Numerical interpolation

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Numerical Methods (6BER03), 2024-2025

Today's outline

- Introduction
- Piecewise constant
- Linear
- Polynomial
- Splines
- Tutorials

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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

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Today's data set

Generate the following data set:

```python
import numpy as np
xdata = np.arange(0,6)
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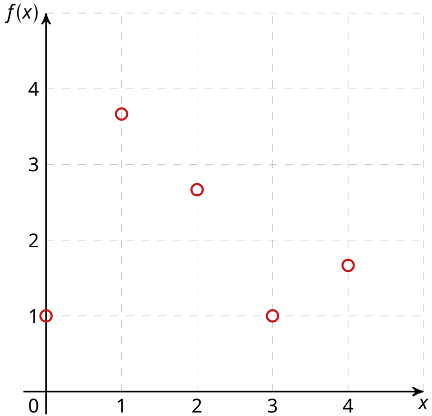
This yields some sample points on which we base our examples:

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

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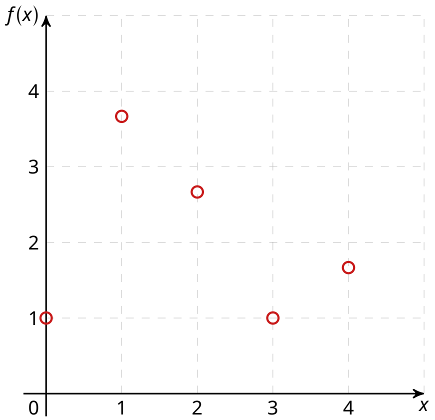

- Nearest-neighbor interpolation in the continuous range $x \in [0, 5]$
- How to treat the point halfway (e.g. at $x = 2.5$)?

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

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

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

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

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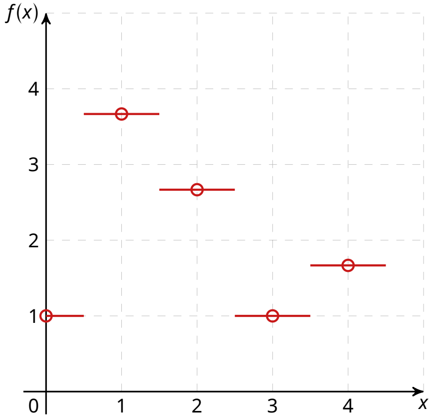

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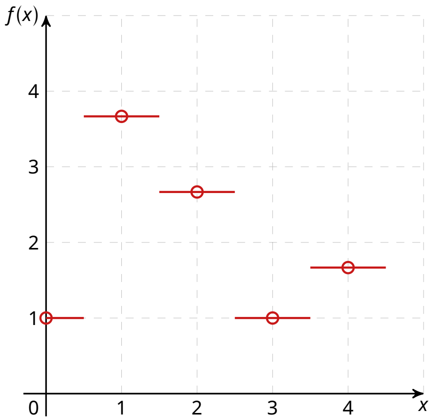

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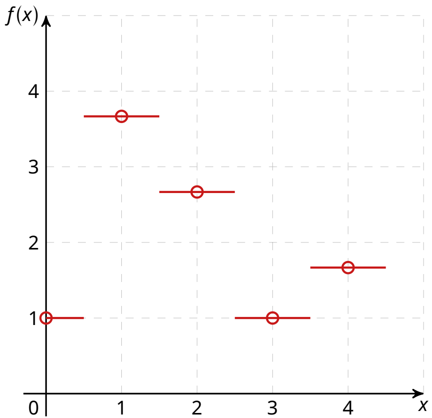

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Linear interpolation

- 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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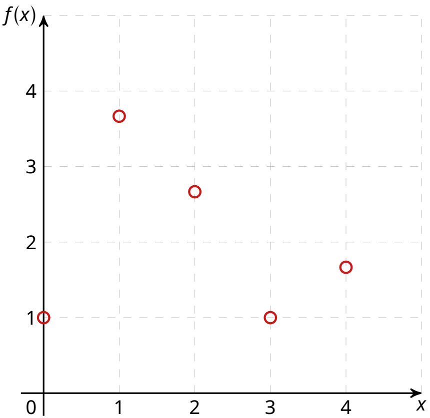

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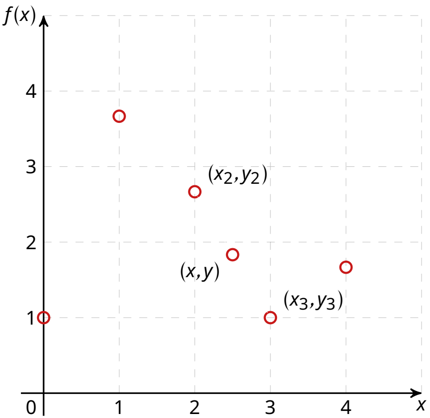

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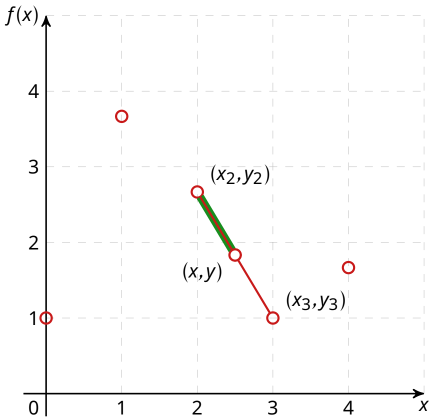

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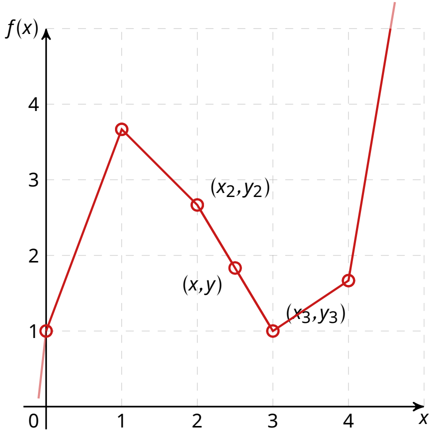

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Interpolation in Python

Interpolation can be done using the SciPy interpolation submodule, e.g.:

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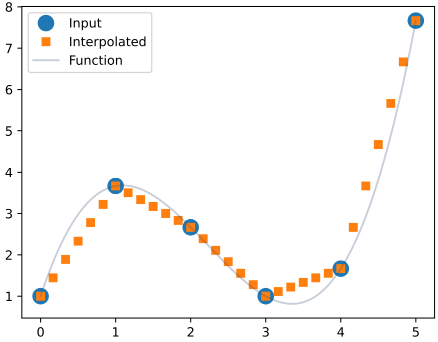
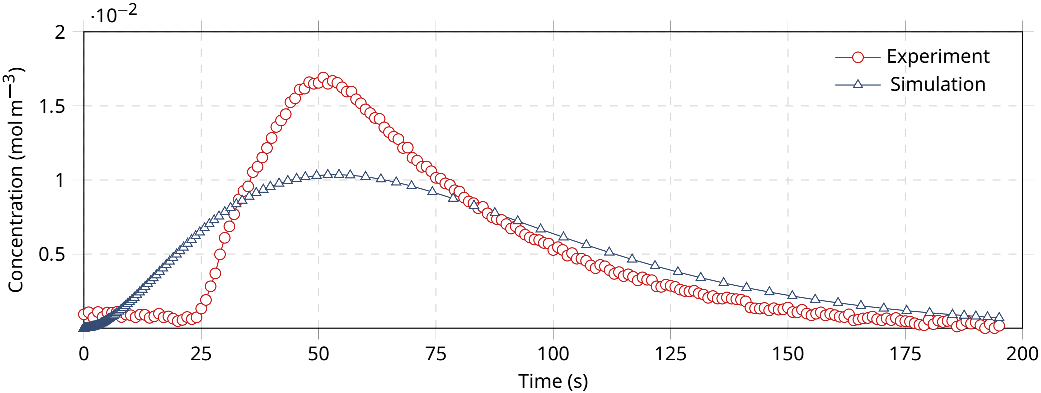


Example: Linear interpolation in Python

Consider the data sets in `exp_data.txt` and `sim_data.txt`, 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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```python
import numpy as np
from scipy.interpolate import interp1d
import matplotlib.pyplot as plt

t_sim, c_sim = np.loadtxt("scripts/interpolation/sim_data.txt").T
t_exp, c_exp = np.loadtxt("scripts/interpolation/exp_data.txt").T

# Linear interpolation
f = interp1d(t_sim, c_sim)
diff = np.abs(c_exp - f(t_exp))

# Plot the solution
plt.subplot(2, 1, 1)
plt.plot(t_exp, c_exp, '-x', label='c_exp')
plt.plot(t_exp, f(t_exp), '-|', label='c_sim_new')
plt.xlabel('Time [s]'); plt.ylabel('Conc [mol m$^{-3}$]')
plt.legend()

plt.subplot(2, 1, 2)
plt.plot(t_exp, diff)
plt.xlabel('Time [s]'); plt.ylabel('Difference [mol m$^{-3}$]')
plt.tight_layout()
# plt.show()
plt.savefig('figures/sim_exp_data_interp.pdf')
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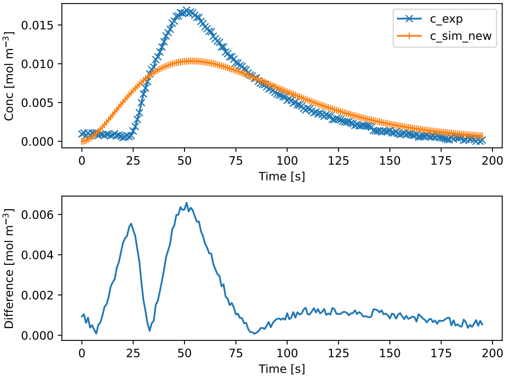

Bi-linear interpolation

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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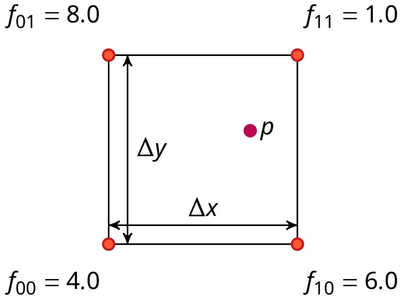

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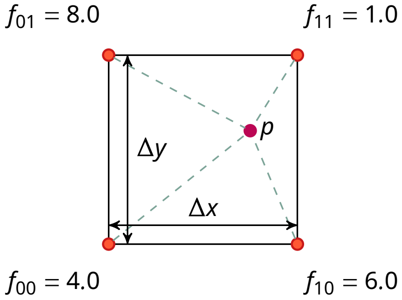

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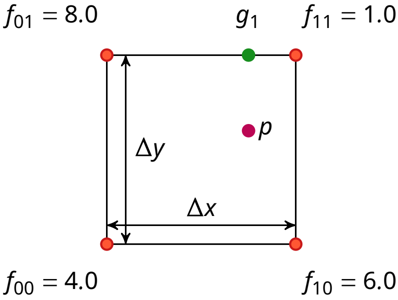

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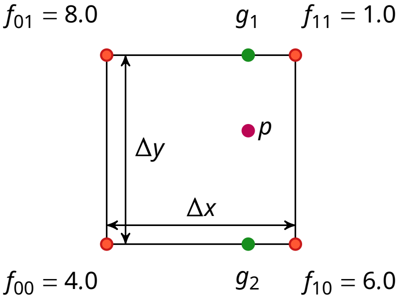

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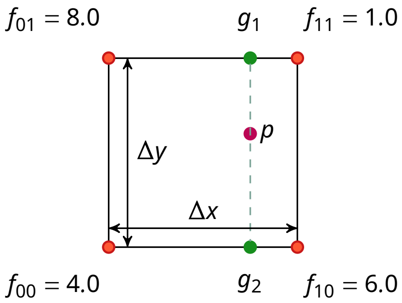

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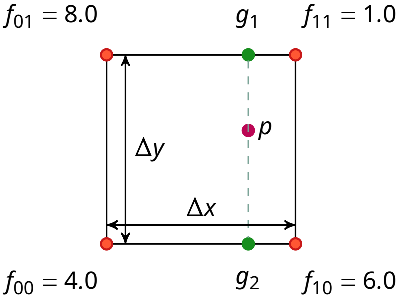
$$g_2 = f_{00}\frac{x_1 - x}{\Delta x} + f_{10}\frac{x - x_0}{\Delta x}$$

$$p = g_2\frac{y_1 - y}{\Delta y} + g_1\frac{y - y_0}{\Delta y}$$

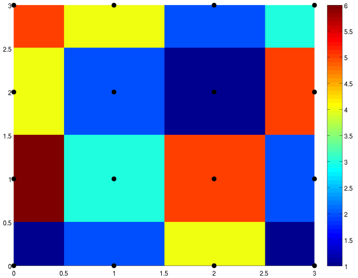


- The order of interpolation (x or y direction first) does not matter; the results are equal

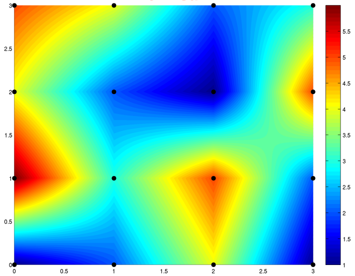
Higher-dimensional field interpolation in Python

2D or higher-dimensional fields of data can be interpolated in Python using the `scipy.interpolate.interp2d`, `scipy.interpolate.interp3d`, or even `scipy.interpolate.RegularGridInterpolator` functions. The method can be adjusted:

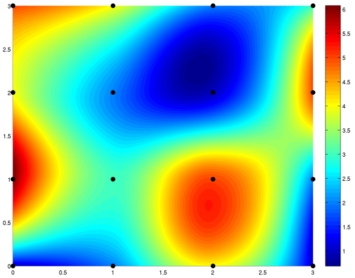
'nearest'



'linear'



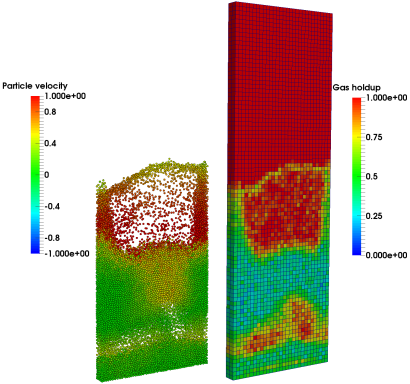
'cubic'



- Also consider tri-linear interpolation (for 3D fields) with `scipy.interpolate.LinearNDInterpolator`, or bicubic interpolation (2D, but third order) with `scipy.interpolate.interp2d`.

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.



Today's outline

- Introduction
- Piecewise constant
- Linear
- Polynomial
- Splines
- Tutorials

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 $(x_1, y_1), (x_2, y_2), \ldots, (x_m, y_m)$, 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 are obtained by solving the linear system $Va = y$.

Polynomial interpolation via Vandermonde matrix

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

```python
import numpy as np
x = np.array([0, 1, 2])
y = np.array([1.0000, 3.6667, 2.6667])
V = np.vander(x, increasing=True)
print(V)
```

```
[ 1. 4.50005 -1.83335]
```

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So we found the equation:

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

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

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	$\frac{8}{3} = 2.67$

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

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

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

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x_k	f_k
x_0	$f[x_0] = f_0$

x_k	f_k
0	1

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

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Construction of Newton polynomials: example

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

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

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Construction of Newton polynomials: example

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

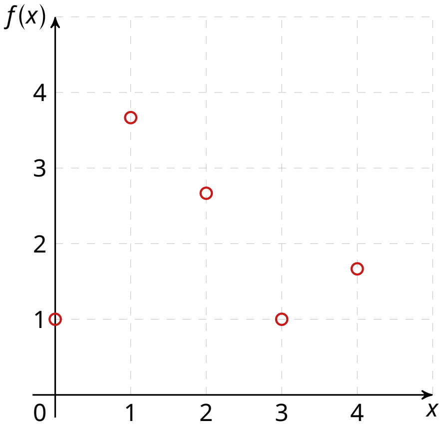
$$p_2(x) = -\frac{11}{6}x^2 + 4\frac{1}{2}x + 1$$

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

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

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

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



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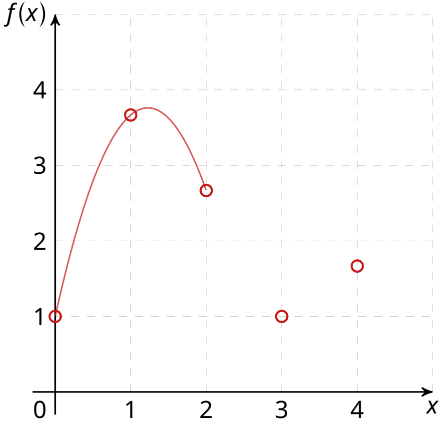

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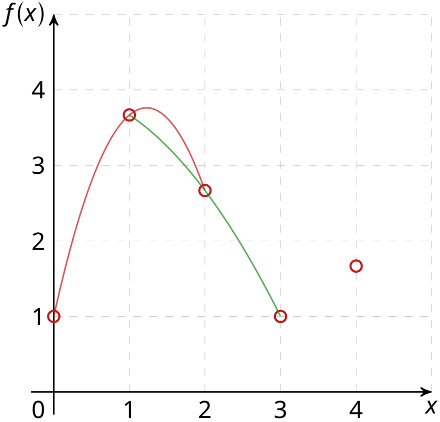

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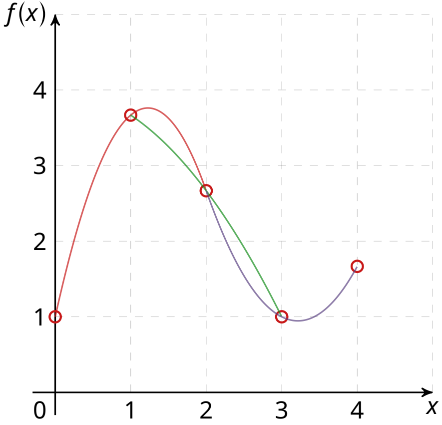

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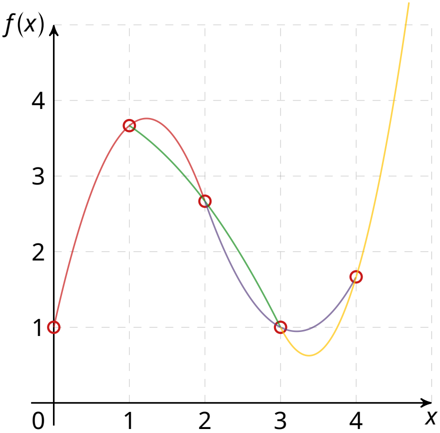

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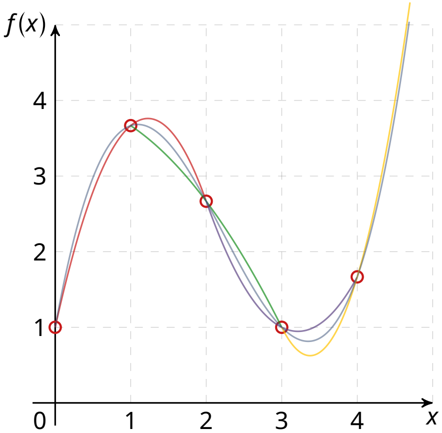

Polynomial fitting in Python: example

Develop the polynomials $p_1(x)$ through $p_5(x)$ using the following data set:

```
import numpy as np
import matplotlib.pyplot as plt
xdata = np.arange(-1,1.5,0.5)
ydata = [x * np.sin(x)/np.sqrt(x+2) if x != 0 else 0.5 for x in xdata]
plt.plot(xdata,ydata,'o')
```

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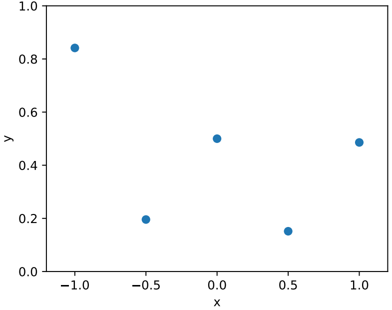


```python
xc = np.linspace(-1.1,1.1,1001,endpoint=True)
for deg in range(1,6):
    # Fit coefficients
    p_coeffs = np.polyfit(xdata,ydata,deg)
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Develop the polynomials $p_1(x)$ through $p_5(x)$ using the following data set:

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xdata = np.arange(-1,1.5,0.5)
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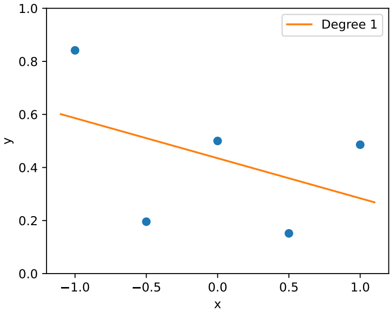


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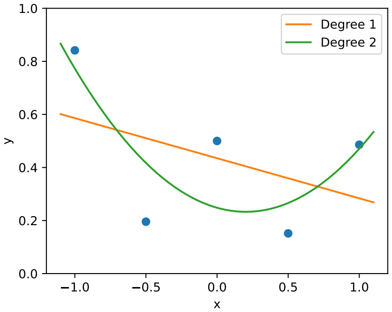


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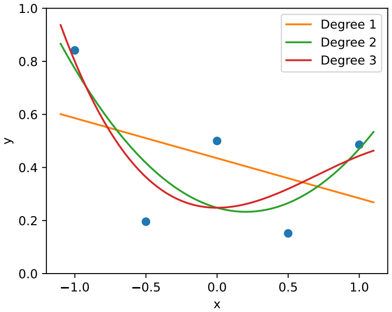


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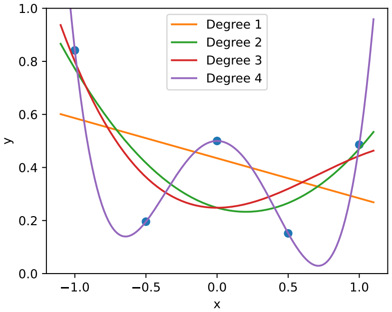


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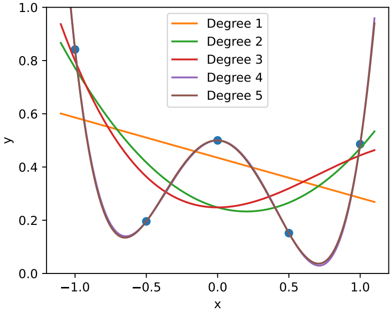


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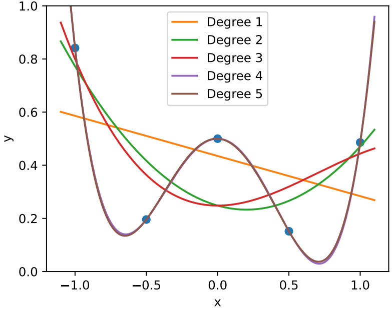


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RankWarning: Polyfit may be poorly conditioned
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Exercise

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

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

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import numpy as np
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f = lambda x: 1/(x**2 + 1/25)
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y4,y10,yinf = f(x4), f(x10), f(xinf)
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```python
# Get coefficients for 4th and 10th order polynomial
p4 = np.polyfit(x4, y4, 4)
p10 = np.polyfit(x10, y10, 10)
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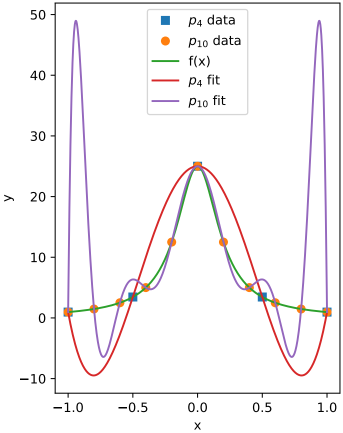

Final thoughts on polynomial interpolation

- 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)
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Today's outline

- Introduction
- Piecewise constant
- Linear
- Polynomial
- **Splines**
- Tutorials

Spline interpolation

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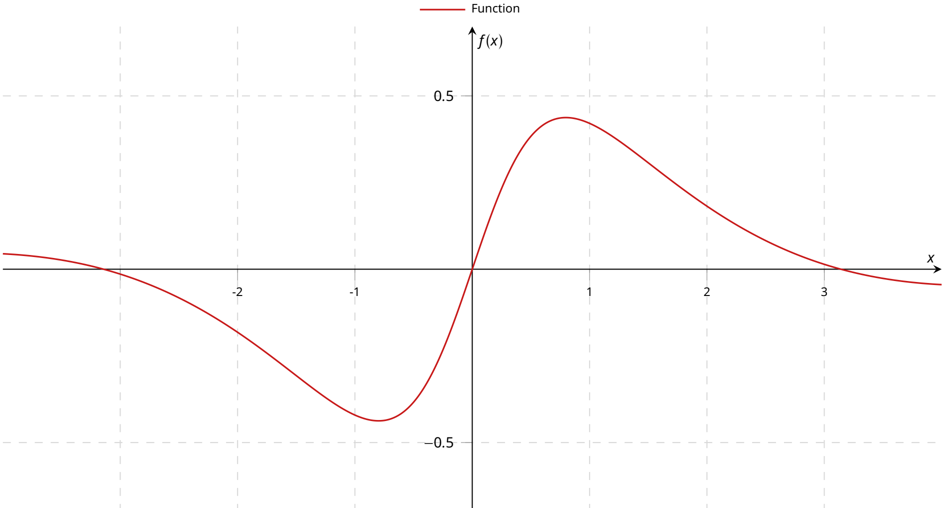
Splines: comparison to other interpolation techniques

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



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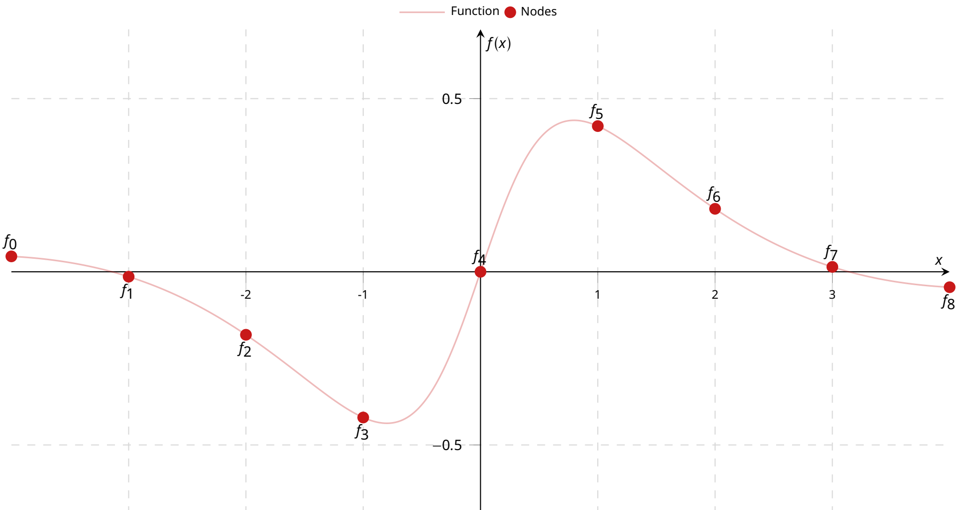

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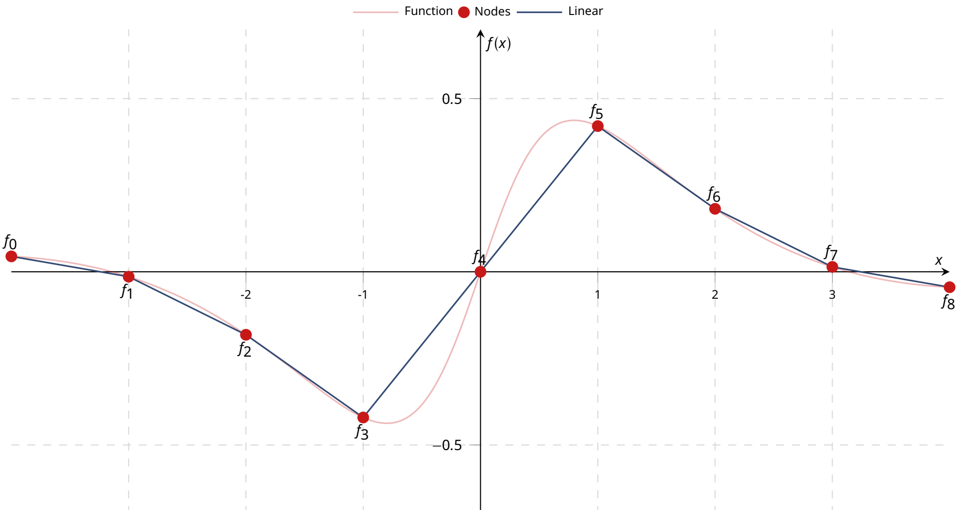

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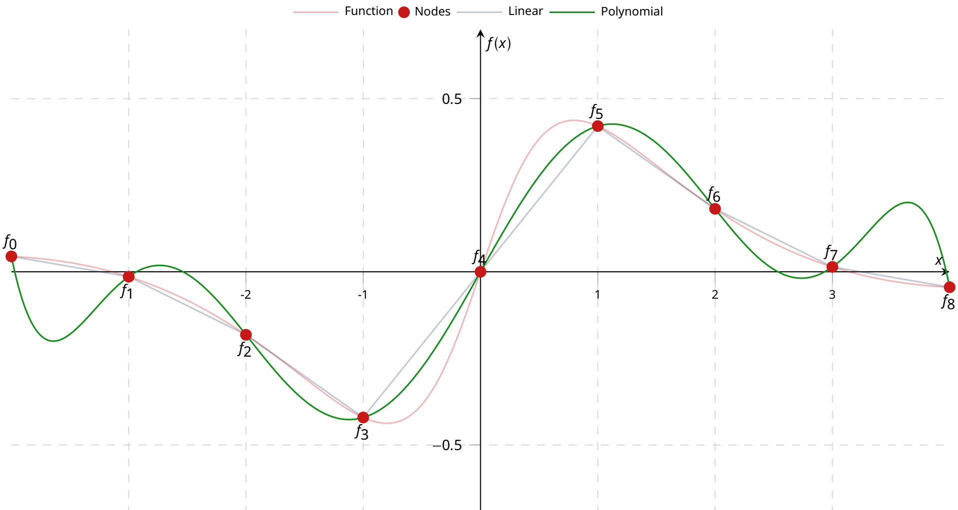

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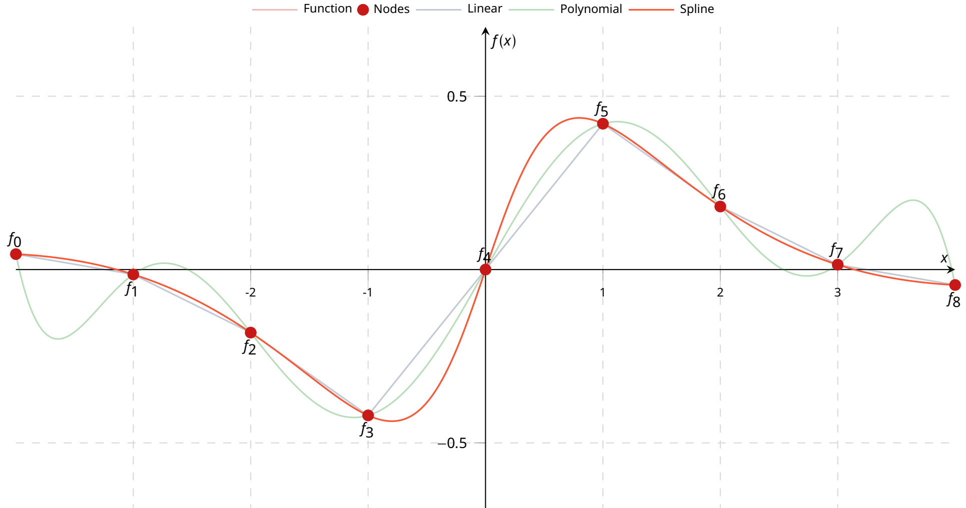

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import numpy as np
import matplotlib.pyplot as plt
from scipy.interpolate import make_interp_spline

# Generate random data set
xdata = np.arange(0, 26)
ydata = np.random.rand(len(xdata))

# Interpolant on a fine mesh
xc = np.linspace(0, 25, 1001)
ifun = make_interp_spline(xdata, ydata)
yc = ifun(xc)

# Plot the data
plt.plot(xdata, ydata, 'o')
plt.plot(xc, yc, '-r')
plt.show()
```

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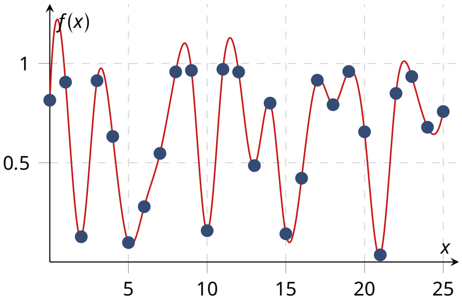

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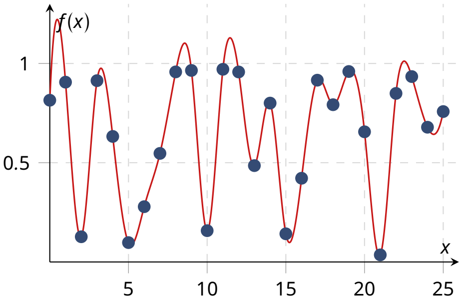

Note: The SciPy Optimize module contains various interpolation methods with a similar interface.

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
- Legendre polynomials: alternative way of performing the polynomial interpolation (not discussed here)

Interpolation tutorials

1. In Python, generate the data:

```
x = np.arange(-4, 6, 1)
y = [0, 0, 0, 1, 1, 1, 0, 0, 0, 0]
```

   Interpolate the data using polynomial interpolation (which order do you use?) and a spline. Plot the results together with the original data in a graph.

2. Do the same exercise for the following data. Can you explain your observations?

```
t = [0, 0.1, 0.499, 0.5, 0.6, 1.0, 1.4, 1.5, 1.899, 1.9, 2.0]
y = [0, 0.06, 0.17, 0.19, 0.21, 0.26, 0.29, 0.29, 0.30, 0.31, 0.31]
```

Hint: Use `scipy.interpolate.interp1d(...,kind="...")` to use different splines.

Numerical integration

Dr.ir. Ivo Roghair, Prof.dr.ir. Martin van Sint Annaland

Chemical Process Intensification group
Eindhoven University of Technology

Numerical Methods (6BER03), 2024-2025

Today's outline

- Introduction
- Riemann integrals
- Trapezoid rule
- Simpson's rule
- Conclusion
- Tutorials

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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
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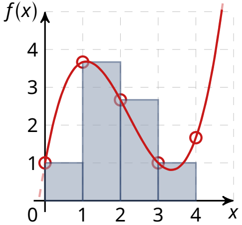

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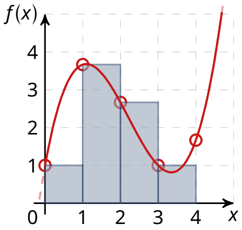

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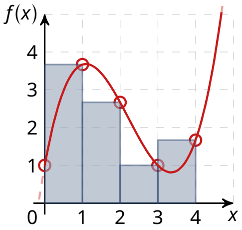

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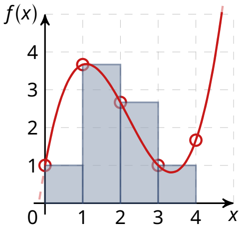

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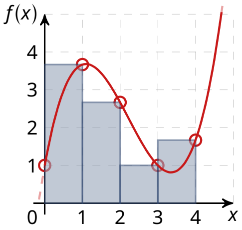

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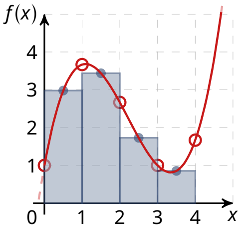
Midpoint rule



$$M_n = \sum_{i=0}^{n-1} f(\bar{x}_i)\Delta x_i$$

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

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Errors in Riemann integrals

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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:

- $|I - L_n| \leq \dfrac{f_{\max}^{(1)}(b-a)^2}{2n}$
- $|I - R_n| \leq \dfrac{f_{\max}^{(1)}(b-a)^2}{2n}$
- $|I - M_n| \leq \dfrac{f_{\max}^{(2)}(b-a)^3}{24n^2}$

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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

- Introduction
- Riemann integrals
- Trapezoid rule
- Simpson's rule
- Conclusion
- Tutorials

Trapezoid rule

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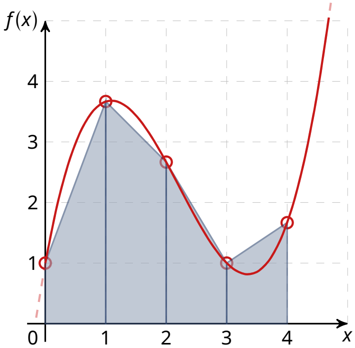

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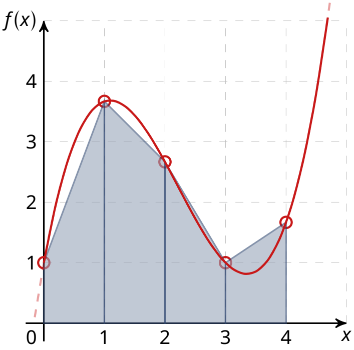
Note that this can be rewritten for equidistant intervals:

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



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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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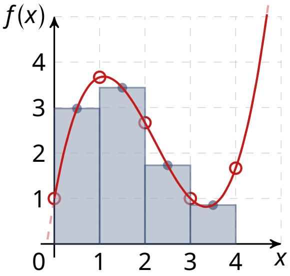
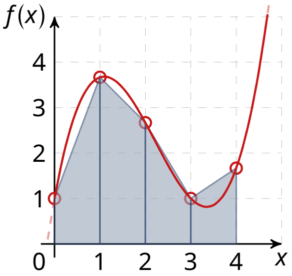
Towards higher-order integration

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

Midpoint rule



Trapezoid rule



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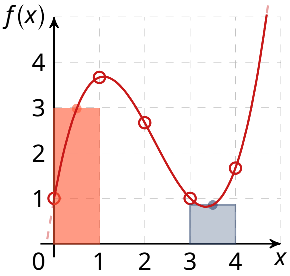

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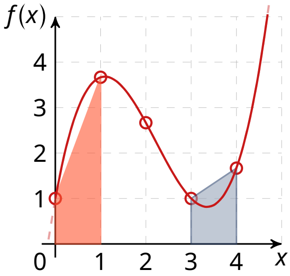

Trapezoid rule

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: $|I - M_n| \leq \dfrac{f^{(2)}_{\max}(b-a)^3}{24n^2}$
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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: $M_i = f(\frac{x_0 + x_2}{2})2\Delta x = f(x_1)2\Delta x$
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- 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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Now we have:

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

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

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If we sum these two intervals we obtain:

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

Simpson's rule

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

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

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The error is given by:

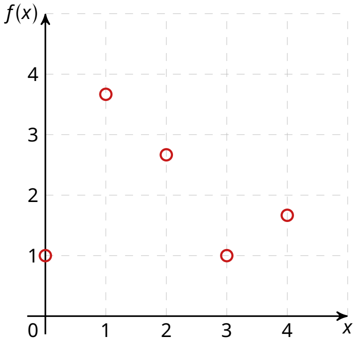
$$|I - S_n| \leq \frac{f_{\max}^{(4)}(b-a)^5}{180n^4}$$

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

Simpson's rule: example

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

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



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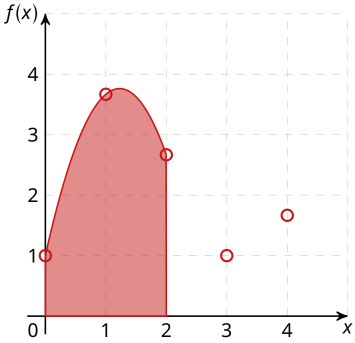

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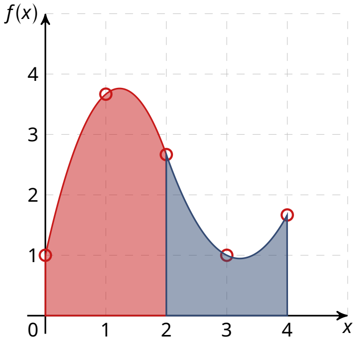

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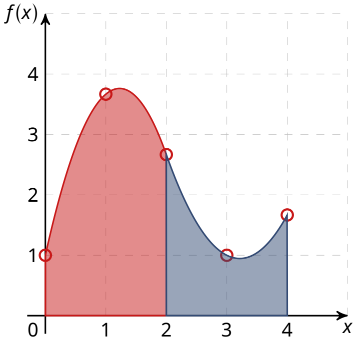

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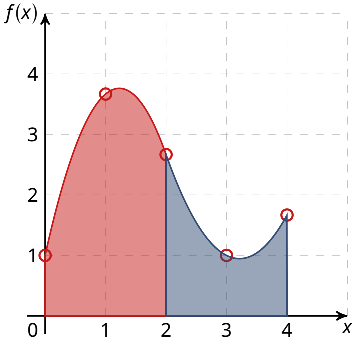

Using Simpson's rule:

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

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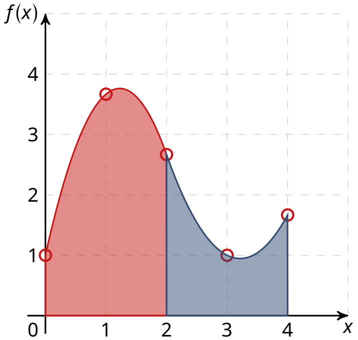

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Simpson's method is of fourth order, and it gives exact approximations of third order polynomials!

Integration in Python

Integration can be done numerically in Python.

- `np.trapz(y, x)` 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.

```
import numpy as np
x = np.linspace(-2, 2, 2001)
y = 1 / (x**2 + 1)
I = np.trapz(y, x) # Or: scipy.integrate.trapezoid
print(I)
```

```
2.214297328921525
```

- Integration of functions can be done using the `quad(func, a, b)` function:

```
import numpy as np
from scipy.integrate import quad
f = lambda x: np.exp(-x**2)
I, err = quad(f, 0, 10)
print(I, err)
```

```
0.886226925452758 1.8483380528941764e-13
```

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What hasn't been discussed?

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

- 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

- Several techniques for numerical integration were discussed:
  - Riemann sums, trapezoid rule, Simpson's rule
  - Upper-bound errors were given for each technique
  - Built-in Python functions were illustrated
- Continue with characterization of convergence of the integration methods in the tutorials!

Integration tutorials

1. Implement a function to integrate a mathematical function for a specific number of integration intervals. Implement it as a function, which can be called with arguments:
   - Function (handle) to integrate
   - Integration boundaries (as separate arguments or as a 2×1 numpy array)
   - Number of integration intervals

   For instance: `def leftrule(func, x0, x1, N):`.
2. Set up a function to integrate:

```python
def myfunction(x):
    return x**2 - 4*x + 6 + np.sin(5*x)
```

3. Integrate the function, e.g. `int_left = leftrule(myfunction, 0, 10, 25)`
4. Assess how the number of intervals affects the deviation from the true integral value.
5. Create a log-log plot of the deviation vs. number of intervals used.
6. Do this for all methods discussed[2] and compare their performance in a graph

[2] Riemann left, right, midpoint, trapezoid, and Simpson