Linear equation solvers Direct methods (elimination methods)

Ivo Roghair, Martin van Sint Annaland

Chemical Process Intensification, Eindhoven University of Technology Introduction

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

Introduction

- Introduction

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
- 2 Gauss elimination
- Partial Pivoting
- 4 LU decomposition
- Summary

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.

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & b_1 \\ A_{21} & A_{22} & A_{23} & b_2 \\ A_{31} & A_{32} & A_{33} & b_3 \end{bmatrix} \longrightarrow \begin{bmatrix} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ A_{31} & A_{32} & A_{33} & b_3 \end{bmatrix}$$

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

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & b_1 \\ A_{21} & A_{22} & A_{23} & b_2 \\ A_{31} & A_{32} & A_{33} & b_3 \end{bmatrix} \longrightarrow \begin{bmatrix} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ A_{31} & A_{32} & A_{33} & b_3 \end{bmatrix}$$

Using row operations

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

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & b_1 \\ A_{21} & A_{22} & A_{23} & b_2 \\ A_{31} & A_{32} & A_{33} & b_3 \end{bmatrix} \longrightarrow \begin{bmatrix} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ A_{31} & A_{32} & A_{33} & b_3 \end{bmatrix}$$

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

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

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & b_1 \\ A_{21} & A_{22} & A_{23} & b_2 \\ A_{31} & A_{32} & A_{33} & b_3 \end{bmatrix} \longrightarrow \begin{bmatrix} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ A_{31} & A_{32} & A_{33} & b_3 \end{bmatrix}$$

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

```
\begin{array}{lll} 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; \end{array}
```

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

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ A_{31} & A_{32} & A_{33} & b_3 \end{bmatrix} \longrightarrow \begin{bmatrix} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ 0 & A'_{32} & A'_{33} & b'_3 \end{bmatrix}$$

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

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ A_{31} & A_{32} & A_{33} & b_3 \end{bmatrix} \longrightarrow \begin{bmatrix} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ 0 & A'_{32} & A'_{33} & b'_3 \end{bmatrix}$$

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

```
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:
```

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

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ 0 & A_{32} & A_{33} & b_3 \end{bmatrix} \longrightarrow \begin{bmatrix} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ 0 & 0 & A''_{33} & b''_3 \end{bmatrix}$$

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

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ 0 & A_{32} & A_{33} & b_3 \end{bmatrix} \longrightarrow \begin{bmatrix} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ 0 & 0 & A''_{33} & b''_3 \end{bmatrix}$$

- $d_{32} \to A_{32}/A'_{22}$
- $A_{32} \rightarrow A_{32} A'_{22}d_{32}$
- $A_{33} \rightarrow A_{33} A'_{23}d_{32}$
- $b_3 \rightarrow b_3 b_2' d_{32}$

$$\begin{array}{lll} d32 &=& A(3,2)/A(2,2);\\ A(3,2) &=& A(3,1) - A(2,2)*d32;\\ A(3,3) &=& A(3,2) - A(2,3)*d32;\\ b(3) &=& b(3) - b(2)*d32; \end{array}$$

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

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ 0 & A_{32} & A_{33} & b_3 \end{bmatrix} \longrightarrow \begin{bmatrix} A_{11} & A_{12} & A_{13} & b_1 \\ 0 & A'_{22} & A'_{23} & b'_2 \\ 0 & 0 & A''_{33} & b''_3 \end{bmatrix}$$

- $d_{32} \to A_{32}/A'_{22}$
- $A_{32} \rightarrow A_{32} A'_{22}d_{32}$
- $A_{33} \rightarrow A_{33} A'_{23}d_{32}$
- $b_3 \rightarrow b_3 b_2' d_{32}$

$$\begin{array}{lll} d32 &=& A(3,2)/A(2,2);\\ A(3,2) &=& A(3,1) - A(2,2)*d32;\\ A(3,3) &=& A(3,2) - A(2,3)*d32;\\ b(3) &=& b(3) - b(2)*d32; \end{array}$$

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

Backsubstitution

The system now reads:

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

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.

$$\begin{array}{l} x_3 = b_3''/A_{33}'' \\ x_2 = (b_2' - A_{23}'x_3)/A_{22}' \\ x_1 = (b_1 - A_{12}x_2 - A_{13}x_3)/A_{11} \end{array} \begin{array}{l} x(3) = b(3) \ / \ A(3,3) \\ x(2) = (b(2) - A(2,3)*x(3)) \ / \ A(2,2) \\ x(1) = (b(1) - A(1,2)*x(2) - A(1,3)*x(3)) \ / \ A(1,1) \end{array}$$

In general:

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

 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,:)
```

```
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
```

```
% 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
```

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

- The function we just made can be found on Canvas
- Use help Gaussian Eliminate 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

- 3 Partial Pivoting

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,:);
```

- 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).

- 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

- 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

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

LU Decomposition

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

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

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 I Ux = 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.

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

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.

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

This finishes the LU decomposition!

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

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

Suppose we have arrived at the situation below, where $A_{32}^{\prime}>A_{22}^{\prime}$:

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

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

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:

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

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

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

$$PA = LU$$

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

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:

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

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. 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 Laccordingly:

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

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:

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

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

$$Ax = b \Rightarrow PAx = Pb \equiv d$$

 $PA = LU \Rightarrow LUx = d$

- Define a new vector y = Ux
 - $Ly = b \Rightarrow Ly = d$
 - 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:

$$x_{N} = \frac{y_{N}}{U_{NN}}$$

$$x_{i} = \frac{y_{i} - \sum_{j=i+1}^{N-1} U_{ij} x_{j}}{U_{ii}}$$

```
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\setminus y
rnorm = norm(A*x - b); % Residual
% Compare results to internal Matlab solver
x = A \setminus b
```

How to use the solver in Matlab

```
A = rand(5,5);
                      % Get random matrix
[L, U, P] = lu(A); % Get L, U and P
                      % Random b vector
b = rand(5,1);
                      % Permute b vector
d = P*b:
y = forwardSub(L,d); % Can also do y=L\d
x = backwardSub(U,y); % Can also do x=U\setminus y
rnorm = norm(A*x - b);  % Residual
% Compare results to internal Matlab solver
x = A \setminus 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

- **5** 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 dont 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