CHEM 3PC3 - Mathematical Tools for Chemical Problems

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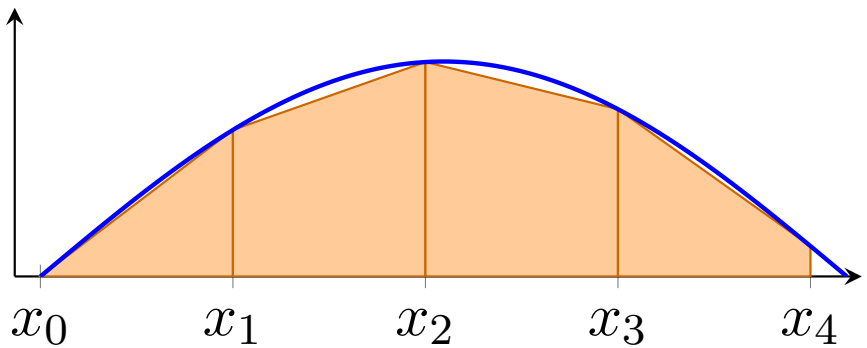
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The composite trapezoidal rule

- One trapezoid is too crude, so we split $[a, b]$ into $N - 1$ intervals of width $h = \frac{b-a}{N-1}$, with grid points $x_i = a + ih$.
- Adding the area of every trapezoid gives

$$\int_a^b f(x)\,dx \approx \frac{h}{2} \sum_{i=0}^{N-2} \Big(f(x_i) + f(x_{i+1}) \Big)$$
$$= h \left[\tfrac{1}{2} f_0 + f_1 + \cdots + f_{N-2} + \tfrac{1}{2} f_{N-1} \right].$$

- Interior points are shared by two trapezoids, so they get weight 1. The two end points get weight $\frac{1}{2}$.



Example: $\displaystyle\int_0^3 x^2\,dx$ with $N = 4$

- Grid: $h = \dfrac{b-a}{N-1} = \dfrac{3}{3} = 1$, so $x_i = 0, 1, 2, 3$ and $f_0 = 0,\ f_1 = 1,\ f_2 = 4,\ f_3 = 9$.
- Apply the rule with $\sum_{i=0}^{N-2} = \sum_{i=0}^{2}$:

$$\int_0^3 x^2\,dx \approx \frac{h}{2}\sum_{i=0}^{2}\Big(f(x_i) + f(x_{i+1})\Big)$$

$$= \tfrac{1}{2}\Big[(0+1) + (1+4) + (4+9)\Big] = \tfrac{19}{2} = 9.5.$$

- Exact: $\displaystyle\int_0^3 x^2\,dx = \frac{x^3}{3}\Big|_0^3 = 9.$
- The estimate overshoots by 0.5: x^2 is convex, so every chord lies **above** the curve. Halving h would quarter the error, since the method is $O(h^2)$.

The trapezoidal rule in Python

- With NumPy arrays, the whole sum is one line:

```
import numpy as np

def trapezoidal_rule(f, h):
    # f: integrand on a uniform grid, h: spacing
    return h / 2 * np.sum(f[:-1] + f[1:])

x = np.linspace(0, np.pi, 11)   # 11 points
h = x[1] - x[0]
print(trapezoidal_rule(np.sin(x), h))  # 1.98352
print(np.trapezoid(np.sin(x), x))      # NumPy
```

- The exact answer is $\int_0^\pi \sin x \, dx = 2$. With only 11 points the error is already below 1%.
- The notebook shows the trapezoids, a convergence test, and a chemistry example.