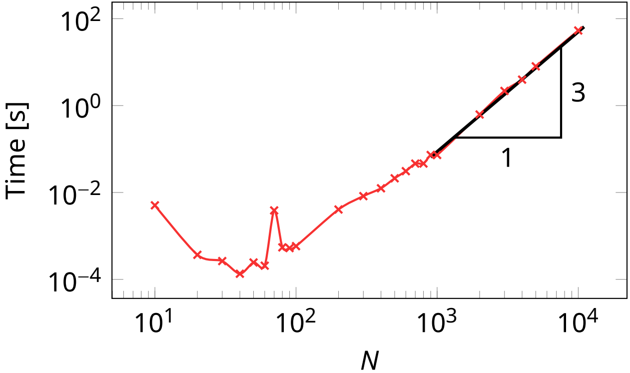
# Exercise: sample results

Each computer produces slightly different results because of background tasks, different matrices, etc. This is especially noticable for small systems.




The time increases by 3 orders of magnitude, for every magnitude in $N$. The *computational complexity* of matrix inversion scales with $\mathcal{O}(N^3)$!

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# Towards larger systems

Computation of determinants and inverses of large matrices in this way is too difficult (slow), so we need other methods to solve large linear systems!

# Towards larger systems

- Determinant of upper triangular matrix:

$$\det\left|M_{\text{tri}}\right| = \prod_{i=1}^{n} a_{ii} \qquad M = \begin{bmatrix} 5 & 3 & 2 \\ 0 & 9 & 1 \\ 0 & 0 & 1 \end{bmatrix} \Rightarrow \det\left|M\right| = 5 \times 9 \times 1 = 45$$

- Matrix multiplication:

$$\det\left|AM\right| = \det\left|A\right| \times \det\left|M\right|$$

- When $A$ is an identity matrix ($\det\left|A\right| = 1$):

$$\det\left|AM\right| = \det\left|A\right| \times \det\left|M\right| = 1 \times \det\left|M\right|$$

- With rules like this, we can use row-operations so that we can compute the determinant more cheaply.

# Solutions of linear systems

Rank of a matrix: the number of linearly independent columns (columns that can not be expressed as a linear combination of the other columns) of a matrix.

$$M = \begin{bmatrix} 5 & 3 & 2 \\ 0 & 9 & 1 \\ 0 & 0 & 1 \end{bmatrix}$$

- 3 independent columns
- In Python:

```
>>> numpy.linalg.matrix_rank(M)
```

$$M = \begin{bmatrix} 1 & 2 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

- col 2 $=2\times$ col 1
- col 4 $=$ col 3 $-$ col 1
- 2 independent columns: rank = 2

# Solutions of linear systems

The solution of a system of linear equations may or may not exist, and it may or may not be unique. Existence of solutions can be determined by comparing the rank of the Matrix $M$ with the rank of the augmented matrix $M_a$:

```
>>> numpy.linalg.matrix_rank(A)
>>> numpy.linalg.matrix_rank(np.column_stack((A,b))) # Concatenated matrices
```

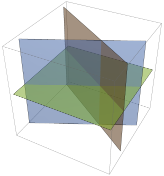
Our system: $Mx = b$

$$M = \begin{bmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{bmatrix}, b = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \Rightarrow M_a = \begin{bmatrix} M_{11} & M_{12} & M_{13} & b_1 \\ M_{21} & M_{22} & M_{23} & b_2 \\ M_{31} & M_{32} & M_{33} & b_3 \end{bmatrix}$$

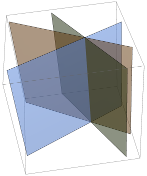
# Existence of solutions for linear systems

For a matrix $M$ of size $n \times n$, and augmented matrix $M_a$:

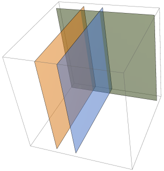
- $\text{Rank}(M) = n$:
  Unique solution

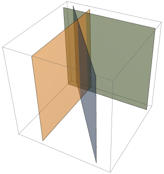


- $\text{Rank}(M) = \text{Rank}(M_a) < n$:
  Infinite number of solutions



- $\text{Rank}(M) < n$, $\text{Rank}(M) < \text{Rank}(M_a)$:
  No solutions





# Two examples

$$M = \begin{bmatrix} 1 & 1 & 2 \\ 0 & 3 & 1 \\ 0 & 0 & 2 \end{bmatrix} \quad b = \begin{bmatrix} 17 \\ 11 \\ 4 \end{bmatrix} \Rightarrow M_a = \begin{bmatrix} 1 & 1 & 2 & 17 \\ 0 & 3 & 1 & 11 \\ 0 & 0 & 2 & 4 \end{bmatrix}$$

$\text{rank}(M) = 3 = n \Rightarrow$ Unique solution

$$M = \begin{bmatrix} 1 & 1 & 2 \\ 0 & 3 & 1 \\ 0 & 0 & 0 \end{bmatrix} \quad b = \begin{bmatrix} 17 \\ 11 \\ 0 \end{bmatrix} \Rightarrow M_a = \begin{bmatrix} 1 & 1 & 2 & 17 \\ 0 & 3 & 1 & 11 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$\text{rank}(M) = \text{rank}(M_a) = 2 < n \Rightarrow$ Infinite number of solutions

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# Summary

- Linear equations can be written as matrices
- Using the inverse, the solution can be determined
  - Inverse via cofactors
  - Inverse and solution in Python
- Introduced the concept of computational complexity: matrix inversion scales with $N^3$
- A solution depends on the rank of a matrix

# Linear equations 2

## Direct methods

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# Overview

## Goals

Today we are going to write a program, which can solve a set of linear equations

- The first method is called Gaussian elimination
- We will encounter some problems with Gaussian elimination
- Then LU decomposition will be introduced

# Today's outline

- Introduction
- **Gauss elimination**
- Partial Pivoting
- LU decomposition
- Summary

# Define the linear system

Consider the system:

$$Ax = b$$

In general:

$$\begin{bmatrix} A_{00} & A_{01} & A_{02} \\ A_{10} & A_{11} & A_{12} \\ A_{20} & A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \end{bmatrix}$$

Desired solution:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_0' \\ b_1' \\ b_2' \end{bmatrix}$$

# Using row operations

- Use row operations to simplify the system. Eliminate element $A_{10}$ by subtracting $A_{10}/A_{00} = d_{10}$ times row 1 from row 2.
- In this case, Row 1 is the pivot row, and $A_{00}$ is the pivot element.

$$\left[\begin{array}{ccc|c} A_{00} & A_{01} & A_{02} & b_0 \\ A_{10} & A_{11} & A_{12} & b_1 \\ A_{20} & A_{21} & A_{22} & b_2 \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} A_{00} & A_{01} & A_{02} & b_0 \\ 0 & A'_{11} & A'_{12} & b'_1 \\ A_{20} & A_{21} & A_{22} & b_2 \end{array}\right]$$

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# Using row operations

Eliminate element $A_{10}$ using $d_{10} = A_{10}/A_{00}$.

$$\left[\begin{array}{ccc|c} A_{00} & A_{01} & A_{02} & b_0 \\ A_{10} & A_{11} & A_{12} & b_1 \\ A_{20} & A_{21} & A_{22} & b_2 \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} A_{00} & A_{01} & A_{02} & b_0 \\ 0 & A'_{11} & A'_{12} & b'_1 \\ A_{20} & A_{21} & A_{22} & b_2 \end{array}\right]$$

- $d_{10} \to A_{10}/A_{00}$
- $A_{10} \to A_{10} - A_{00} d_{10}$
- $A_{11} \to A_{11} - A_{01} d_{10}$
- $A_{12} \to A_{12} - A_{02} d_{10}$
- $b_1 \to b_1 - b_0 d_{10}$

```
d10 = A[1,0] / A[0,0]

A[1,0] = A[1,0] - A[0,0] * d10
A[1,1] = A[1,1] - A[0,1] * d10
A[1,2] = A[1,2] - A[0,2] * d10

b[1] = b[1] - b[0] * d10
```

# Using row operations

Eliminate element $A_{20}$ using $d_{20} = A_{20}/A_{00}$.

$$\left[\begin{array}{ccc|c} A_{00} & A_{01} & A_{02} & b_0 \\ 0 & A'_{11} & A'_{12} & b'_1 \\ A_{20} & A_{21} & A_{22} & b_2 \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} A_{00} & A_{01} & A_{02} & b_0 \\ 0 & A'_{11} & A'_{12} & b'_1 \\ 0 & A'_{21} & A'_{22} & b'_2 \end{array}\right]$$

- $d_{20} \to A_{20}/A_{00}$
- $A_{20} \to A_{20} - A_{00}d_{20}$
- $A_{21} \to A_{21} - A_{01}d_{20}$
- $A_{22} \to A_{22} - A_{02}d_{20}$
- $b_2 \to b_2 - b_0d_{20}$

```
d20 = A[2, 0] / A[0, 0]

A[2, 0] = A[2, 0] - A[0, 0] * d20
A[2, 1] = A[2, 1] - A[0, 1] * d20
A[2, 2] = A[2, 2] - A[0, 2] * d20
b[2] = b[2] - b[0] * d20
```

# Using row operations

Eliminate element $A'_{21}$ using $d_{21} = A'_{21}/A'_{11}$. Note that now the second row has become the pivot row.

$$\left[\begin{array}{ccc|c} A_{00} & A_{01} & A_{02} & b_0 \\ 0 & A'_{11} & A'_{12} & b'_1 \\ 0 & A'_{21} & A'_{22} & b'_2 \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} A_{00} & A_{01} & A_{02} & b_0 \\ 0 & A'_{11} & A'_{12} & b'_1 \\ 0 & 0 & A''_{22} & b''_2 \end{array}\right]$$

- $d_{21} \to A_{21}/A'_{11}$
- $A_{21} \to A_{21} - A'_{11} d_{21}$
- $A_{22} \to A_{22} - A'_{12} d_{21}$
- $b_2 \to b_2 - b'_2 d_{21}$

```
d21 = A[2, 1] / A[1, 1]
A[2, 1] = A[2, 1] - A[1, 1] * d21
A[2, 2] = A[2, 2] - A[1, 2] * d21
b[2] = b[2] - b[1] * d21
```

The matrix is now a triangular matrix — the solution can be obtained by back-substitution.

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# Backsubstitution

The system now reads:

$$\begin{bmatrix} A_{00} & A_{01} & A_{02} \\ 0 & A'_{11} & A'_{12} \\ 0 & 0 & A''_{22} \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_0 \\ b'_1 \\ b''_2 \end{bmatrix}$$

Start at the last row $N$, and work upward until row 1.

$$x_2 = b''_2 / A''_{22}$$
$$x_1 = (b'_1 - A'_{12} x_2)/A'_{11}$$
$$x_0 = (b_0 - A_{01} x_1 - A_{02} x_2)/A_{00}$$

```
x = np.empty_like(b)
x[2] = b[2] / A[2,2]
x[1] = (b[1] - A[1,2] * x[2]) / A[1,1]
x[0] = (b[0] - A[0,1] * x[1] - A[0,2] * x[2]) / A[0,0]
```

In general:

$$x_N = \frac{b_N}{A_{NN}} \qquad x_i = \frac{b_i - \sum_{j=i+1}^{N} A_{ij} x_j}{A_{ii}}$$

# Writing the program

- Create a function that provides the framework: take matrix $A$ and vector $b$ as an input, and return the solution $x$ as output:

```python
def gaussian_eliminate(A, b):
    pass  # Your implementation here
```

- We will use *for-loops* instead of typing out each command line.
- Useful Python (with NumPy) shortcuts:
    - `A[0, :]` = $[A_{00}, A_{01}, A_{02}]$
    - `A[:, 1]` = $[A_{01}, A_{11}, A_{21}]$
    - `A[0, 1:]` = $[A_{01}, A_{02}]$
- A row operation could look like:

```python
A[i, :] = A[i, :] - d * A[0, :]
```

# The program: elimination step

An initial draft could look like:

```python
def gaussian_eliminate_draft(A,b):
    """Perform elimination to obtain an upper triangular matrix"""
    A = np.array(A,dtype=np.float64)
    b = np.array(b,dtype=np.float64)

    assert A.shape[0] == A.shape[1], "Coefficient matrix should be square"

    N = len(b)
    for col in range(N-1):                  # Select pivot
        for row in range(col+1,N):          # Loop over rows below pivot
            d = A[row,col] / A[col,col]     # Choose elimination factor
            for element in range(row,N):    # Elements from diagonal to right
                A[row,element] = A[row,element] - d * A[col,element]
            b[row] = b[row] - d * b[col]

    return A,b
```

# The program: elimination step

Employing some of the row operations to create `gaussian_eliminate_v1`:

```python
for element in range(row,N):
    A[row,element] = A[row,element] - d * A[col,element]
```

```python
A[row,:] = A[row,:] - d * A[col,:]
```

```python
def gaussian_eliminate_v1(A,b):
    A = np.array(A,dtype=np.float64)
    b = np.array(b,dtype=np.float64)

    assert A.shape[0] == A.shape[1], "Coefficient matrix should be square"

    N = len(b)
    for col in range(N-1):
        for row in range(col+1,N):
            d = A[row,col] / A[col,col]
            A[row,:] = A[row,:] - d * A[col,:]
            b[row] = b[row] - d * b[col]

    return A,b
```

# Testing

Let's try to eliminate our linear system! If you create/downloaded our file `gaussjordan.py`, you can access the functions by importing them. The file should be stored where your own code/notebook is:

```
from gaussjordan import gaussian_eliminate_draft,gaussian_eliminate_v1
import numpy as np

A = np.array([[1, 1, 1], [2, 1, 3], [3, 1, 6]])
b = np.array([4, 7, 5])

Aprime,bprime = gaussian_eliminate_draft(A,b)
print(Aprime)
print(bprime)
```

# The program: Backsubstitution

Now we have elimination working, let's create a back substitution algorithm too. Recall:

$$x_N = \frac{b_N}{A_{NN}} \qquad x_i = \frac{b_i - \sum_{j=i+1}^{N} A_{ij}x_j}{A_{ii}}$$

```python
def backsubstitution_draft(A, b):
    """Back substitutes an upper triangular matrix to
          find x in Ax=b"""
    x = np.copy(b)
    N = len(b)

    for row in range(N-1, -1, -1):
        for i in range(row+1, N):
            x[row] = x[row] - A[row, i] * x[i]
        x[row] = x[row] / A[row, row]

    return x
```

```python
def backsubstitution_v1(A,b):
    """Back substitutes an upper triangular matrix to find x in Ax=b"""
    x = np.empty_like(b)
    N = len(b)

    for row in range(N)[::-1]:
        x[row] = (b[row] - np.sum(A[row,row+1:] * x[row+1:])) / A[row,row]

    return x
```

# A full Gauss Elimination solver

- The functions we just built are distributed via Canvas too
- Use `help GaussianEliminate` to find out how it works
- Solve the following system of equations:

$$\begin{bmatrix} 9 & 9 & 5 & 2 \\ 6 & 7 & 1 & 3 \\ 6 & 4 & 3 & 5 \\ 2 & 6 & 2 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 7 \\ 4 \\ 10 \\ 1 \end{bmatrix}$$

- Compare your solution with `np.linalg.solve(A,b)`

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# Partial pivoting

- Now try to run the algorithm with the following system:

$$\begin{bmatrix} 0 & 2 & 1 \\ 3 & 2 & 1 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 4 \\ 3 \\ 10 \end{bmatrix}$$

- It does not work! Division by zero, due to $A_{11} = 0$.
- Solution: Swap rows to move largest element to the diagonal.

# Partial pivoting: implementing row swaps

- Find maximum element row below pivot in current column

```
index = np.argmax(np.abs(A[col:, col])) + col
```

- Store current row

```
temp = A[column,:]
```

- Swap pivot row and desired row in `A`

```
A[column,:] = A[index,:]
A[index,:] = temp
```

- Do the same for `b` — store and swap

```
temp = b[column]
b[column] = b[index]
b[index] = temp
```

# Adding the partial pivoting rules

```python
def gaussian_eliminate_partial_pivot(A,b):
    A = np.array(A,dtype=np.float64)
    b = np.array(b,dtype=np.float64)

    assert A.shape[0] == A.shape[1], "Coefficient matrix should be square"

    N = len(b)
    for col in range(N-1):
        index = np.argmax(np.abs(A[col:, col])) + col
        temp = A[col,:]
        A[col,:] = A[index,:]
        A[index,:] = temp

        temp = b[col]
        b[col] = b[index]
        b[index] = temp
        for row in range(col+1,N):
            d = A[row,col] / A[col,col]
            A[row,:] = A[row,:] - d * A[col,:]
            b[row] = b[row] - d * b[col]

    return A,b
```

# Improve the program by using re-usable functions

```python
def swap_rows(mat,i1,i2):
    """Swap two rows in a matrix/vector"""
    temp = mat[i1,...].copy()
    mat[i1,...] = mat[i2,...]
    mat[i2,...] = temp
```

```python
def gaussian_eliminate_v2(A,b):
    A = np.array(A,dtype=np.float64)
    b = np.array(b,dtype=np.float64)

    assert A.shape[0] == A.shape[1], "Coefficient matrix should be square"

    N = len(b)
    for col in range(N-1):
        index = np.argmax(np.abs(A[col:, col])) + col
        swap_rows(A,col,index)
        swap_rows(b,col,index)
        for row in range(col+1,N):
            d = A[row,col] / A[col,col]
            A[row,:] = A[row,:] - d * A[col,:]
            b[row] = b[row] - d * b[col]

    return A,b
```

# Alternatives to this program

- Python can compute the solution to Ax=b with `scipy.linalg.solve` or `numpy.linalg.solve` solvers (more efficient)
- Too many loops. Loops make Python slow.
- There are fundamental problems with Gaussian elimination
  - You can add a counter to the algorithm to see how many subtraction and multiplication operations it performs for a given size of matrix A.
  - The number of operations to perform Gaussian elimination is $\mathcal{O}(2N^3)$ (where $N$ is the number of equations)
  - Exercise: verify this for our script
  - LU decomposition takes $\mathcal{O}(2N^3/3)$ flops, 3 times less!
  - Forward and backward substitution each take $\mathcal{O}(N^2)$ flops (both cases)

# Today's outline



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# LU Decomposition

Suppose we want to solve the previous set of equations, but with several right hand sides:

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} \begin{bmatrix} \vdots & \vdots & \vdots \\ x_1 & x_2 & x_3 \\ \vdots & \vdots & \vdots \end{bmatrix} = \begin{bmatrix} \vdots & \vdots & \vdots \\ b_1 & b_2 & b_3 \\ \vdots & \vdots & \vdots \end{bmatrix}$$

Factor the matrix A into two matrices, L and U, such that $A = LU$:

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ \times & 1 & 0 \\ \times & \times & 1 \end{bmatrix} \begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \end{bmatrix}$$

Now we can solve for each right hand side, using only a forward followed by a backward substitution!

# Substitutions

- Define a lower and upper matrix $L$ and $U$ so that $A = LU$
- Therefore $LUx = b$
- Define a new vector $y = Ux$ so that $Ly = b$
- Solve for $y$, use $L$ and forward substitution
- Then we have $y$, solve for $x$, use $Ux = y$
- Solve for $x$, use $U$ and backward substitution
- But how to get L and U?

# Decomposing the matrix (1)

When we eliminate the element $A_{21}$ we can keep multiplying by a matrix that undoes this row operations, so that the product remains equal to $A$.

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ d_{21} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ 0 & A_{22} - d_{21}A_{12} & A_{23} - d_{21}A_{13} \\ A_{31} & A_{32} & A_{33} \end{bmatrix}$$

# Decomposing the matrix (2)

When we eliminate the element $A_{31}$ we can keep multiplying by a matrix that undoes this row operations, so that the product remains equal to $A$.

$$A = \begin{bmatrix} 1 & 0 & 0 \\ d_{21} & 1 & 0 \\ d_{31} & 0 & 1 \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ 0 & A'_{22} = A_{22} - d_{21}A_{12} & A'_{23} = A_{23} - d_{21}A_{13} \\ 0 & A'_{32} = A_{32} - d_{31}A_{12} & A'_{33} = A_{33} - d_{31}A_{21} \end{bmatrix}$$

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# Decomposing the matrix (3)

When we eliminate the element $A_{32}$ we can keep multiplying by a matrix that undoes this row operations, so that the product remains equal to $A$.

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ d_{21} & 1 & 0 \\ d_{31} & d_{32} & 1 \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ 0 & A'_{22} & A'_{23} \\ 0 & 0 & A''_{33} = A'_{33} - d_{32}A'_{23} \end{bmatrix}$$

We now have a lower matrix $L$ and an upper matrix $U$. This finishes the LU decomposition!

# Pivoting during decomposition

Suppose we have arrived at the situation below, where $A'_{32} > A'_{22}$:

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ d_{21} & 1 & 0 \\ d_{31} & 0 & 1 \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ 0 & A'_{22} & A'_{23} \\ 0 & A'_{32} & A'_{33} \end{bmatrix}$$

Exchange rows 2 and 3 to get the largest value on the main diagonal. Use a permutation matrix to store the swapped rows:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ d_{31} & 0 & 1 \\ d_{21} & 1 & 0 \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ 0 & A'_{32} & A'_{33} \\ 0 & A'_{22} & A'_{23} \end{bmatrix}$$

Multiplying with a permutation matrix will swap the rows of a matrix. The permutation matrix is just an identity matrix, whose rows have been interchanged.

# Recipe for LU decomposition

When decomposing matrix $A$ into $A = LU$, it may be beneficial to swap rows to get the largest values on the diagonal of $U$ (pivoting). A permutation matrix $P$ is used to store row swapping such that:

$$PA = LU$$

- Write down a permutation matrix and the linear system
- Promote the largest value in the column diagonal
- Eliminate all elements below diagonal
- Move on to the next column and move largest elements to diagonal
- Eliminate elements below diagonal
- Repeat 5 and 6
- Write down L,U and P

# LU decomposition example (1)

Write down a permutation matrix, which starts as the identity matrix, and the linear system:

$$PA = LU$$

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

Promote the largest value into the diagonal of column 1 — swap row 1 and 2:

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

# LU decomposition example (2)

Eliminate all elements below the diagonal — row 2 already contains a zero in column 1, row 3 = row 3 - 0.5 row 1. Record the multiplier 0.5 in $L$:

$$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 & 1 \\ 2 & 1 & 1 \\ 1 & 2 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0.5 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & 1.5 & -0.5 \end{bmatrix}$$

Elimination of column 1 is done. Now step to the next column, and move the largest value below/on the diagonal to the diagonal (swap rows 2 and 3). Adjust $P$ and the lower triangle of $L$ accordingly:

$$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 1 \\ 2 & 1 & 0 \\ 1 & 2 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0.5 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 \\ 0 & 1.5 & -0.5 \\ 0 & 1 & 1 \end{bmatrix}$$

# LU decomposition example (3)

Eliminate all elements below the diagonal —
row 3 = row 3 - $\frac{2}{3}$row 2. Record the multiplier $\frac{2}{3}$ in $L$:

$$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 1 \\ 2 & 1 & 0 \\ 1 & 2 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0.5 & 1 & 0 \\ 0 & \frac{2}{3} & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 \\ 0 & 1.5 & -0.5 \\ 0 & 0 & \frac{4}{3} \end{bmatrix}$$

We have obtained the matrices from $PA = LU$:

$$P = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \quad L = \begin{bmatrix} 1 & 0 & 0 \\ 0.5 & 1 & 0 \\ 0 & \frac{2}{3} & 1 \end{bmatrix} \quad U = \begin{bmatrix} 2 & 1 & 1 \\ 0 & 1.5 & -0.5 \\ 0 & 0 & \frac{4}{3} \end{bmatrix}$$

Proceed with solving for $x$.

# Substitutions

$$Ax = b \quad \Rightarrow \quad PAx = Pb \equiv d$$
$$PA = LU \quad \Rightarrow \quad LUx = d$$

- Define a new vector $y = Ux$
  - $Ly = b \quad \Rightarrow \quad Ly = d$
  - Solve for $y$, forward substitution:

$$y_0 = \frac{d_0}{L_{00}}$$
$$y_i = \frac{d_i - \sum_{j=0}^{i} L_{ij} y_j}{L_{ii}}$$

- Then solve $Ux = y$:
  - Solve for $x$, backward substitution:

$$x_N = \frac{y_N}{U_{NN}}$$
$$x_i = \frac{y_i - \sum_{j=i+1}^{N} U_{ij} x_j}{U_{ii}}$$

# How to use the solver in Python

```python
import numpy as np
from scipy.linalg import lu
from gaussjordan import backsubstitution_v1 as backwardSub
from gaussjordan import forwardsubstitution as forwardSub

# Example usage
A = np.random.rand(5, 5)  # Get random matrix
P, L, U = lu(A)           # Get L, U and P
b = np.random.rand(5)     # Random b vector
d = P @ b                 # Permute b vector
y = forwardSub(L, d)      # Can also do y=L\d
x = backwardSub(U, y)     # Can also do x=U\y
rnorm = np.linalg.norm(A @ x - b)  # Residual
```

- Use this as a basis to create a function that takes $A$ and $b$, and returns $x$.
- Use the function to check the performance for various matrix sizes and inspect the performance.

# Today's outline

- Introduction
- Gauss elimination
- Partial Pivoting
- LU decomposition
- Summary

# Summary

- This lecture covered direct methods using elimination techniques.
- Gaussian elimination can be slow ($\mathcal{O}(N^3)$)
- Back substitution is often faster ($\mathcal{O}(N^2)$)
- LU decomposition means that we don't have to do Gaussian elimination every time (saves time and effort), but the matrix has to stay the same.
- Python's libraries have built in routines for solving linear equations and LU decomposition.
- Advanced techniques such as (preconditioned) conjugate gradient or biconjugate gradient solvers are also available.
- Next part covers iterative approaches