Numerical Integration

Numerical Integration Problems

- Basic 1D numerical integration
  - Given ability to evaluate $f(x)$ for any x, find

$$\int_a^b f(x)\,dx$$

  - Goal: best **accuracy** with fewest **samples**
  - Classic problem – even analytic functions not necessarily integrable in closed form

$$G(x) = \int_{-\infty}^{x} e^{-t^2}\,dt$$

Related Topics

- Multi-dimensional integration
- Ordinary differential equations
- Partial differential equations

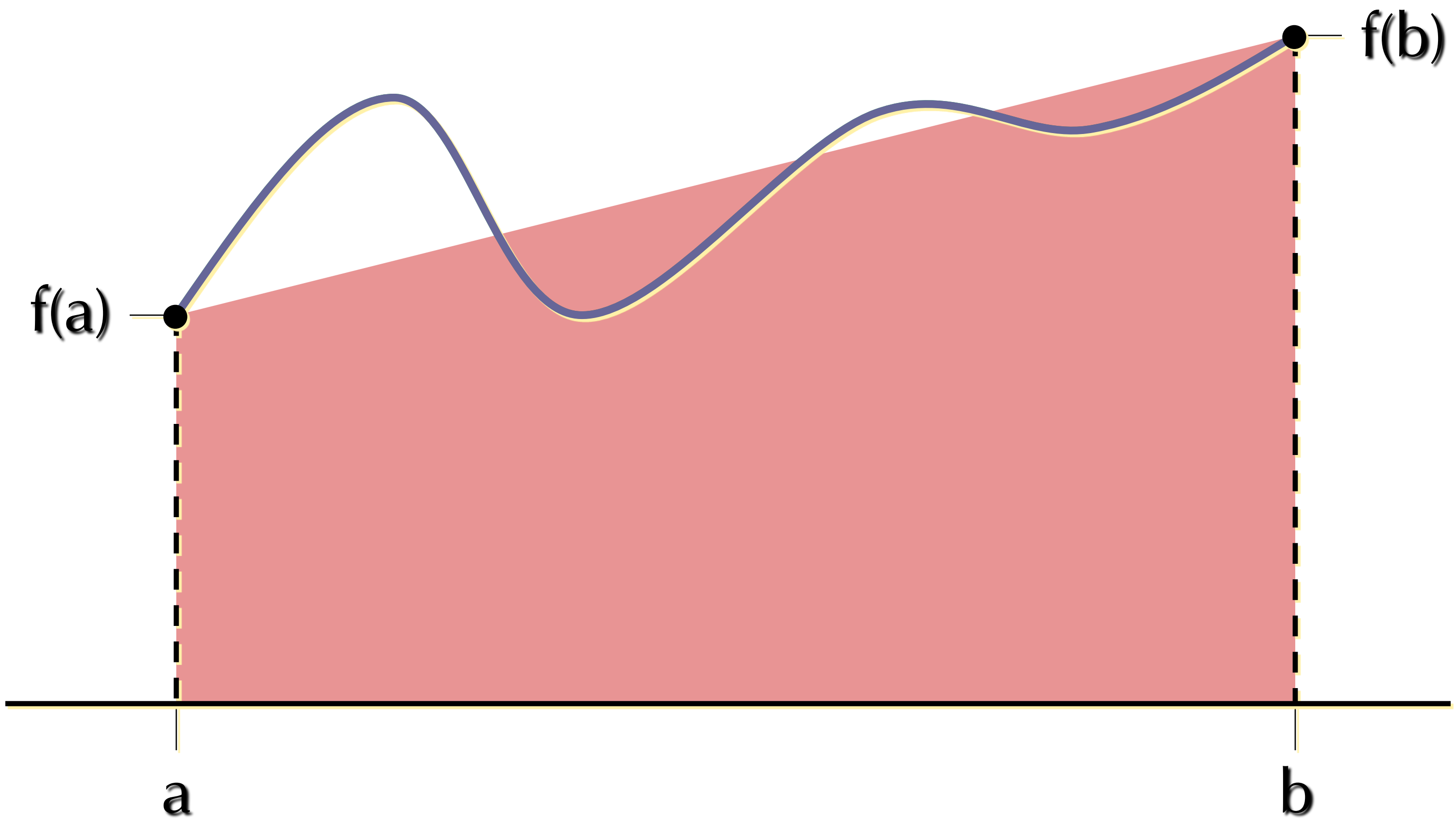
Quadrature

1. Sample $f(x)$ at a set of points
2. Approximate by a friendly function
3. Integrate approximating function

- Choices:
  - Which approximating function?
  - Which sampling points? ("nodes")
    - Even vs. uneven spacing?
  - Fit single function vs. multiple (piecewise)?

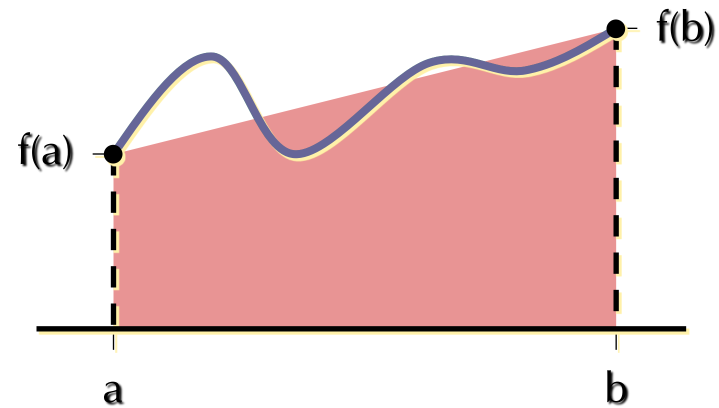
Trapezoidal Rule

- Approximate function by trapezoid



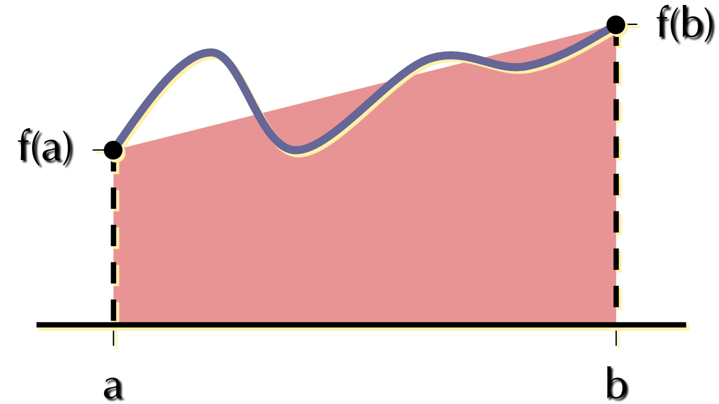
Trapezoidal Rule

$$\int_a^b f(x)\,dx \approx (b-a)\frac{f(a)+f(b)}{2}$$

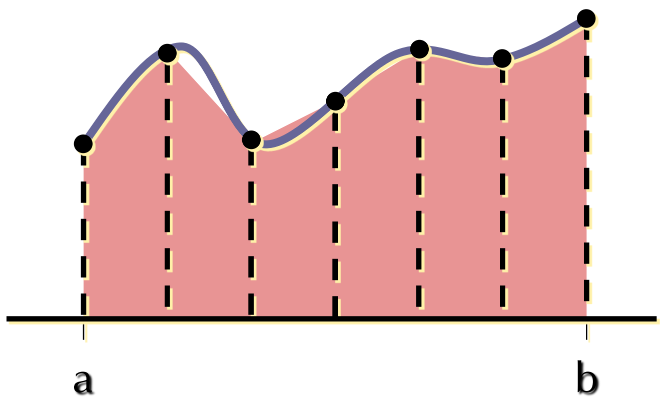


Extended Trapezoidal Rule

$$\int_a^b f(x)\,dx \approx (b-a)\frac{f(a)+f(b)}{2}$$



Divide into segments of width h, piecewise trapezoidal approximation



$$\int_a^b f(x)\,dx \approx h\left(\tfrac{1}{2}f(a)+f(x_1)+\cdots+f(x_{n-1})+\tfrac{1}{2}f(b)\right)$$

Trapezoidal Rule Error Analysis (for a single segment)

- How accurate is this approximation?

$$\int_a^b f(x)\,dx \approx \frac{(b-a)}{2}\big(f(a)+f(b)\big)+\mathscr{E}$$

- Start with Taylor series for $f(x)$ around midpoint m:

$$f(x) \approx f(m)+(x-m)\,f'(m)+\tfrac{1}{2}(x-m)^2\,f''(m)+$$
$$\tfrac{1}{6}(x-m)^3\,f'''(m)+\tfrac{1}{24}(x-m)^4\,f^{(4)}(m)+\cdots$$

Trapezoidal Rule Error Analysis

- Expand LHS:

$$\int_a^b f(x)\,dx \approx (b-a)\,f(m) + 0 + \tfrac{1}{24}(b-a)^3\, f''(m) +$$

$$0 + \tfrac{1}{1920}(b-a)^5\, f^{(4)}(m) + \cdots$$

- Expand RHS:

$$\frac{(b-a)}{2}\big(f(a)+f(b)\big) + \mathscr{E} = \tfrac{1}{2}(b-a)\Big[2f(m) + 0 + \tfrac{1}{4}(b-a)^2\, f''(m) +$$

$$0 + \tfrac{1}{192}(b-a)^4\, f^{(4)}(m) + \cdots\Big] + \mathscr{E}$$

Trapezoidal Rule Error Analysis

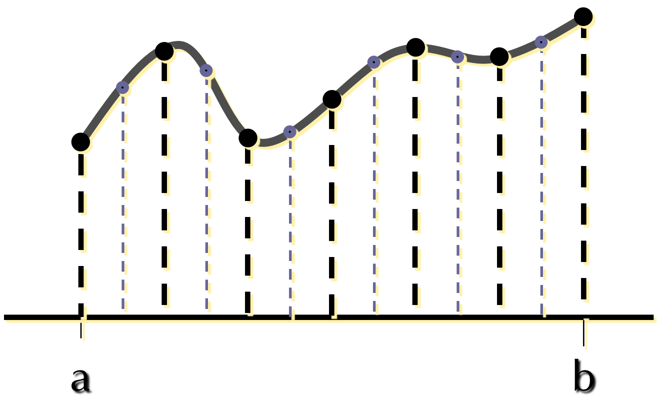
- So,

$$\mathscr{E} = -\tfrac{1}{12}(b-a)^3 f''(m) - \tfrac{1}{480}(b-a)^5 f^{(4)}(m) + \cdots$$

- In general, error for a *single* segment proportional to h^3
- Error for subdividing entire a→b interval proportional to h^2
  - "Cubic local accuracy, quadratic global accuracy"
  - Exact for linear functions
  - Note that only even-power terms in error: h^2, h^4, etc.

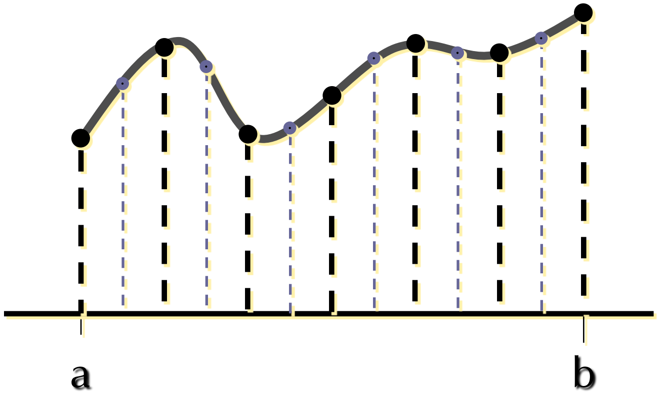
Determining Step Size

- Can't necessarily compute $f^{(2)}$, so can't compute error directly
- Can estimate error:
  1. $I(h_1) =$ quadrature with width h_1
  2. $I(h_2) =$ quadrature with width $h_2 = .5h_1$
  3. Estimate error $\cong I(h_2) - I(h_1)$



Progressive Qudrature

- Re-use nodes from Q_{n1} to compute Q_{n2}
- For Trapezoidal rule:
  - Cut each interval in half
  - Evaluate only additional needed samples



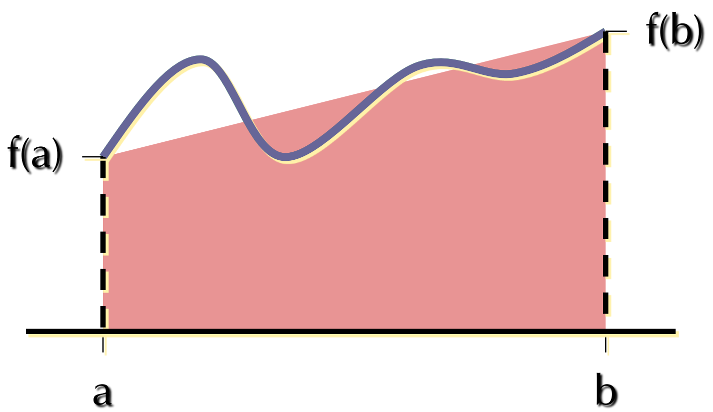
Quadrature: General Formulation

- n-point qudarature rule:

$$Q_n(f) = \sum_{i=1}^{n} w_i \, f(x_i)$$

- **Closed** if $a = x_1$, $x_n = b$; open if $a < x_1$, $x_n < b$

$$\int_a^b f(x)\,dx \approx (b-a)\frac{f(a)+f(b)}{2}$$



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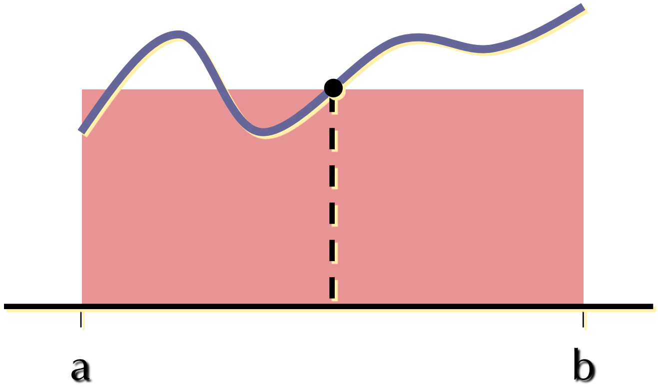
$$Q_n(f) = \sum_{i=1}^{n} w_i \, f(x_i)$$

- Closed if a = x_1, x_n = b; **open** if a < x_1, x_n < b

$$\int_a^b f(x)\,dx \approx (b-a)\,f\left(\tfrac{a+b}{2}\right)$$



Open Methods

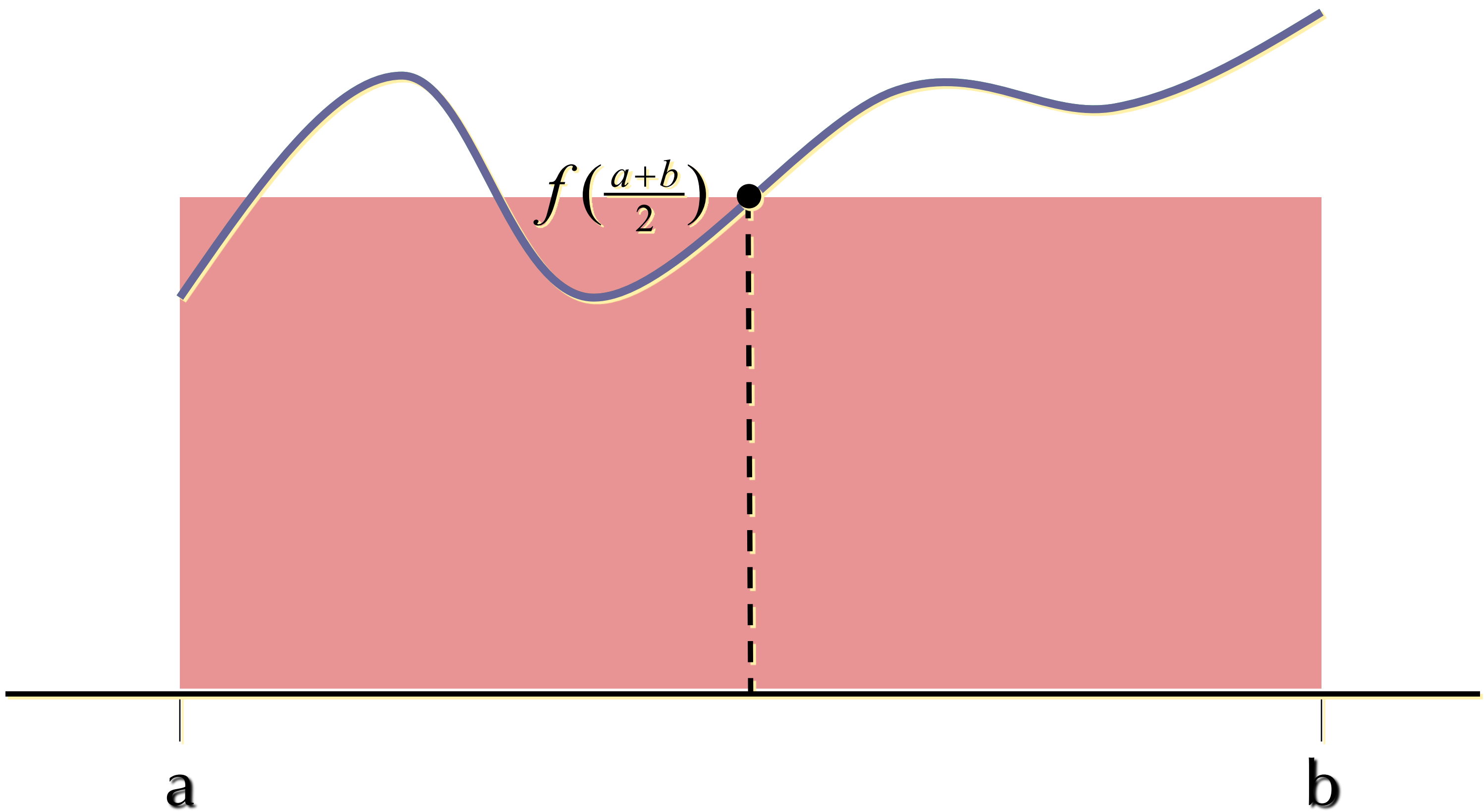
- Trapezoidal rule won't work if function undefined at one of the points where evaluating
  - Most often: function infinite at an endpoint

$$\int_0^1 \frac{dx}{x^2}$$

- Open methods only evaluate function on the *open* interval (i.e., not at endpoints)

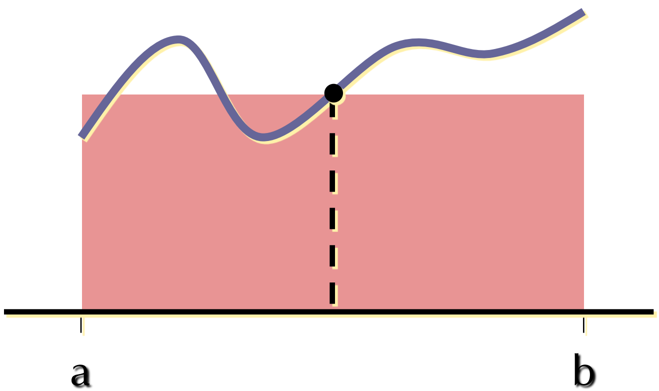
Midpoint Rule

- Approximate function by rectangle evaluated at midpoint

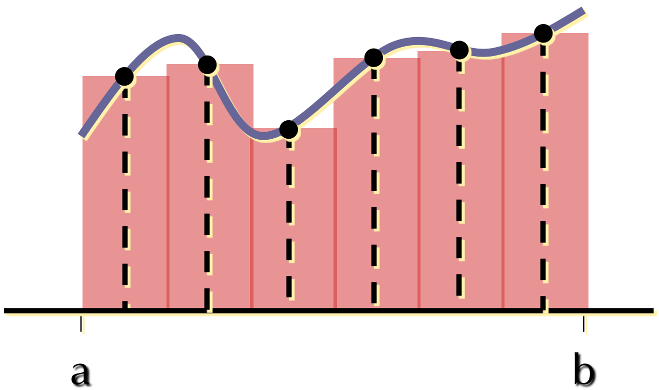


Extended Midpoint Rule

$$\int_a^b f(x)\,dx \approx (b-a)\,f\left(\tfrac{a+b}{2}\right)$$



Divide into segments of width h:



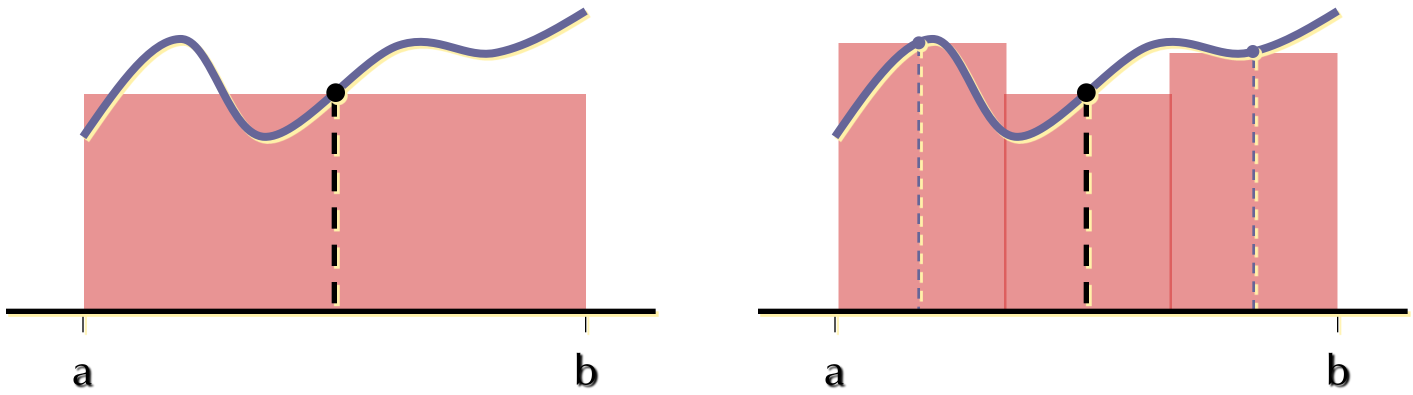
$$\int_a^b f(x)\,dx \approx h\Big(f\left(a+\tfrac{h}{2}\right)+f\left(a+\tfrac{3h}{2}\right)+\cdots+f\left(b-\tfrac{h}{2}\right)\Big)$$

Midpoint Rule Error Analysis

- Following similar analysis to trapezoidal rule, find that local accuracy is cubic, quadratic global accuracy
  - Surprisingly, leading-order constant is ½ as big!
  - Better than trapezoidal rule with fewer samples…
- Formula suitable for progressive quadrature, but can’t halve intervals without wasting samples

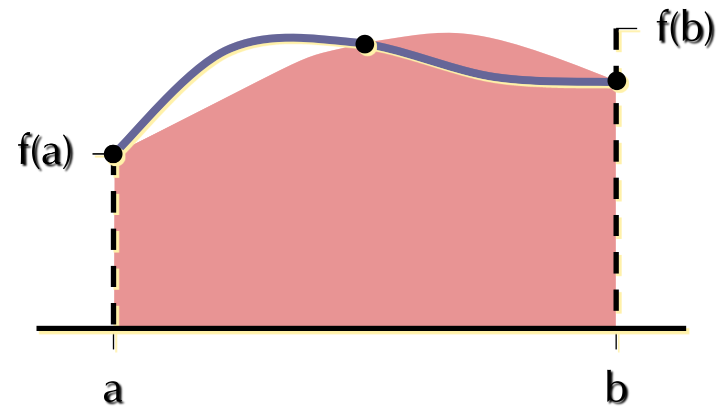
Extended / Adaptive Midpoint Rule

- Can cut interval into *thirds*:



Simpson's Rule

- Approximate integral by using parabola through three points

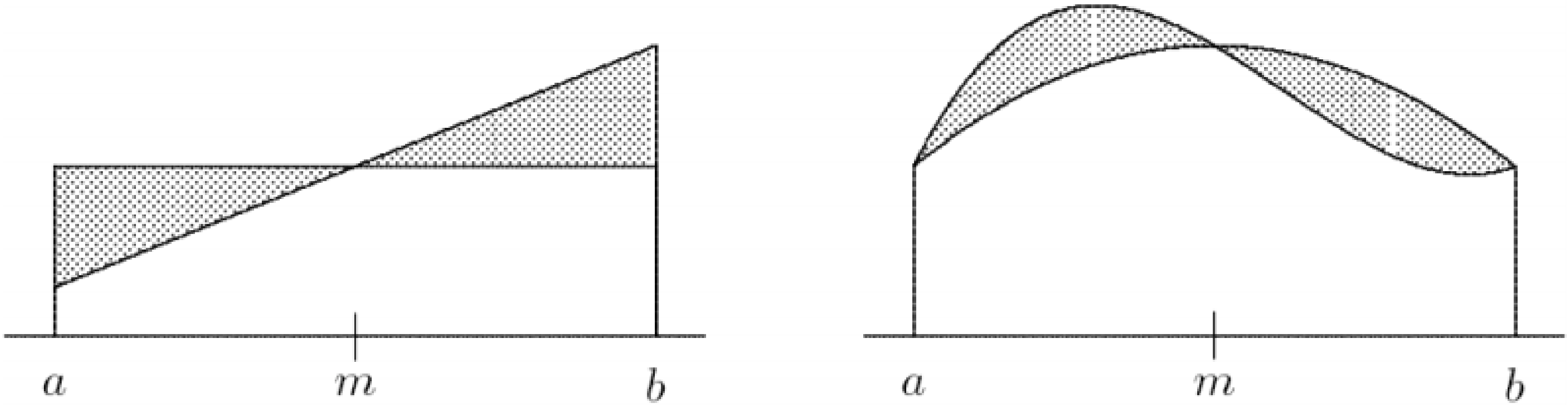


$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left(f(a) + 4f\left(\tfrac{a+b}{2}\right) + f(b)\right) + O(h^5)$$

Simpson's Rule Error

- Better accuracy than midpoint or trapezoid
  - Global error $O(h^4)$, exact for cubic (!) functions

Surprise benefits of odd-point rules



- Errors cancel exactly if true function is polynomial of odd degree

Simpson's Rule Error

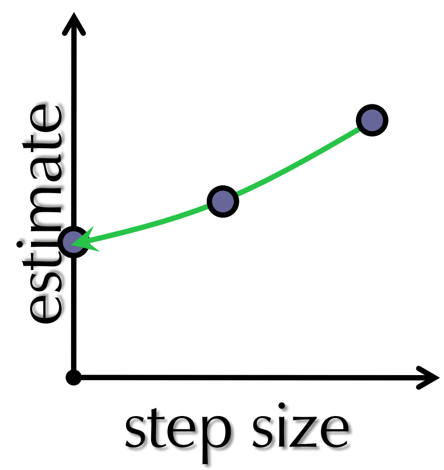
- Better accuracy than midpoint or trapezoid
  - Global error $O(h^4)$, exact for cubic (!) functions
- Higher-order polynomials (Newton-Cotes):
  - Global error $O(h^{k+1})$ for k odd, $O(h^{k+2})$ for k even
  - Fits polynomial of degree k for k points, *k* **odd**
  - Or polynomial of degree k-1 for k points, k **even**
  - **However:** solution becomes increasingly ill-conditioned

Richardson Extrapolation

- Better way of getting higher accuracy for a given # of samples
- Suppose we've evaluated integral for step size *h* and step size *h*/2 using trapezoidal rule:

$$F_h = F + \alpha h^2 + \beta h^4 + \cdots$$

$$F_{h/2} = F + \alpha\left(\tfrac{h}{2}\right)^2 + \beta\left(\tfrac{h}{2}\right)^4 + \cdots$$

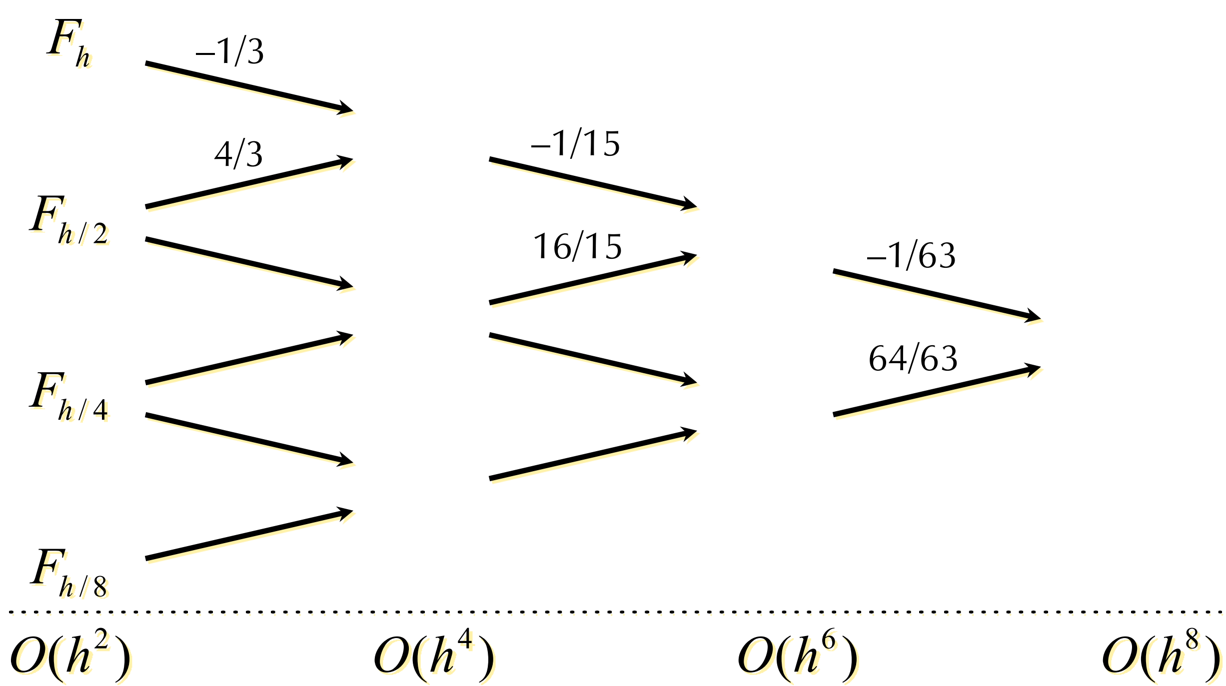


- Then

$$\tfrac{4}{3}F_{h/2} - \tfrac{1}{3}F_h = F + O(h^4)$$

Richardson Extrapolation

- This treats the approximation as a function of h and "extrapolates" the result to h=0
- Can repeat:



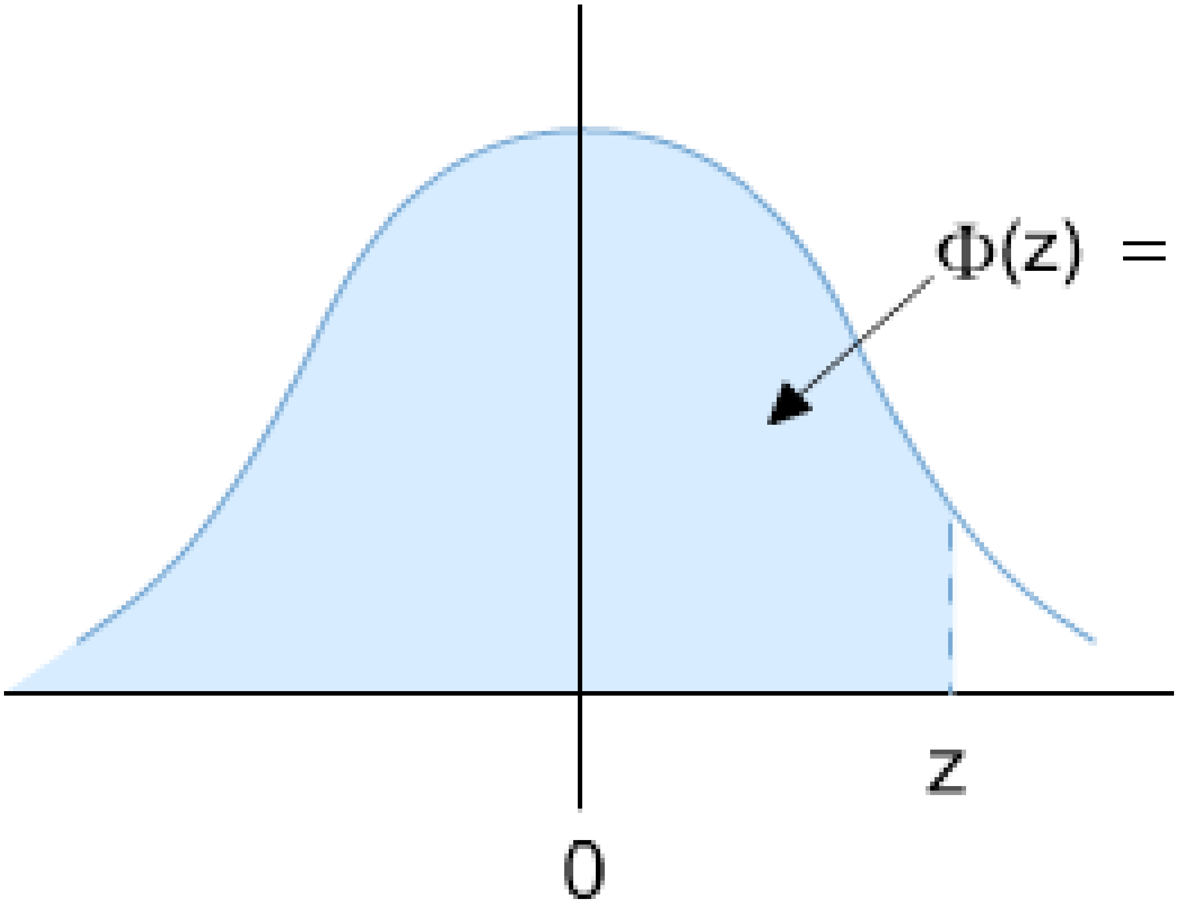
Limits at Infinity

- Usual trick: change of variables

$$\int_a^b f(x)\,dx = \int_{1/a}^{1/b} \frac{1}{t^2} f\left(\tfrac{1}{t}\right) dt$$

- Works with *a*, *b* same sign, one of them infinite
  - Otherwise, split into multiple pieces
- Also requires *f* to decrease faster than $1/x^2$
  - Else need different change of variables, if possible!

Example: Standard normal distribution

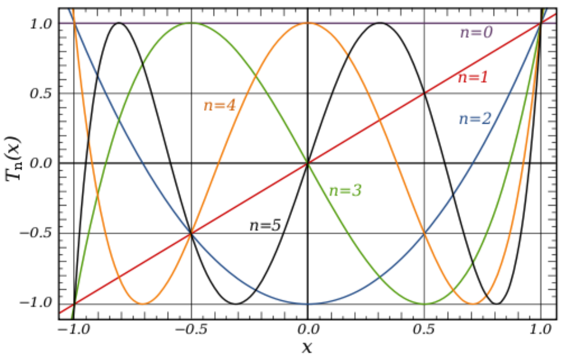


$$\Phi(z) = \int_{-\infty}^{z} \frac{1}{\sqrt{2\pi}} e^{-x^2/2}\,dx$$

$P(Z \leqslant z)$

Other Quadrature Rules

- Nonuniform sampling: complexity vs. accuracy
- Clenshaw-Curtis: Chebyshev polynomials
  - Change of variables: $x = \cos\theta$
  - Sample at extrema of polynomials
  - FFT-based algorithm to find weights

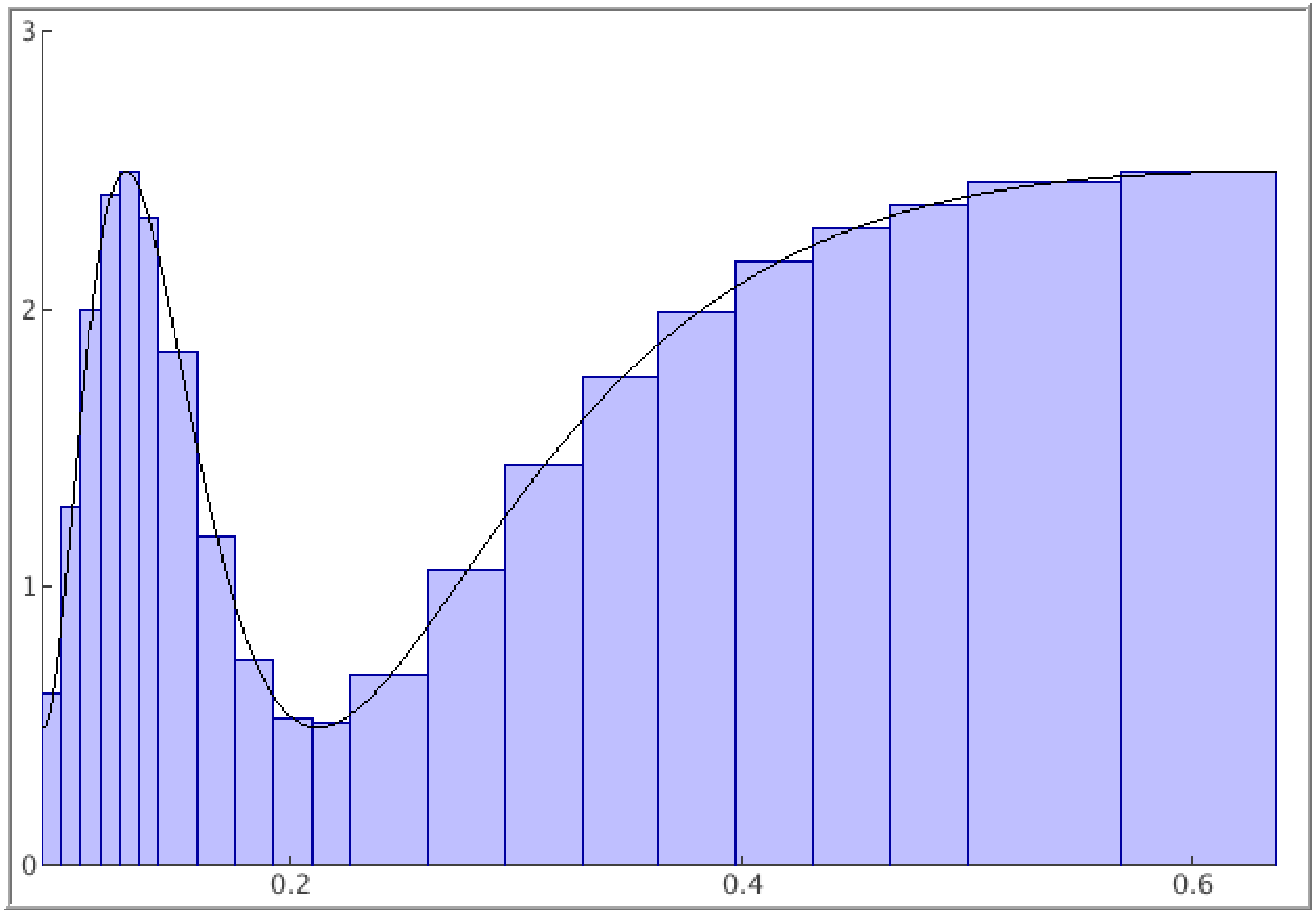


- Gaussian quadrature
  - Optimize sampling locations to get highest possible accuracy: $O(h^{2n})$ for n sampling points

Discontinuities

- All the above error analyses assumed nice (continuous, differentiable) functions
- In the presence of a discontinuity, all methods revert to accuracy proportional to h
  - In general, if the k-th order derivative is discontinuous, can do no better than $O(h^{k+1})$
- Locally-adaptive methods: do not subdivide all intervals equally, focus on those with large error (estimated from change with a single subdivision)

Adaptive Quadrature



http://www.cse.illinois.edu/iem/integration/adaptivq/