Numerical interpolation and integration

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Part I

Numerical interpolation

Today's outline

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5 Splines

Interpolation problem

Definition

Given a set of points x_k, $k = 0, \ldots, n$, $x_i \neq x_j$ with associated function values f_k, $k = 0, \ldots, n$, 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:

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

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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 requires additionally some way of computing the error between function (curve) and data

- Curve-fitting does not strictly enforce the function to match the data exactly

- Curve-fitting may be done on multiple datapoints at one position

- Curve-fitting is much more expensive to do, requires optimisation

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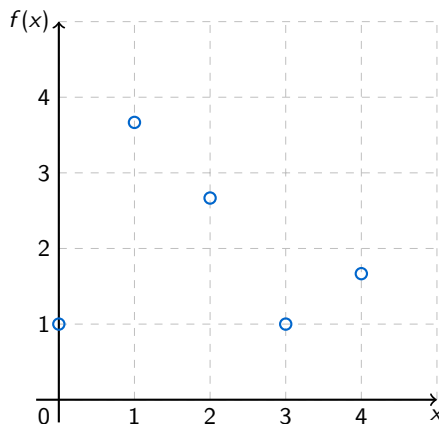`interpolation-dataset.mat`,
which contains multiple data sets.

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Today's data set

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`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 o at discrete
intervals $x_n \in \{0, 5\}$

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Piecewise constant interpolation

- Nearest-neighbor interpolation in the continuous range $x \in [0, 5]$

- How to treat the point halfway (e.g. at $x = 2.5$)?

  $x \in [0, 0.5] \quad \rightarrow f(x) = f(0)$
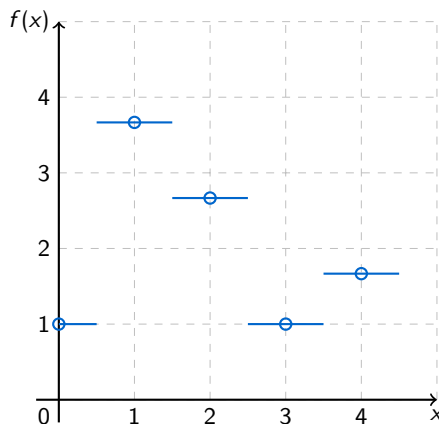 $x \in]0.5, 1.5] \quad \rightarrow f(x) = f(1)$
  $x \in]1.5, 2.5] \quad \rightarrow f(x) = f(2)$
  $x \in]2.5, 3.5] \quad \rightarrow f(x) = f(3)$
  $x \in]3.5, 4.5] \quad \rightarrow f(x) = f(4)$

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

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

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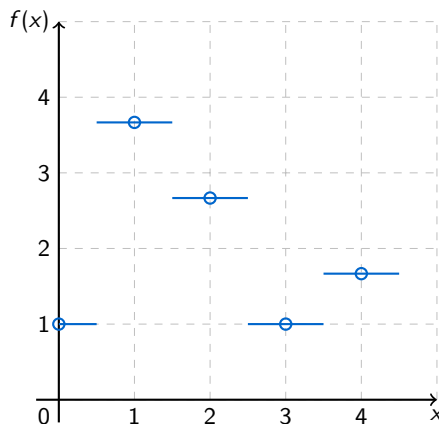 $x \in]0.5, 1.5] \quad \rightarrow f(x) = f(1)$
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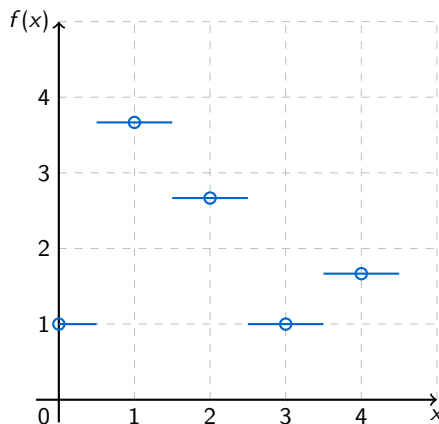
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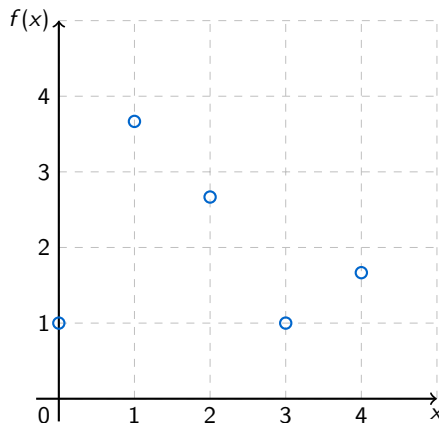
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Linear interpolation

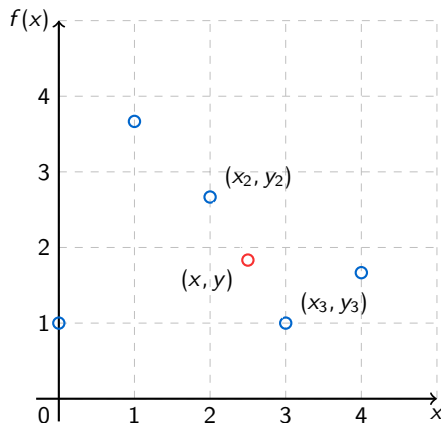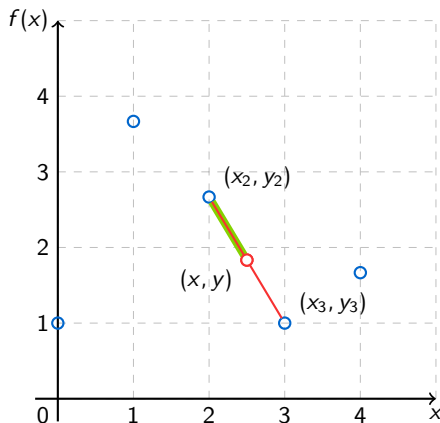Data set $f_n(x_n)$ represented by ○ at discrete intervals $x_n \in \{0, 5\}$

- 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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Linear interpolation

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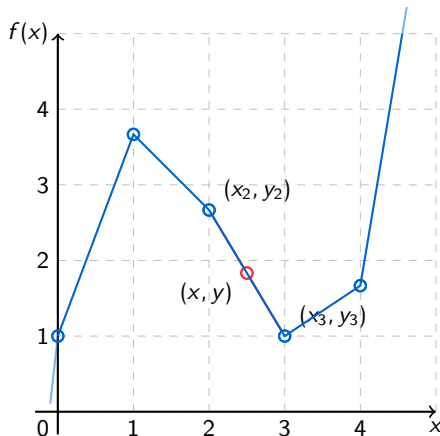
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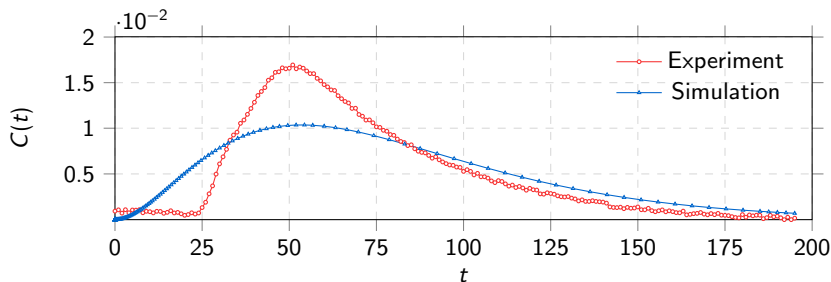
Linear interpolation

- While linear interpolation is fast, and relatively easy to program, it is not very accurate

- At the nodes, the derivatives are discontinuous i.e. not differentiable

- Error is proportional to the square of the distance between nodes

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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.

Example: Linear interpolation in Matlab

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```matlab
% 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}.
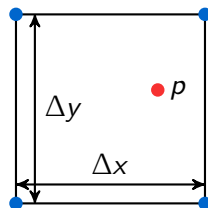
$$g_1 = f_{01}\frac{x_1 - x}{x_1 - x_0} + f_{11}\frac{x - x_0}{x_1 - x_0}$$
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$f_{01} = 8.0$ $f_{11} = 1.0$

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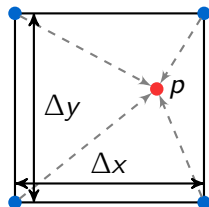
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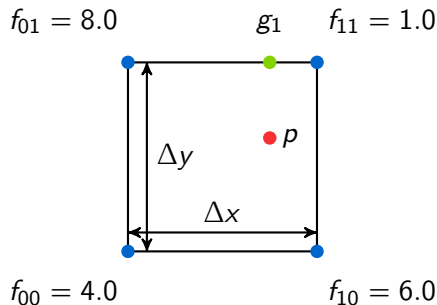

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$\bullet\, p$

Δy

Δx
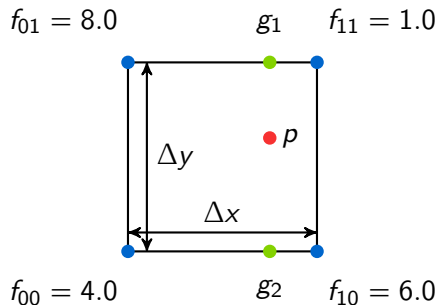
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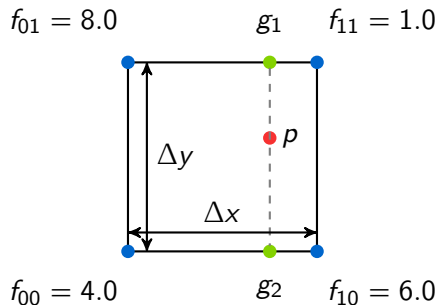$f_{00} = 4.0 \qquad g_2 \quad f_{10} = 6.0$

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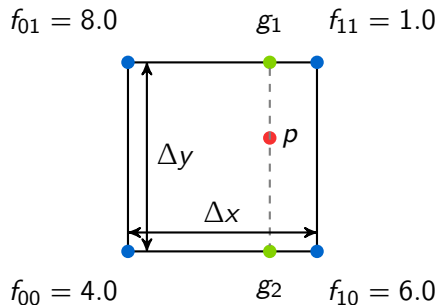$f_{00} = 4.0$ g_2 $f_{10} = 6.0$

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p

Δy

Δx

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

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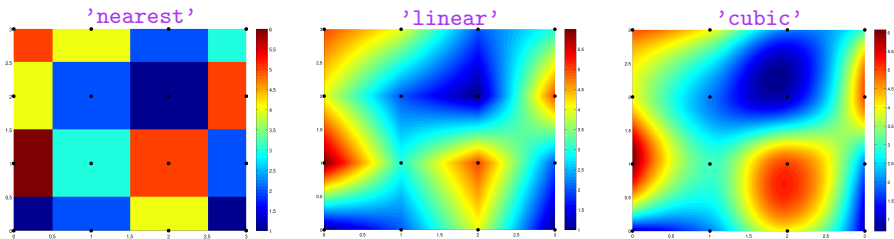
- Similar to 1D linear interpolation, the derivatives are
  discontinuous on the grid nodes
- Also consider tri-linear interpolation (for 3D fields), or bicubic
  interpolation (2D, but third order)

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.
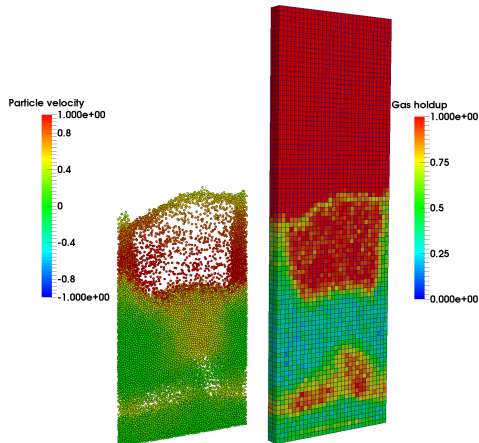
Polynomial interpolation

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:

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

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

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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
```

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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So we found the equation:

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

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    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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Construction of Newton polynomials

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The polynomial terms are computed via:

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

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

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

Construction of Newton polynomials

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$$w_m(x) = (x - x_0) \cdot (x - x_1) \cdots (x - x_{m-1}) = w_{m-1} \cdot (x - x_{m-1})$$
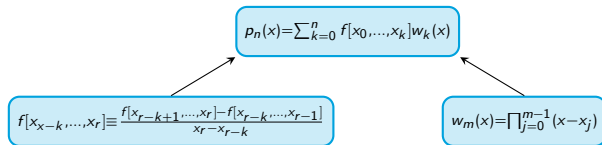$$w_m(x) = \prod_{j=0}^{m-1} (x - x_j), \qquad m = 0, \ldots, n$$

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

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

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Construction of Newton polynomials: example

Sample data

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

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

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

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Construction of Newton polynomials: example

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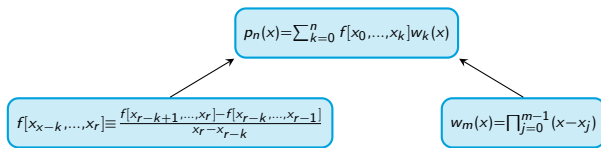
$$w_m(x) = \prod_{j=0}^{m-1} (x - x_j)$$

x_k	f_k
x_0	$f[x_0] = f_0$

x_k	f_k
0	1

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Construction of Newton polynomials: example

Sample data

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

Construction of Newton polynomials: example

Sample data

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

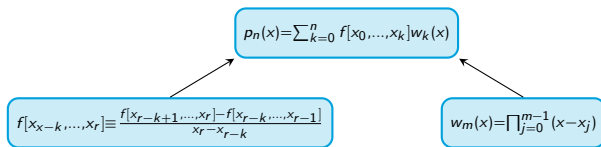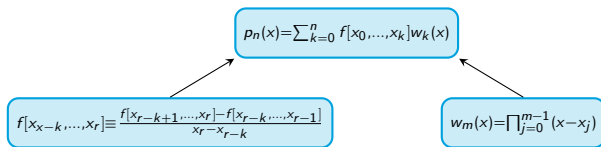| x_k	f_k		
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Construction of Newton polynomials: example

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

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Construction of Newton polynomials: example

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Construction of Newton polynomials: example

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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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Construction of Newton polynomials: example

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

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Construction of Newton polynomials: example

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

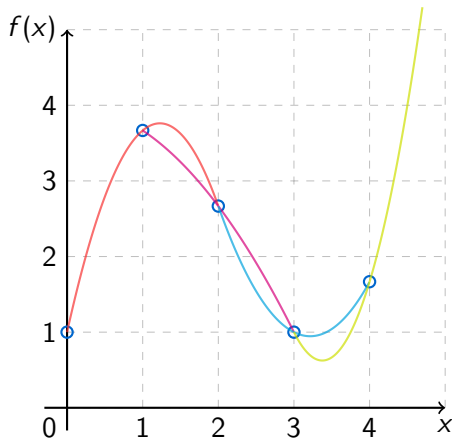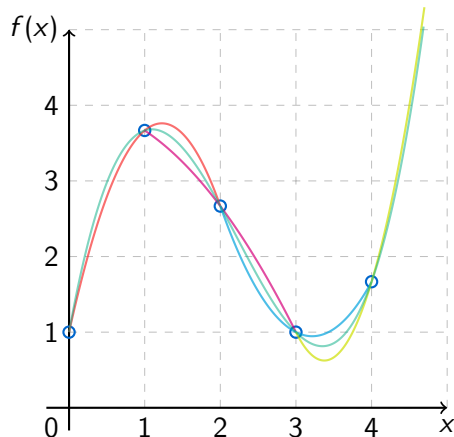## Construction of Newton polynomials: example

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

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

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

$$p_2(x) = \frac{7x^2}{6} - 7\frac{1}{2}x + 13$$
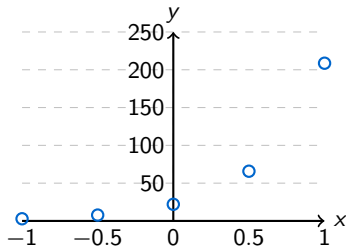
$$p_2(x) = \frac{8}{3}x^2 - 18x + 31$$

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Construction of Newton polynomials: example

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Construction of Newton polynomials: example

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Construction of Newton polynomials: example

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Construction of Newton polynomials: example

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

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

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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Polynomial fitting in Matlab: example

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

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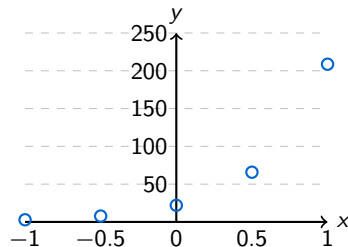
Polynomial fitting in Matlab: example

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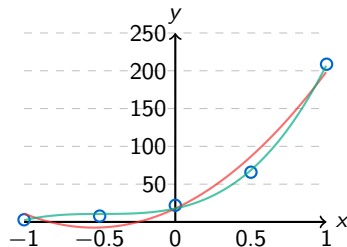| x_k	y_k
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1.0	208.6744

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

Develop the $p_2(x)$, $p_3(x)$ and $p_4(x)$
from the following data set
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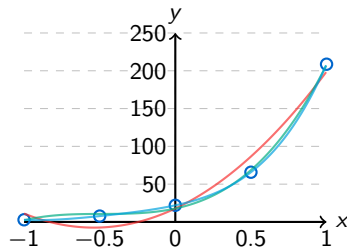| x_k	y_k
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0.0	22.0000
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1.0	208.6744

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);
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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Polynomial fitting in Matlab: example

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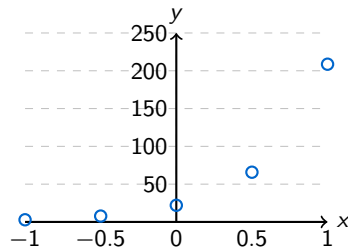
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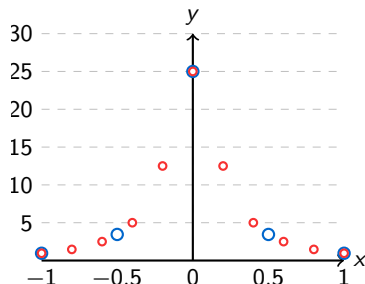
```
x_cont = linspace(-1,1,1001);
p2 = polyfit(x2,y2,2);
p3 = polyfit(x2,y2,3);
p4 = polyfit(x2,y2,4);
y_cont2 = polyval(p2,x_cont);
y_cont3 = polyval(p3,x_cont);
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plot(x2,y2,'o',x_cont,y_cont2,x_cont,y_cont3,
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```

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

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);
y_cont2 = polyval(p2,x_cont);
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plot(x2,y2,'o',x_cont,y_cont2,x_cont,y_cont3,
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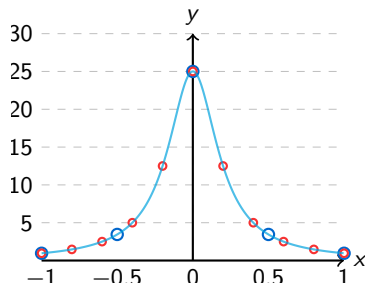
Exercise

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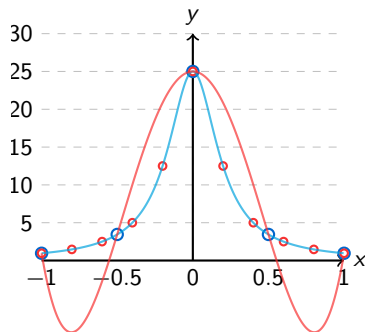
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x_cont = linspace(-1,1,1001);
p4 = polyfit(x3a,y3a,4);
p10 = polyfit(x3b,y3b,10);
y_cont4 = polyval(p4,x_cont);
y_cont10 = polyval(p10,x_cont);
ezplot('1./(x.^2+(1/25))',[-1 1]); hold on;
plot(x3a,y3a,'o',x3b,y3b,'x',x_cont,y_cont4,x_cont,
    y_cont10);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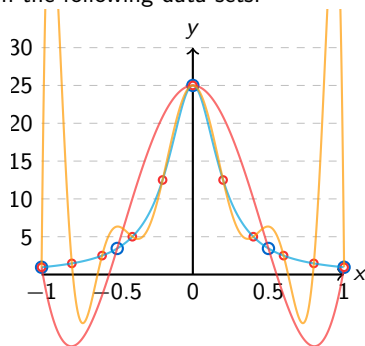
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```

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Final thoughts on polynomial interpolation

Final thoughts on polynomial interpolation

- 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)

- Matlab functions `polyfit(x,y,n)` and `polyval(p,x_new)` were demonstrated.

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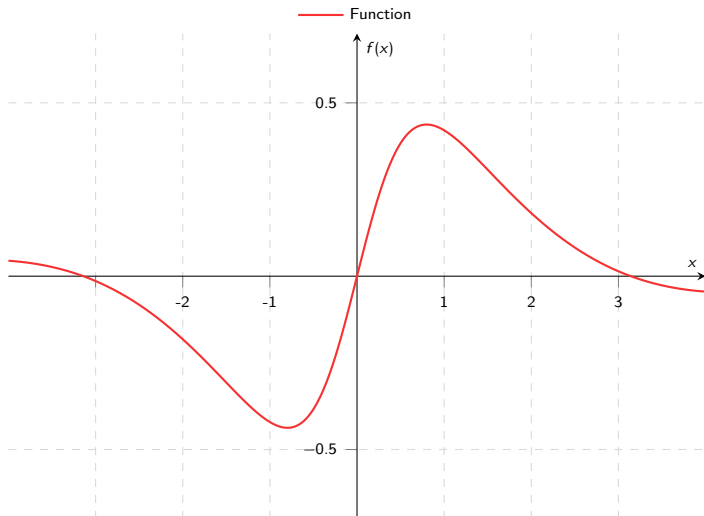# Spline interpolation

A spline is a numerical function that represents a smooth, higher order, piecewise polynomial interpolants of a data set.

Spline interpolation

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- Smooth: the interpolant is continuous in the first and second derivatives

- Higher order: The most common type of splines uses third-order polynomials (cubic splines)

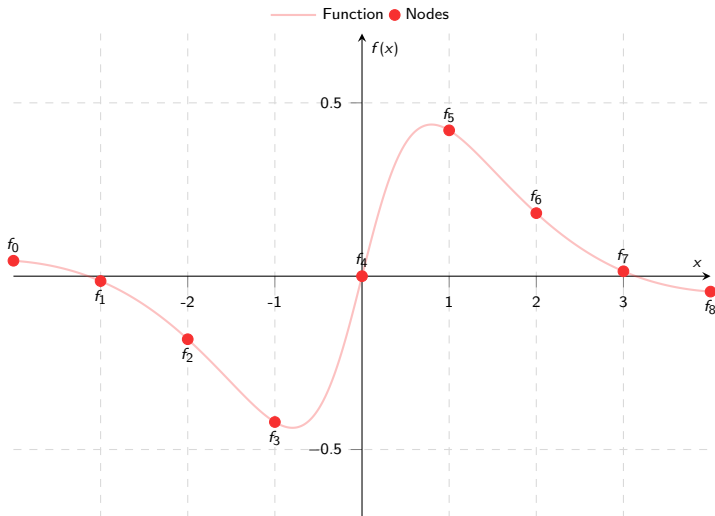- Piecewise polynomial: The interpolant is constructed between each two consecutive tabulated points

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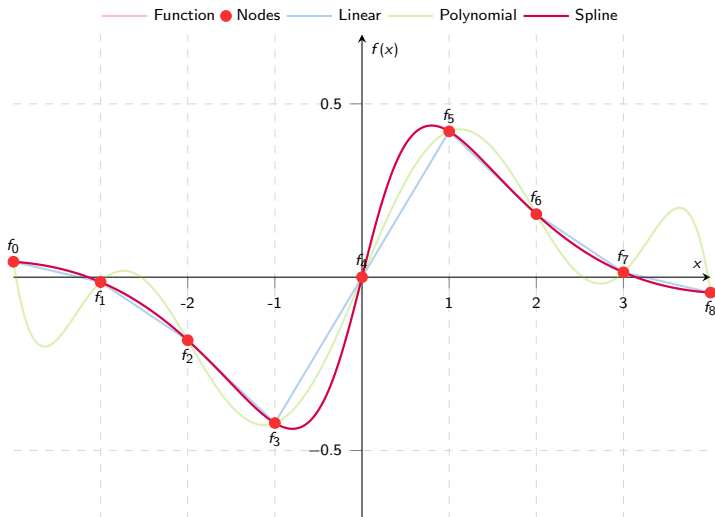oo

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Splines: comparison to other interpolation techniques

Interpolation of $f(x) = \dfrac{\sin x}{1 + x^2}$

Splines: comparison to other interpolation techniques
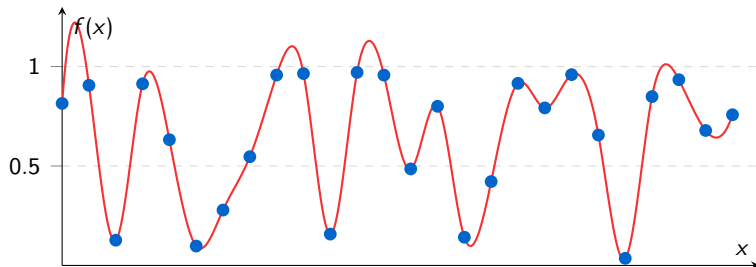
Interpolation of $f(x) = \dfrac{\sin x}{1 + x^2}$

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Splines: comparison to other interpolation techniques

Interpolation of $f(x) = \dfrac{\sin x}{1 + x^2}$

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Splines: comparison to other interpolation techniques

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Splines: comparison to other interpolation techniques

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Spline interpolation in Matlab

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

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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')
```

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Part II

Numerical integration

Today's outline

Today's outline

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
- 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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Riemann integrals

> 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.
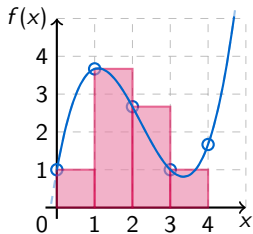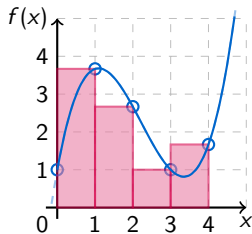
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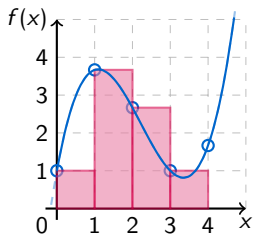
Left endpoint rule

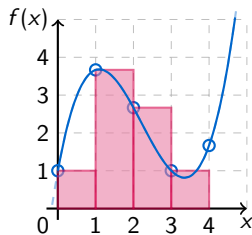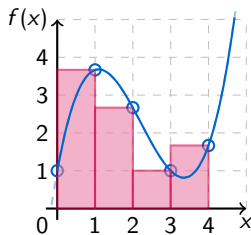$$L_n = \sum_{i=1}^{n} f(x_{i-1})\Delta x_i$$

Riemann integrals

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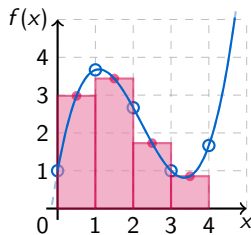
Left endpoint rule

Right endpoint rule

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Left endpoint rule

Right endpoint rule

Midpoint rule

$$L_n = \sum_{i=1}^{n} f(x_{i-1})\Delta x_i$$

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

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

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

Errors in Riemann integrals

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:

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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!

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⑧ Trapezoid rule

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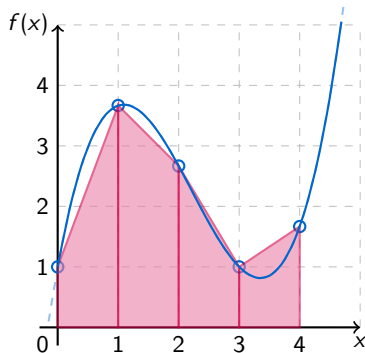
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Trapezoid rule

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Note that this can be rewritten for equidistant intervals:

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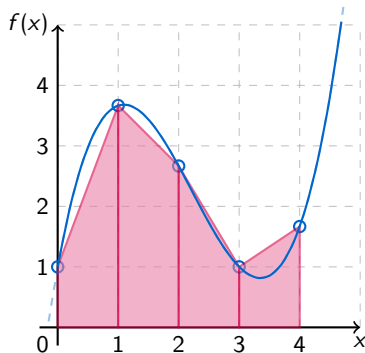
Error in trapezoid integration

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.

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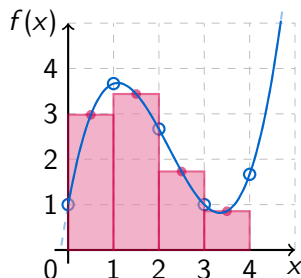
7 Riemann integrals

8 Trapezoid rule

9 Simpson's rule
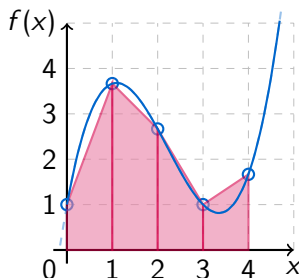
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Towards higher-order integration

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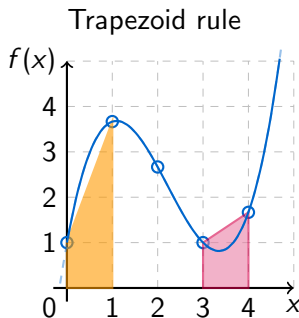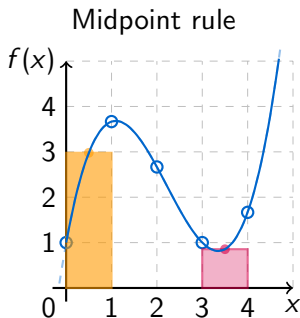

Midpoint rule

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).

Introduction
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Riemann integrals
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Trapezoid rule
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Simpson's rule
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Conclusion
ooo

Towards higher-order integration

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

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

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

Towards higher-order integration

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For a quadratic function, the errors relate as:

$$|I - M_n| = \frac{1}{2}|I - T_n|$$

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For a quadratic function, the errors relate as:

$$|I - M_n| = \frac{1}{2}|I - T_n|$$

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

- Trapezoid: $T_i = \dfrac{f(x_0) + f(x_2)}{2}2\Delta x$

- Simpson: $S_i = \dfrac{2}{3}M_i + \dfrac{1}{3}T_i$

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

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

Now we have:

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

Simpson's rule

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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:

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

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:

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

$$= \frac{\Delta x}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + f4)$$

Simpson's rule

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

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

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

Simpson's rule

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

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

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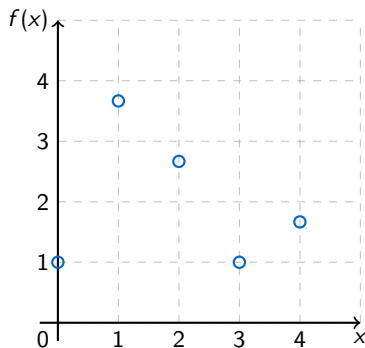
The error is given by:

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

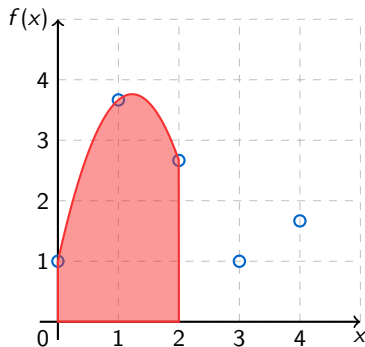if integrand f is differentiable on $[a, b]$.

Simpson's rule: example

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

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

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

Simpson's rule: example

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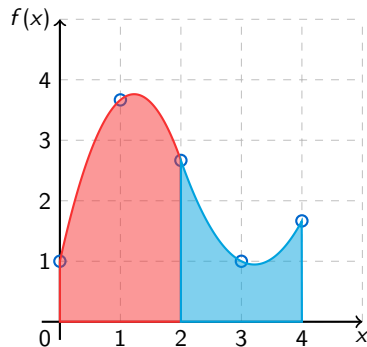- Interpolating x_0, x_1 and x_2:
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  $\int_0^2 p_{2a} = \frac{55}{9} \approx 6.1111$

- Interpolating x_2, x_3 and x_4:
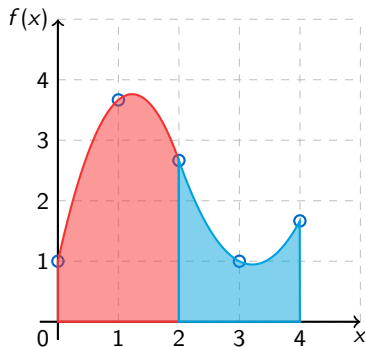 $p_{2b}(x) = \frac{7x^2}{6} - 7\frac{1}{2}x + 13$
  $\int_2^4 p_{2b} = \frac{25}{9} \approx 2.777\ldots$

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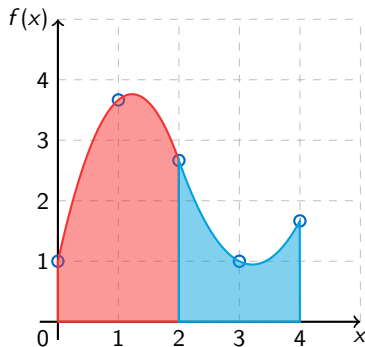
- Interpolating x_0, x_1 and x_2:
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- Adding the separate integrals:
  $\int_0^2 p_{2a} + \int_2^4 p_{2b} = \frac{80}{9}$

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- Adding the separate integrals:
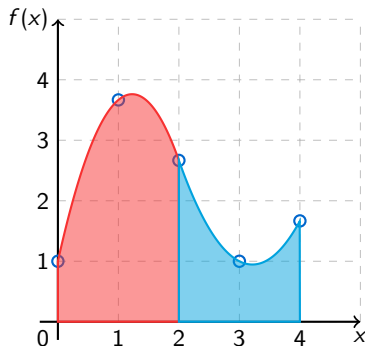 $\int_0^2 p_{2a} + \int_2^4 p_{2b} = \frac{80}{9}$

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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$\frac{1}{3}(1 + 4 \cdot 3.6667 + 2 \cdot 2.6667 + 4 \cdot 1.0000 + 1.6667) = 8.88888 = \frac{80}{9}$

> 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
```

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Riemann integrals
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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