Numerical Differentiation

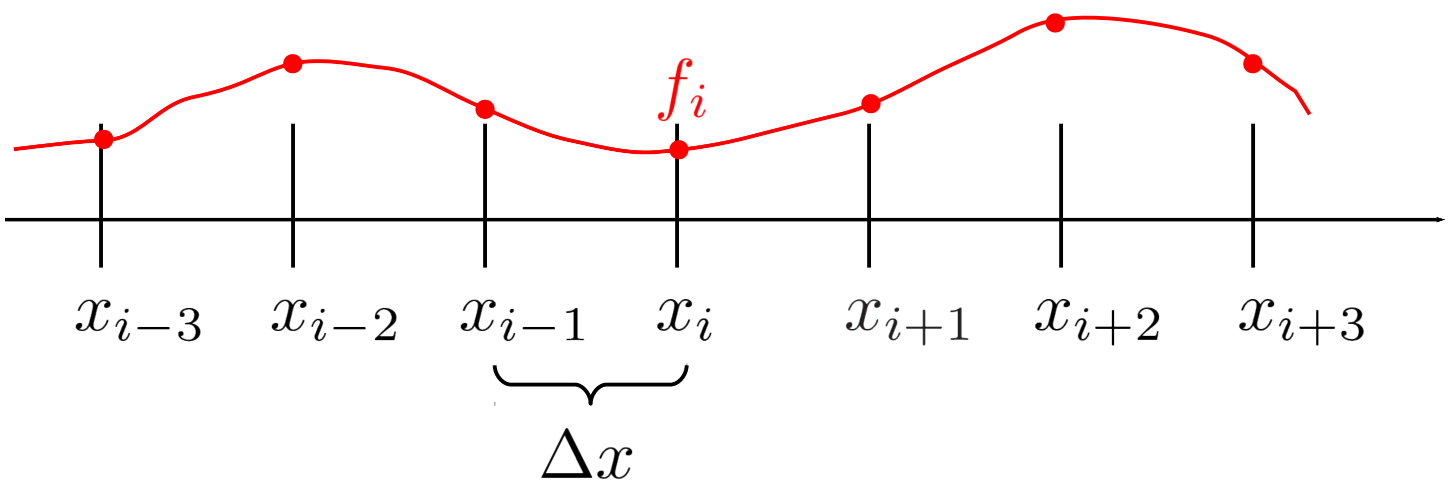
- We'll follow the discussion in Pang (Ch. 3) with some additions along the way
- Numerical differentiation approximations are key for:
  - Solving ODEs
  - PDEs

Numerical Differentiation

- We can imagine 2 situations
  - We have our function f(x) defined only at a set of (possibly regularly spaced) points
    - Generally speaking, asking for greater accuracy involves using more of the discrete points in the approximation for f'
  - We have an analytic expression for f(x) and want to compute the derivative numerically
    - Usually it would be better to take the analytic derivative of f(x), but we can learn something about error estimation in this case.
    - Used, for example, in computing the numerical Jacobian for integrating a system of ODEs (we'll see this later)

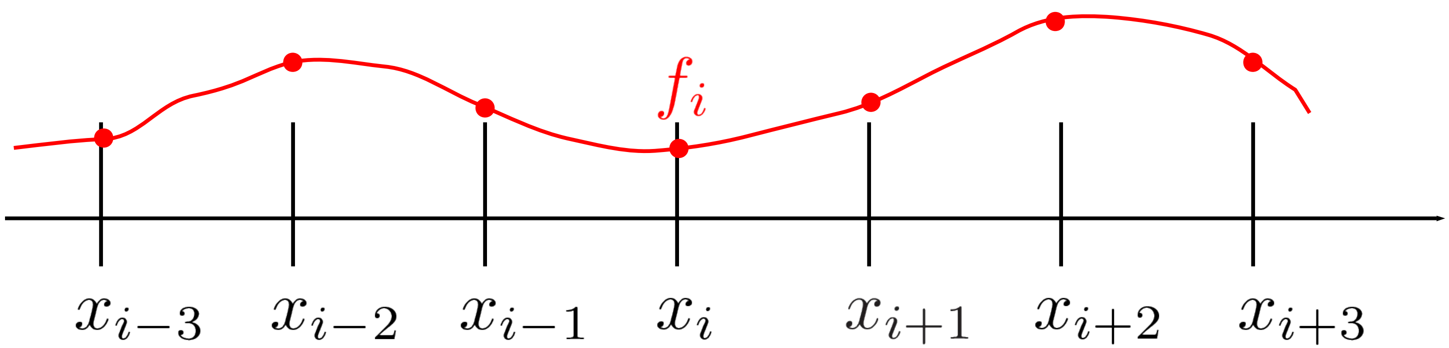
Gridded Data

- Discretized data is represented at a finite number of locations
  - Integer subscripts are used to denote the position (index) on the grid
  - Structured/regular: spacing is constant



  - Data is known only at the grid points: $f_i = f(x_i)$

First Derivative / Order of Accuracy



- Taylor expansion:

$$f_{i+1} = f(x_i + \Delta x) = f_i + \left.\frac{\partial f}{\partial x}\right|_{x_i} \Delta x + \frac{1}{2} \left.\frac{\partial^2 f}{\partial x^2}\right|_{x_i} \Delta x^2 + \ldots$$

- Solving for the first derivative:

$$\underbrace{\left.\frac{\partial f}{\partial x}\right|_{x_i} = \frac{f_{i+1} - f_i}{\Delta x}}_{\text{Discrete approximation to } f'} \underbrace{- \frac{1}{2} \left.\frac{\partial^2 f}{\partial x^2}\right|_{x_i} \Delta x}_{\text{Leading term in the truncation error}} + \ldots$$

First Derivative / Order of Accuracy

- This is a first-order accurate expression for the derivative at point i
  - Alternately, we can use the point to the left (blackboard)
  - The are called difference or finite-difference formulae
- Shorthand: $\mathcal{O}(\Delta x)$
  - “big-O notation”

- How can we get higher order?

First Derivative / Order of Accuracy

- First derivative approximations:
  - First-order (one-sided):

$$f' = \frac{f_i - f_{i-1}}{\Delta x} \qquad f' = \frac{f_{i+1} - f_i}{\Delta x}$$

2-point stencil

  - Second-order (centered):

$$f' = \frac{f_{i+1} - f_{i-1}}{2\Delta x}$$

3-point stencil

  - Fourth-order:

$$f' = \frac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12\Delta x}$$

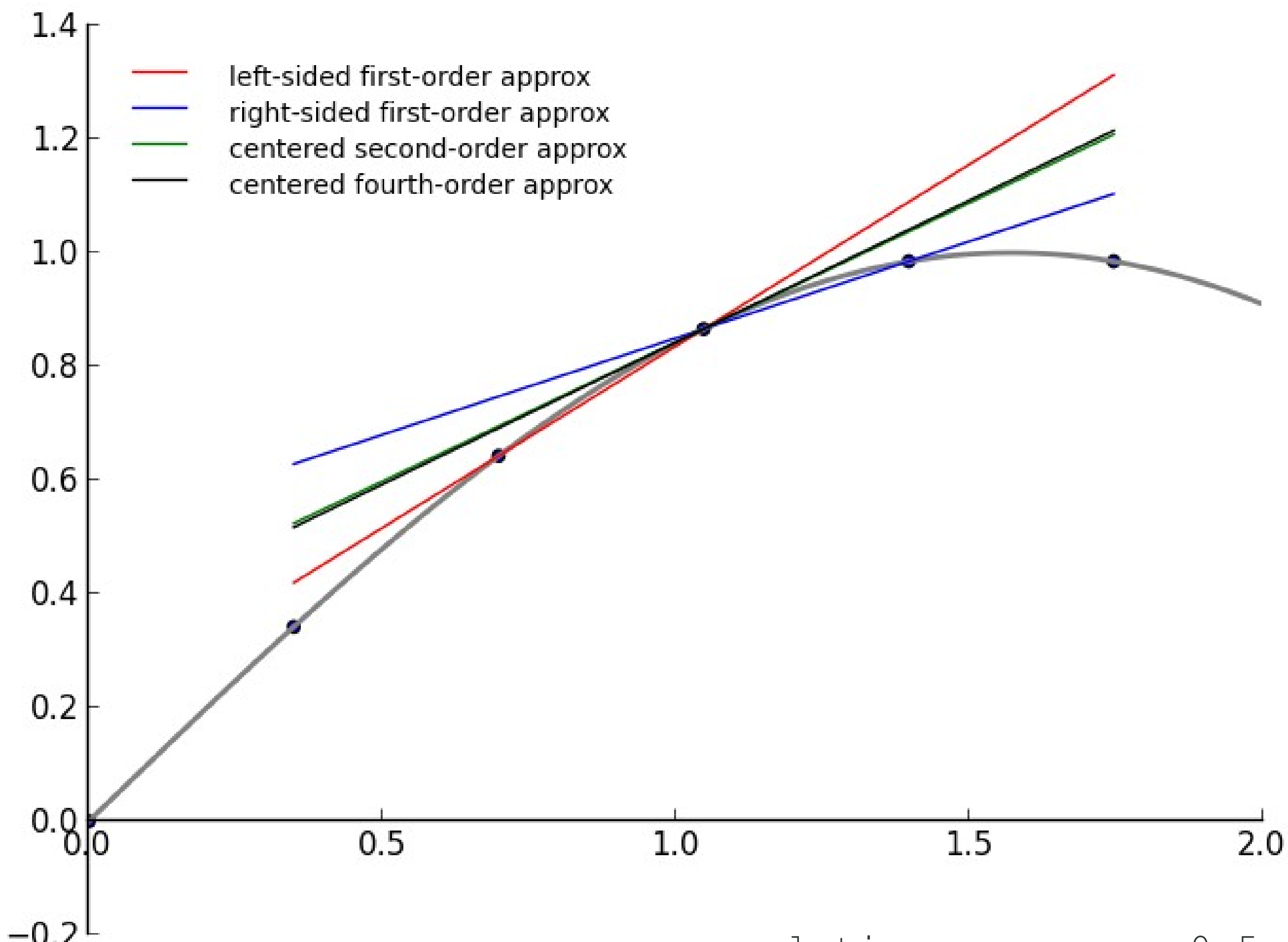
5-point stencil

- Range of points involved is called the stencil
  - Some points may have a '0' coefficient

First Derivative / Order of Accuracy

- General trend: more points = higher accuracy
  - Found via Taylor expanding from greater distances and algebra
- What happens at the boundaries of our finite-gridded data?
  - Can interpolate past the last point to use the same stencil
  - Can switch to one-sided stencils
- Practically speaking: the first and second order approximations are the ones that are used the most often.

First Derivative Comparison




```
analytic:             0.5
left-sided O(dx):     0.639529171481
right-sided O(dx):    0.34028636457
centered O(dx**2):    0.489907768026
centered O(dx**4):    0.499756119208
```

Roundoff vs. Truncation Error

(Yakowitz & Szidarovszky)

- Just evaluating f at our gridded points introduces round-off error:
  - $\overline{f}_{i+1}$ is an approximation to $f_{i+1} = f(x_{i+1})$
  - Assume some bound: $|f_{i+1} - f_i| \le \delta$
  - Error is (blackboard):

$$\left| f' - \frac{\overline{f}_{i+1} - \overline{f}_i}{\Delta x} \right| \le \underbrace{\frac{|f''|h}{2}}_{\text{truncation}} + \underbrace{\frac{2\delta}{h}}_{\text{roundoff}}$$

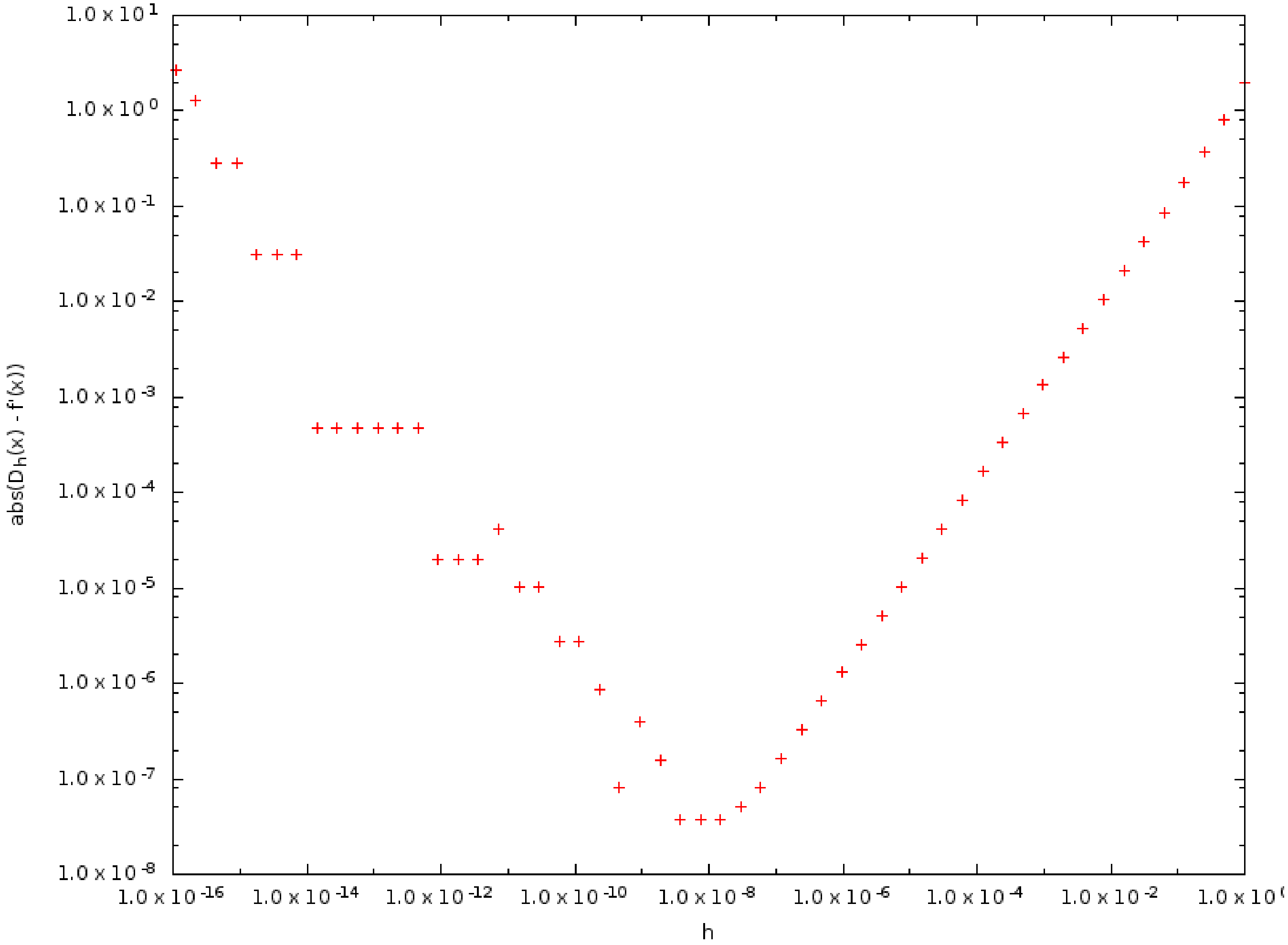
This should be near machine ε

As h → ε, the roundoff term becomes O(1)

Another thing to consider: with roundoff, is $(x + \Delta x) - x = \Delta x$?

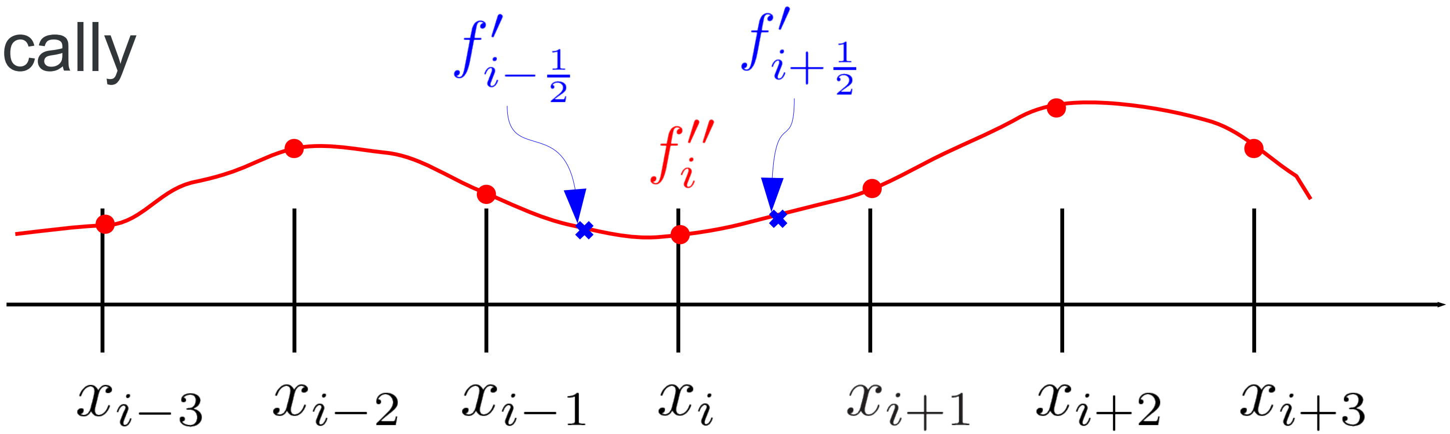
Round-off vs. Truncation Error

- exp(x)



Higher-Derivatives

- Graphically



$$f'_{i+1/2} = \frac{f_{i+1} - f_i}{\Delta x}$$

This is 2nd order at the midpoint between the two points

$$f''_i = \frac{f'_{i+1/2} - f'_{i-1/2}}{\Delta x}$$

This is a centered difference (derivative) of the derivatives = second derivative

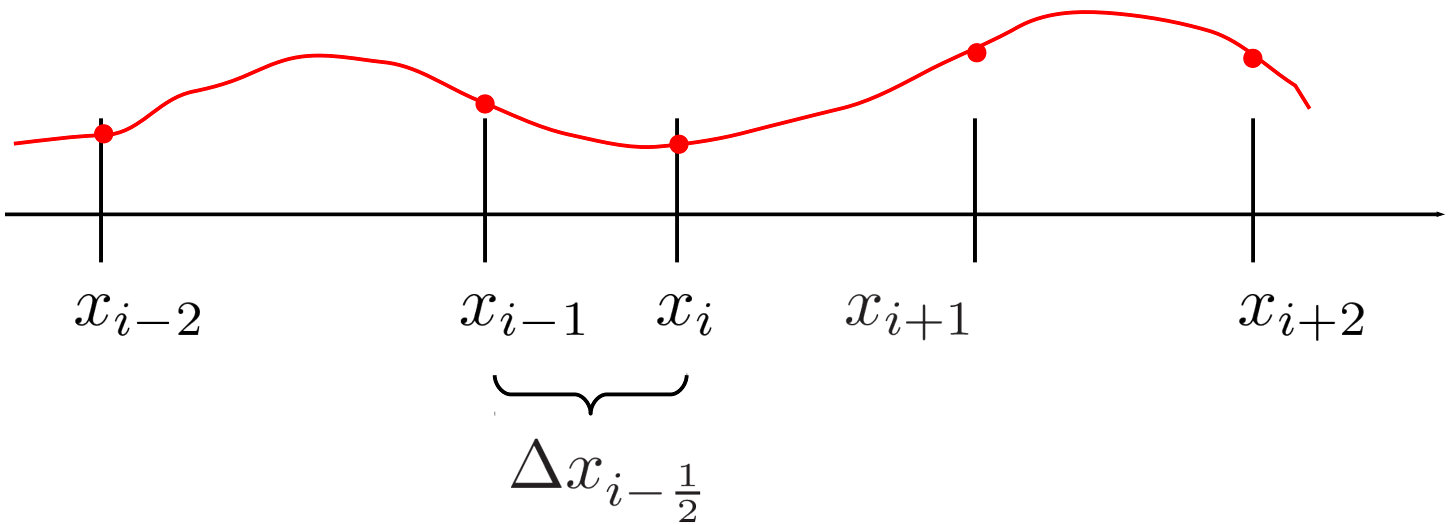
$$= \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2}$$

Second-order accurate

- Also via Taylor expansion (blackboard)

Non-Uniform Data

- Two choices:
  - Interpolate to a uniform grid
  - Re-derive our expressions for a non-uniform grid (preferred)



$$f' = \frac{\Delta x^2_{i-\frac{1}{2}} f_{i+1} + (\Delta x^2_{i+\frac{1}{2}} - \Delta x^2_{i-\frac{1}{2}}) f_i - \Delta x^2_{i+\frac{1}{2}} f_{i-1}}{\Delta x_{i-\frac{1}{2}} \Delta x_{i+\frac{1}{2}} (\Delta x_{i+\frac{1}{2}} + \Delta x_{i-\frac{1}{2}})} + \mathcal{O}(\Delta x^2_{i-\frac{1}{2}}) + \mathcal{O}(\Delta x^2_{i+\frac{1}{2}})$$

(blackboard derivation...)

Analytic f Given

- If we have f(x) available analytically, we can make estimates of the error
  - This will come into play with ODEs, where we have the analytic righthand side
- Controlling accuracy
  - Consider:

$$\Delta_1(h) \equiv \frac{f(x+h) - f(x-h)}{2h}$$

  - We are free to choose h
  - Compare $\Delta_1(h)$ to $\Delta_1(h/2)$ estimate error

Analytic f Given

- Iteratively build more accurate approximations
  - $f(x \pm h) = f(x) \pm h f' + \frac{1}{2} h^2 f'' \pm \frac{1}{3!} h^3 f''' + \frac{1}{4!} h^4 f^{(4)} \pm \frac{1}{5!} h^5 f^{(5)} + \ldots$
  - This gives:

$$\Delta_1(h) = f' + \frac{1}{6} h^2 f''' + \mathcal{O}(h^4)$$

  - Consider: $$\Delta_1(h/2) = f' + \frac{1}{6}\frac{1}{4} h^2 f''' + \mathcal{O}(h^4)$$

  - Combine: $$f' = -\frac{\Delta_1(h) - 4\Delta_1(h/2)}{3} + \mathcal{O}(h^4)$$

  - This is an example of Richardson extrapolation—we'll see this more when we go to ODEs

Numerical Integration

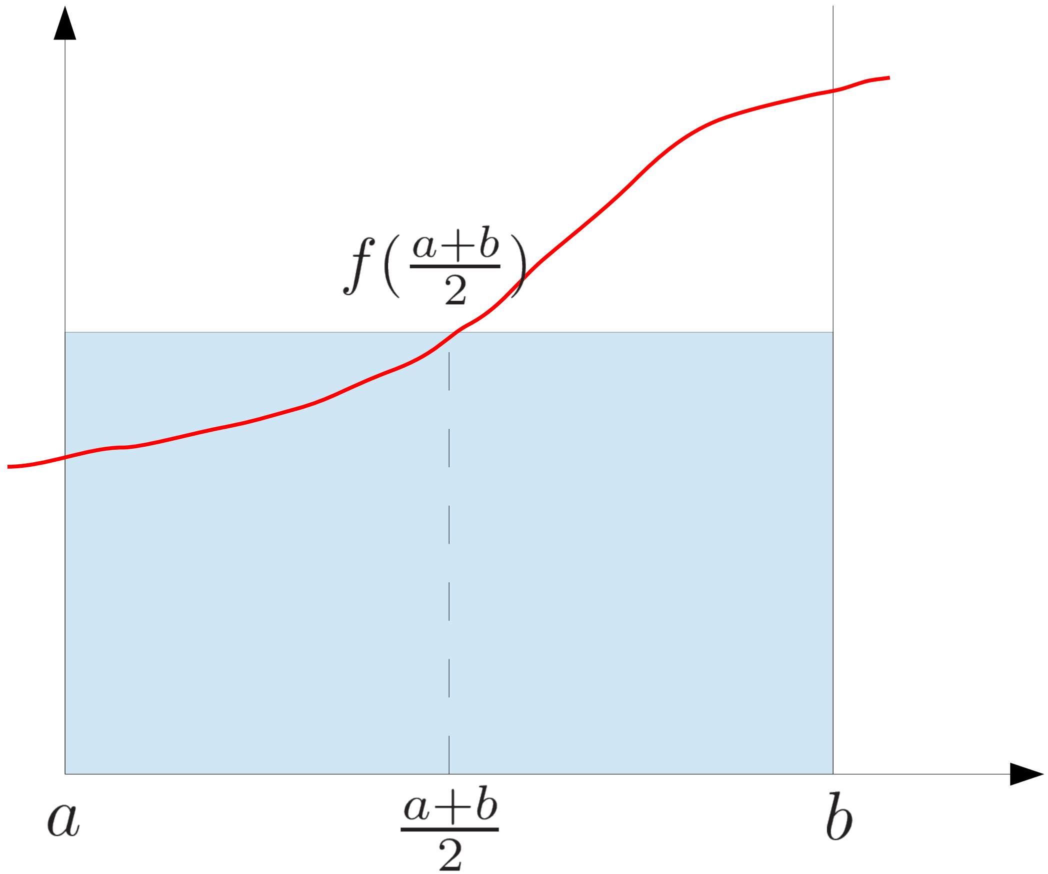
- We want to solve:

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

- Again, we have two distinct cases:
  - f(x) is provided at discrete points on a grid
  - We have an analytic expression for f(x)
- We'll follow the discussion in Pang and also that of Garcia

Numerical Integration

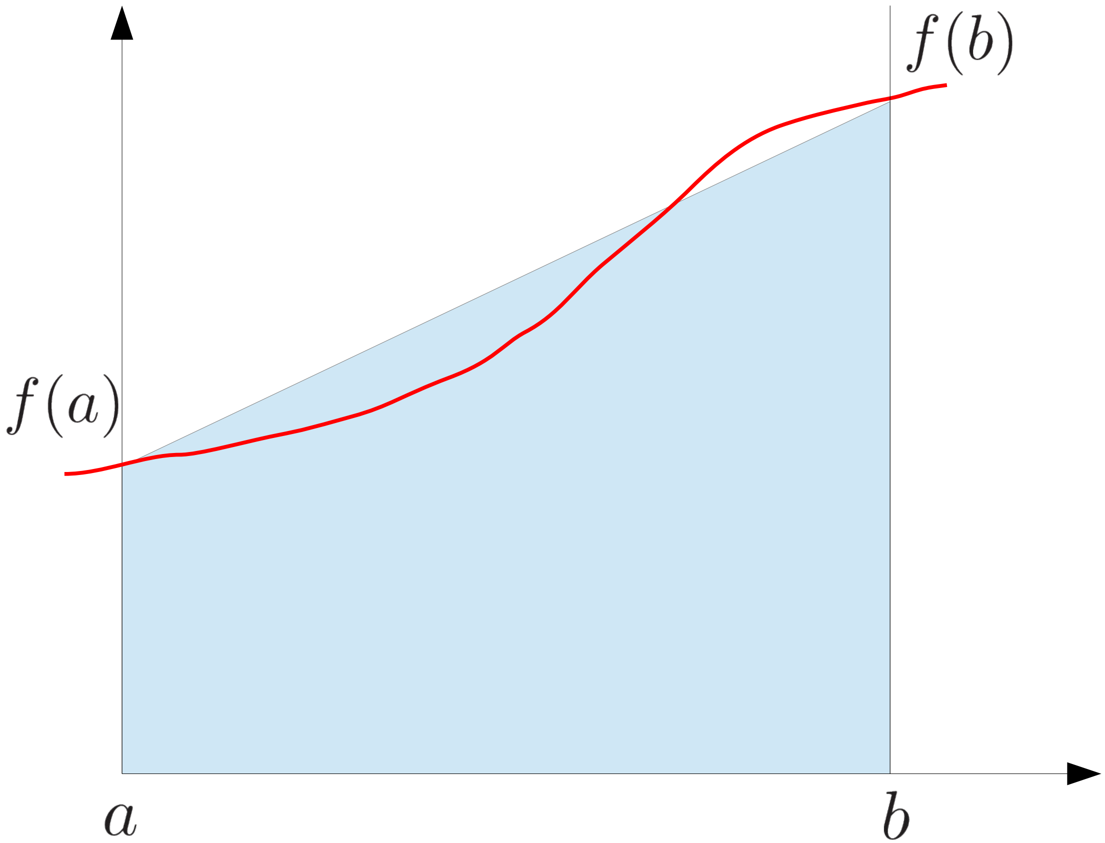
- Simplest case: piecewise constant interpolant (midpoint rule)



$$I \approx (b-a) f\left(\frac{a+b}{2}\right)$$

Numerical Integration

- One step up: piecewise linear interpolant (trapezoid rule)



$$I \approx (b-a)\frac{f(b)+f(a)}{2}$$

This is just the area of a trapezoid

Numerical Integration

- As you might expect, the accuracy gets better the higher-order the interpolating polynomial
  - Trapezoid rule will integrate a linear f(x) perfectly
- What about a parabola?
  - For now, we'll stick with equally spaced locations at which we evaluate f(x)

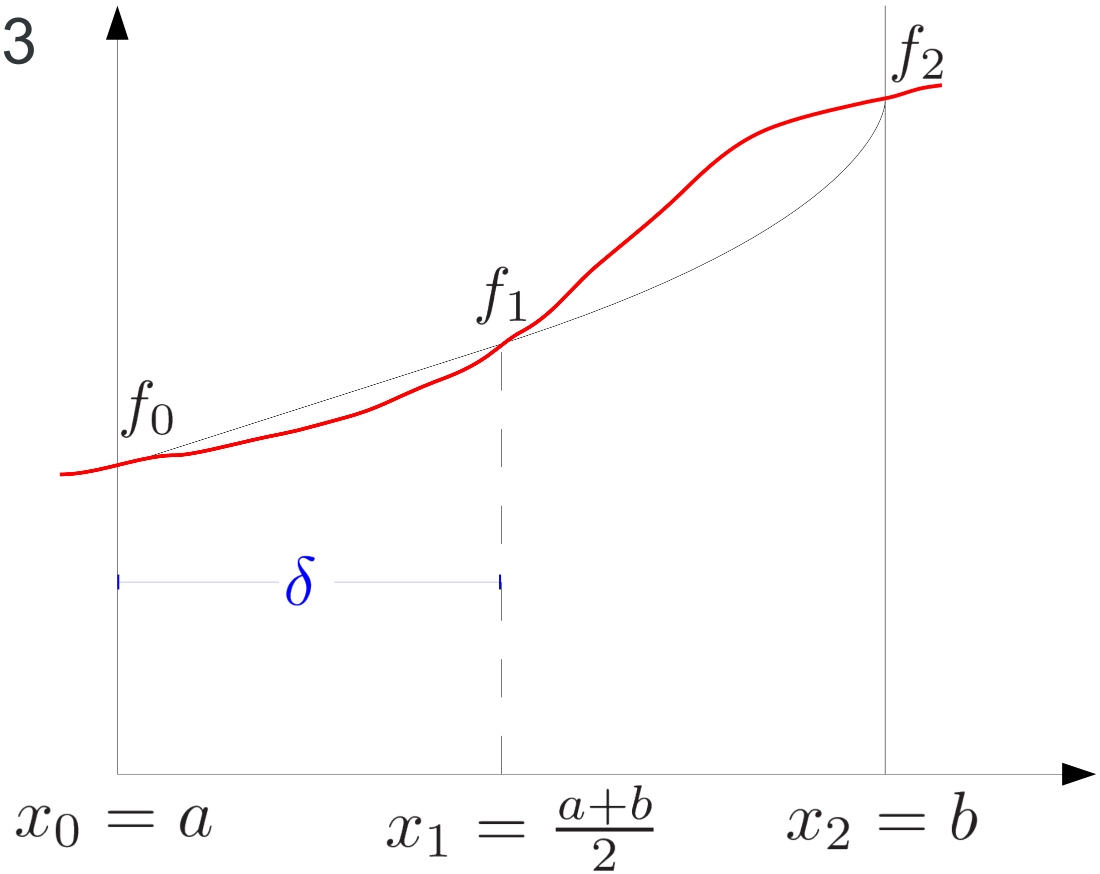
Simpson's Rule

- Piecewise linear interpolant (Simpson's rule)
  - 3 unknowns (A, B, C) and 3 points
  - Blackboard algrebra...

$$A = \frac{f_0 - 2f_1 + f_2}{2\delta^2}$$

$$B = -\frac{f_2 - 4f_1 + 3f_0}{2\delta}$$

$$C = f_0$$



$$f(x) = A(x - x_0)^2 + B(x - x_1) + C$$

Simpson's Rule

- Then integrate under the parabola

$$I = \int_{x_0}^{x_2} [A(x - x_0)^2 + B(x - x_0) + C] dx$$

$$= \frac{\delta}{3}(f_0 + 4f_1 + f_2)$$

Summary of Simple Rules

(Yakowitz & Szidarovszky)

- Error estimates
  - Actually rather complicated to derive (see a math text on Numerical Methods)
  - Simple trapezoidal:

$$\int_a^b f(x) \approx \frac{\delta}{2}(f(a) + f(b)) - \frac{\delta^3}{12} f''(\zeta) \qquad \delta = b - a$$

  - Simple Simpson's:

$$\int_a^b f(x)dx \approx \frac{\delta}{3}(f(a) + 4f(\tfrac{a+b}{2}) + f(b)) - \frac{\delta^5}{90} f^{(4)}(\zeta) \qquad \delta = \frac{b-a}{2}$$

  - Note the only way to reduce the error here is to make [a, b] smaller
  - Here, ζ is some unknown point in [a, b]

Summary of Simple Rules

- Any numerical integration method that represents the integral as a (weighted) sum at a discrete number of points is called a quadrature rule
- Fixed spacing between points (what we've seen so far): Newton-Cotes quadrature

Open Integration Rules

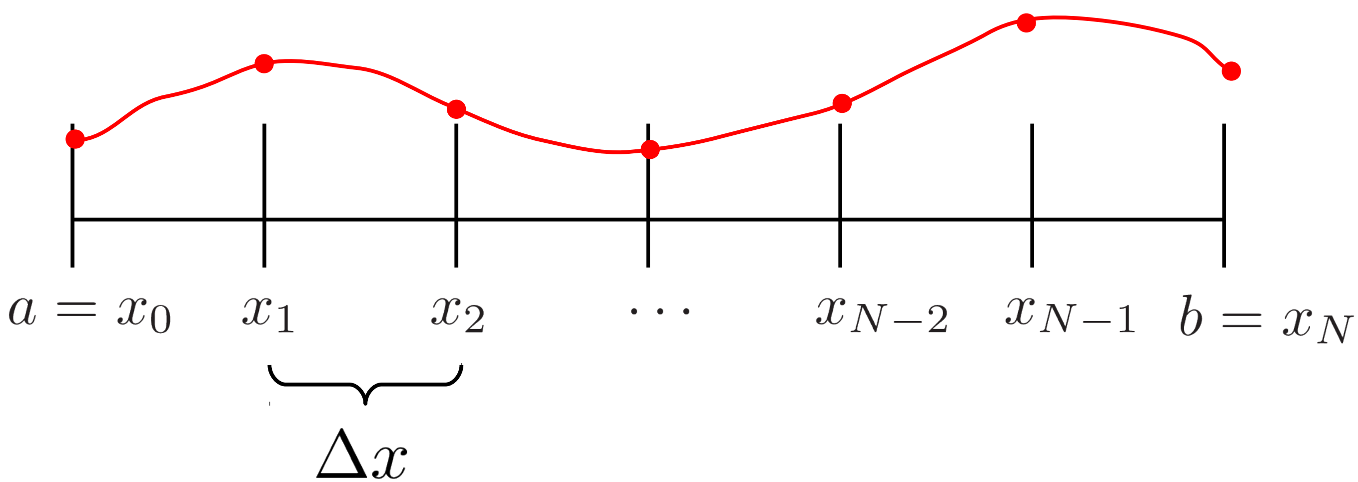
- Forms of these exist where the end-points of the interval are not used—these are open integration rules
  - Usually not very desirable
  - See, for example, Numerical Recipes

Compound Integration

- Mid-point, trapezoidal, and Simpson's integration as we wrote them are ok when [a,b] is small.
- Integrating over large domain is not very accurate
  - We could keep adding terms to our polynomials (getting higher and higher degree), or we could string together our current expressions
    - More points = more accuracy
  - Compound integration—break domain into sub-domains and use these rules in each sub-domain.

Compound Integration

- Break interval into chunks



$$I \equiv \int_a^b f(x)dx = \sum_{i=0}^{N-1} \underbrace{\int_{x_i}^{x_{i+1}} f(x)dx}_{\text{Integral over a single slab}}$$

Compound Integration

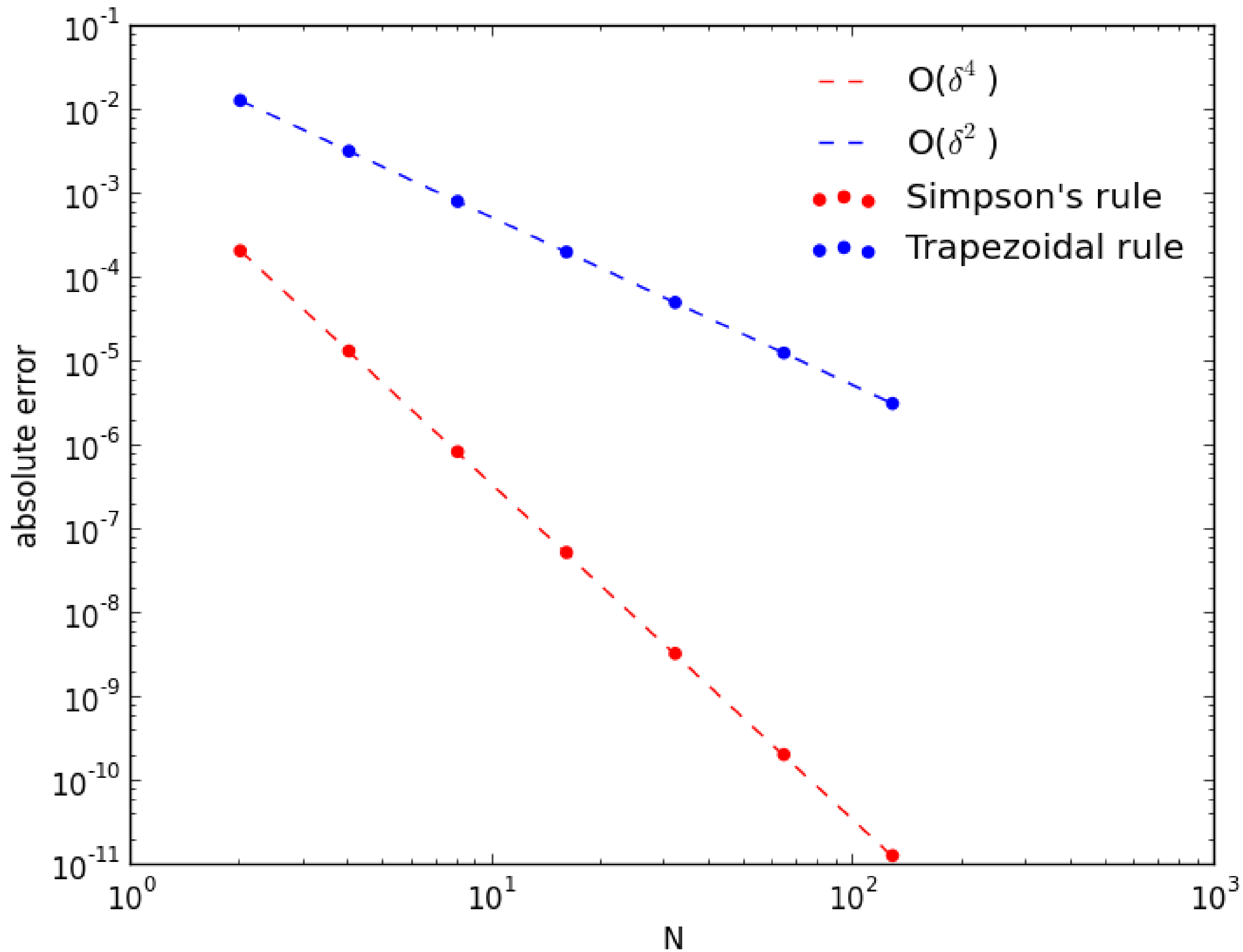
- Compound Trapezoidal

$$\int_a^b f(x)dx = \frac{\Delta x}{2} \sum_{i=0}^{N-1} (f_i + f_{i+1}) + \mathcal{O}(\Delta x^2)$$

- Compound Simpson's
  - Integrate pairs of slabs together (requires even number of slabs)

$$\int_a^b f(x)dx = \frac{\Delta x}{3} \sum_{i=0}^{N/2-1} (f_{2i} + 4f_{2i+1} + f_{2i+2}) + \mathcal{O}(\Delta x^4)$$

Compound Integration



$$\int_0^1 e^{-x}dx$$

Always a good idea to check the convergence rate!

Adaptive Integration

- If you know the analytic form of f(x), then you can estimate the error by increasing N
  - Can make use of previous function evaluations (see Garcia)
- Recover Simpson's rule from adaptive trapezoidal (see NR)

Gaussian Quadrature

- Instead of fixed spacing, what if we strategically pick the spacings?
  - We want to express

$$\int_a^b f(x)dx \approx w_1 f(x_1) + \ldots w_N f(x_N)$$

  - w's are weights. We will choose the location of points x_i

Gaussian Quadrature

(Garcia, Ch. 10)

- Gaussian quadrature: fundamental theorem
  - q(x) is a polynomial of degree N, such that

$$\int_a^b q(x)\rho(x)x^k\,dx = 0$$

  - k = 0, ..., N-1 and ρ(x) is a specified weight function.
  - Choose x_1, x_2, ... x_N as the roots of the polynomial q(x)
  - We can write

$$\int_a^b f(x)\rho(x)dx \approx w_1 f(x_1) + \ldots w_N f(x_N)$$

  and there will be a set of w's for which the integral is exact if f(x) is a polynomial of degree < 2N!

Gaussian Quadrature

(Garcia, Ch. 10)

- The amazing result of this theorem is that by picking the points strategically, we are exact for polynomials up to degree 2N-1
  - With a fixed grid, of N points, we can fit an N-1 degree polynomial
    - Exact integration for f(x) only if it is a polynomial of degree N-1 or less
  - If our f(x) is closely approximated by a polynomial of degree 2N-1, then this will be very accurate.
- Many choices of weighting function, ρ(x), leading to different q's and x's and w's.

Gaussian Quadrature

(Garcia, Ch. 10)

- Example from Garcia:
  - 3-point quadrature
    - This means 3 roots, so q(x) is a cubic
  - Weight function ρ(x) = 1
  - Work in the interval [-1, 1]
    - Easy to transform from [a, b] to [-1, 1]:

$$x = \frac{1}{2}(b+a) + \frac{1}{2}(b-a)z$$

$$z = \frac{x - \frac{1}{2}(b+a)}{\frac{1}{2}(b-a)} \, ; \qquad dx = \tfrac{1}{2}(b-a)dz$$

$$\int_a^b f(x)dx = \frac{b-a}{2}\int_{-1}^{1} f(z)dz$$

Gaussian Quadrature

(Garcia, Ch. 10)

- 3-point quadrature:
  - $q(x) = c_0 + c_1 x + c_2 x^2 + c_3 x^3$
- Step 1: Apply the theorem to find the c's:

$$\left.\begin{aligned} \int_{-1}^{1} q(x) &= 0 \\ \int_{-1}^{1} x q(x) &= 0 \\ \int_{-1}^{1} x^2 q(x) &= 0 \end{aligned}\right\}$$

This can give 3 equations for the c's, allowing us to find q(x) up to some arbitrary factor.

Alternately, these are the conditions for the Legendre polynomials (the Gram-Schmidt orthogonalization)

$$q(x) = P_3(x) = \frac{5}{2}x^3 - \frac{3}{2}x$$

Gaussian Quadrature

(Garcia, Ch. 10)

- Step 2: find the roots (those are our quadrature points)
  - For

$$q(x) = P_3(x) = \frac{5}{2}x^3 - \frac{3}{2}x$$

    we can easily factor this:

$$x = 0, \pm\sqrt{\frac{3}{5}}$$

  - This means that our quadrature becomes:

$$\int_{-1}^{1} f(x)dx \approx w_1 f(-\sqrt{3/5}) + w_2 f(0) + w_3 f(\sqrt{3/5})$$

Gaussian Quadrature

(Garcia, Ch. 10)

- Step 3: find the weights
  - The theorem tells us that with the x's as the roots, then the proper choice of weights makes the integration exact for polynomials up to degree 2N-1

$$f(x) = 1 : \int_{-1}^{1} dx = w_1 + w_2 + w_3$$

Note the "="—this is exact

this is: $2 = w_1 + w_2 + w_3$

$$f(x) = x : \int_{-1}^{1} x dx = -\sqrt{\tfrac{3}{5}} w_1 + \sqrt{\tfrac{3}{5}} w_3 = 0$$

$$f(x) = x^2 : \int_{-1}^{1} x^2 dx = \tfrac{3}{5} w_1 + \tfrac{3}{5} w_3 = \tfrac{2}{3}$$

Gaussian Quadrature

(Garcia, Ch. 10)

- These three equations can be solved to find the weights:

$$w_1 = \frac{5}{9}; w_2 = \frac{8}{9}; w_3 = \frac{5}{9}$$

- Therefore, our 3-point quadrature is:

$$\int_{-1}^{1} f(x)dx \approx \frac{5}{9} f(-\sqrt{3/5}) + \frac{8}{9} f(0) + \frac{5}{9} f(\sqrt{3/5})$$

Our choice of weight function and integration interval results in the Gauss-Legendre method

Gaussian Quadrature

(Garcia, Ch. 10)

- Example:

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-y^2} dy$$

```
erf(1) (exact):            0.84270079295
3-point trapezoidal:       0.825262955597 -0.017437837353
3-point Simpson's:         0.843102830043 0.000402037093266
3-point Gauss-Legendre:    0.842690018485 -1.0774465204e-05
```

Notice how well the Gauss-Legendre does for this integral.

Gaussian Quadrature

- Other quadratures exist:

Interval	ω(x)	Orthogonal polynomials	A & S	For more information, see ...
[−1, 1]	1	Legendre polynomials	25.4.29	Section *Gauss–Legendre quadrature*, above
(−1, 1)	$(1-x)^\alpha(1+x)^\beta, \quad \alpha, \beta > -1$	Jacobi polynomials	25.4.33 ($\beta = 0$)	Gauss–Jacobi quadrature
(−1, 1)	$\frac{1}{\sqrt{1-x^2}}$	Chebyshev polynomials (first kind)	25.4.38	Chebyshev–Gauss quadrature
[−1, 1]	$\sqrt{1-x^2}$	Chebyshev polynomials (second kind)	25.4.40	Chebyshev–Gauss quadrature
[0, ∞)	e^{-x}	Laguerre polynomials	25.4.45	Gauss–Laguerre quadrature
[0, ∞)	$x^\alpha e^{-x}$	Generalized Laguerre polynomials		Gauss–Laguerre quadrature
(−∞, ∞)	e^{-x^2}	Hermite polynomials	25.4.46	Gauss–Hermite quadrature

(Wikipedia)

- In practice, the roots and weights are tabulated for these out to many numbers of points, so there is no need to compute them.

Multi-dimensional Integration

- For multi-dimensional integration, Monte Carlo methods may be faster (less function evaluations)