

# Numerical integration

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# 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  $x = b$ .

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

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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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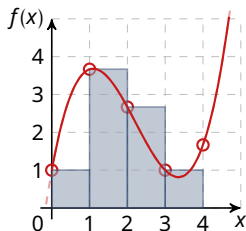
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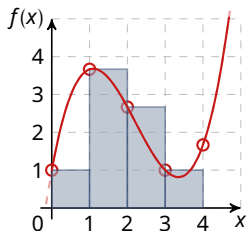


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# Riemann integrals

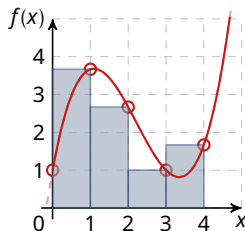
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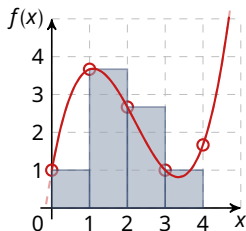


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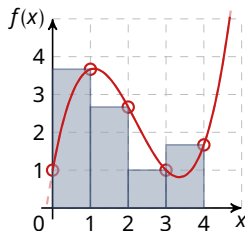
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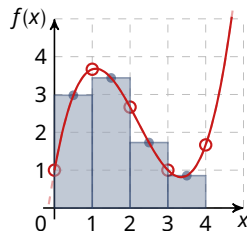
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$$R_n = \sum_{i=1}^n f(x_i) \Delta x_i$$

Midpoint rule



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

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

# Errors in Riemann integrals

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



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

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

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# Trapezoid rule

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

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

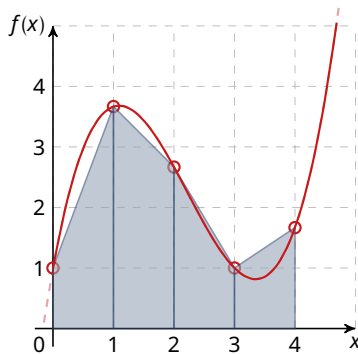
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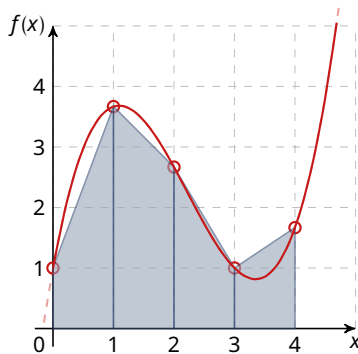
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Note that this can be rewritten for equidistant intervals:

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





# Error in trapezoid integration

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

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

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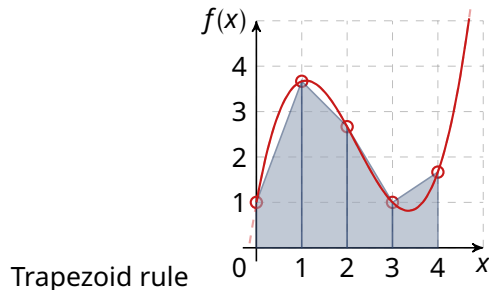
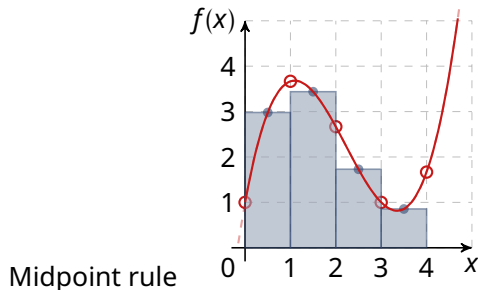
The midpoint rule approximation has lower error bounds than the trapezoid rule. A linear function is, however, better approximated by the trapezoid rule.

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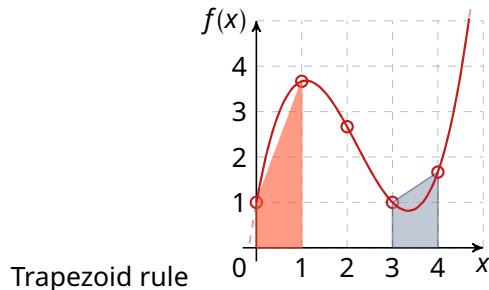
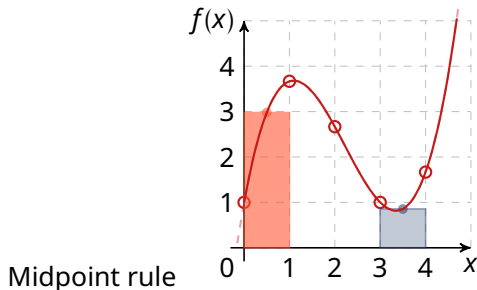
# Towards higher-order integration

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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).

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

- Midpoint:  $|I - M_n| \leq \frac{f_{\max}^{(2)}(b-a)^3}{24n^2}$
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For a quadratic function, the errors relate as:

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

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

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

# Simpson's rule

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

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

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

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If we sum these two intervals we obtain:

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

# Simpson's rule

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

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



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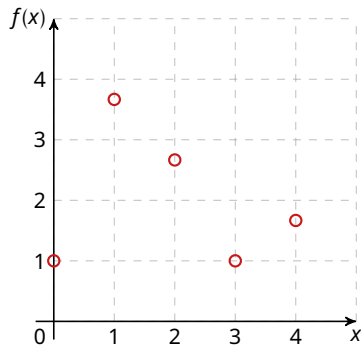
$$|I - S_n| \leq \frac{f_{\max}^{(4)}(b-a)^5}{180n^4}$$

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

# Simpson's rule: example

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

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



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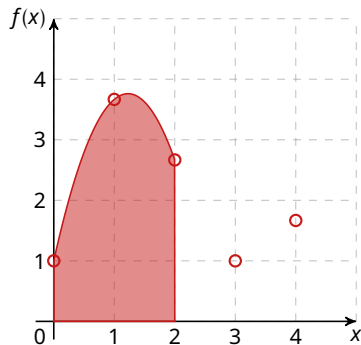
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- Interpolating  $x_0, x_1$  and  $x_2$ :

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

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



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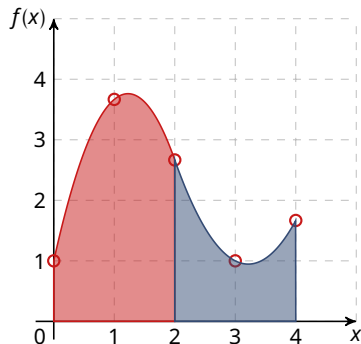
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$$p_{2b}(x) = \frac{7x^2}{6} - 7\frac{1}{2}x + 13$$

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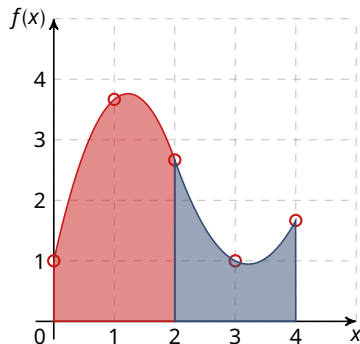
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- Adding the separate integrals:

$$\int_0^2 p_{2a} + \int_2^4 p_{2b} = \frac{80}{9}$$



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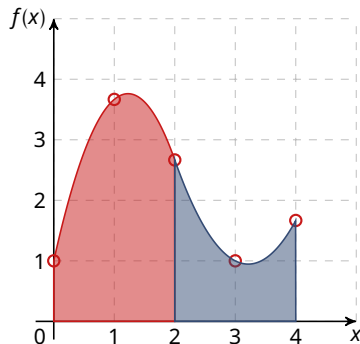
- Interpolating  $x_2, x_3$  and  $x_4$ :

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

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

- Adding the separate integrals:

$$\int_0^2 p_{2a} + \int_2^4 p_{2b} = \frac{80}{9}$$



Using Simpson's rule:

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

# Simpson's rule: example

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

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

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

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

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

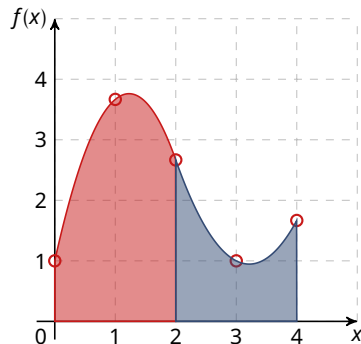
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$$p_{2b}(x) = \frac{7x^2}{6} - 7\frac{1}{2}x + 13$$

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Using Simpson's rule:

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

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.

```
1 >> import numpy as np
2 >> x = np.linspace(-2, 2, 2001)
3 >> y = 1 / (x**2 + 1)
4 >> I = np.trapz(y, x)
5 >> I
6 2.214297328921525
```

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

```
1 >> import numpy as np
2 >> from scipy.integrate import quad
3 >> def func(x):
4 >> return np.exp(-x**2)
5 >> I, err = quad(func, 0, 10)
6 >> I
7 0.8862269254527579
```



# Today's outline

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

# 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  $2 \times 1$  numpy array)
  - Number of integration intervals

For instance: `def leftrule(func, x0, x1, N):.`

- 2 Set up a function to integrate:

```
1 def myfunction(x):  
2     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<sup>1</sup> and compare their performance in a graph

<sup>1</sup>Riemann left, right, midpoint, trapezoid, and Simpson