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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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:

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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

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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`,
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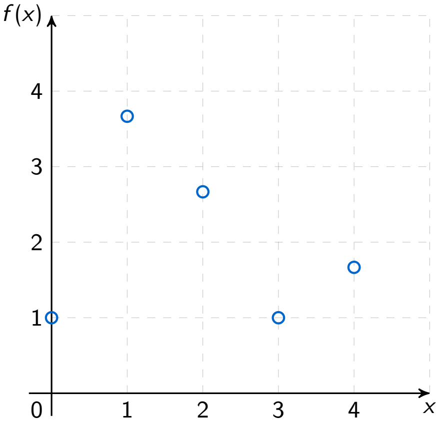
We start with `x1` and `y1`:

x_k	f_k
0	1.00
1	$\frac{11}{3} = 3.67$
2	$\frac{8}{3} = 2.67$
3	1.00
4	$\frac{5}{3} = 1.67$
5	$\frac{23}{3} = 7.67$

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 $x = 2.5$)?

$$\begin{aligned} x \in& [0, 0.5] && \rightarrow f(x) = f(0) \\ x \in&]0.5, 1.5] && \rightarrow f(x) = f(1) \\ x \in&]1.5, 2.5] && \rightarrow f(x) = f(2) \\ x \in&]2.5, 3.5] && \rightarrow f(x) = f(3) \\ x \in&]3.5, 4.5] && \rightarrow f(x) = f(4) \end{aligned}$$

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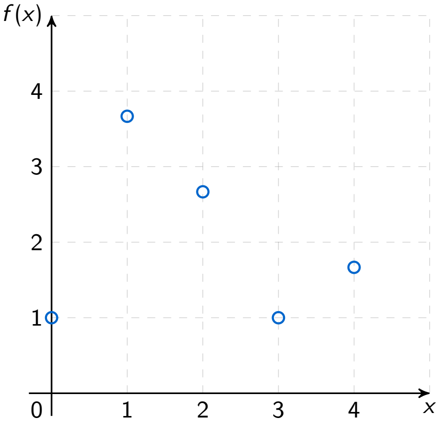

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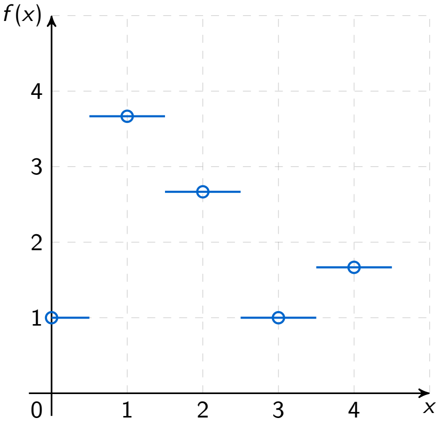

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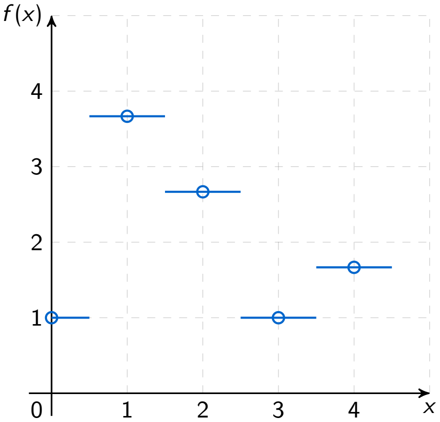

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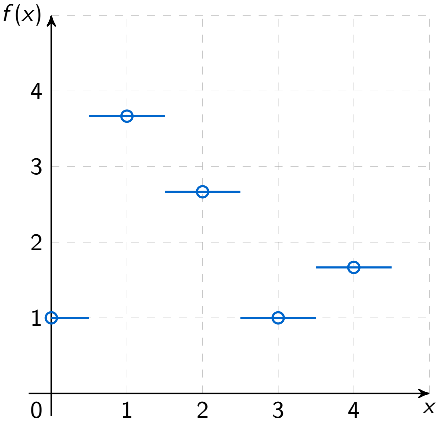

Linear interpolation

- 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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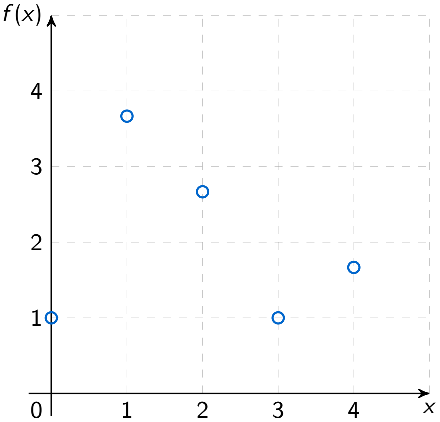

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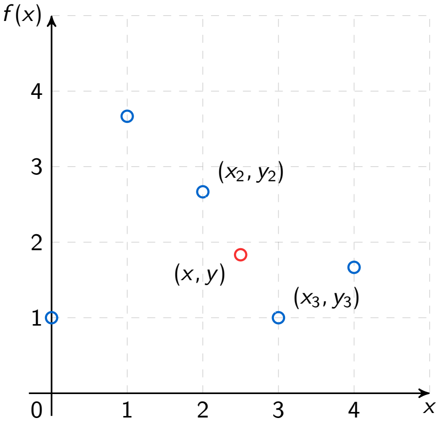

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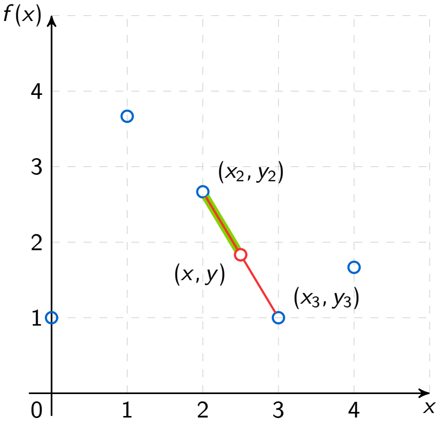

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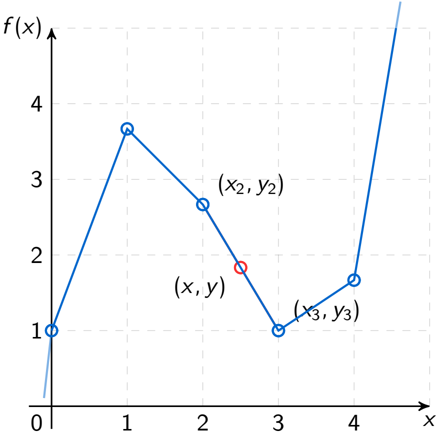

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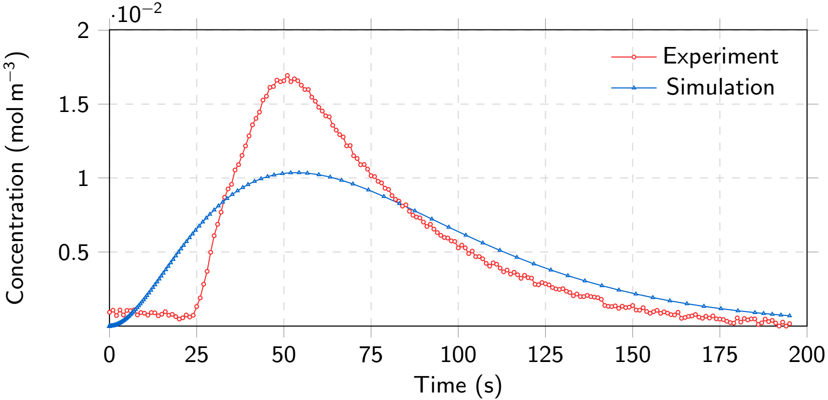
Example: Linear interpolation in Matlab

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}.

$$g_1 = f_{01}\frac{x_1 - x}{x_1 - x_0} + f_{11}\frac{x - x_0}{x_1 - x_0}$$
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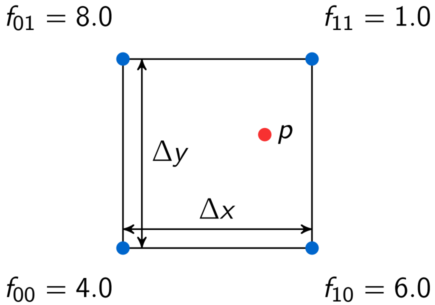

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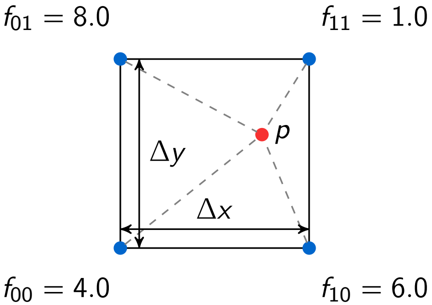

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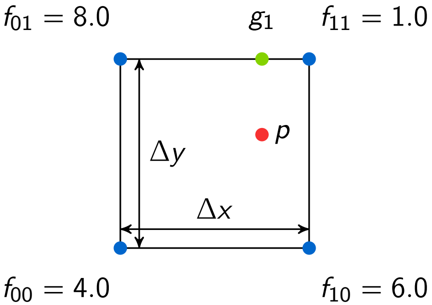

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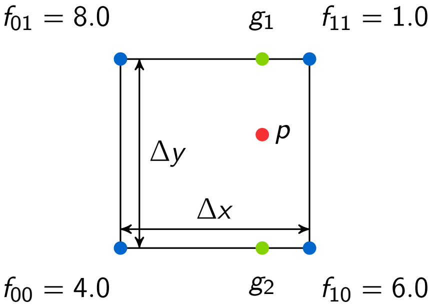

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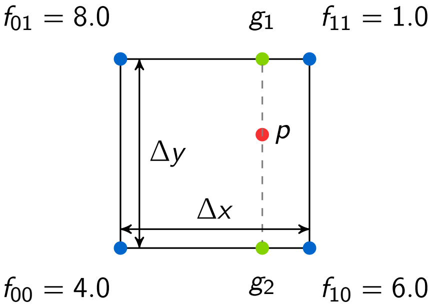

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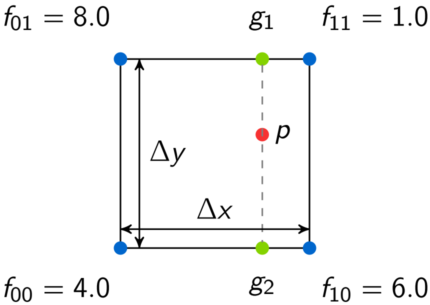
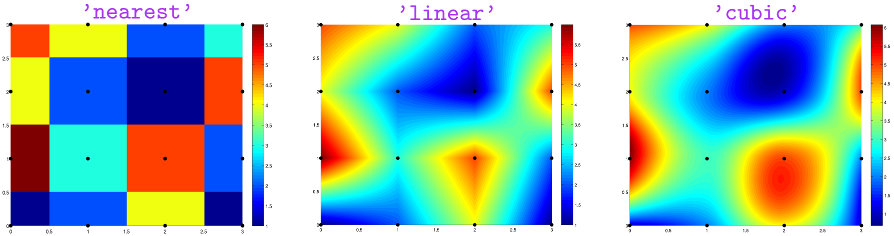


- The order of interpolation (x or y direction first) does not matter; the results are equal

Higher-dimensional field interpolation in Matlab

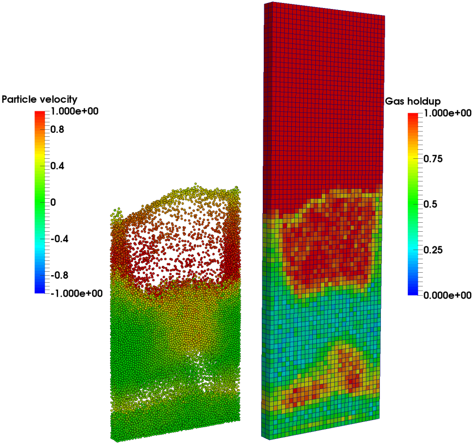
2D or higher-dimensional fields of data can be interpolated in Matlab using the `interp2`, `interp3` or even `interpn` functions, the method can be adjusted:



- 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:

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

Polynomial interpolation via Vandermonde matrix

Consider the data points (x_1, y_1), (x_2, y_2), ..., (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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```
>> x = [0 1 2];
>> y = [1.0000; 3.6667;
     2.6667];
>> V = vander(x);
>> a = V\y
a =
   -1.8333
     4.5000
     1.0000
```

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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 $f[x_0, \ldots, x_k]$ and polynomial terms $w_m(x)$:

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

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The polynomial terms are computed via:

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

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

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

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

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

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

Construction of Newton polynomials: example

Sample data

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

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x_k	f_k
x_0	$f[x_0] = f_0$

x_k	f_k
0	1

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

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

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

x_k	f_k		
0	1		
1	3.67	$\frac{\frac{11}{3} - 1}{1 - 0} = \frac{8}{3}$	
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$$f[x_{x-k},\dots,x_r]\equiv\frac{f[x_{r-k+1},\dots,x_r]-f[x_{r-k},\dots,x_{r-1}]}{x_r-x_{r-k}}$$

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

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

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$$= 1 \cdot 1 + \frac{8}{3} \cdot (x - 0) + \left(-\frac{11}{6}\right) \cdot (x - 0)(x - 1) = -\frac{11}{6}x^2 + 4\frac{1}{2}x + 1$$

Construction of Newton polynomials: example

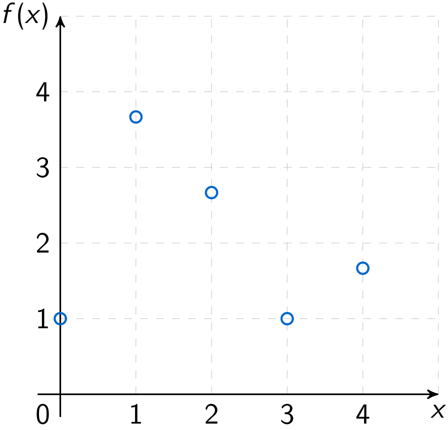
For each three points, a new polynomial interpolant can be derived:

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

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

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

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



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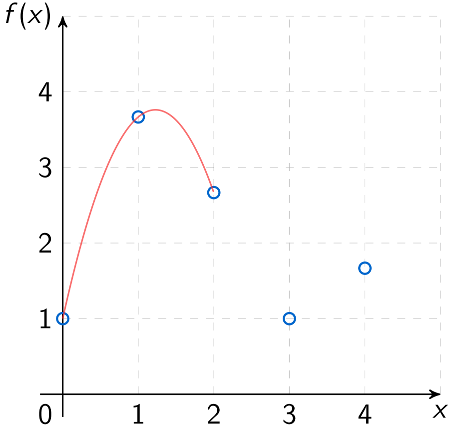

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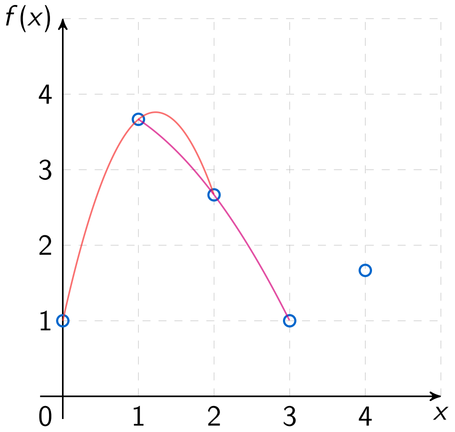

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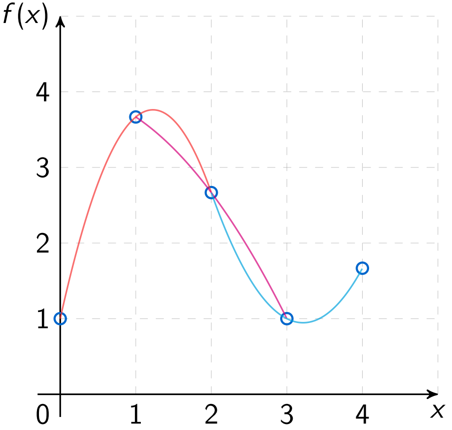

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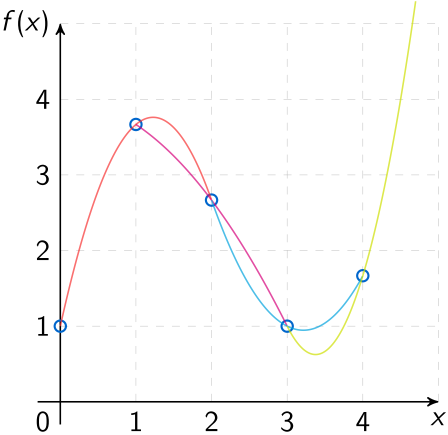

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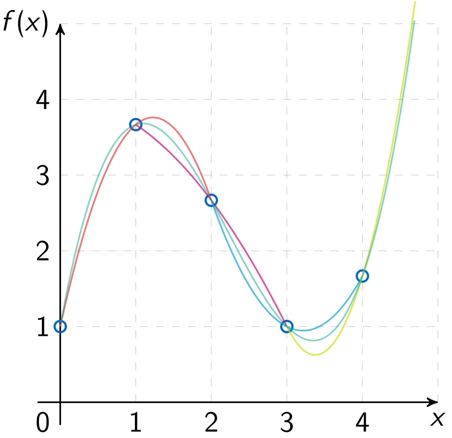
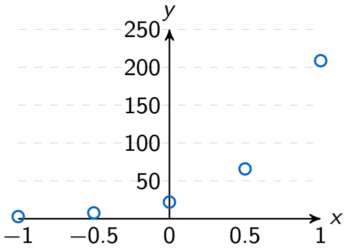


$$f(x) = \frac{x^3}{2} - \frac{10x^2}{3} + \frac{11x}{2} + 1$$

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



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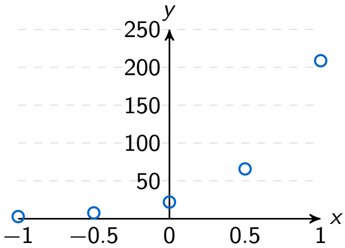

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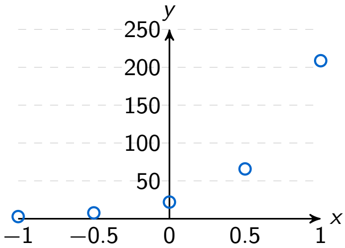

We use the built-in polyfit(x,y,n) and polyval(p,x) functions:

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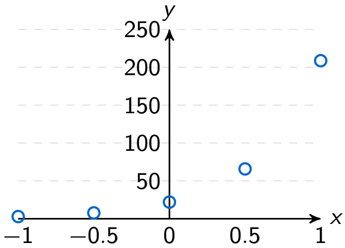

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y_cont2 = polyval(p2,x_cont);
y_cont3 = polyval(p3,x_cont);
y_cont4 = polyval(p4,x_cont);
plot(x2,y2,'o',x_cont,y_cont2,x_cont,y_cont3,
    x_cont,y_cont4)
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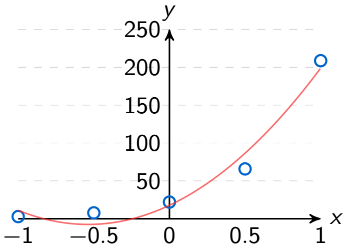

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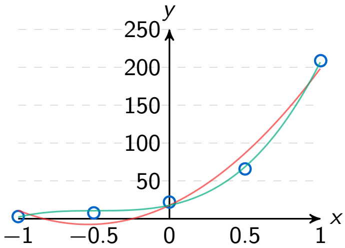

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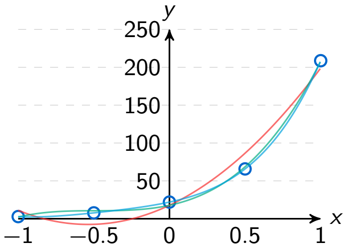

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y_cont4 = polyval(p4,x_cont);
plot(x2,y2,'o',x_cont,y_cont2,x_cont,y_cont3,
    x_cont,y_cont4)
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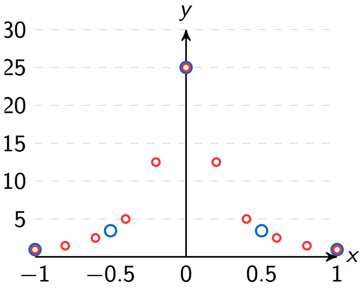
Exercise

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

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

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



Exercise

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

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

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x3a = linspace(-1 , 1 , 5);
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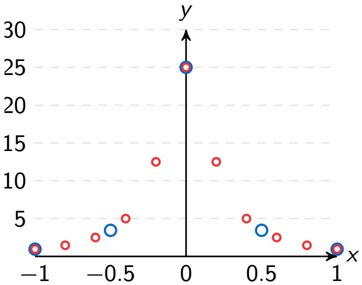


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x_cont = linspace(-1,1,1001);
p4 = polyfit(x3a,y3a,4);
p10 = polyfit(x3b,y3b,10);
y_cont4 = polyval(p4,x_cont);
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ezplot('1./(x.^2+(1/25))',[-1 1]); hold on;
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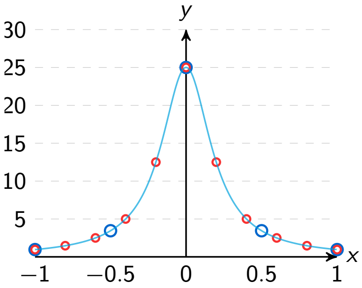


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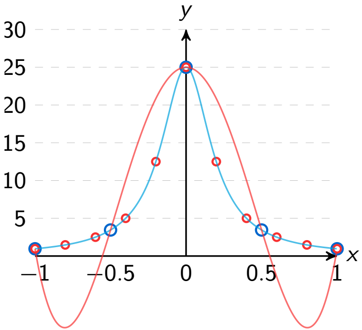


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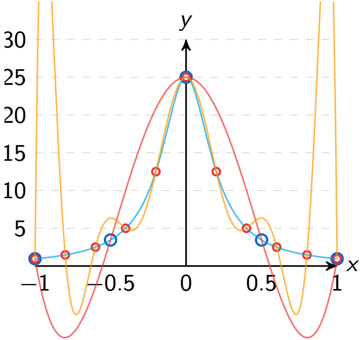


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Final thoughts on polynomial interpolation

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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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Splines: comparison to other interpolation techniques

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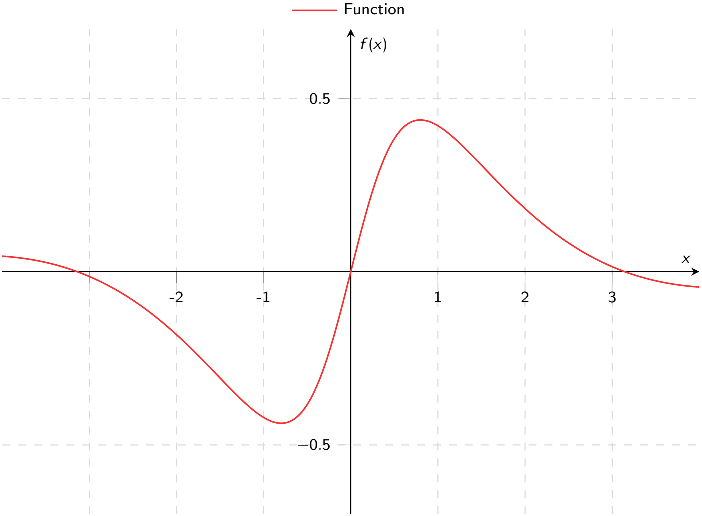

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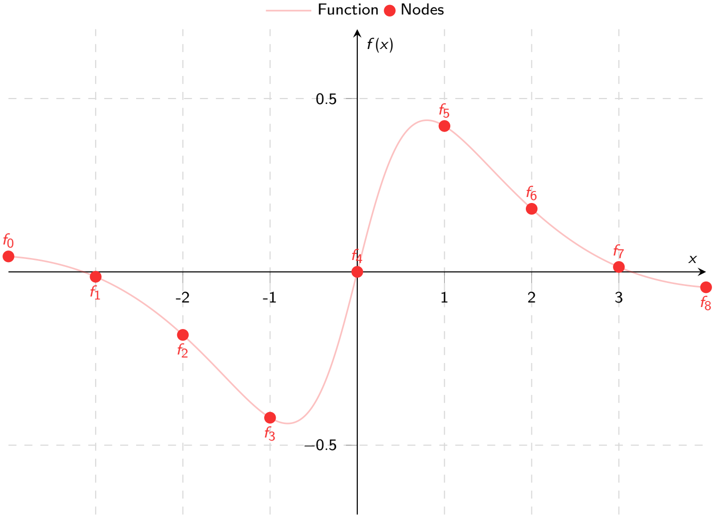

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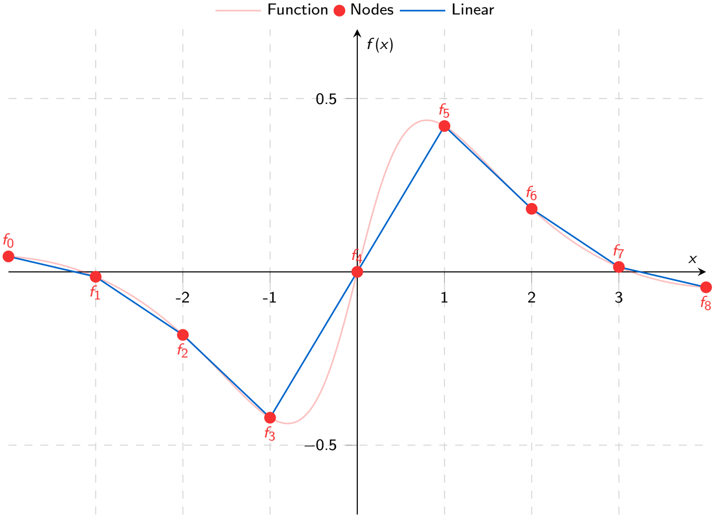

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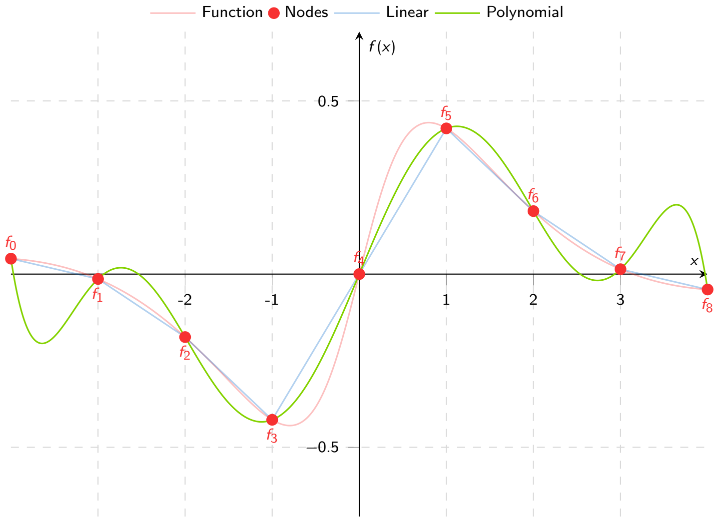

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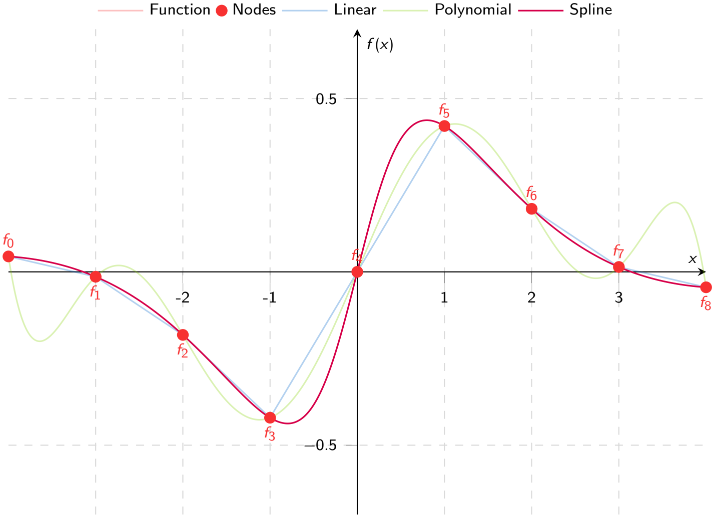

Spline interpolation in Matlab

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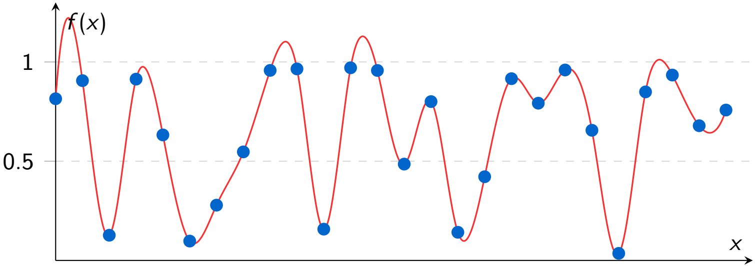
```
% Generate random data set
x=0:25;
y = rand(size(x));
% Interpolant on a fine mesh
xc = linspace(0,25,1001);
yc = interp1(x,y,xc,'spline');
plot(x,y,'o',xc,yc,'-r')
```



Part II

Numerical integration

Today's outline

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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 $x = b$.

$$I(x) = \int_a^b f(x)dx$$

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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
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Basic idea: Subdivide the interval $[a, b]$ into n subintervals of equal length $\Delta x = \frac{b-a}{n}$ and use the sum of area to approximate the integral.

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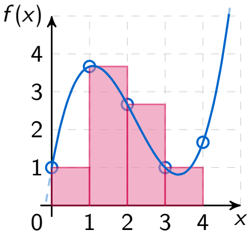

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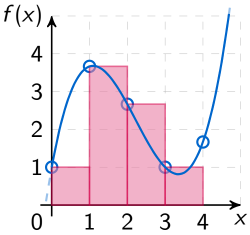

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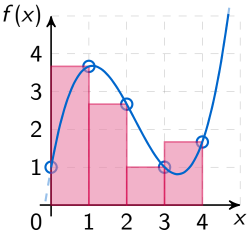

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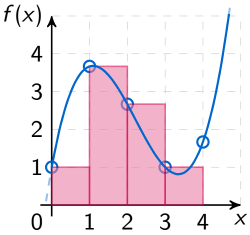

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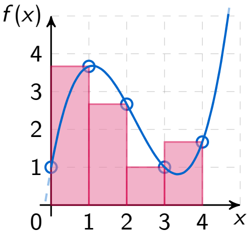

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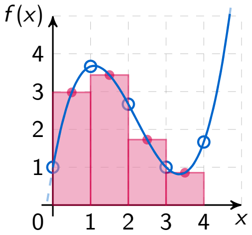

$$M_n = \sum_{i=1}^{n} f(\bar{x}_i)\Delta x_i$$

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

Errors in Riemann integrals

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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

Trapezoid rule

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

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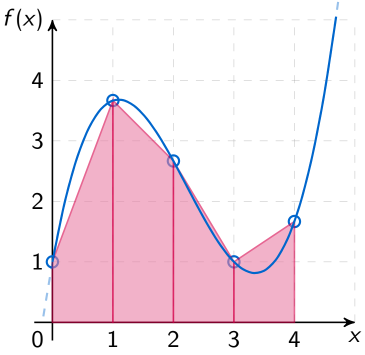

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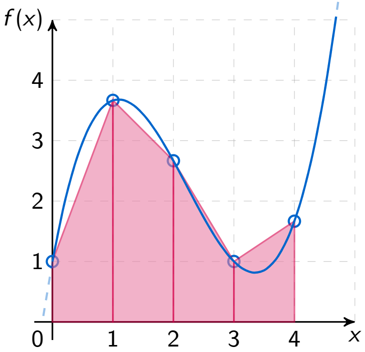
Note that this can be rewritten for equidistant intervals:

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



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:

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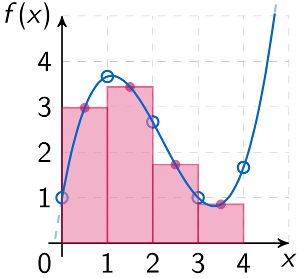
The midpoint rule approximation has lower error bounds than the trapezoid rule. A linear function is, however, better approximated by the trapezoid rule.

Today's outline

Towards higher-order integration

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

Midpoint rule



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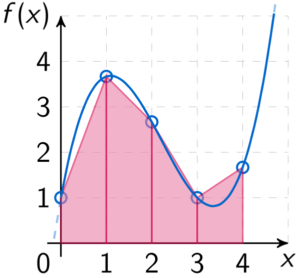

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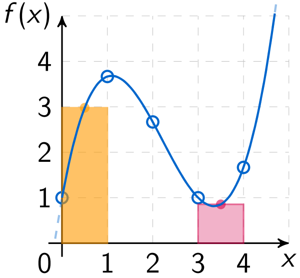

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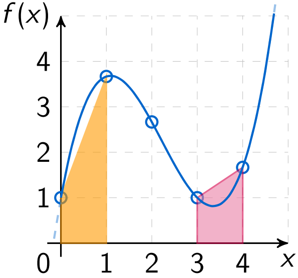

In convex parts (bending down), the midpoint rule tends to overestimate the integral (trapezoid underestimates).
In concave parts (bending up), the midpoint rule tends to underestimate the integral (trapezoid overestimates).

Towards higher-order integration

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

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

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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: $M_i = f(\frac{x_0 + x_2}{2})2\Delta x = f(x_1)2\Delta x$
- 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 $x_2 - x_0 = 2\Delta x$.

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- Midpoint: $M_i = f(\frac{x_0 + x_2}{2})2\Delta x = f(x_1)2\Delta x$
- 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:

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

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

Simpson's rule

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

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

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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:

$$\begin{aligned} I \approx S_i + S_j &= \left[\frac{\Delta x}{3}\left(f_0 + 4f_1 + f_2\right)\right] + \left[\frac{\Delta x}{3}\left(f_2 + 4f_3 + f_4\right)\right] \\ &= \frac{\Delta x}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + f4\right) \end{aligned}$$

Simpson's rule

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

$$\int_a^b f(x)dx \approx \sum_{\substack{k=2 \\ k \text{ even}}}^{n} \frac{\Delta x}{3}\left(f_{k-2} + 4f_{k-1} + f_k\right)$$

$$= \frac{\Delta x}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \ldots + 2f_{n-2} + 4f_{n-1} + f_n\right)$$

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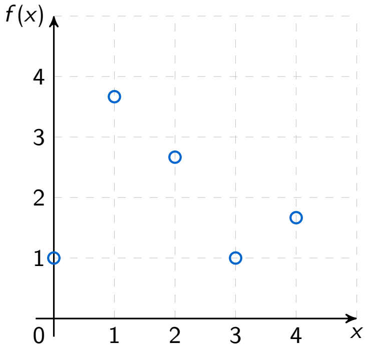
The error is given by:

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

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

Simpson's rule: example

Recall our example data, described by $f(x) = \frac{x^3}{2} - \frac{10x^2}{3} + \frac{11x}{2} + 1$
$I = \int_0^4 \frac{x^3}{2} - \frac{10x^2}{3} + \frac{11x}{2} + 1 = \frac{80}{9} \approx 8.888\ldots$



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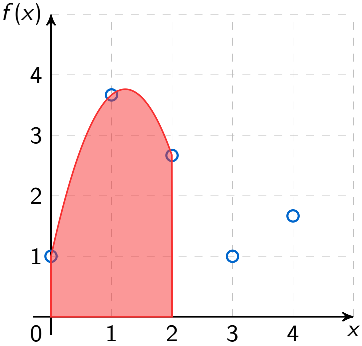
- Interpolating x_0, x_1 and x_2:
  $p_{2a}(x) = -\frac{11}{6}x^2 + 4\frac{1}{2}x + 1$
  $\int_0^2 p_{2a} = \frac{55}{9} \approx 6.1111$



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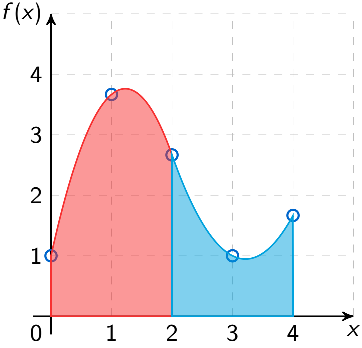

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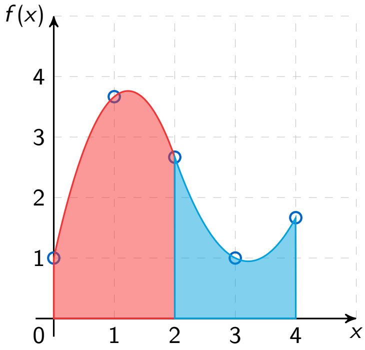

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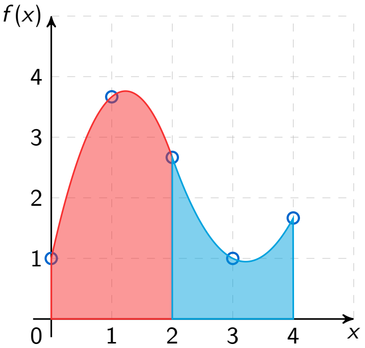

Using Simpson's rule: $I \approx \frac{\Delta x}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + f_4\right) =$
$\frac{1}{3}\left(1 + 4 \cdot 3.6667 + 2 \cdot 2.6667 + 4 \cdot 1.0000 + 1.6667\right) = 8.88888 = \frac{80}{9}$

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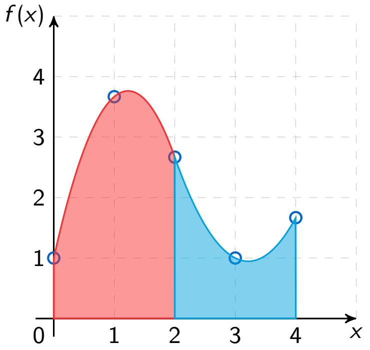

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Simpson's method is of third order: it gives exact approximations of third order polynomials!

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

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