Numerical Integration

Algorithm:

- Trapezoidal Rule
- Simpson’s Rule
- Gaussian Quadrature

- Analytical differentiation is easy, but analytical integration is “hard”:

  more of an art than a science

  - Led to the development of numerical techniques, even back in the 18th Century
  - Even simple classical methods are still useful

- Numerical integration is always equivalent to the solution of a differential equation:

If $y = \int f(x)\, dx$ then $dy/dx = f(x)$

There are several modern algorithms for solving differential equations (that are particularly useful when f(x) is not smooth)

INTEGRATING A SPECTRUM (PROBLEM)

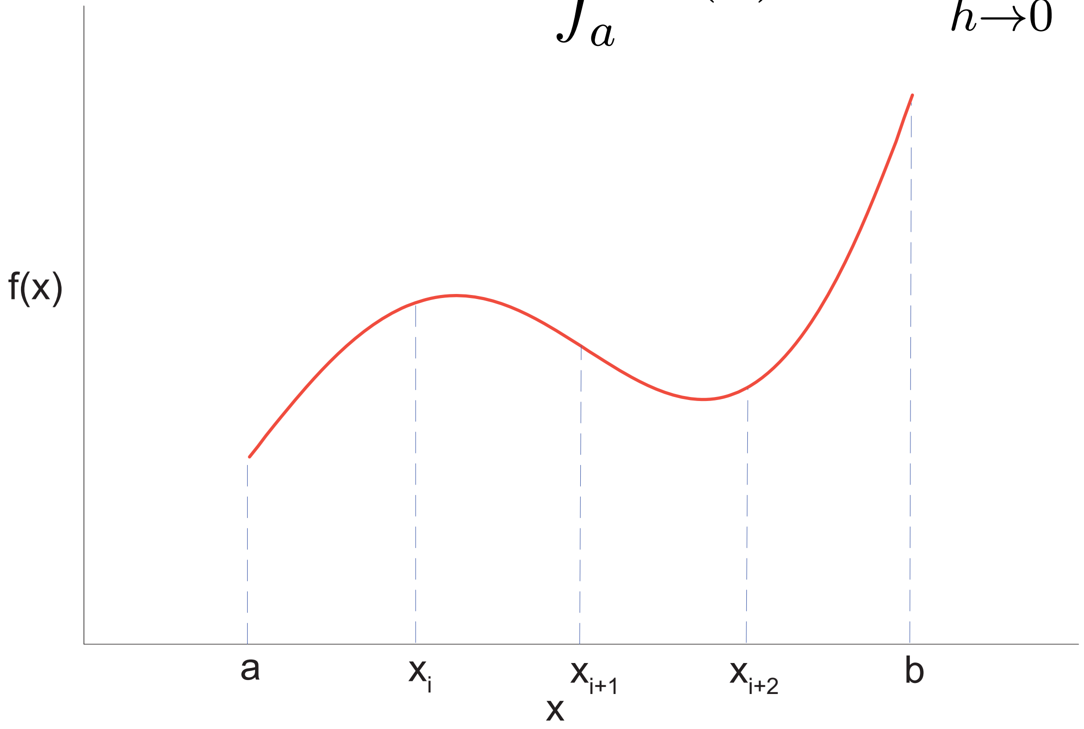
Problem: An experiment has measured $dN(t)/dt$, the number of particles per unit time entering a counter. Your **problem** is to integrate this spectrum to obtain the number of particles $N(1)$ that entered the counter in the first second for an arbitrary decay rate

$$N(1) = \int_0^1 \frac{dN(t)}{dt}\, dt.$$

- Analytical Integration may require some cleverness. However, it is relatively straightforward on a computer (numerical)
- Numerical Quadrature: count the number of boxes laying below a curve

Reimann definition of Integral

$$\int_a^b f(x)\,dx = \lim_{h\to 0}\left[h \sum_{i=1}^{(b-a)/h} f(x_i)\right].$$



$$\int_a^b f(x)\,dx \simeq \sum_{i=1}^{N} f(x_i) w_i$$

- First consider methods that use a constant step size ($\Delta x_i = h$ for all i)

Trapezoidal rule

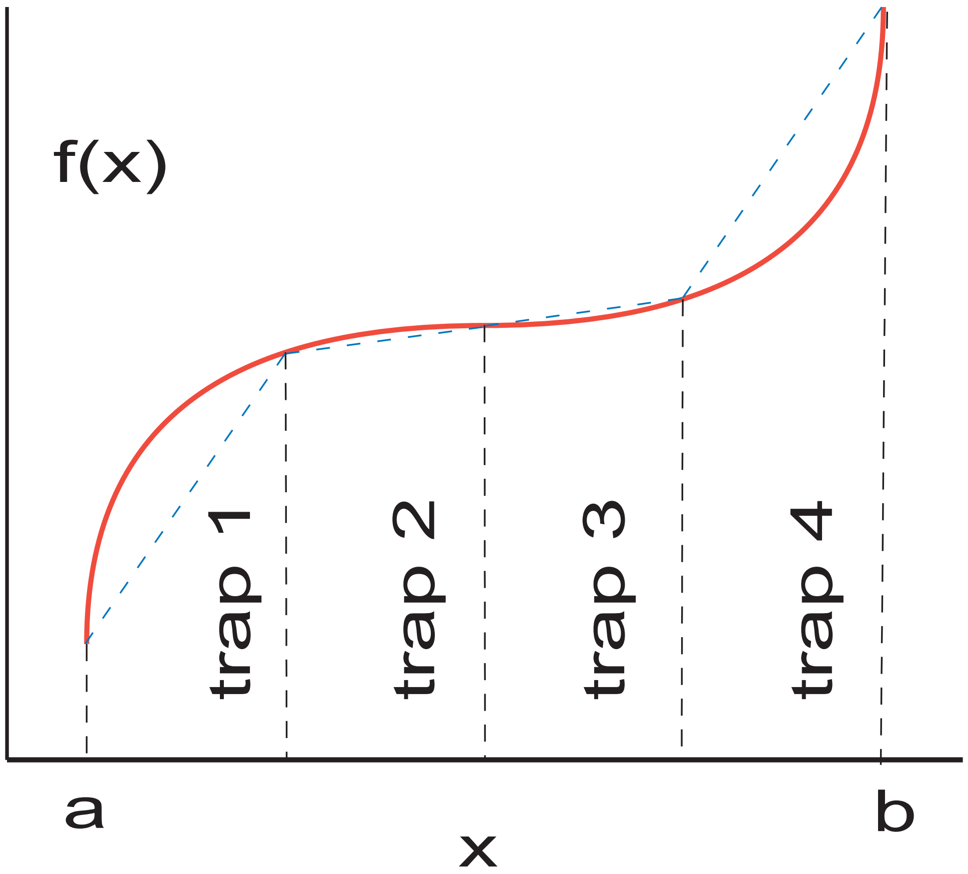
- Break integral into N –1 equally spaced intervals

  $$I = h\left(\tfrac{1}{2}f_1 + f_2 + f_3 + \ldots + f_{N-1} + \tfrac{1}{2}f_N\right) + h^2\left(f_1' - f_N'\right)/12 + \ldots.$$

  with stepsize $h = (x_b - x_a)/(N - 1)$

- Error is proportional to $h^2 \propto 1/N^2$
  - Need to cover regions where f'' is large with high density of points

Trapezoidal rule



The area of each such trapezoid

$$\int_{x_i}^{x_i+h} f(x)\,dx \simeq \frac{h(f_i + f_{i+1})}{2} = \frac{1}{2}hf_i + \frac{1}{2}hf_{i+1}.$$

$$\int_a^b f(x)\,dx \simeq \frac{h}{2}f_1 + hf_2 + hf_3 + \cdots + hf_{N-1} + \frac{h}{2}f_N.$$

Simpson's rule

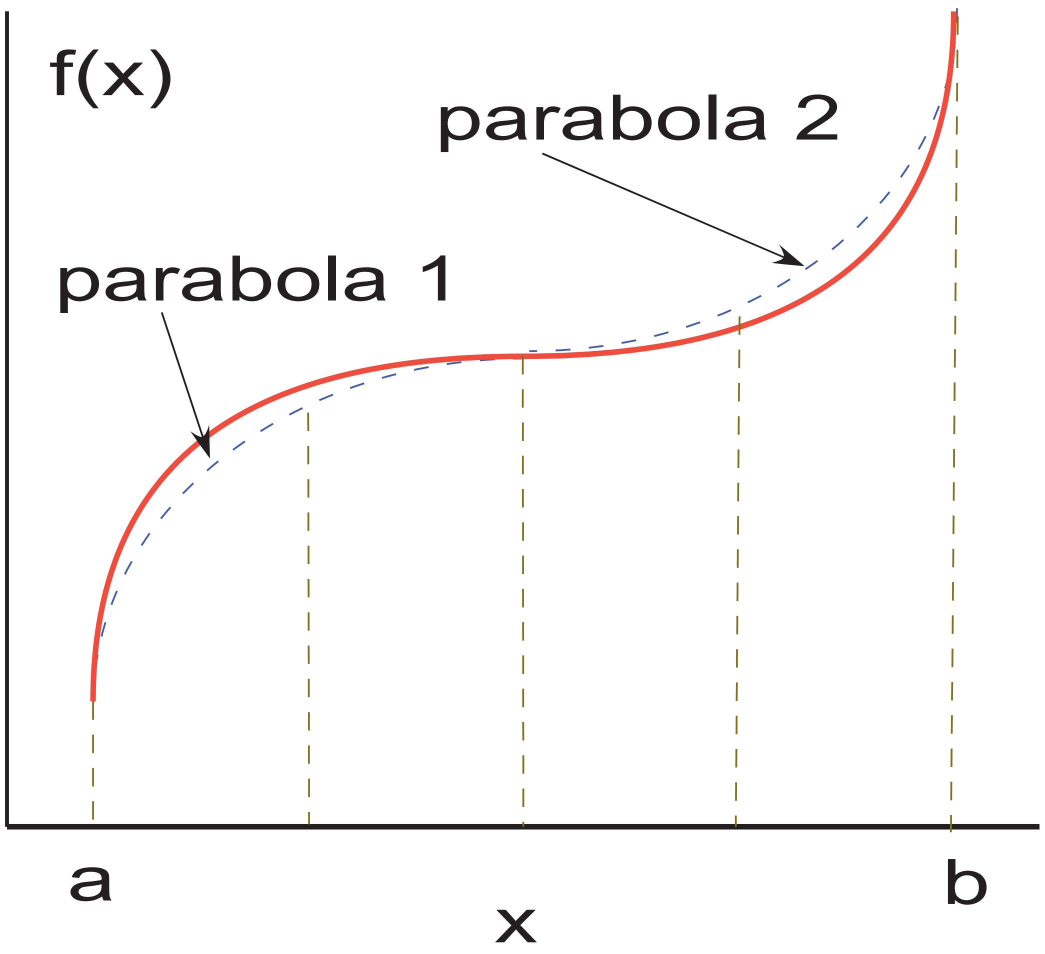
- Slightly better performer for fairly *smooth* functions
- Again, break integral into N –1 equally spaced intervals, but now use

$$I = h\,(f_1 + 4f_2 + 2f_3 + 4f_4 + 2f_5 + \ldots 2f_{N-2} + 4f_{N-1} + f_N)/3 + h^4\,(f_1'' - f_N'')\,/\,180 + \ldots.$$

  with N odd

- Now error is proportional to f'''/N^4

Simpson’s rule



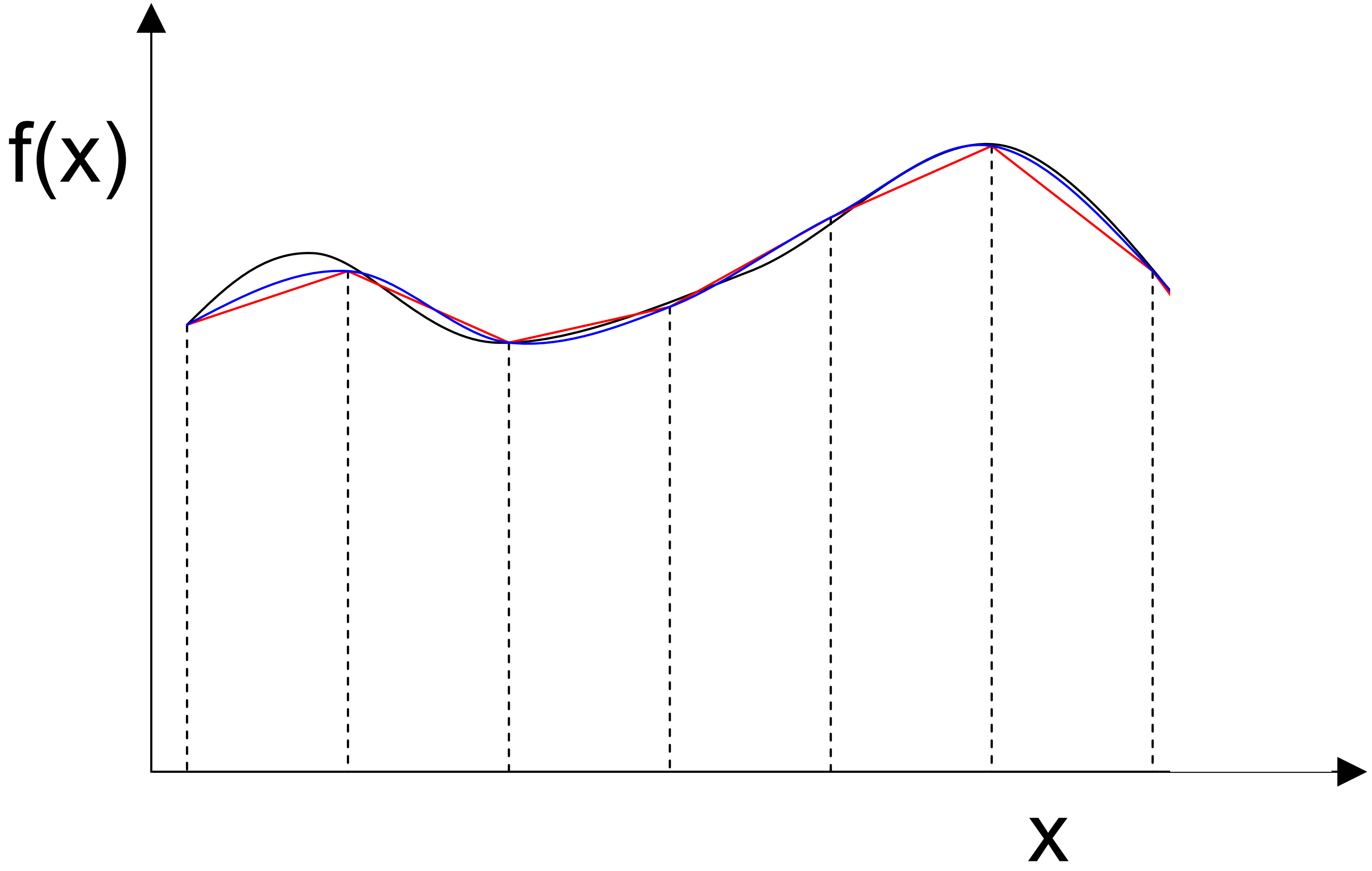
$$f(x) \simeq \alpha x^2 + \beta x + \gamma$$

The area under the parabola for each interval:

$$\int_{x_i}^{x_i+h} (\alpha x^2 + \beta x + \gamma)\, dx = \frac{\alpha x^3}{3} + \frac{\beta x^2}{2} + \gamma x \Big|_{x_i}^{x_i+h} .$$

Geometric interpretation

- Black – integrand; red – trapezoid; blue – Simpson's



Control of truncation errors

- The choice of N must reflect the obvious tradeoff between

  accuracy ($\propto 1/N^2$ or $1/N^4$) and

  computational expense ($\propto N$)

- We keep increasing N until the answer stops changing (or changes only by an acceptably small amount)

- For the trapezoid and Simpson rules:

$$\mathcal{E}_t = O\left(\frac{[b-a]^3}{N^2}\right) f^{(2)}, \quad \mathcal{E}_s = O\left(\frac{[b-a]^5}{N^4}\right) f^{(4)}$$