Linear equations 1

Linear algebra basics

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Numerical Methods (6E5X0), 2022-2023

Today's outline

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

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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:

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

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 $Mx = b$:

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

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- 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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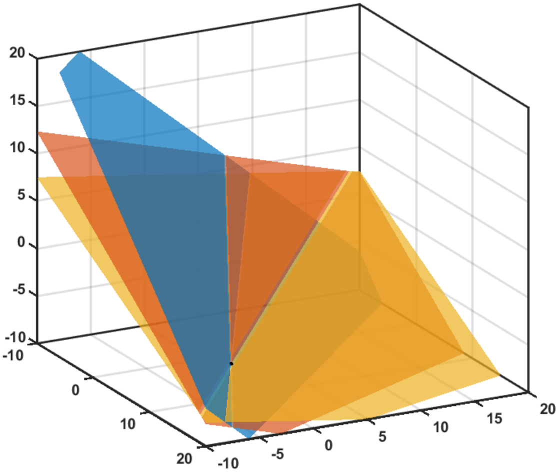

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Inverse of a matrix

- 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^{th} element in M.

Computing the co-factors

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

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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 ± 1, depending on the position.

$$\begin{bmatrix} 1 & \times & \times \\ \times & 1 & 3 \\ \times & 1 & 6 \end{bmatrix}$$

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$$\begin{bmatrix} \boxed{1} & \times & \times \\ \times & 1 & 3 \\ \times & 1 & 6 \end{bmatrix} \qquad \begin{bmatrix} \boxed{+} & - & + \\ - & + & - \\ + & - & + \end{bmatrix}$$

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

Computing the co-factors

Back to our example:

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

Computing the co-factors

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- 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:

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

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:

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

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- The solution is:

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

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

Solving a linear system in Matlab using the inverse

- Create the matrix:

```
>> A = [1 1 1; 2 1 3; 3 1 6];
```

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>> Ainv = inv(A);
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>> x = Ainv * b
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- Matlab's internal direct solver:

```
>> x = 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 $N \in \{10, 20, 50, 100, 200, \dots, 5000, 10000\}$). 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.

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```
% Generate random matrices of various sizes 's'.
% Invert the matrices and store the time required
% for the inversion. Plot the times vs 's'
s = [10:10:90 100:100:1000 2000:1000:5000 10000]
for n = 1:length(s)
```

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    s(n)
    A = rand(s(n));
```

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```
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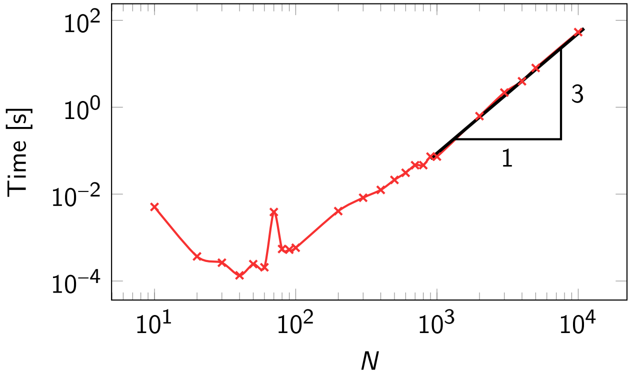
s = [10:10:90 100:100:1000 2000:1000:5000 10000]
for n = 1:length(s)
    s(n)
    A = rand(s(n));
    tic;
    Ainv = inv(A);
    t_inv(n) = toc;
end
loglog(s,t_inv)
xlabel('N')
ylabel('Time [s]')
```

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 $\mathcal{O}(N^3)$!

Solving a linear system in Excel using the inverse

$$Ax = b \qquad \begin{bmatrix} 1 & 1 & 1 \\ 2 & 1 & 3 \\ 3 & 1 & 6 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 4 \\ 7 \\ 5 \end{bmatrix}$$

- Create matrix A in 3×3 cells
- Create right hand side vector b in 3 vertical cells

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- Create matrix A in 3×3 cells
- Create right hand side vector b in 3 vertical cells
- Compute the inverse I :
  - Select an empty area of 3×3 cells
  - Type `=MINVERSE( B2:D4 )` (In Dutch Excel: `INVERSEMAT`)
  - Close with Ctrl+Shift+Enter

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  - Type `=MINVERSE(B2:D4)` (In Dutch Excel: `INVERSEMAT`)
  - Close with Ctrl+Shift+Enter
- Solution:
  - Select 3 vertical cells
  - Type `=MMULT(H2:J4;B6:B8)` (In Dutch Excel: `PRODUCTMAT`. The semicolon may be a comma.)
  - Close with Ctrl+Shift+Enter

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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 Matlab:

```
>> rank(M)
```

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

- col 2 = 2× 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:

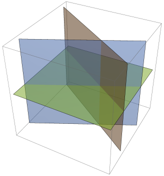
```
>> rank(A)
>> rank([A b])
```

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

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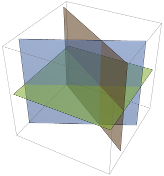
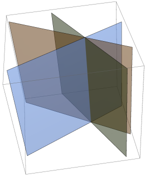


- $\text{Rank}(M) = \text{Rank}(M_a) < n$:
  Infinite number of solutions



Existence of solutions for linear systems

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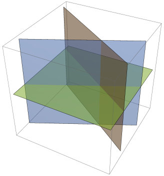

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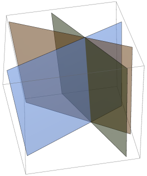
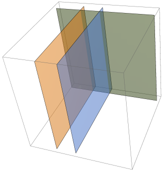
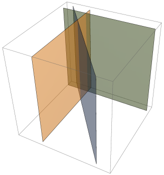


- Rank$(M) < n$, Rank$(M) <$ Rank(M_a):
  No solutions





Two examples

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

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

Two examples

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

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$\mathrm{rank}(M) = \mathrm{rank}(M_a) = 2 < n \Rightarrow$ 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 Matlab
  - Inverse and solution in Excel
- 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

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Define the linear system

Consider the system:

$$Ax = b$$

In general:

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

Desired solution:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1' \\ b_2' \\ b_3' \end{bmatrix}$$

Using row operations

- Use row operations to simplify the system. Eliminate element A_{21} by subtracting $A_{21}/A_{11} = d_{21}$ times row 1 from row 2.
- In this case, Row 1 is the pivot row, and A_{11} is the pivot element.

$$\left[\begin{array}{ccc|c} A_{11} & A_{12} & A_{13} & b_1 \\ A_{21} & A_{22} & A_{23} & b_2 \\ A_{31} & A_{32} & A_{33} & b_3 \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ A_{31} & A_{32} & A_{33} & b_3 \end{array}\right]$$

Using row operations

Eliminate element A_{21} using $d_{21} = A_{21}/A_{11}$.

$$\left[\begin{array}{ccc|c} A_{11} & A_{12} & A_{13} & b_1 \\ A_{21} & A_{22} & A_{23} & b_2 \\ A_{31} & A_{32} & A_{33} & b_3 \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ A_{31} & A_{32} & A_{33} & b_3 \end{array}\right]$$

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- $d_{21} \rightarrow A_{21}/A_{11}$
- $A_{21} \rightarrow A_{21} - A_{11}d_{21}$
- $A_{22} \rightarrow A_{22} - A_{12}d_{21}$
- $A_{23} \rightarrow A_{23} - A_{13}d_{21}$
- $b_2 \rightarrow b_2 - b_1 d_{21}$

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Using row operations

Eliminate element A_{21} using $d_{21} = A_{21}/A_{11}$.

$$\left[\begin{array}{ccc|c} A_{11} & A_{12} & A_{13} & b_1 \\ A_{21} & A_{22} & A_{23} & b_2 \\ A_{31} & A_{32} & A_{33} & b_3 \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ A_{31} & A_{32} & A_{33} & b_3 \end{array}\right]$$

- $d_{21} \to A_{21}/A_{11}$
- $A_{21} \to A_{21} - A_{11} d_{21}$
- $A_{22} \to A_{22} - A_{12} d_{21}$
- $A_{23} \to A_{23} - A_{13} d_{21}$
- $b_2 \to b_2 - b_1 d_{21}$

```
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;
A(2,3) = A(2,3) - A(1,3)*d21;
b(2) = b(2) - b(1)*d21;
```

Using row operations

Eliminate element A_{31} using $d_{31} = A_{31}/A_{11}$.

$$\left[\begin{array}{ccc|c} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ A_{31} & A_{32} & A_{33} & b_3 \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ 0 & A'_{32} & A'_{33} & b'_3 \end{array}\right]$$

Using row operations

Eliminate element A_{31} using $d_{31} = A_{31}/A_{11}$.

$$\left[\begin{array}{ccc|c} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ A_{31} & A_{32} & A_{33} & b_3 \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ 0 & A'_{32} & A'_{33} & b'_3 \end{array}\right]$$

- $d_{31} \to A_{31}/A_{11}$
- $A_{31} \to A_{31} - A_{11} d_{31}$
- $A_{32} \to A_{32} - A_{12} d_{31}$
- $A_{33} \to A_{33} - A_{13} d_{31}$
- $b_3 \to b_3 - b_1 d_{31}$

```
d31 = A(3,1)/A(1,1);
A(3,1) = A(3,1) - A(1,1)*d31;
A(3,2) = A(3,2) - A(1,2)*d31;
A(3,3) = A(3,3) - A(1,3)*d31;
b(3) = b(3) - b(1)*d31;
```

Using row operations

Eliminate element A_{32} using $d_{32} = A_{32}/A'_{22}$. Note that now the second row has become the pivot row.

$$\left[\begin{array}{ccc|c} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ 0 & A_{32} & A_{33} & b_3 \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ 0 & 0 & A''_{33} & b''_3 \end{array}\right]$$

Using row operations

Eliminate element A_{32} using $d_{32} = A_{32}/A'_{22}$. Note that now the second row has become the pivot row.

$$\left[\begin{array}{ccc|c} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ 0 & A_{32} & A_{33} & b_3 \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ 0 & 0 & A''_{33} & b''_3 \end{array}\right]$$

- $d_{32} \to A_{32}/A'_{22}$
- $A_{32} \to A_{32} - A'_{22} d_{32}$
- $A_{33} \to A_{33} - A'_{23} d_{32}$
- $b_3 \to b_3 - b'_2 d_{32}$

```
d32 = A(3,2)/A(2,2);
A(3,2) = A(3,1) - A(2,2)*d32;
A(3,3) = A(3,2) - A(2,3)*d32;
b(3) = b(3) - b(2)*d32;
```

Using row operations

Eliminate element A_{32} using $d_{32} = A_{32}/A'_{22}$. Note that now the second row has become the pivot row.

$$\left[\begin{array}{ccc|c} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ 0 & A_{32} & A_{33} & b_3 \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ 0 & 0 & A''_{33} & b''_3 \end{array}\right]$$

- $d_{32} \to A_{32}/A'_{22}$
- $A_{32} \to A_{32} - A'_{22} d_{32}$
- $A_{33} \to A_{33} - A'_{23} d_{32}$
- $b_3 \to b_3 - b'_2 d_{32}$

```
d32 = A(3,2)/A(2,2);
A(3,2) = A(3,1) - A(2,2)*d32;
A(3,3) = A(3,2) - A(2,3)*d32;
b(3) = b(3) - b(2)*d32;
```

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

Backsubstitution

The system now reads:

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ 0 & A'_{22} & A'_{23} \\ 0 & 0 & A''_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b'_2 \\ b''_3 \end{bmatrix}$$

Backsubstitution

The system now reads:

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ 0 & A'_{22} & A'_{23} \\ 0 & 0 & A''_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b'_2 \\ b''_3 \end{bmatrix}$$

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

$$x_3 = b''_3 / A''_{33}$$
$$x_2 = (b'_2 - A'_{23}x_3)/A'_{22}$$
$$x_1 = (b_1 - A_{12}x_2 - A_{13}x_3)/A_{11}$$

Backsubstitution

The system now reads:

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ 0 & A'_{22} & A'_{23} \\ 0 & 0 & A''_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b'_2 \\ b''_3 \end{bmatrix}$$

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

$$x_3 = b''_3 / A''_{33}$$
$$x_2 = (b'_2 - A'_{23} x_3)/A'_{22}$$
$$x_1 = (b_1 - A_{12} x_2 - A_{13} x_3)/A_{11}$$

```
x(3) = b(3) / A(3,3)
x(2) = (b(2) - A(2,3)*x(3)) /A(2,2)
x(1) = (b(1) - A(1,2)*x(2) - A(1,3)*x(3)) / A(1,1)
```

In general:

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

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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:

```
function [x,A,b] = GaussianEliminate(A,b)
```

- We will use *for-loops* instead of typing out each command line.
- Useful Matlab shortcuts:
  - `A(1,:)` $= [A_{11}, A_{12}, A_{13}]$
  - `A(:,2)` $= [A_{12}, A_{22}, A_{32}]^T$
  - `A(1,2:end)` $= [A_{12}, A_{13}]$
- A row operation could look like:

```
A(i,:) = A(i,:) - d*A(1,:)
```

The program: elimination

```
function [x,A,b] = GaussianEliminate(A,b)

% Perform elimination to obtain an upper triangular matrix
N = length(b);
for column=1:(N-1) % Select pivot
    for row=(column+1):N % Loop over subsequent rows (below pivot)
        d=A(row,column)/A(column,column);
        A(row,:)=A(row,:)-d*A(column,:);
        b(row)= b(row)-d*b(column);
    end
end
```

The program: Backsubstitution

```
% Assign b to x
x=b;

% Perform backsubstitution
for row=N:-1:1
    x(row) = b(row);
    for i =(row+1):N
        x(row)=x(row)-A(row,i)*x(i);
    end
    x(row)=x(row)/A(row,row);
end
```

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

Exercise: Gaussian Elimination

- The function we just made can be found on Canvas
- 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 `A\b`

Today's outline

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

Partial pivoting

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

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

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

```
[dummy,index] = max(abs(A(column:end,column)));
Index = index+column-1;
```

Partial pivoting: implementing row swaps

- Find maximum element row below pivot in current column
- Store current row

```
[dummy,index] = max(abs(A(column:end,column)));
Index = index+column-1;
```

```
temp = A(column,:);
```

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Partial pivoting: implementing row swaps

- Find maximum element row below pivot in current column
- Store current row
- Swap pivot row and desired row in A

```
[dummy,index] = max(abs(A(column:end,column)));
Index = index+column-1;
```

```
temp = A(column,:);
```

```
A(column,:) = A(index,:);
A(index,:) = temp;
```

Partial pivoting: implementing row swaps

- Find maximum element row below pivot in current column
- Store current row
- Swap pivot row and desired row in A
- Do the same for b: store and swap

```
[dummy,index] = max(abs(A(column:end,column)));
Index = index+column-1;
```

```
temp = A(column,:);
```

```
A(column,:) = A(index,:);
A(index,:) = temp;
```

```
temp = b(column);
b(column) = b(index);
b(index) = temp;
```

Improve the program by using re-usable functions

```
function [x] = GaussianEliminate(A,b)
% GaussianEliminate(A,b): solves x in Ax=b
N = length(b);
for c=1:(N-1)
    [dummy,index]=max(abs(A(c:end,c)));
    index=index+c-1;
    A = SWAP(A,c,index); % Created swap function
    b = SWAP(b,c,index);
    for row=(column+1):N
        d=A(row,column)/A(column,column);
        A(row,:)=A(row,:)-d*A(column,:);
        b(row)= b(row)-d*b(column);
    end
end
x = backwardSub(A,b); % Created BS function
return
```

This function is also provided (named GaussianEliminate_v2 and GaussianEliminate_v3 on Canvas).

Alternatives to this program

- MATLAB can compute the solution to Ax=b with its own solvers (more efficient) `A\b`
- Too many loops. Loops make MATLAB slow.
- There are fundamental problems with Gaussian elimination

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  - 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

Alternatives to this program

- MATLAB can compute the solution to Ax=b with its own solvers (more efficient) `A\b`
- Too many loops. Loops make MATLAB 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

LU Decomposition

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

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

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.

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

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.

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

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 $A'_{32} > A'_{22}$:

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

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

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

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

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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:

$$PA = LU$$

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

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:

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

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

Elimination of column 1 is done. 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 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:

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

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:

$$y_1 = \frac{d_1}{L_{11}}$$
$$y_i = \frac{d_i - \sum_{j=1}^{i-1} L_{ij} y_j}{L_{ii}}$$

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

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

How to use the solver in Matlab

```
A = rand(5,5);              % Get random matrix
[L, U, P] = lu(A);          % Get L, U and P
b = rand(5,1);              % 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 = norm(A*x - b);      % Residual

% Compare results to internal Matlab solver
x = A\b
```

How to use the solver in Matlab

```
A = rand(5,5);              % Get random matrix
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rnorm = norm(A*x - b);      % Residual

% Compare results to internal Matlab solver
x = A\b
```

- 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.
- Matlab has build in routines for solving linear equations (backslash operator \) and LU decomposition (`lu`).
- Advanced techniques such as (preconditioned) conjugate gradient or biconjugate gradient solvers are also available.
- Next part covers iterative approaches

Linear equations 3

Iterative methods

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Chemical Process Intensification group
Eindhoven University of Technology

Numerical Methods (6E5X0), 2022-2023

Today's outline

- Introduction
- Sparse matrices
- Laplace's equation
- Creating a sparse system
- Iterative methods
- Summary

Today's outline

Sparse matrices

- In many engineering cases, we deal with sparse matrices (as opposed to dense matrices)
- A matrix is sparse when it mostly consists of zeros
- Linear systems where equations depend on a limited number of variables (e.g. spatial discretization)
- Storing zeros is not very efficient:

```
>> A = eye(10000);
>> whos A
>> S = sparse(A);
>> whos S
```

- Can you think of a way to achieve this?
- Sparse matrix formats: Yale, CRS, CCS

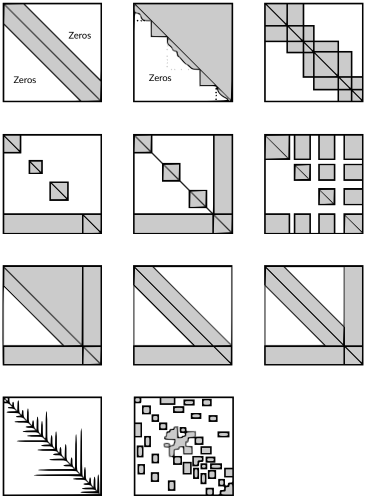
Sparse matrix storage format

- Example: Yale storage format, storing 3 vectors:
  - `A = [5 8 3 6]`
  - `IA = [0 1 2 3 4]`
  - `JA = [0 1 2 1]`

$$A = \begin{bmatrix} 5 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 6 & 0 & 0 \end{bmatrix}$$

- `A` stores the non-zero values
- `IA` stores the index in A of the first non-zero in row i
- `JA` stores the column index
- Note: zero-based indices are used here!

Sparse matrix layout examples



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Today's outline

- Introduction
- Sparse matrices
- Laplace's equation
- Creating a sparse system
- Iterative methods
- Summary

Laplace's equation

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$$

$$T = \text{Temperature}$$

$$\alpha = \text{Thermal diffusivity}$$

Laplace's equation

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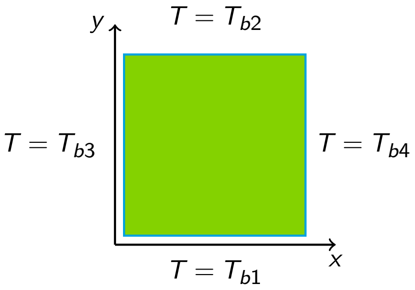


Laplace's equation

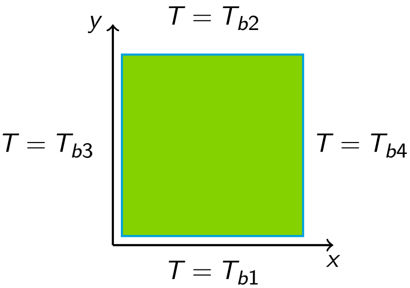
$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$$

$T =$ Temperature

$\alpha =$ Thermal diffusivity

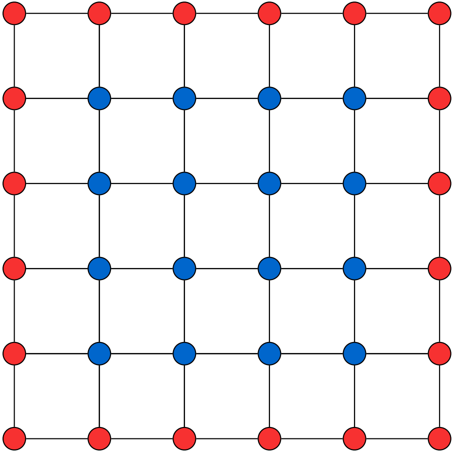
In steady state:

$$\nabla^2 T = 0$$



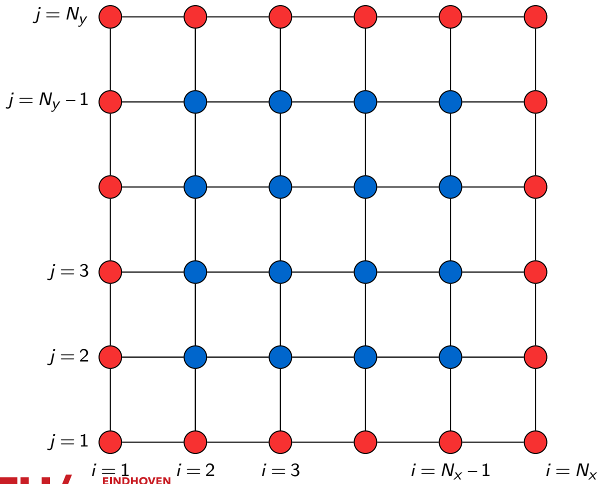
$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

Discretization of Laplace's equation (I)



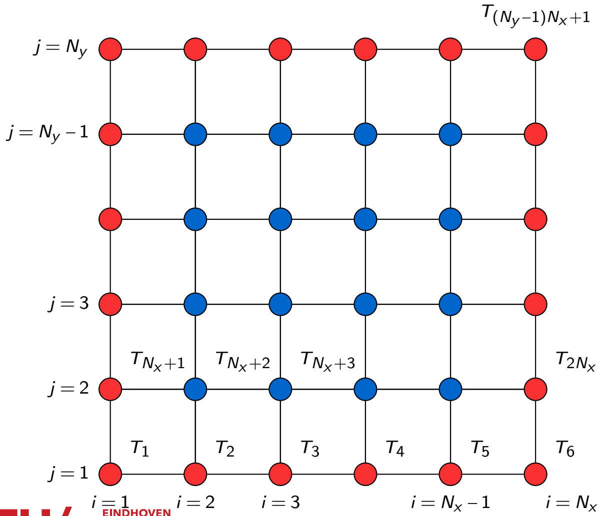
- Define a grid of points in x and y

Discretization of Laplace's equation (I)



- Define a grid of points in x and y
- Index of the grid points using 2D coordinates i and j

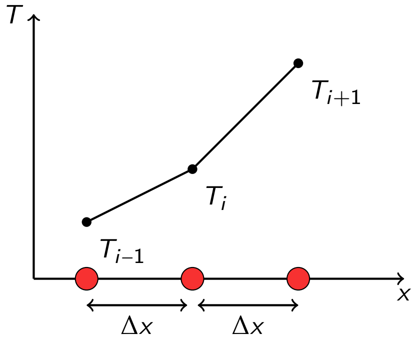
Discretization of Laplace's equation (I)



- Define a grid of points in x and y
- Index of the grid points using 2D coordinates i and j
- Set up the equations using a 1D index system: $T_{i,j} = T_{i+N_x(j-1)}$

Discretization of Laplace's equation (II)

Estimate the second-order differentials: assume a piece-wise linear profile in the temperature:



Discretization of Laplace's equation (II)

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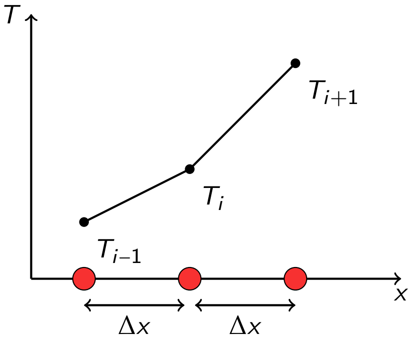

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{\left.\frac{\partial T}{\partial x}\right|_{i+\frac{1}{2}} - \left.\frac{\partial T}{\partial x}\right|_{i-\frac{1}{2}}}{\Delta x}$$

$$\approx \frac{\frac{\left(T_{i+1,j} - T_{i,j}\right)}{\Delta x} - \frac{\left(T_{i,j} - T_{i-1,j}\right)}{\Delta x}}{\Delta x}$$

$$= \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{(\Delta x)^2}$$

Discretization of Laplace's equation (III)

The y-direction is derived analogously, so that the 2D Laplace's equation is discretized as:

$$\frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{(\Delta x)^2} + \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{(\Delta y)^2} = 0$$

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Use a single index counter $k = i + N_x(j-1)$, so that the equation becomes:

$$\frac{T_{k+1} - 2T_k + T_{k-1}}{(\Delta x)^2} + \frac{T_{k+N_x} - 2T_k + T_{k-N_x}}{(\Delta y)^2} = 0$$

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Use a single index counter $k = i + N_x(j-1)$, so that the equation becomes:

$$\frac{T_{k+1} - 2T_k + T_{k-1}}{(\Delta x)^2} + \frac{T_{k+N_x} - 2T_k + T_{k-N_x}}{(\Delta y)^2} = 0$$

For an equal spaced grid $\Delta x = \Delta y = 1$:

$$T_{k-N_x} + T_{k-1} - 4T_k + T_{k+1} + T_{k+N_x} = 0$$

$$\Rightarrow AT = b$$

Today's outline

- Introduction
- Sparse matrices
- Laplace's equation
- Creating a sparse system
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- Summary

Creating the linear system

$$T_{k-N_x} + T_{k-1} - 4T_k + T_{k+1} + T_{k+N_x} = 0$$

Create a *banded* matrix A: the main diagonal k contains -4, whereas the bands at $k-1$, $k+1$, $k-N_x$ and $k+N_x$ contain a 1. Boundary cells just contain a 1 on the main diagonal so that the temperature is equal to T_b (e.g. $T_1 = 1T_b$).

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \cdots & 1 & \cdots & 1 & -4 & 1 & \cdots & 1 & \ddots & 0 \\ 0 & \cdots & 1 & \cdots & 1 & -4 & 1 & \cdots & 1 & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_k \\ T_k + 1 \\ \vdots \\ T_{(N_y-1)N_x} \\ T_{(N_y-1)N_x+1} \end{bmatrix} = \begin{bmatrix} T_b \\ T_b \\ \vdots \\ 0 \\ 0 \\ \vdots \\ T_b \\ T_b \end{bmatrix}$$

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Creating the linear system

$$T_{k-N_x} + T_{k-1} - 4T_k + T_{k+1} + T_{k+N_x} = 0$$

Create a *banded* matrix A in Matlab, by setting the coefficients for the internal cells:

```
Nx=5;  %number of points along x direction
Ny=5;  %number of points in the y direction
Nc=Nx*Ny; % Total number of points

e = ones(Nc,1);
A = spdiags([e,e,-4*e,e,e],[-Nx,-1,0,1,Nx],Nc,Nc);
b = zeros(Nc,1);
```

The function `spdiags` uses the following arguments:

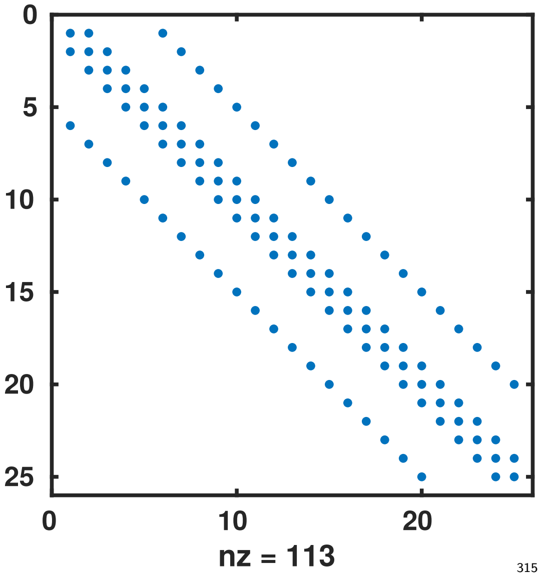
- The coefficients that have to be put on the diagonals arranged as columns in a matrix
- The position of the bands with respect to the main diagonal
- Size of the resulting matrix (in our case square $N_x N_y \times N_x N_y$)

Matrix sparsity

- Let's check the matrix layout:

```
>> spy(A)
```

- This command shows the non-zero values of a matrix
- Apart from the main diagonal, there are offset bands!



About boundary conditions

- For the nodes on the boundary, we have a simple equation:

$$T_{k,\text{boundary}} = \text{Some fixed value}$$

- However, we have set all nodes to be a function of their neighbors...
- Find the boundary node indices using $k = i + Nx(j-1)$
  - `i = 1, j = 1:Ny`
  - `i = Nx, j = 1:Ny`
  - `j = 1, i = 1:Nx`
  - `j = Ny, i = 1:Nx`
- Reset the row in A to zeros, set $A_{kk} = 1$
- Set value in rhs: $b_k = T_{k,\text{boundary}}$
- Boundary conditions are often more elaborate to implement! See `setBoundaryConditions.m`.

Partial implementation of the boundary conditions

See `setBoundaryConditions.m`.

```
function [A,b] = setBoundaryConditions(A,b,Tb,Nx,Ny)

% Set boundary conditions over x-direction
for i=1:Nx
    j = 1;
    ind = i + Nx * (j-1);
    A(ind,:) = 0;    % Reset matrix for boundary cells
    A(ind,ind) = 1; % Add a 1 on the diagonal
    b(ind) = Tb(1);
    j = Ny;
    ind = i + Nx * (j-1);
    A(ind,:) = 0;    % Reset matrix for boundary cells
    A(ind,ind) = 1; % Add a 1 on the diagonal
    b(ind) = Tb(2);
end

%% Repeat for y-direction
```

How applying boundary conditions affects the linear system

```
function [A,b] = setBoundaryConditions(A,b,Tb,Nx,Ny)
```

How applying boundary conditions affects the linear system

```
function [A,b] = setBoundaryConditions(A,b,Tb,Nx,Ny)
```

- Make sure that matrix `A` and right hand side vector `b` are in your workspace, as well as `Nx` and `N_y`
- Create a vector that holds the temperature at each boundary:

```
>> T = [10 20 30 40];
```

- Call the function, store A and b in new variables:

```
>> [A2,b2] = setBoundaryConditions(A,b,T,Nx,Ny);
```

- Check the new structure of the matrix and the right hand side:

```
>> subplot(1,2,1); spy(A2);
>> subplot(1,2,2); spy(b2);
```

A full program, including solver

The program and auxiliary functions are on Canvas (`solveLaplaceEq.m`)

```
function [x,y,T,A] = solveLaplaceEq(Nx,Ny)
% Solves the steady-state Laplace equation

Tb = [10 20 30 40]; % Fixed boundary temperatures

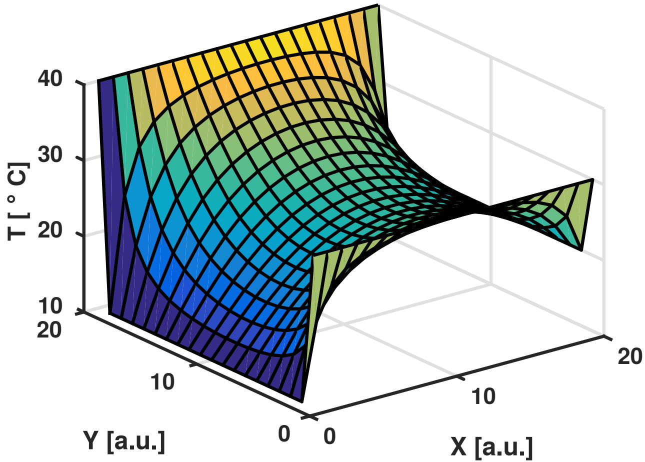
% Fill sparse matrix with [1 1 -4 1 1]
e = ones(Nx*Ny,1);
A = spdiags([e,e,-4*e,e,e],[-Nx,-1,0,1,Nx],Nx*Ny,Nx*Ny);
b = zeros(Nx*Ny,1);

[A,b] = setBoundaryConditions(A,b,Tb,Nx,Ny);

T = A\b;  % Solve matrix
Tc = reshape(T,[Nx,Ny]); % Reshape x-vec to mat Nx,Ny
[xc yc] = meshgrid(1:Nx,1:Ny); % Get position arrays
surf(xc,yc,Tc); % Surface plot
```

Sample results

Solved for a 20×20 system with $T_b = [10\ 20\ 30\ 40]$.



Exercise: Verify the numerical solution using Fourier-series

A Fourier-series expansion for the steady-state heat conduction in a flat plate is given for a domain: $x, y \in [0,1]$, with fixed-temperature boundaries $T\big|_{x=0} = T\big|_{x=1} = T\big|_{y=0} = 0$ and $T\big|_{y=1} = 1$:

$$T = \frac{4}{\pi}\sum_{n=1}^{\infty}\frac{\sin(m\pi x)\sinh(m\pi y)}{m\sinh(m\pi)} \quad \text{with} \quad m = 2n-1$$

Compute and plot the exact temperature profile in the 2D plate, and compare it with the numerical solution:

Hints:

- Use meshgrid to create a mesh in x and y
- Compute the temperature using the Fourier series, use vectorised computations over x and y so that only 1 loop (over n) is required.
- Solve the numerics for the same problem (note the boundary conditions)
- Compare the numerical and exact solutions (e.g. a plot).

Exercise: Verify the numerical solution using Fourier-series

```
% Generate the mesh
Nx = 35; Ny = 35;
[x y] = meshgrid(linspace(0,1,Nx),linspace(0,1,Ny));
T = zeros(size(x));
```

Exercise: Verify the numerical solution using Fourier-series

```
% Generate the mesh
Nx = 35; Ny = 35;
[x y] = meshgrid(linspace(0,1,Nx),linspace(0,1,Ny));
T = zeros(size(x));
% Fourier series expansion
for n = 1:100
    m = 2*n-1;
    T = T + (sin(m*pi*x).*sinh(m*pi*y))./(m*sinh(m*pi));
end
Tex = T*4/pi;
```

Exercise: Verify the numerical solution using Fourier-series

```
% Generate the mesh
Nx = 35; Ny = 35;
[x y] = meshgrid(linspace(0,1,Nx),linspace(0,1,Ny));
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% Fourier series expansion
for n = 1:100
    m = 2*n-1;
    T = T + (sin(m*pi*x).*sinh(m*pi*y))./(m*sinh(m*pi));
end
Tex = T*4/pi;
% Compute numerical solution and post-process

% First plot is created inside solveLaplaceEq, which also returns Tnum
figure; subplot(1,3,1)
[xc,yc,Tnum] = solveLaplaceEq(Nx,Ny)

% Plot exact (Fourier)
subplot(1,3,2); surf(x,y,Tex);
xlabel('x'); ylabel('y'); zlabel('T')

% Plot difference
subplot(1,3,3); surf(x,y,Tex-Tnum);
xlabel('x'); ylabel('y'); zlabel('T')
```

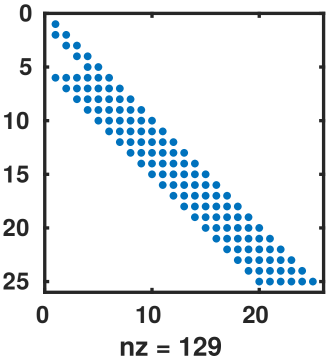
LU decomposition of a sparse matrix

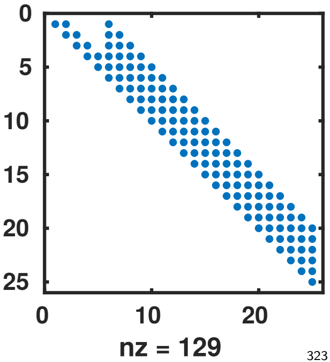
```
>> [L,U,P] = lu(A)
>> subplot(1,2,1)
>> spy(L)
>> subplot(1,2,2)
>> spy(U)
```

LU decomposition of a sparse matrix

- With LU decomposition we produce matrices that are less sparse than the original matrix.
- Sparse storage often required, and also numerical techniques that fully utilizes this!

```
>> [L,U,P] = lu(A)
>> subplot(1,2,1)
>> spy(L)
>> subplot(1,2,2)
>> spy(U)
```





LU decomposition

- LU decomposition and Gaussian elimination on a matrix like A requires more memory (with 3D problems, the offset in the diagonal would even be bigger!)
- In general extra memory allocation will not be a problem for MATLAB
- MATLAB is clever, in that sense that it attempts to reorder equations, to move elements closer to the diagonal)

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- In general extra memory allocation will not be a problem for MATLAB
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Alternatives for elimination methods

- Use iterative methods when systems are large and sparse.
- Often such systems are encountered when we want to solve PDE's of higher dimensions

Today's outline

Examples of iterative methods

- Jacobi method
- Gauss-Seidel method
- Succesive over relaxation

- `bicg` — Bi-conjugate gradient method
- `pcg` — preconditioned conjugate gradient method
- `gmres` — generalized minimum residuals method
- `bicgstab` — Bi-conjugate gradient method

The Jacobi method

- In our example we derived the following equation:

$$T_{k-N_x} + T_{k-1} - 4T_k + T_{k+1} + T_{k+N_x} = 0$$

- Rearranging gives:

$$T_k = \frac{T_{k-N_x} + T_{k-1} + T_{k+1} + T_{k+N_x}}{4}$$

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- In the Jacobi scheme the iteration proceeds as follows:
  1. Start with an initial guess for the values of T at each node
  2. Compute updated values and store a new vector:

$$T_k^{\text{new}} = \frac{T_{k-N_x}^{\text{old}} + T_{k-1}^{\text{old}} + T_{k+1}^{\text{old}} + T_{k+N_x}^{\text{old}}}{4}$$

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  3. Do this for all nodes

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  3. Do this for all nodes
  4. Repeat the procedure until converged

Jacobi method for Laplace's equation

See `laplace_jacobi.m` (from Canvas)

```
% Grid size
nx = 40; ny = 40;
```

Jacobi method for Laplace's equation

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% Grid size
nx = 40; ny = 40;
% The temperature field + boundaries at old and new times
T = zeros(nx,ny);
T(1,:) = 40;  % Left
T(nx,:) = 60; % Right
T(:,1) = 20;  % Bottom
T(:,ny) = 30; % Top
```

Jacobi method for Laplace's equation

See `laplace_jacobi.m` (from Canvas)

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% For plotting
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Tnew = T;
% For plotting
[x y] = meshgrid(1:nx, 1:ny);
for iter = 1:1000
  for i = 2:nx-1
    for j = 2:ny-1
      Tnew(i,j) = (T(i-1,j)+T(i+1,j)+T(i,j-1)+T(i,j+1))/4.0;
    end
  end
```

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    end
  end
  surf(x,y,Tnew);
  title(['Iteration: ' num2str(iter)]);
  drawnow
  T = Tnew; % Update T
end
```

About the straightforward implementation

- The method as implemented works fine for a simple Laplace equation
- For generic systems of linear equations, the implementation cannot be used.

About the straightforward implementation

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- For generic systems of linear equations, the implementation cannot be used.

> We will now introduce the Jacobi method so it can be used for generic systems of linear equations.

The Jacobi method with matrices

We can split our (banded) matrix A into a diagonal matrix D and a remainder R:

$$A \quad = \quad D \quad + \quad R$$

$$\begin{bmatrix}
\times & \times & & & & & \times & & \\
\times & \times & \times & & & & & \times & \\
& \times & \times & \times & & & & & \times \\
& & \times & \times & \times & & & & \\
& & & \times & \times & \times & & & \\
& & & & \times & \times & \times & & \\
\times & & & & & \times & \times & \times & \\
& \times & & & & & \times & \times & \times \\
& & \times & & & & & \times & \times
\end{bmatrix}
=
\begin{bmatrix}
\times & & & & & & & & \\
& \times & & & & & & & \\
& & \times & & & & & & \\
& & & \times & & & & & \\
& & & & \times & & & & \\
& & & & & \times & & & \\
& & & & & & \times & & \\
& & & & & & & \times & \\
& & & & & & & & \times
\end{bmatrix}
+
\begin{bmatrix}
& \times & & & & & \times & & \\
\times & & \times & & & & & \times & \\
& \times & & \times & & & & & \times \\
& & \times & & \times & & & & \\
& & & \times & & \times & & & \\
& & & & \times & & \times & & \\
\times & & & & & \times & & \times & \\
& \times & & & & & \times & & \times \\
& & \times & & & & & \times &
\end{bmatrix}$$

Jacobi method: solving a system

- We can solve $AT = b$, now written generally as $Ax = b$, by:

$$
\begin{aligned}
Ax &= b \\
(D+R)x &= b \\
Dx &= b - Rx \\
Dx^{\text{new}} &= b - Rx^{\text{old}} \\
x^{\text{new}} &= D^{-1}(b - Rx^{\text{old}})
\end{aligned}
$$

- Using the n and $n+1$ notation for old and new time steps, we find in general:

$$x^{n+1} = D^{-1}(b - Rx^n)$$

$$x_i^{n+1} = \frac{1}{A_{ii}}\left(b_i - \sum_{j\neq i} A_{ij}x_j^n\right)$$

Diagram of the Jacobi method

Set T^{old} $=$ a guess

Diagram of the Jacobi method

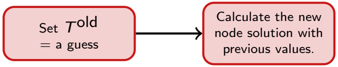
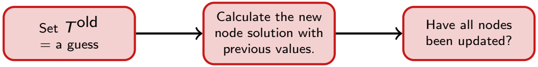


Diagram of the Jacobi method



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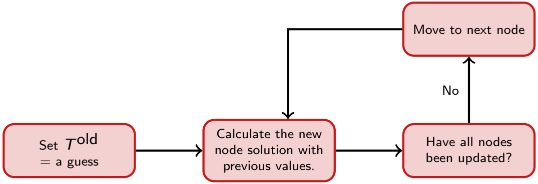

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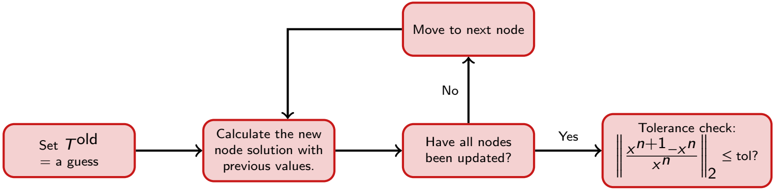

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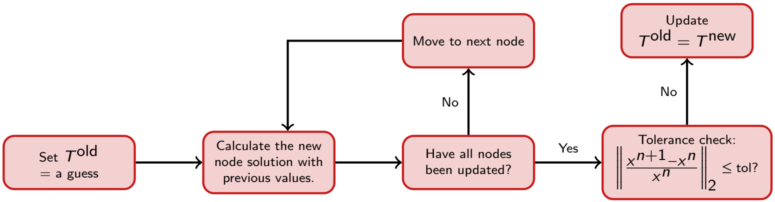

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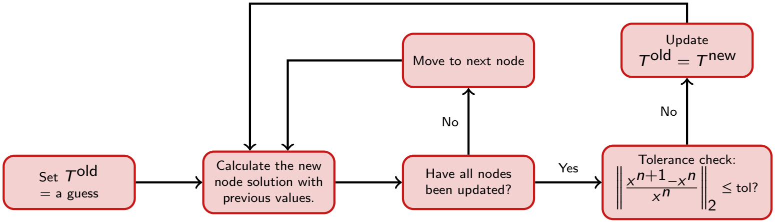

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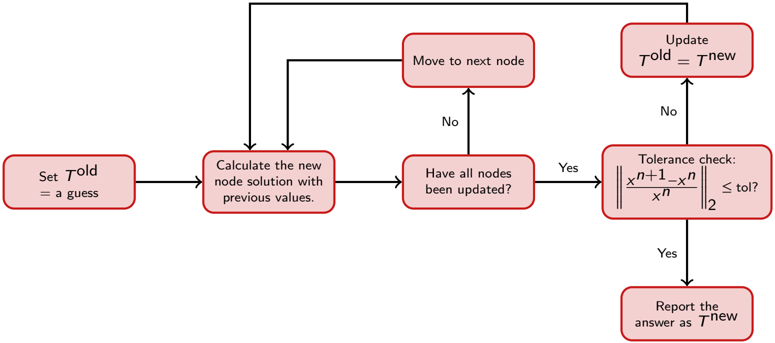

The core of the solver

The full file is on Canvas, `solveJacobi.m`.

```
  while ( xDiff > tol && it_jac < 1000 )
    x_old = x;
    for i=1:N
        s = 0;
        for j = 1:N
            if (j ~= i)
                s = s+A(i,j)*x_old(j);
            end
        end
        x(i) = (b(i)-s)/A(i,i);
    end
    it_jac = it_jac+1;
    xDiff = norm((x-x_old)./x,2);
end
it_jac
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```

Try to call it from the `solveLaplaceEq.m` file, instead of using `\`.

A few details on this algorithm

- The while loop holds two aspects
  - A convergence criterion (`norm((x-x_old)./x,2)> tol`). Some considerations are:
    - L_1-norm (sum)
    - L_2-norm (Euclidian distance)
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  - Protection against infinite loops (no convergence)
- Reset the sum for each row, before summing for the new unknown node

- Start vector x is not shown in the example, but should be there!
- It can have huge impact on performance!
- The for-loops also have a large performance penalty!

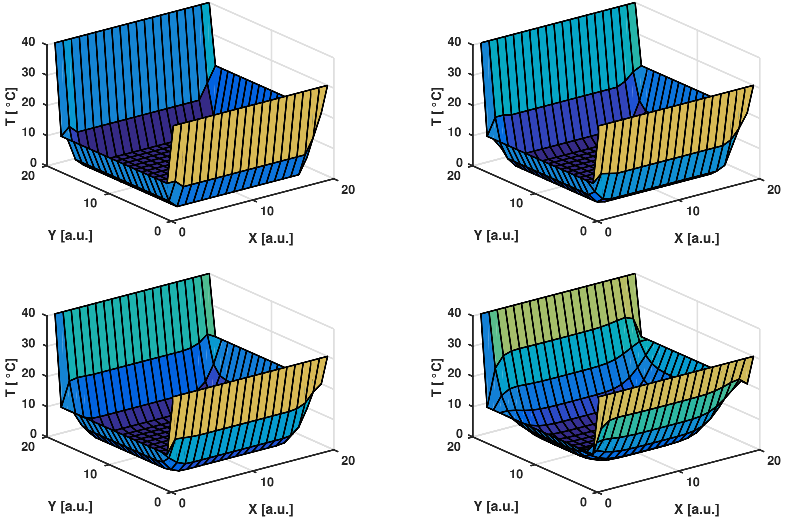
The solver using array indices

Make a copy of the Jacobian solver, and replace the for-loop by a vector-operation:

```
% While not converged or max_it not reached
while ( xDiff > tol && it_jac < 1000 )
  x_old = x;
  for i=1:N
    % Sum off-diagonal*x_old
    offDiagonalIndex = [1:(i-1) (i+1):N];
    Aij_Xj = A(i,offDiagonalIndex)*x_old(offDiagonalIndex);

    % Compute new x value
    x(i) = (b(i)-Aij_Xj)/A(i,i);
  end
  it_jac = it_jac+1;
  xDiff = norm((x-x_old)./x,2);
end
```

Iterations 1, 2, 3 and 10



Gauss-Seidel method

The Gauss-Seidel method is quite similar to Jacobi method

- The only difference is that the new estimate x^{new} is returned to the solution x^{old} as soon as it is completed
- For following nodes, the updated solution is used immediately

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- Our straightforward script (from the Jacobi method) is therefore changed easily:
  - Do not create a `Tnew` array (save memory!)
  - Do not store the solution in `Tnew`, but simply in `T`
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  - See `laplace_gaussseidel.m` for the algorithm.

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- Our straightforward script (from the Jacobi method) is therefore changed easily:
  - Do not create a `Tnew` array (save memory!)
  - Do not store the solution in `Tnew`, but simply in `T`
  - Do not perform the update step `T=Tnew`
  - See `laplace_gaussseidel.m` for the algorithm.
- The straightforward script works well for the current Laplace equation, but we define the generic Gauss-Seidel algorithm on the following slides.

Gauss-Seidel method

- Define a lower and strictly upper triangular matrix, such that $A = L + U$
- Now we can solve AT=b by:

$$
\begin{aligned}
(L+U)T &= b \\
LT &= b - UT \\
LT^{\text{new}} &= b - UT^{\text{old}} \\
T^{\text{new}} &= L^{-1}(b - UT^{\text{old}})
\end{aligned}
$$

- Using the n and $n+1$ notation for old and new time steps, we find in for the general Gauss-Seidel method:

$$x^{n+1} = L^{-1}(b - Ux^{n})$$

$$x_i^{n+1} = \frac{1}{A_{ii}} \left(b_i - \sum_{j<i} A_{ij} x_j^{n+1} - \sum_{j>i} A_{ij} x_j^{n} \right)$$

Today's outline

Summary

- Partial differential equations can be discretized into sparse systems of linear equations
- Sparse matrices can be stored in memory efficiently using specialised formats (e.g. compressed row storage)
- The Jacobi and Gauss–Seidel methods were introduced as iterative methods; other methods are based on the same principle (successive over-relaxation method, for example)
- Various implementation issues were discussed, e.g. vectorised computing, convergence tolerances

Direct methods vs. Iterative methods

- Iterative methods converge *gradually* to a solution while direct methods (possibly with partial pivoting) factorise a (set of) matrix(ces) which allow to compute the solution by *substitution*.
- Direct methods generally use more memory, since they need to store also the result matrices.
- A strictly (or irreducibly) diagonally dominant matrix is a prerequisite for convergence of the Jacobi and Gauss-Seidel method.
- For real-life situations; 1D problems are generally solved with direct methods (LU decomposition). If you have systems of more than 1 dimension, a direct method still can be used, if there are no memory issues, otherwise an iterative method would be more attractive.