

# Numerical interpolation and integration

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## Part I

# Numerical interpolation

# Today's outline

- ① Introduction
- ② Piecewise constant
- ③ Linear
- ④ Polynomial
- ⑤ Splines

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## ① Introduction

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# Interpolation problem

## Definition

Given a set of points  $x_k$ ,  $k = 0, \dots, n$ ,  $x_i \neq x_j$  with associated function values  $f_k$ ,  $k = 0, \dots, n$ , or simply:  $\{x_k, f_k\}_{k=0}^n$ . The interpolation problem is defined as: find a polynomial  $p_n$  such that this interpolates the values of  $f_k$  on the points  $x_k$ :

$$p_n(x_k) = f_k, \quad k = 0, \dots, n$$

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## Theorem

*The interpolation problem for  $\{x_k, f_k\}_{k=0}^n$  has a unique solution when  $x_i \neq x_j$  for  $i \neq j$ . Note that we cannot allow multiple function values  $f_k$  for the same value of  $x_k$ .*

# What is interpolation?

Interpolation means constructing additional data points within the range of, and using, a discrete set of known data points.

It is typically performed on a uniformly spread data set, but this is not strictly necessary for all methods

# Is interpolation the same as curve fitting?



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- Curve-fitting does not strictly enforce the function to match the data exactly
- Curve-fitting may be done on multiple datapoints at one position
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# Why do chemical engineers need interpolation?

- Comparison of two data sets which are given at different positions
  - An experimental data set may have been recorded at a constant rate, but the numerical solution is computed at irregular intervals
- Reconstruction of field values distant of computing nodes
  - A CFD simulation on a regular grid containing structures that are not grid-conformant requires interpolation to the structures
- Calculation of a physical property at a condition between those of a lookup table
  - The viscosity of a substance may have been measured at 20°C and 30°C, but not at the desired 28.5°C

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# General

Several important numerical interpolation methods are discussed today:

- Piecewise constant interpolation
- Linear interpolation
  - Bilinear interpolation
- Polynomial interpolation (Newton's method)
- Spline interpolation

# Today's data set

Download the datafile  
`interpolation-dataset.mat`,  
which contains multiple data sets.

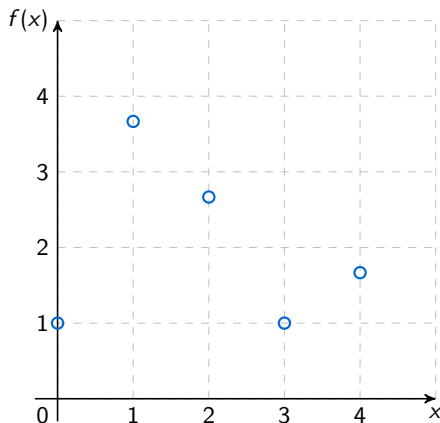
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We start with  $x_1$  and  $y_1$ :

$x_k$	$f_k$
0	1.00
1	$\frac{11}{3} = 3.67$
2	$\frac{5}{2} = 2.50$
3	1.00
4	$\frac{5}{3} = 1.67$
5	$\frac{20}{3} = 6.67$

Data set  $f_n(x_n)$  represented by ○ at discrete intervals  $x_n \in \{0, 5\}$



# Piecewise constant interpolation

- Nearest-neighbor interpolation in the continuous range  $x \in [0, 5]$
- How to treat the point halfway (e.g. at  $x = 2.5$ )?

$$x \in [0, 0.5] \rightarrow f(x) = f(0)$$

$$x \in [0.5, 1.5] \rightarrow f(x) = f(1)$$

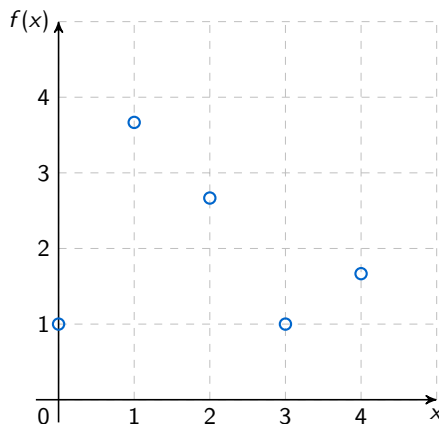
$$x \in [1.5, 2.5] \rightarrow f(x) = f(2)$$

$$x \in [2.5, 3.5] \rightarrow f(x) = f(3)$$

$$x \in [3.5, 4.5] \rightarrow f(x) = f(4)$$

- Not often used for simple problems, but e.g. for 2D (Voronoi)

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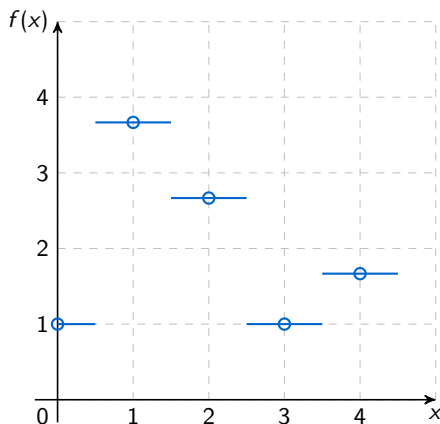
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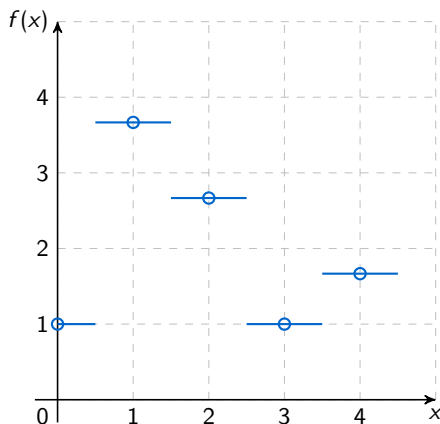
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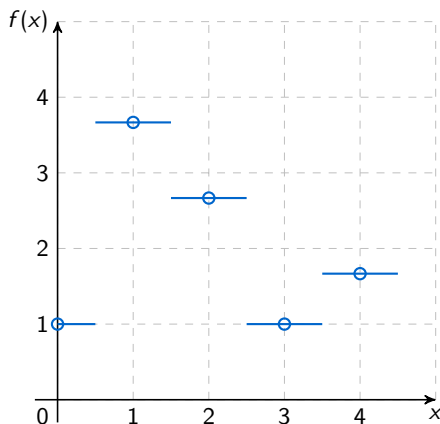
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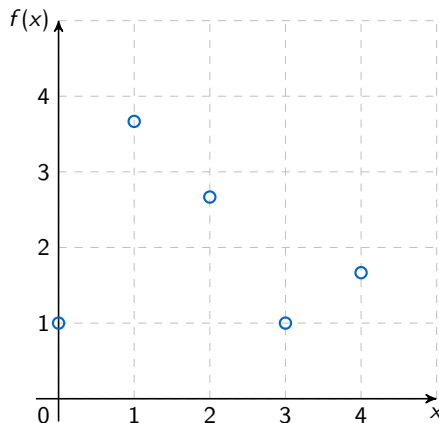
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- Linear interpolation to  $(x, y)$  between 2 data points  $(x_2, y_2)$  and  $(x_3, y_3)$ :

$$\frac{y - y_2}{x - x_2} = \frac{y_3 - y_2}{x_3 - x_2}$$

- Reordered, and more formally:

$$y = y_n + (y_{n+1} - y_n) \frac{x - x_n}{x_{n+1} - x_n}$$





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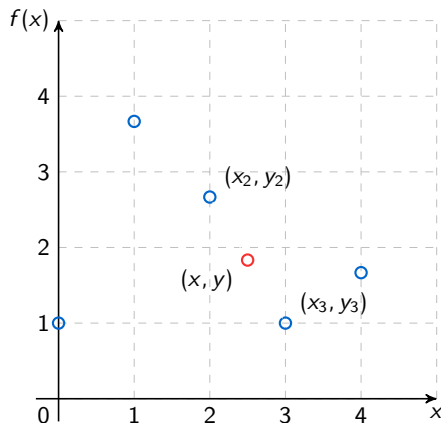
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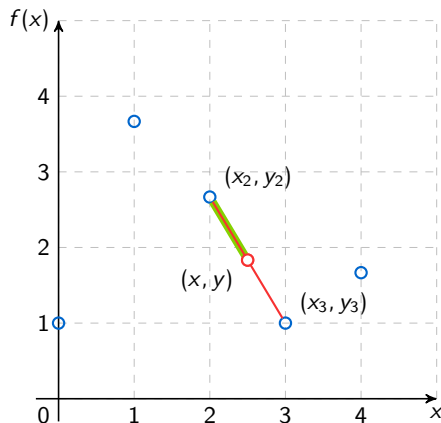
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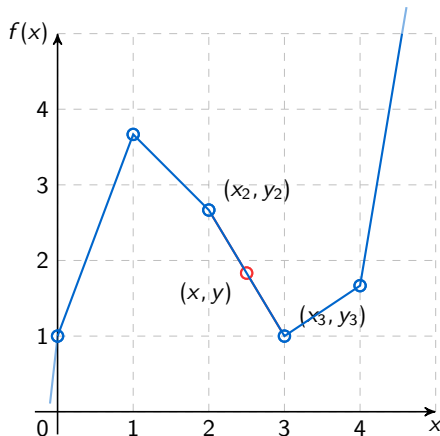
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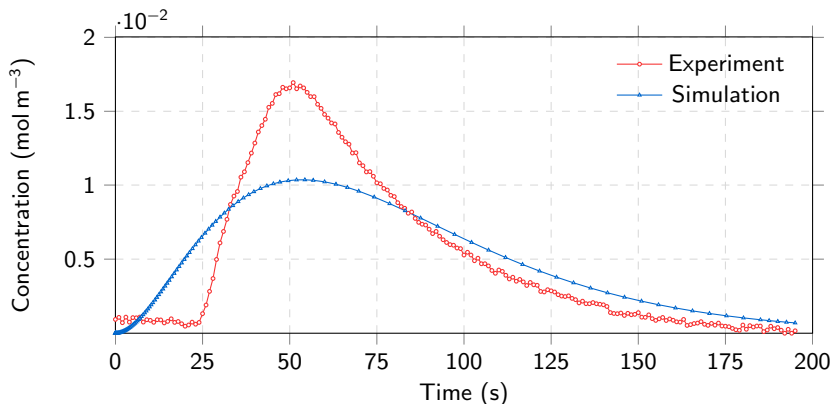
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## Example: Linear interpolation in Matlab

Consider the data set in `sim_exp_dataset.mat`, containing a normalized concentration and time vector for an experiment and a simulation. The simulation was performed with adaptive node distance to save computation time, thus the concentration is not known at the same times. We are not able to compare yet.



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```
% Linear interpolation
c_sim_new = interp1(t_sim,c_sim,t_exp,'linear');
diff = abs(c_exp-c_sim_new);
% Plot the solution
subplot(2,1,1);
plot(t_exp,c_exp,'b-x',t_exp,c_sim_new,'r-o');
subplot(2,1,2);
stem(t_exp,diff);
% Compute the L2-norm
norm(diff)
```



# Bi-linear interpolation

When a 2D field of some quantity is known, we can interpolate the solution to an arbitrary position in the 2D domain  $p(x, y)$  using 4 field values  $f_{00}$ ,  $f_{10}$ ,  $f_{01}$  and  $f_{11}$ .

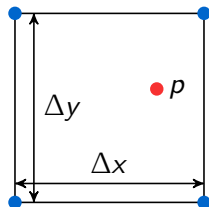
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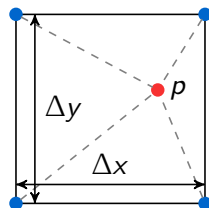
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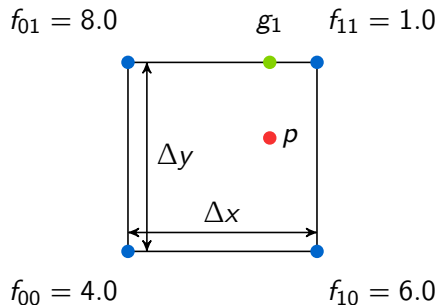
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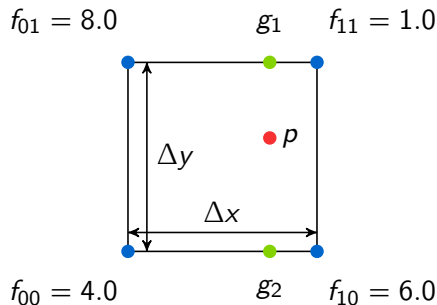
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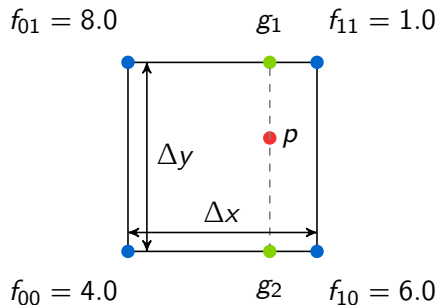
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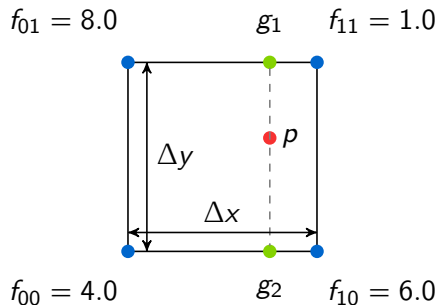
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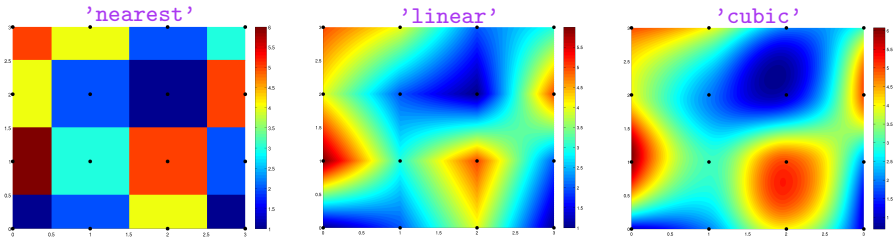
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- The order of interpolation ( $x$  or  $y$  direction first) does not matter; the results are equal

# Higher-dimensional field interpolation in Matlab

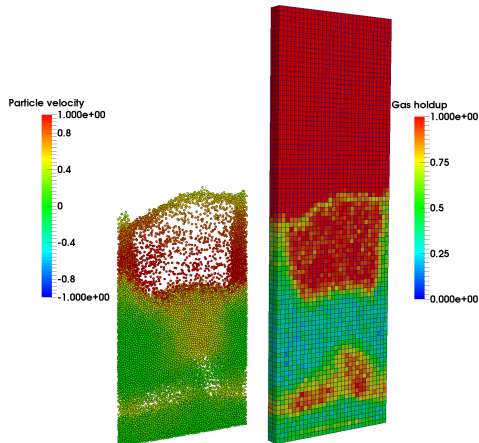
2D or higher-dimensional fields of data can be interpolated in Matlab using the `interp2`, `interp3` or even `interpn` functions, the method can be adjusted:



- Similar to 1D linear interpolation, the derivatives are discontinuous on the grid nodes
- Also consider tri-linear interpolation (for 3D fields), or bicubic interpolation (2D, but third order)

# A practical example

Field interpolation is used in e.g. CFD simulations, e.g. a fluidized bed simulation using a *discrete particle model*, where particles are found in between the grid nodes used for velocity computation.





# Polynomial interpolation

The examples that we have seen, are simplified forms of *Newton polynomials*. We can interpolate our data with a polynomial of degree  $n$ :

$$p_n(x) = a_n x^n + a_{n-1} x^{n-1} + \dots + a_2 x^2 + a_1 x + a_0$$

# Polynomial interpolation via Vandermonde matrix

Consider the data points  $(x_1, y_1), (x_2, y_2), \dots, (x_m, y_m)$ , the Vandermonde matrix  $V$ , coefficient vector  $a$  and function value vector  $y$ :

$$V_{m,n} = \begin{pmatrix} x_1^0 & x_1^1 & x_1^2 & \cdots & x_1^{n-1} \\ x_2^0 & x_2^1 & x_2^2 & \cdots & x_2^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_m^0 & x_m^1 & x_m^2 & \cdots & x_m^{n-1} \end{pmatrix} \quad a = \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{n-1} \end{pmatrix} \quad y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix}$$

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>> y = [1.0000; 3.6667;  
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>> V = vander(x);  
>> a = V\y  
a =  
    -1.8333  
     4.5000  
     1.0000
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     1.0000
```

So we found the equation:

$$p_2(x) = -1.8333x^2 + 4.5x - 1$$

# Polynomial interpolation via Vandermonde matrix

Consider the data points  $(x_1, y_1), (x_2, y_2), \dots, (x_m, y_m)$ , the Vandermonde matrix  $V$ , coefficient vector  $a$  and function value vector  $y$ :

$$V_{m,n} = \begin{pmatrix} x_1^0 & x_1^1 & x_1^2 & \cdots & x_1^{n-1} \\ x_2^0 & x_2^1 & x_2^2 & \cdots & x_2^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_m^0 & x_m^1 & x_m^2 & \cdots & x_m^{n-1} \end{pmatrix} \quad a = \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{n-1} \end{pmatrix} \quad y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix}$$

The coefficients of a polynomial through the data points can be obtained by solving the linear system  $Va = y$ .

```
>> x = [0 1 2];  
>> y = [1.0000; 3.6667;  
        2.6667];  
>> V = vander(x);  
>> a = V \ y  
a =  
   -1.8333  
    4.5000  
    1.0000
```

So we found the equation:

$$p_2(x) = -1.8333x^2 + 4.5x - 1$$

These Vandermonde-systems are often *ill-conditioned*, so we need another, more stable, method!

# Construction of Newton polynomials

Formally, the polynomials  $p_n(x)$  are described using prefactors  $f[x_0, \dots, x_k]$  and polynomial terms  $w_m(x)$ :

$$p_n(x) = \sum_{k=0}^n f[x_0, \dots, x_k] w_k(x)$$

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The polynomial terms are computed via:

$$w_0(x) = 1, \quad w_1(x) = (x - x_0), \quad w_2(x) = (x - x_0) \cdot (x - x_1),$$

$$w_m(x) = (x - x_0) \cdot (x - x_1) \cdots (x - x_{m-1}) = w_{m-1} \cdot (x - x_{m-1})$$

$$w_m(x) = \prod_{j=0}^{m-1} (x - x_j), \quad m = 0, \dots, n$$

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$$w_m(x) = \prod_{j=0}^{m-1} (x - x_j), \quad m = 0, \dots, n$$

The prefactors are *forward divided differences*, which can be computed as:

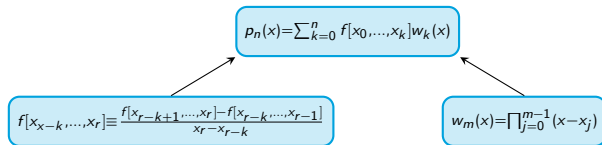
$$f[x_{x-k}, \dots, x_r] \equiv \frac{f[x_{r-k+1}, \dots, x_r] - f[x_{r-k}, \dots, x_{r-1}]}{x_r - x_{r-k}}$$



# Construction of Newton polynomials: example

Sample data

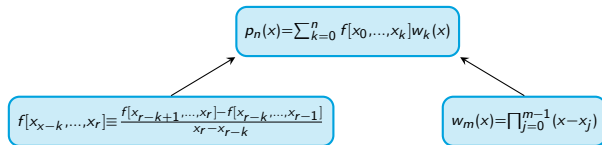
$x_k$	$f_k$
0	1.00
1	$\frac{11}{3} = 3.67$
2	$\frac{8}{3} = 2.67$



# Construction of Newton polynomials: example

Sample data

$x_k$	$f_k$
0	1.00
1	$\frac{11}{3} = 3.67$
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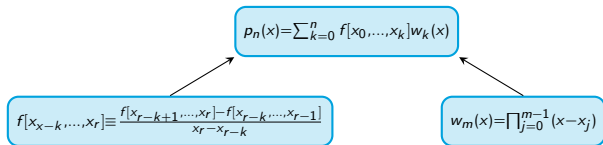
$x_k$	$f_k$
$x_0$	$f[x_0] = f_0$

$x_k$	$f_k$
0	1

# Construction of Newton polynomials: example

Sample data

$x_k$	$f_k$
0	1.00
1	$\frac{11}{3} = 3.67$
2	$\frac{8}{3} = 2.67$



$x_k$	$f_k$
$x_0$	$f[x_0] = f_0$
$x_1$	$f[x_1] = f_1 \quad f[x_0, x_1] = \frac{f_1 - f_0}{x_1 - x_0}$

$x_k$	$f_k$
0	1
1	$3.67 \quad \frac{\frac{11}{3} - 1}{1 - 0} = \frac{8}{3}$

# Construction of Newton polynomials: example

Sample data

$x_k$	$f_k$
0	1.00
1	$\frac{11}{3} = 3.67$
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$$p_n(x) = \sum_{k=0}^n f[x_0, \dots, x_k] w_k(x)$$

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$$w_m(x) = \prod_{j=0}^{m-1} (x - x_j)$$

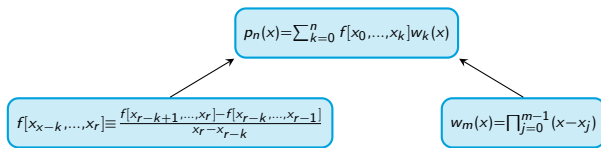
$x_k$	$f_k$
$x_0$	$f[x_0] = f_0$
$x_1$	$f[x_1] = f_1 \quad f[x_0, x_1] = \frac{f_1 - f_0}{x_1 - x_0}$
$x_2$	$f[x_2] = f_2 \quad f[x_1, x_2] = \frac{f_2 - f_1}{x_2 - x_1} \quad f[x_0, x_1, x_2] = \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0}$

$x_k$	$f_k$
0	1
1	3.67 $\frac{\frac{11}{3} - 1}{1 - 0} = \frac{8}{3}$
2	2.67 $\frac{\frac{8}{3} - \frac{11}{3}}{2 - 1} = \frac{-1}{1} = -1 \quad \frac{(-1) - \frac{8}{3}}{2 - 0} = -\frac{11}{6}$

# Construction of Newton polynomials: example

Sample data

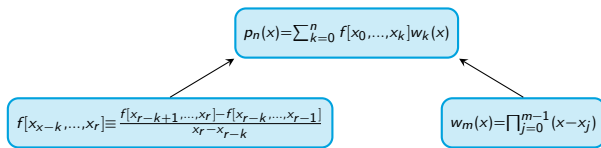
$x_k$	$f_k$
0	1.00
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# Construction of Newton polynomials: example

Sample data

$x_k$	$f_k$
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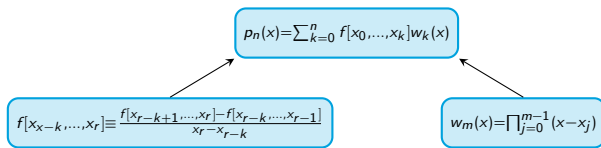


$x_k$	$f_k$
0	1
1	3.67 $\frac{\frac{11}{3} - 1}{1 - 0} = \frac{8}{3}$
2	2.67 $\frac{\frac{8}{3} - \frac{11}{3}}{2 - 1} = \frac{-1}{1} = -1$ $\frac{(-1) - \frac{8}{3}}{2 - 0} = -\frac{11}{6}$

# Construction of Newton polynomials: example

Sample data

$x_k$	$f_k$
0	1.00
1	$\frac{11}{3} = 3.67$
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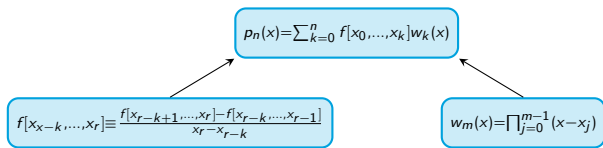
$x_k$	$f_k$
0	1
1	3.67 $\frac{\frac{11}{3} - 1}{1 - 0} = \frac{8}{3}$
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$$p_2(x) = 1 \cdot w_m(0) + \frac{8}{3} \cdot w_m(1) + \left(-\frac{11}{6}\right) \cdot w_m(2)$$

# Construction of Newton polynomials: example

Sample data

$x_k$	$f_k$
0	1.00
1	$\frac{11}{3} = 3.67$
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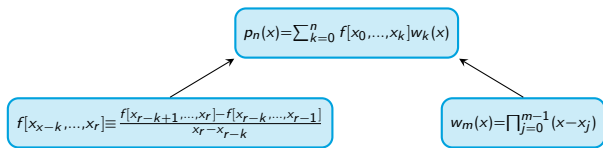
$$\begin{aligned}
 p_2(x) &= 1 \cdot w_m(0) + \frac{8}{3} \cdot w_m(1) + \left(-\frac{11}{6}\right) \cdot w_m(2) \\
 &= 1 \cdot 1 + \frac{8}{3} \cdot (x - 0) + \left(-\frac{11}{6}\right) \cdot (x - 0)(x - 1)
 \end{aligned}$$



# Construction of Newton polynomials: example

Sample data

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$x_k$	$f_k$
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1	3.67 $\frac{\frac{11}{3}-1}{\frac{1}{3}-0} = \frac{8}{3}$
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$$\begin{aligned}
 p_2(x) &= 1 \cdot w_m(0) + \frac{8}{3} \cdot w_m(1) + \left(-\frac{11}{6}\right) \cdot w_m(2) \\
 &= 1 \cdot 1 + \frac{8}{3} \cdot (x - 0) + \left(-\frac{11}{6}\right) \cdot (x - 0)(x - 1) = -\frac{11}{6}x^2 + 4\frac{1}{2}x + 1
 \end{aligned}$$

# Construction of Newton polynomials: example

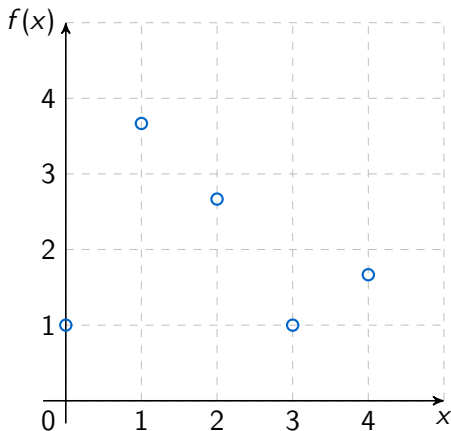
For each three points, a new polynomial interpolant can be derived:

$$p_2(x) = -\frac{11}{6}x^2 + 4\frac{1}{2}x + 1$$

$$p_2(x) = 4 - \frac{x^2}{3}$$

$$p_2(x) = \frac{7x^2}{6} - 7\frac{1}{2}x + 13$$

$$p_2(x) = \frac{8}{3}x^2 - 18x + 31$$



# Construction of Newton polynomials: example

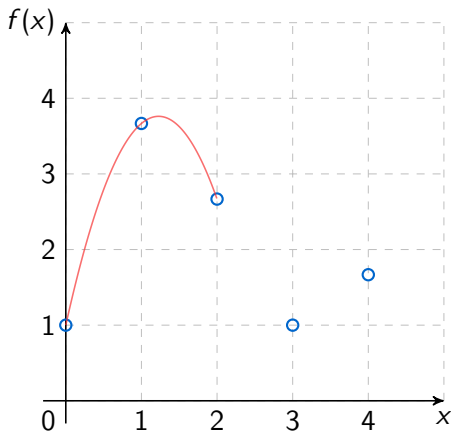
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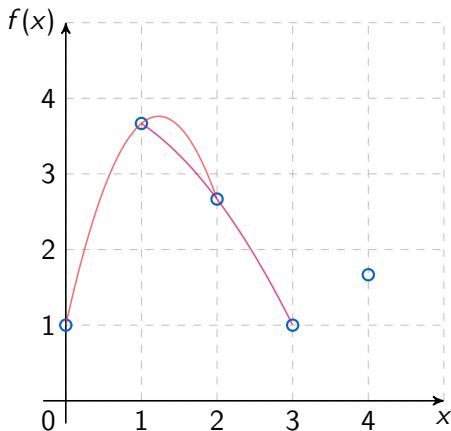
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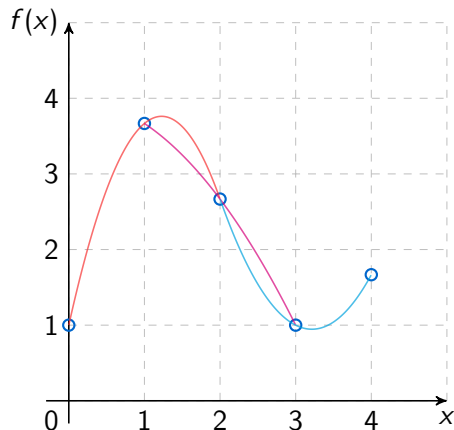
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# Construction of Newton polynomials: example

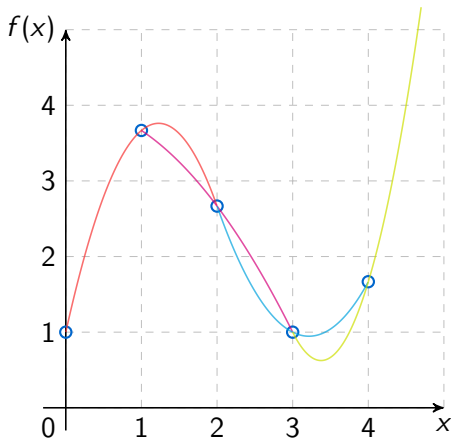
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# Construction of Newton polynomials: example

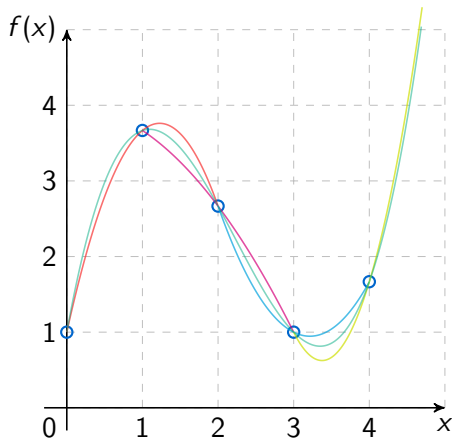
For each three points, a new polynomial interpolant can be derived:

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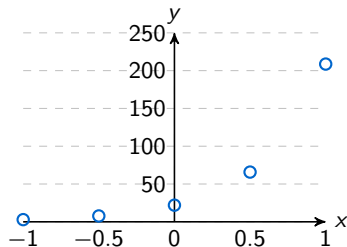


$$f(x) = \frac{x^3}{2} - \frac{10x^2}{3} + \frac{11x}{2} + 1$$

## Polynomial fitting in Matlab: example

Develop the  $p_2(x)$ ,  $p_3(x)$  and  $p_4(x)$   
from the following data set  
(example data x2 and y2):

$x_k$	$y_k$
-1.0	2.8677
-0.5	7.7530
0.0	22.0000
0.5	65.7863
1.0	208.6744

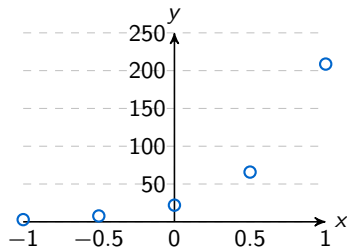




# Polynomial fitting in Matlab: example

Develop the  $p_2(x)$ ,  $p_3(x)$  and  $p_4(x)$  from the following data set (example data `x2` and `y2`):

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1.0	208.6744

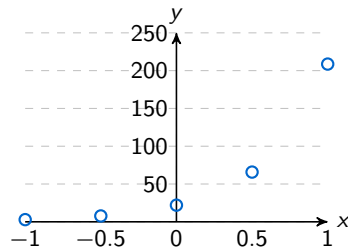


We use the built-in `polyfit(x,y,n)` and `polyval(p,x)` functions:

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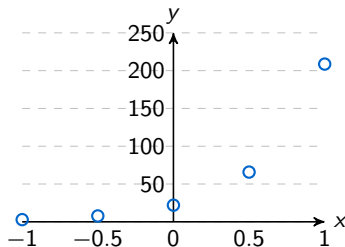
We use the built-in `polyfit(x,y,n)` and `polyval(p,x)` functions:

```
x_cont = linspace(-1,1,1001);  
p2 = polyfit(x2,y2,2);  
p3 = polyfit(x2,y2,3);  
p4 = polyfit(x2,y2,4);
```

# Polynomial fitting in Matlab: example

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$x_k$	$y_k$
-1.0	2.8677
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0.0	22.0000
0.5	65.7863
1.0	208.6744



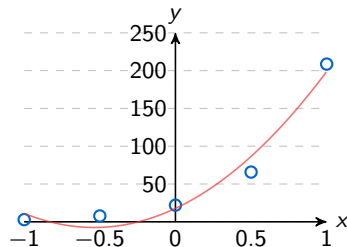
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```
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p2 = polyfit(x2,y2,2);  
p3 = polyfit(x2,y2,3);  
p4 = polyfit(x2,y2,4);  
y_cont2 = polyval(p2,x_cont);  
y_cont3 = polyval(p3,x_cont);  
y_cont4 = polyval(p4,x_cont);  
plot(x2,y2,'o',x_cont,y_cont2,x_cont,y_cont3,  
      x_cont,y_cont4)
```

# Polynomial fitting in Matlab: example

Develop the  $p_2(x)$ ,  $p_3(x)$  and  $p_4(x)$  from the following data set (example data x2 and y2):

$x_k$	$y_k$
-1.0	2.8677
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0.0	22.0000
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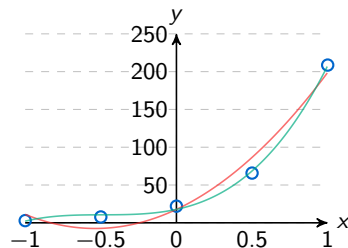
We use the built-in `polyfit(x,y,n)` and `polyval(p,x)` functions:

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p3 = polyfit(x2,y2,3);  
p4 = polyfit(x2,y2,4);  
y_cont2 = polyval(p2,x_cont);  
y_cont3 = polyval(p3,x_cont);  
y_cont4 = polyval(p4,x_cont);  
plot(x2,y2,'o',x_cont,y_cont2,x_cont,y_cont3,  
      x_cont,y_cont4)
```

# Polynomial fitting in Matlab: example

Develop the  $p_2(x)$ ,  $p_3(x)$  and  $p_4(x)$  from the following data set (example data x2 and y2):

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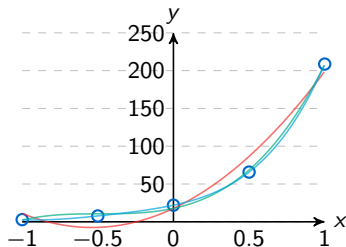
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```
x_cont = linspace(-1,1,1001);  
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p3 = polyfit(x2,y2,3);  
p4 = polyfit(x2,y2,4);  
y_cont2 = polyval(p2,x_cont);  
y_cont3 = polyval(p3,x_cont);  
y_cont4 = polyval(p4,x_cont);  
plot(x2,y2,'o',x_cont,y_cont2,x_cont,y_cont3,  
      x_cont,y_cont4)
```

# Polynomial fitting in Matlab: example

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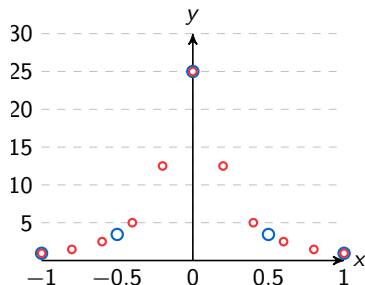
```
x_cont = linspace(-1,1,1001);  
p2 = polyfit(x2,y2,2);  
p3 = polyfit(x2,y2,3);  
p4 = polyfit(x2,y2,4);  
y_cont2 = polyval(p2,x_cont);  
y_cont3 = polyval(p3,x_cont);  
y_cont4 = polyval(p4,x_cont);  
plot(x2,y2,'o',x_cont,y_cont2,x_cont,y_cont3,  
      x_cont,y_cont4)
```

# Exercise

Develop the  $p_4(x)$  and  $p_{10}(x)$  interpolants from the following data sets:

$$f(x) = \frac{1}{x^2 + \frac{1}{25}} \quad x \in [-1, 1]$$

```
x3a = linspace(-1 , 1 , 5);  
x3b = linspace(-1 , 1 , 11);  
y3a = 1 ./ (x3a.^2 + (1/25));  
y3b = 1 ./ (x3b.^2 + (1/25));
```



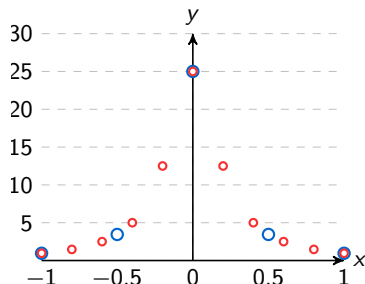
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$$f(x) = \frac{1}{x^2 + \frac{1}{25}} \quad x \in [-1, 1]$$

```
x3a = linspace(-1 , 1 , 5);  
x3b = linspace(-1 , 1 , 11);  
y3a = 1 ./ (x3a.^2 + (1/25));  
y3b = 1 ./ (x3b.^2 + (1/25));
```

```
x_cont = linspace(-1,1,1001);  
p4 = polyfit(x3a,y3a,4);  
p10 = polyfit(x3b,y3b,10);  
y_cont4 = polyval(p4,x_cont);  
y_cont10 = polyval(p10,x_cont);  
ezplot('1./(x.^2+(1/25))',[-1 1]); hold on;  
plot(x3a,y3a,'o',x3b,y3b,'x',x_cont,y_cont4,x_cont,  
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```





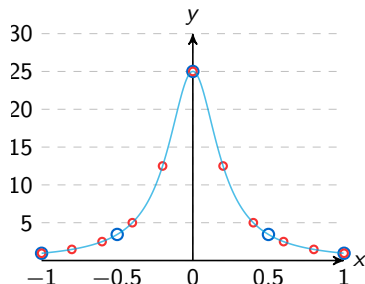
# Exercise

Develop the  $p_4(x)$  and  $p_{10}(x)$  interpolants from the following data sets:

$$f(x) = \frac{1}{x^2 + \frac{1}{25}} \quad x \in [-1, 1]$$

```
x3a = linspace(-1 , 1 , 5);  
x3b = linspace(-1 , 1 , 11);  
y3a = 1 ./ (x3a.^2 + (1/25));  
y3b = 1 ./ (x3b.^2 + (1/25));
```

```
x_cont = linspace(-1,1,1001);  
p4 = polyfit(x3a,y3a,4);  
p10 = polyfit(x3b,y3b,10);  
y_cont4 = polyval(p4,x_cont);  
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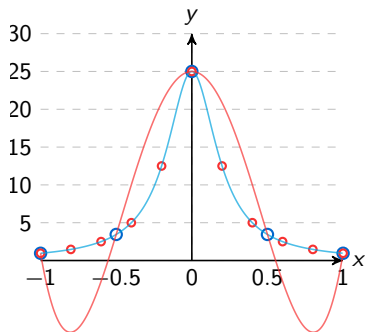
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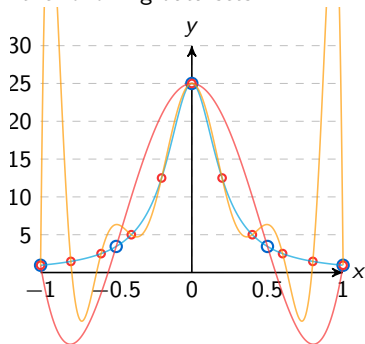
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## Final thoughts on polynomial interpolation

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- An polynomial interpolant of order  $n$  requires  $n + 1$  data points
  - More data points: interpolant does *not always* cross the points
  - Fewer data points: interpolant is not unique
- Higher-degree polynomials at equidistant points may cause strong oscillatory behaviour (Runge's phenomenon)
  - Mitigation of the problem on Chebyshev (i.e. non uniform grid)...
  - ... or by performing piecewise interpolation (next topic)
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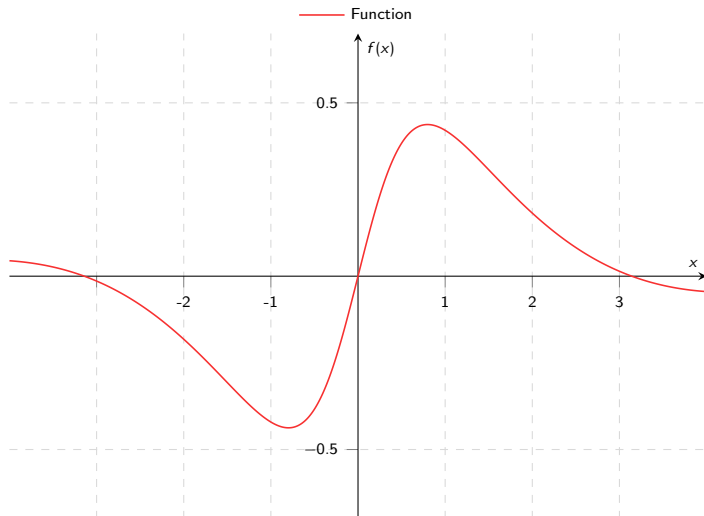
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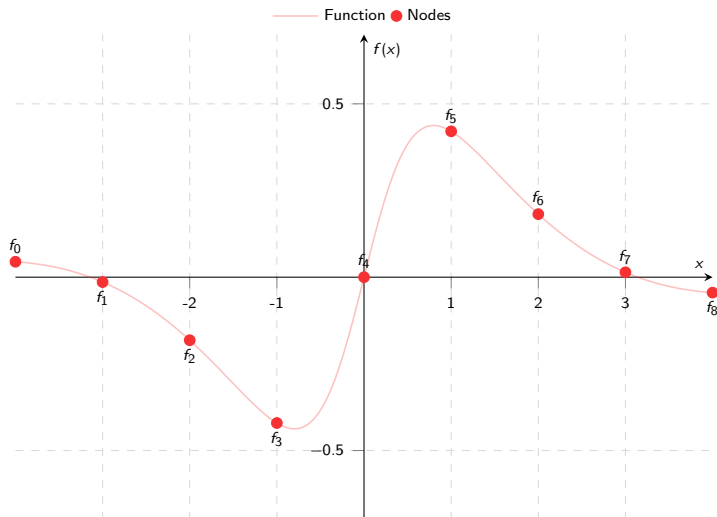
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Interpolation of  $f(x) = \frac{\sin x}{1 + x^2}$



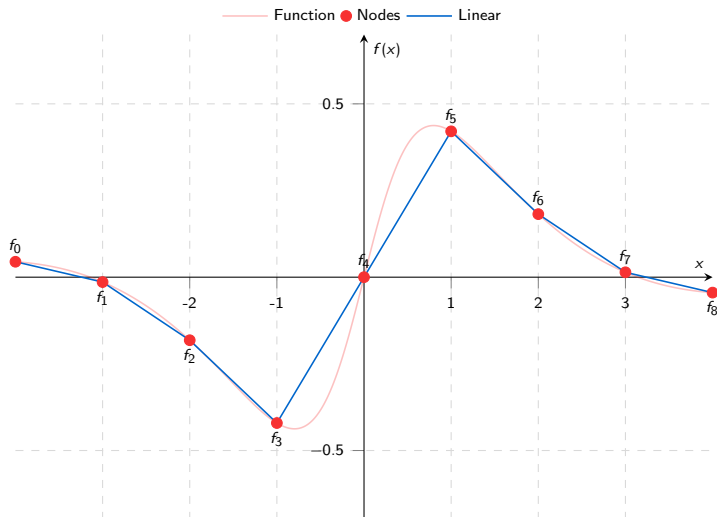
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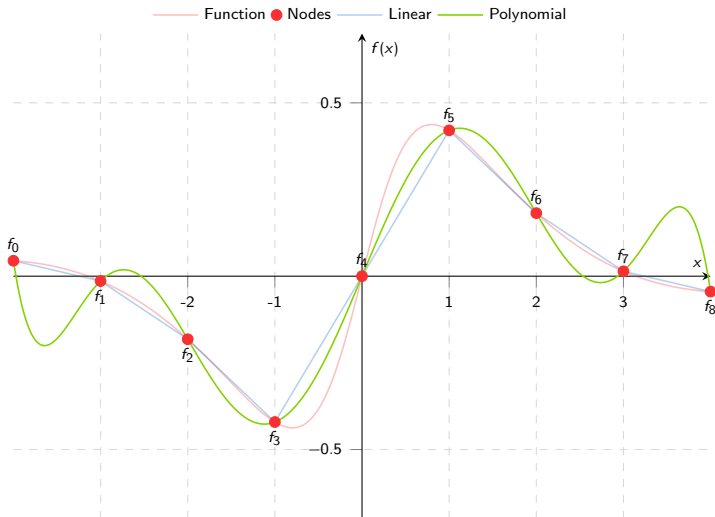
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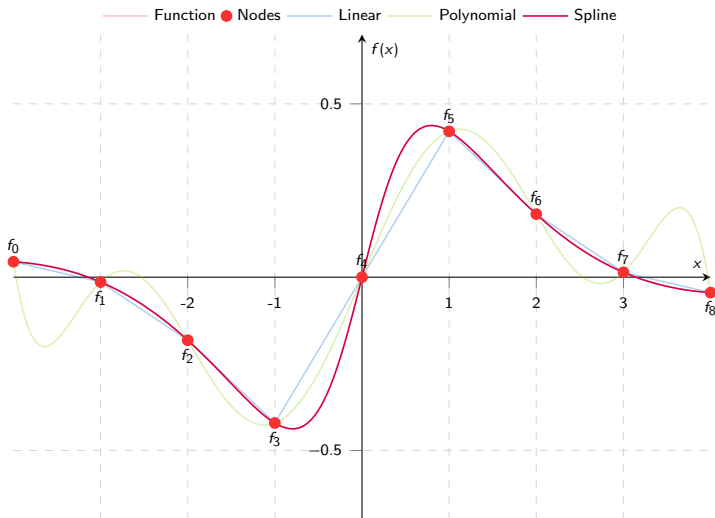
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# Spline interpolation in Matlab

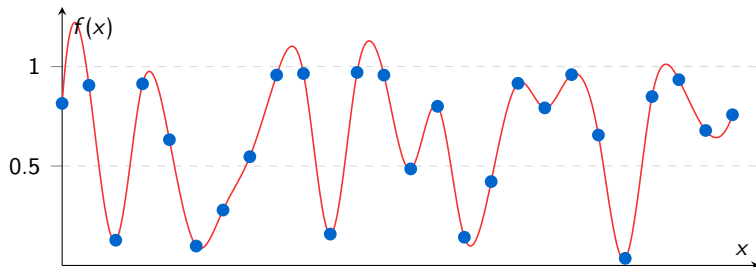
We can generate a random data set, and interpolate using `interp1`:



# Spline interpolation in Matlab

We can generate a random data set, and interpolate using `interp1`:

```
% Generate random data set  
x=0:25;  
y = rand(size(x));  
% Interpolant on a fine mesh  
xc = linspace(0,25,1001);  
yc = interp1(x,y,xc,'spline');  
plot(x,y,'o',xc,yc,'-r')
```



## Part II

# Numerical integration

# Today's outline

⑥ Introduction

⑦ Riemann integrals

⑧ Trapezoid rule

⑨ Simpson's rule

⑩ Conclusion

# Today's outline

## ⑥ Introduction

## ⑦ Riemann integrals

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# What is numerical integration?

To determine the integral  $I(x)$  of an integrand  $f(x)$ , which can be used to compute the area underneath the integrand between  $x = a$  and  $x = b$ .

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Today we will outline different numerical integration methods.

- Riemann integrals
- Trapezoidal rule
- Simpson's rule

# Why do chemical engineers need integration?

- Obtaining the cumulative particle size distribution from a particle size distribution
- The concentration outflow over time may be integrated to yield the residence time distribution
- Integration of a varying product outflow yields the total product outflow
- Quantitative analysis of mixture components via e.g. GC/MS
- Not all function have an explicit antiderivative, e.g.  $\int e^{x^2} dx$  or  $\int \frac{1}{\ln x} dx$

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⑥ Introduction

⑦ Riemann integrals

⑧ Trapezoid rule

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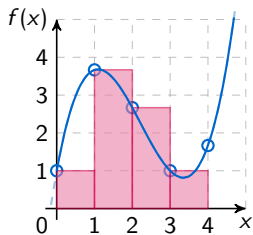
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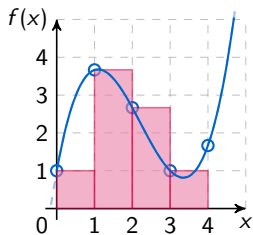


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# Riemann integrals

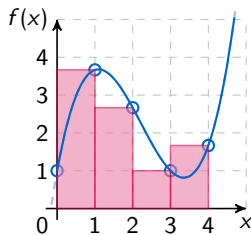
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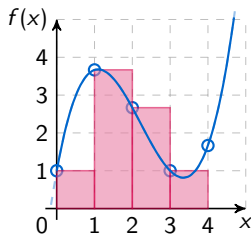


$$R_n = \sum_{i=1}^n f(x_i) \Delta x_i$$

# Riemann integrals

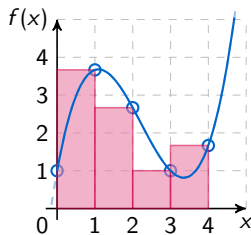
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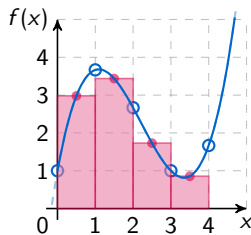
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$$R_n = \sum_{i=1}^n f(x_i)\Delta x_i$$

Midpoint rule



$$M_n = \sum_{i=1}^n f(\bar{x}_i)\Delta x_i$$

$$\text{with } \bar{x}_i = \frac{x_{i-1} + x_i}{2}$$



## Errors in Riemann integrals

We define the exact integral as  $I = \int_a^b f(x)dx$ , and  $L_n$ ,  $R_n$  and  $M_n$  represent the left, right and midpoint rule approximations of  $I$  based on  $n$  intervals.

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Writing  $f_{\max}^{(k)}$  for the maximum value of the  $k$ -th derivative, the upper-bounds of the errors by Riemann integrals are:

- $|I - L_n| \leq \frac{f_{\max}^{(1)}(b-a)^2}{2n}$
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Note that while  $|I - L_n|$  and  $|I - R_n|$  give the same *upper-bounds* of the error, this does not mean the same error. Rather, the error is of opposite sign!

# Today's outline

⑥ Introduction

⑦ Riemann integrals

⑧ Trapezoid rule

⑨ Simpson's rule

⑩ Conclusion

# Trapezoid rule

Since the sign of the approximation error of the left and right endpoint rules is opposite, we can take the average of these approximations:

$$T_n = \frac{L_n + R_n}{2}$$

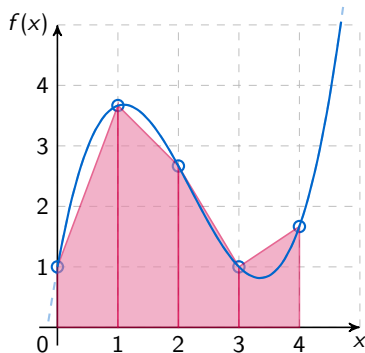
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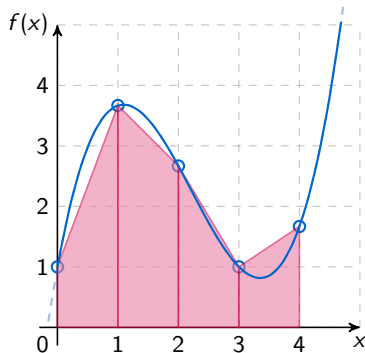
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Note that this can be rewritten for equidistant intervals:

$$T_n = \frac{b-a}{2n} (f(x_0) + 2f(x_1) + \dots + 2f(x_{n-1}) + f(x_n))$$



## Error in trapezoid integration

The trapezoid rule result over  $n$  intervals  $T_n$  approximates the exact integral  $I = \int_a^b f(x)dx$ . The upper-bounds of the error is given as:

$$|I - T_n| \leq \frac{f_{\max}^{(2)}(b-a)^3}{12n^2}$$

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The midpoint rule approximation has lower error bounds than the trapezoid rule. A linear function is, however, better approximated by the trapezoid rule.

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⑦ Riemann integrals

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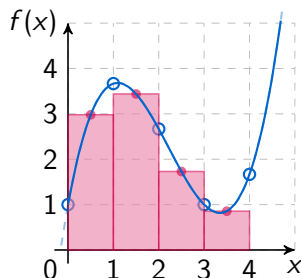
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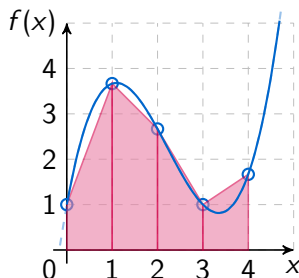
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Compare how the midpoint and trapezoid functions behave on convex and concave parts of a graph.

Midpoint rule

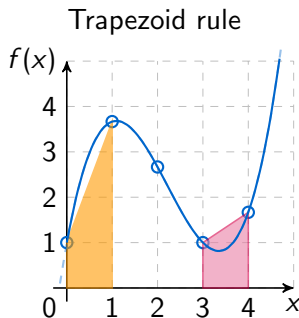
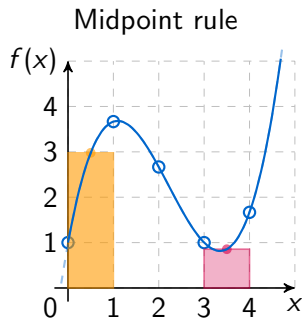


Trapezoid rule



# Towards higher-order integration

Compare how the midpoint and trapezoid functions behave on convex and concave parts of a graph.



In convex parts (bending down), the midpoint rule tends to overestimate the integral (trapezoid underestimates).

In concave parts (bending up), the midpoint rule tends to underestimate the integral (trapezoid overestimates).

## Towards higher-order integration

The errors of the midpoint rule and trapezoid rule behave in a similar way, but have opposite signs.

- Midpoint:  $|I - M_n| \leq \frac{f_{\max}^{(2)}(b-a)^3}{24n^2}$
- Trapezoid:  $|I - T_n| \leq \frac{f_{\max}^{(2)}(b-a)^3}{12n^2}$



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Taking the weighted average of these two yields the Simpson's rule:

$$S_{2n} = \frac{2}{3}M_n + \frac{1}{3}T_n$$

The  $2n$  means we have  $2n$  subintervals: the  $n$  trapezoid intervals are subdivided by the midpoint rule.

# Simpson's rule

Consider the interval  $i \in [x_0, x_2]$ , subdivided in three equidistant interpolation points:  $x_0, x_1, x_2$ .

- Midpoint:  $M_i = f\left(\frac{x_0 + x_2}{2}\right)2\Delta x = f(x_1)2\Delta x$
- Trapezoid:  $T_i = \frac{f(x_0) + f(x_2)}{2}2\Delta x$
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Note that  $M_i$  and  $T_i$  were computed on interval  $x_2 - x_0 = 2\Delta x$ .

Now we have:

$$\begin{aligned} S_i &= \frac{2}{3}[f(x_1)2\Delta x] + \frac{1}{3}\left[\frac{f(x_0) + f(x_2)}{2}2\Delta x\right] \\ &= \frac{4\Delta x}{3}f(x_1) + \frac{\Delta x}{3}f(x_0) + f(x_2) \end{aligned}$$

## Simpson's rule

Consider the interval  $i \in [x_0, x_2]$ , subdivided in three equidistant interpolation points:  $x_0, x_1, x_2$ .

- Midpoint:  $M_i = f\left(\frac{x_0 + x_2}{2}\right)2\Delta x = f(x_1)2\Delta x$
- Trapezoid:  $T_i = \frac{f(x_0) + f(x_2)}{2}2\Delta x$
- Simpson:  $S_i = \frac{2}{3}M_i + \frac{1}{3}T_i$

Note that  $M_i$  and  $T_i$  were computed on interval  $x_2 - x_0 = 2\Delta x$ .

Now we have:

$$\begin{aligned} S_i &= \frac{2}{3}[f(x_1)2\Delta x] + \frac{1}{3}\left[\frac{f(x_0) + f(x_2)}{2}2\Delta x\right] \\ &= \frac{4\Delta x}{3}f(x_1) + \frac{\Delta x}{3}f(x_0) + f(x_2) = \frac{\Delta x}{3}(f(x_0) + 4f(x_1) + f(x_2)) \end{aligned}$$

# Simpson's rule

We write  $f(x_k) = f_k$ . The integral of an interval  $i \in [x_0, x_2]$  is approximated as:

$$S_i = \frac{\Delta x}{3} (f_0 + 4f_1 + f_2)$$

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The next interval,  $S_j$  with  $j \in [x_2, x_4]$  with midpoint  $x_3 = \frac{x_2+x_4}{2}$  is approximated as:

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If we sum these two intervals we obtain:

$$\begin{aligned} I \approx S_i + S_j &= \left[ \frac{\Delta x}{3} (f_0 + 4f_1 + f_2) \right] + \left[ \frac{\Delta x}{3} (f_2 + 4f_3 + f_4) \right] \\ &= \frac{\Delta x}{3} (f_0 + 4f_1 + 2f_2 + 4f_3 + f_4) \end{aligned}$$



# Simpson's rule

In general, Simpson's rule can be written as:

$$\begin{aligned}\int_a^b f(x) dx &\approx \sum_{\substack{k=2 \\ k \text{ even}}}^n \frac{\Delta x}{3} (f_{k-2} + 4f_{k-1} + f_k) \\ &= \frac{\Delta x}{3} (f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \dots + 2f_{n-2} + 4f_{n-1} + f_n)\end{aligned}$$

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The error is given by:

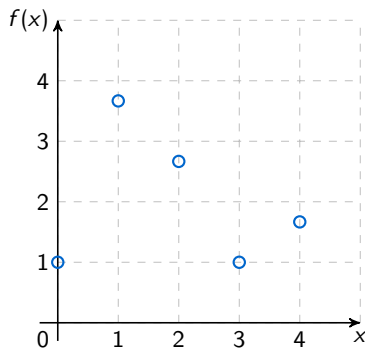
$$|I - S_n| \leq \frac{f_{\max}^{(4)}(b-a)^5}{180n^4}$$

if integrand  $f$  is differentiable on  $[a, b]$ .

## Simpson's rule: example

Recall our example data, described by  $f(x) = \frac{x^3}{2} - \frac{10x^2}{3} + \frac{11x}{2} + 1$

$$I = \int_0^4 \frac{x^3}{2} - \frac{10x^2}{3} + \frac{11x}{2} + 1 = \frac{80}{9} \approx 8.888\dots$$



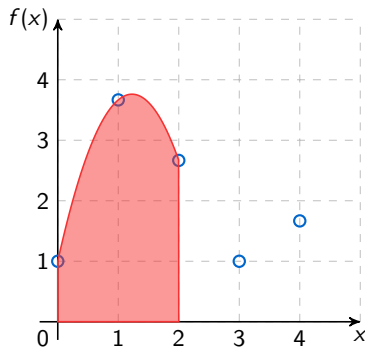
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- Interpolating  $x_0, x_1$  and  $x_2$ :

$$p_{2a}(x) = -\frac{11}{6}x^2 + 4\frac{1}{2}x + 1$$

$$\int_0^2 p_{2a} = \frac{55}{9} \approx 6.1111$$



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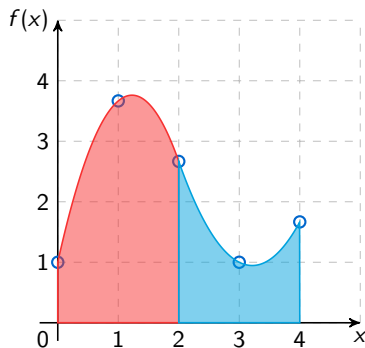
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- Interpolating  $x_2, x_3$  and  $x_4$ :

$$p_{2b}(x) = \frac{7x^2}{6} - 7\frac{1}{2}x + 13$$

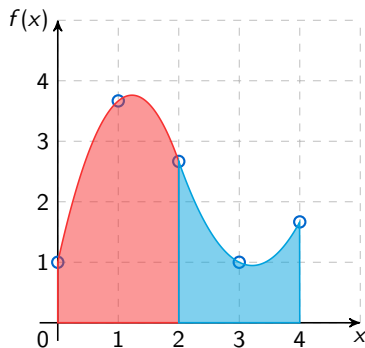
$$\int_2^4 p_{2b} = \frac{25}{9} \approx 2.777\dots$$



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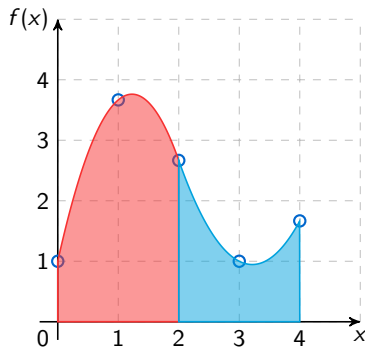
- Interpolating  $x_0, x_1$  and  $x_2$ :  
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 $\int_2^4 p_{2b} = \frac{25}{9} \approx 2.777\dots$
- Adding the separate integrals:  
 $\int_0^2 p_{2a} + \int_2^4 p_{2b} = \frac{80}{9}$



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 $p_{2b}(x) = \frac{7x^2}{6} - 7\frac{1}{2}x + 13$   
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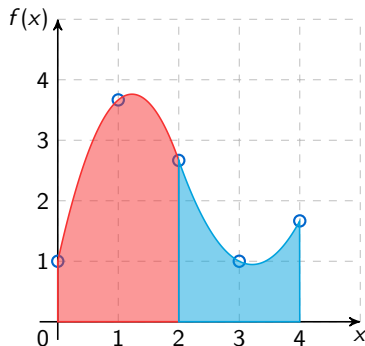


Using Simpson's rule:  $I \approx \frac{\Delta x}{3} (f_0 + 4f_1 + 2f_2 + 4f_3 + f_4) =$   
 $\frac{1}{3} (1 + 4 \cdot 3.6667 + 2 \cdot 2.6667 + 4 \cdot 1.0000 + 1.6667) = 8.88888 = \frac{80}{9}$

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Recall our example data, described by  $f(x) = \frac{x^3}{2} - \frac{10x^2}{3} + \frac{11x}{2} + 1$   
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 $\frac{1}{3} (1 + 4 \cdot 3.6667 + 2 \cdot 2.6667 + 4 \cdot 1.0000 + 1.6667) = 8.88888 = \frac{80}{9}$

Simpson's method is of third order: it gives exact approximations of third order polynomials!



# Integration in Matlab

Integration can be done numerically in Matlab.

- `trapz(x,y)` uses the trapezoid rule to integrate the data. Make sure you use the `x` variable if your data is not spaced with  $\Delta x = 1$ . Can handle non-equidistant data.
- Integration of functions can be done using the `integral(fun,xmin,xmax)` function:

```
fun = @(x) exp(-x.^2);  
I = integral(fun,0,10)  
I =  
    0.886226925452758
```

# Today's outline

⑥ Introduction

⑦ Riemann integrals

⑧ Trapezoid rule

⑨ Simpson's rule

⑩ Conclusion

# What hasn't been discussed?

This course is by no means complete, and further reading is possible.

- Legendre polynomials: Another way of performing the polynomial interpolation
- Gaussian quadrature: A third-order integration method that requires only two base points (in contrast to the third order Simpson's method, which requires three points)
- Adaptive techniques: Parts of a function that are relatively steady (no wild oscillations) and differentiable can be integrated with much larger step sizes than other parts of the function.
- Simpson's 3/8-rule: Yet another integration technique, requiring an additional data point

# Summary

- Interpolation is used to obtain data between existing data points
  - (Bi-)Linear, polynomial and spline interpolation methods
  - Construction of Newton polynomials
  - Oscillations of high-order polynomials
- Several techniques for numerical integration were discussed:
  - Riemann sums, trapezoid rule, Simpson's rule
  - Upper-bound errors were given for each technique