Differentiation / Integration

Numerical Differentiation

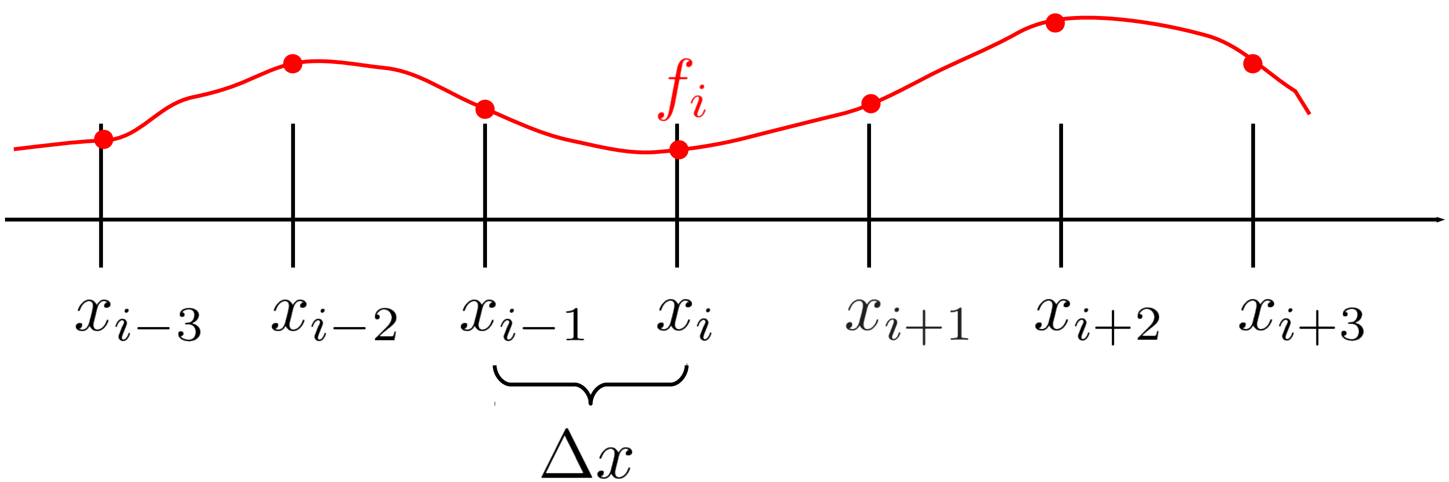
- We'll follow the discussion in Pang (Ch. 3) with some additions along the way
- Numerical differentiation approximations are key for:
  - Solving ODEs
  - PDEs

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)

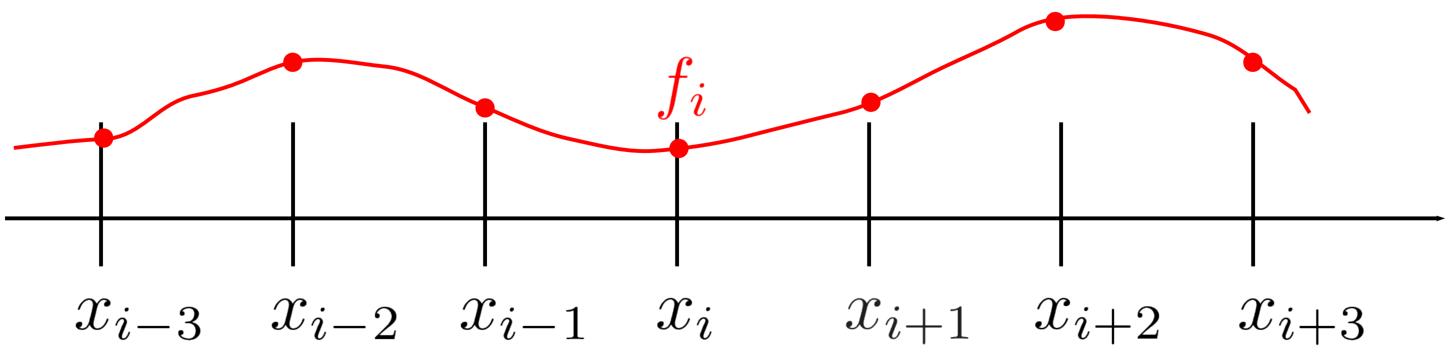
Gridded Data

- 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:

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

- Solving for the first derivative:

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

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)
  - These 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.

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: $|\bar{f}_i - f_i| \leq \delta$
  - Error is (blackboard):

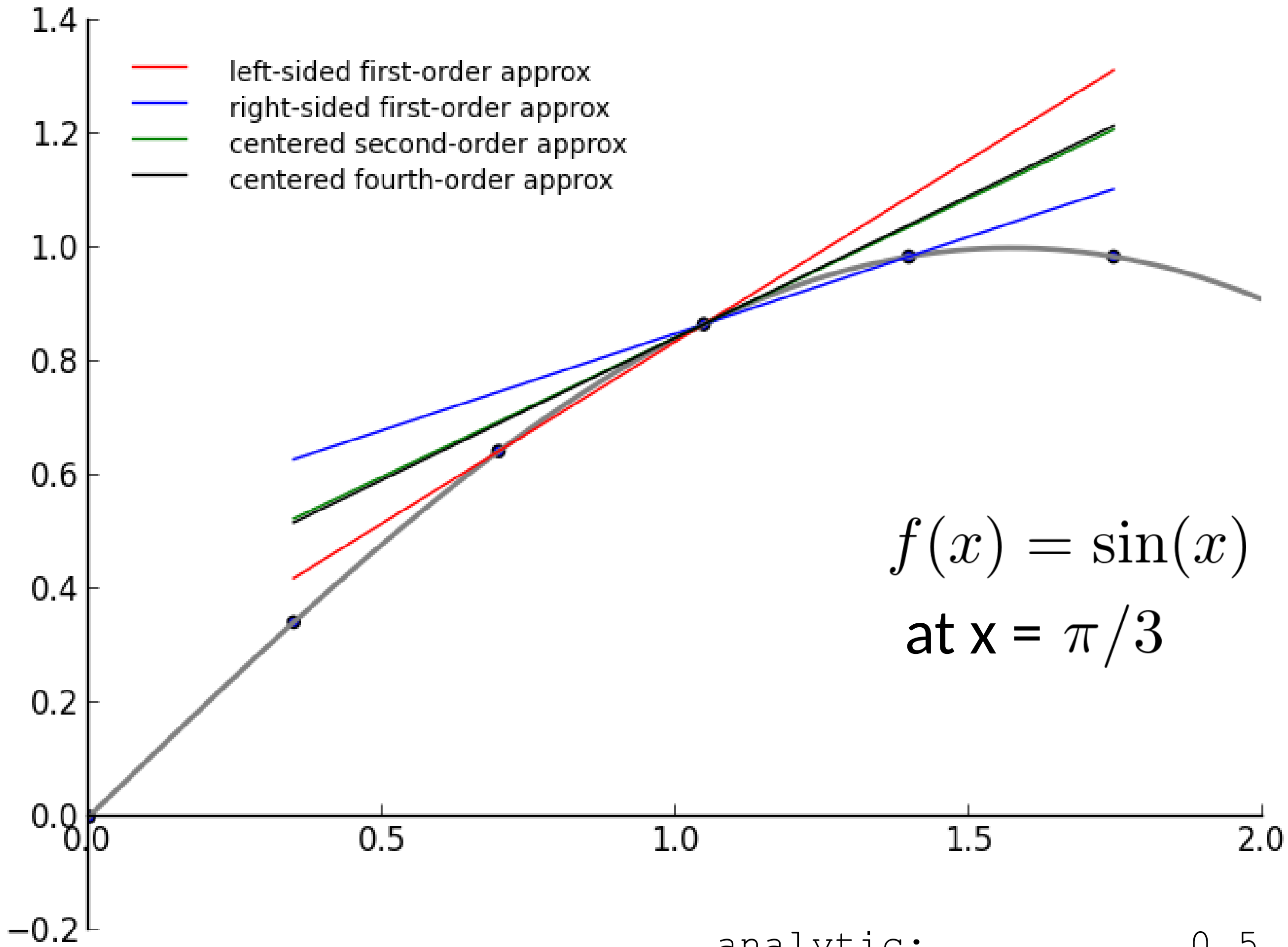
$$\left| f' - \frac{\overline{f}_{i+1} - \overline{f}_i}{\Delta x} \right| \leq \underbrace{\frac{|f''|\Delta x}{2}}_{\text{truncation}} + \underbrace{\frac{2\delta}{\Delta x}}_{\text{roundoff}}$$

This should be near machine ε

As $\Delta x \rightarrow$ ε, the roundoff term becomes O(1)

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

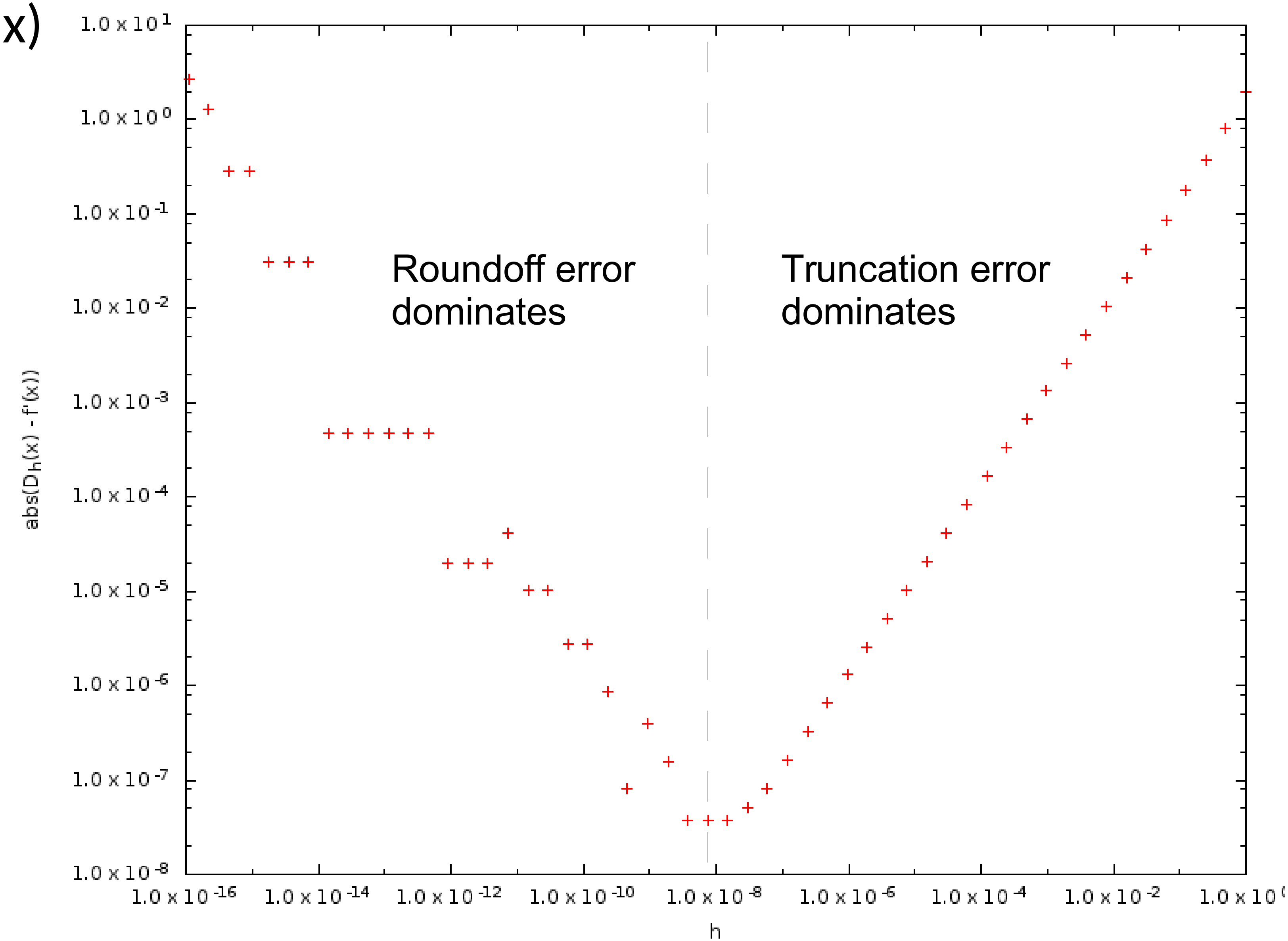
First Derivative Comparison




```
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
```

Round-off vs. Truncation Error

- exp(x)



Differentiation / Integration

First Derivative / Order of Accuracy

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

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2-point stencil

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5-point stencil

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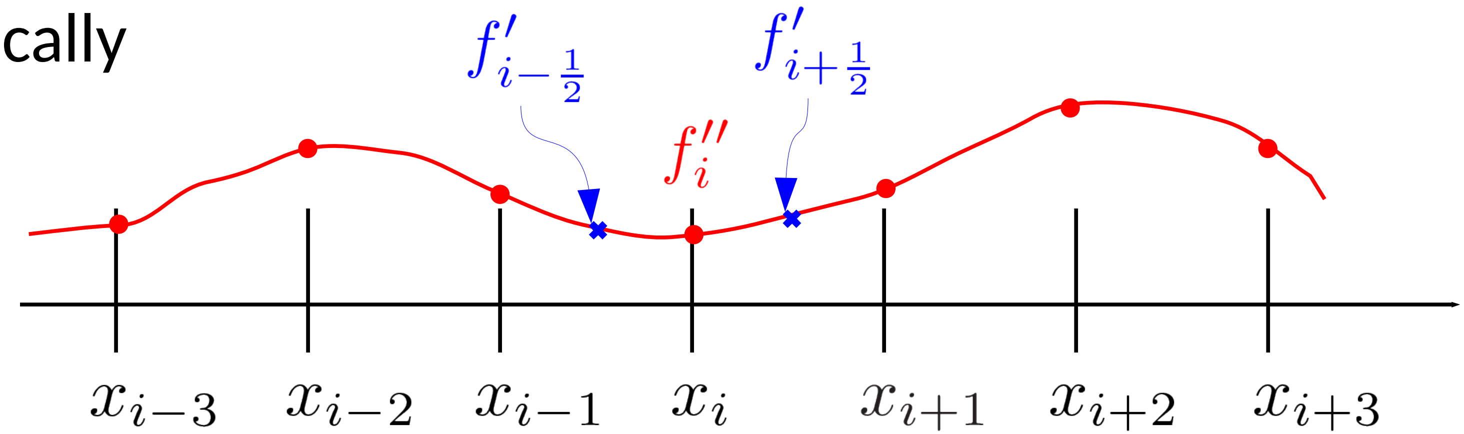
Higher-Derivatives

- 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

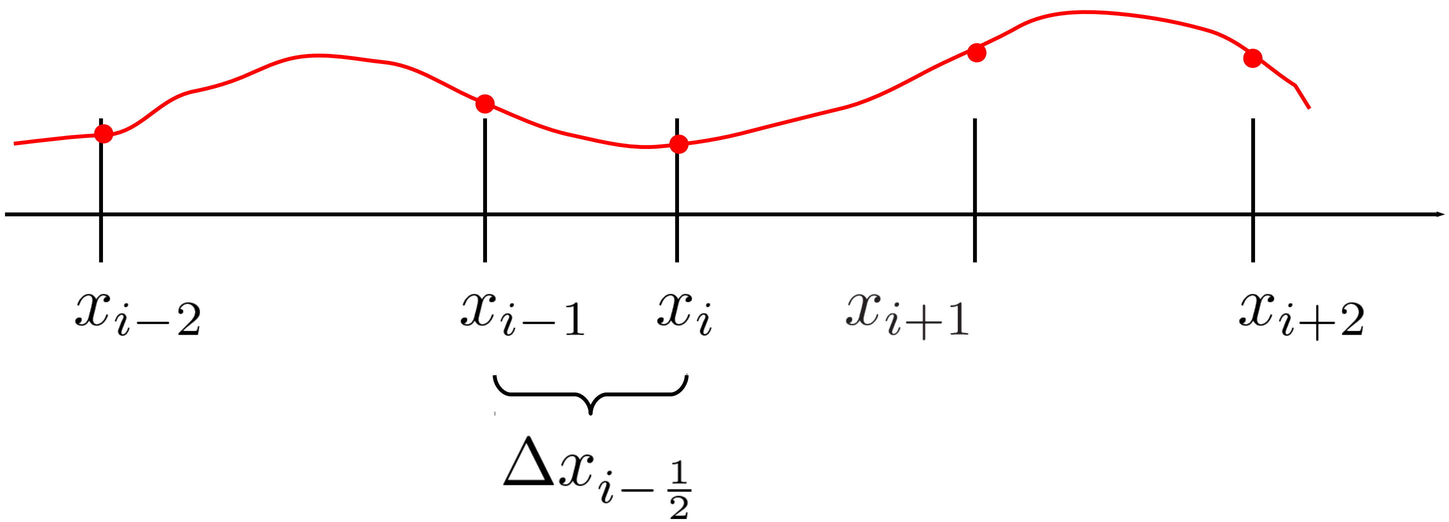
$$= \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2}$$

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)



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

(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
  - $f(x \pm h) = f(x) \pm hf' + \frac{1}{2}h^2 f'' \pm \frac{1}{3!}h^3 f''' + \frac{1}{4!}h^4 f^{(4)} \pm \frac{1}{5!}h^5 f^{(5)} + \ldots$
  - 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

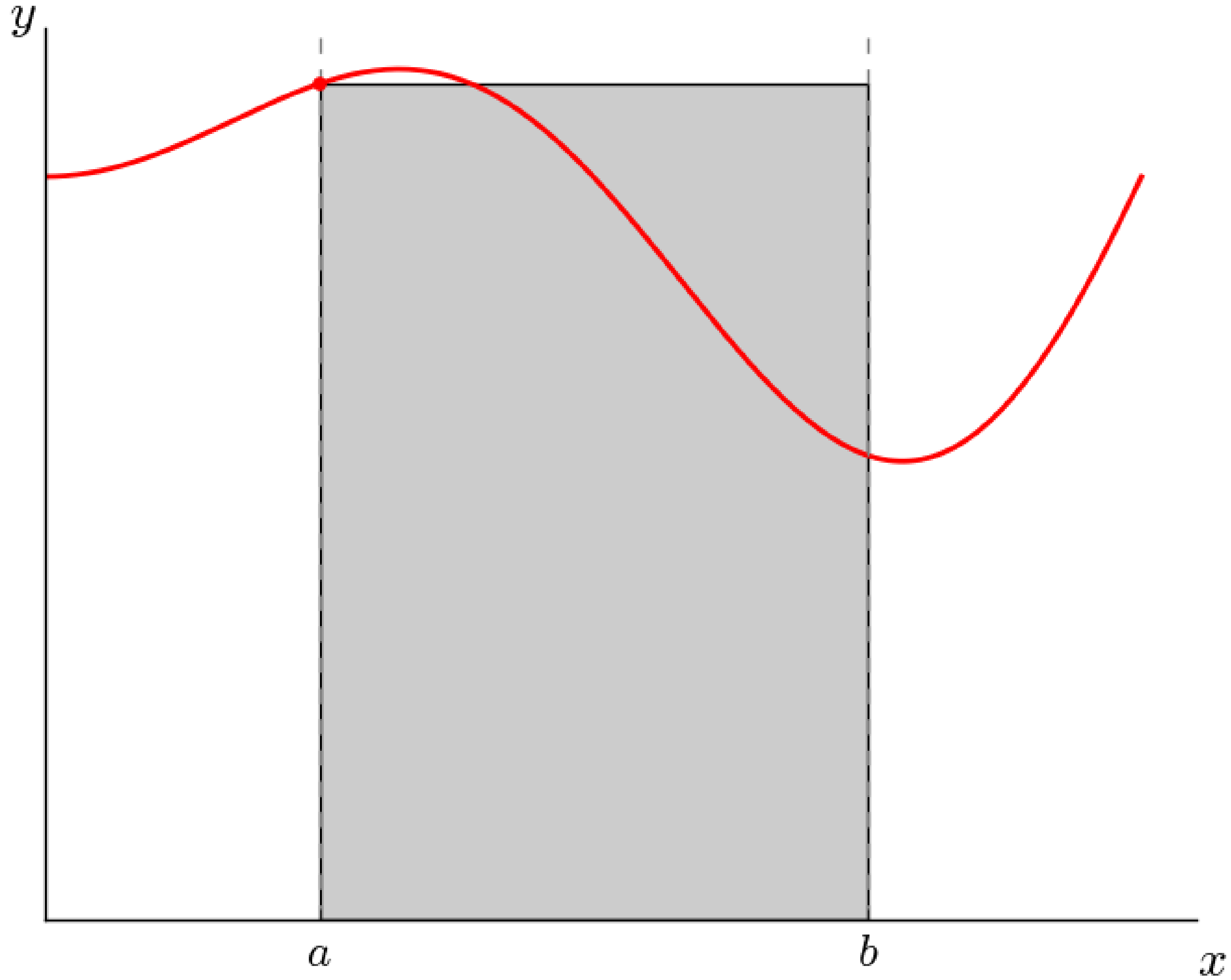
- We want to solve:

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

- 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

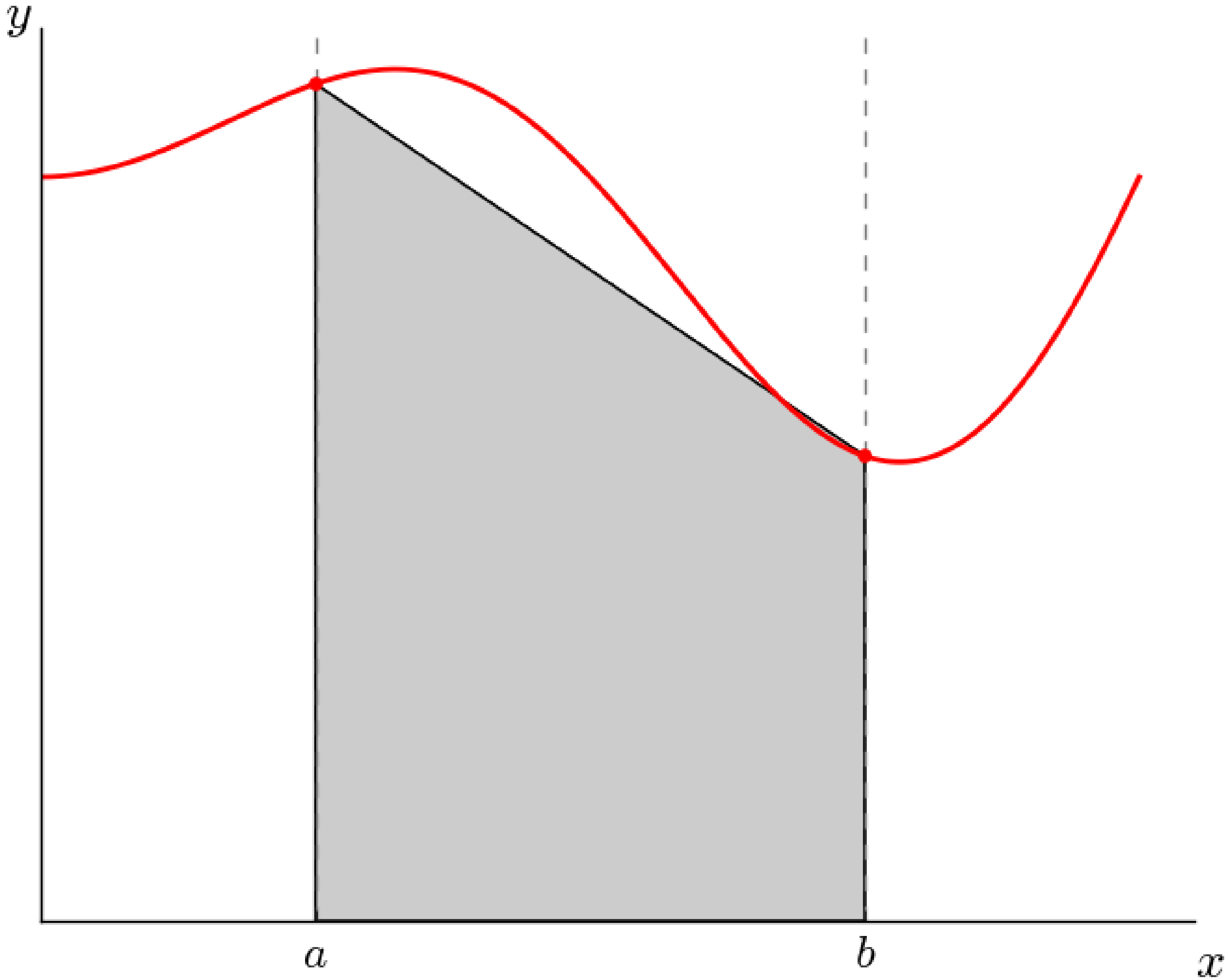
- Simplest case: piecewise constant interpolant (rectangle rule)



$$I \approx (b - a) f(a)$$

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)

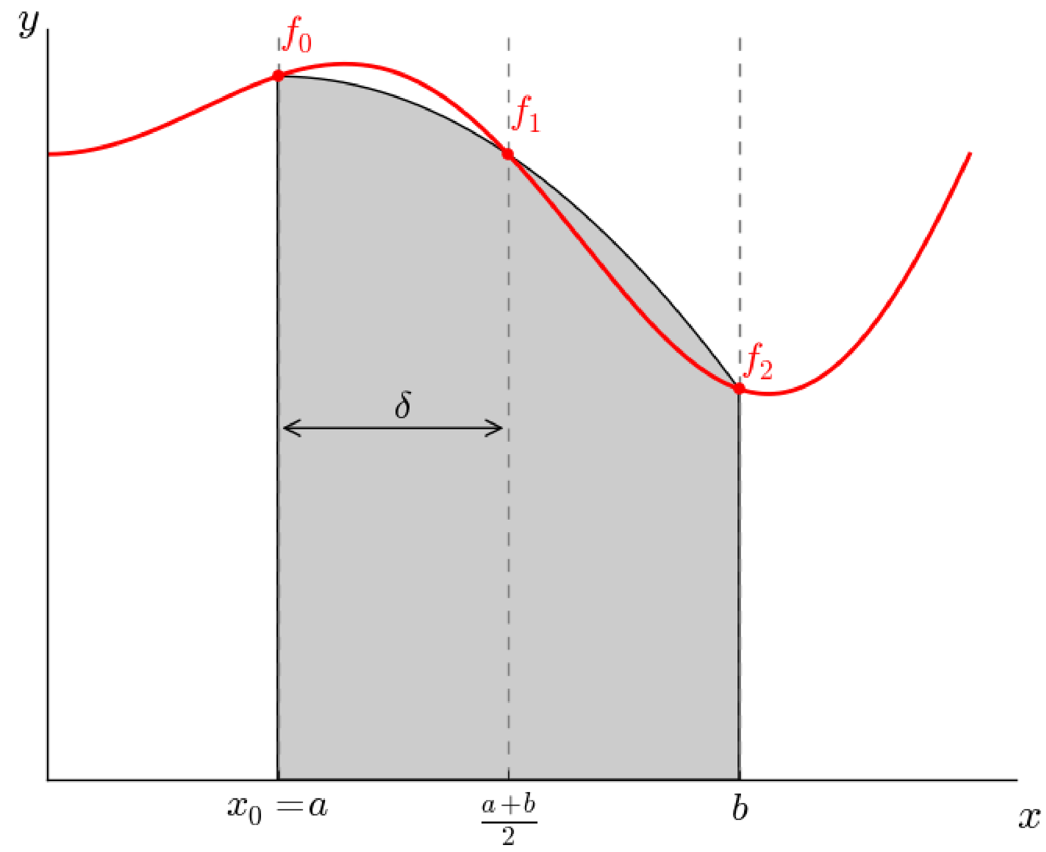
Simpson's Rule

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

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

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

$$C = f_0$$



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

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

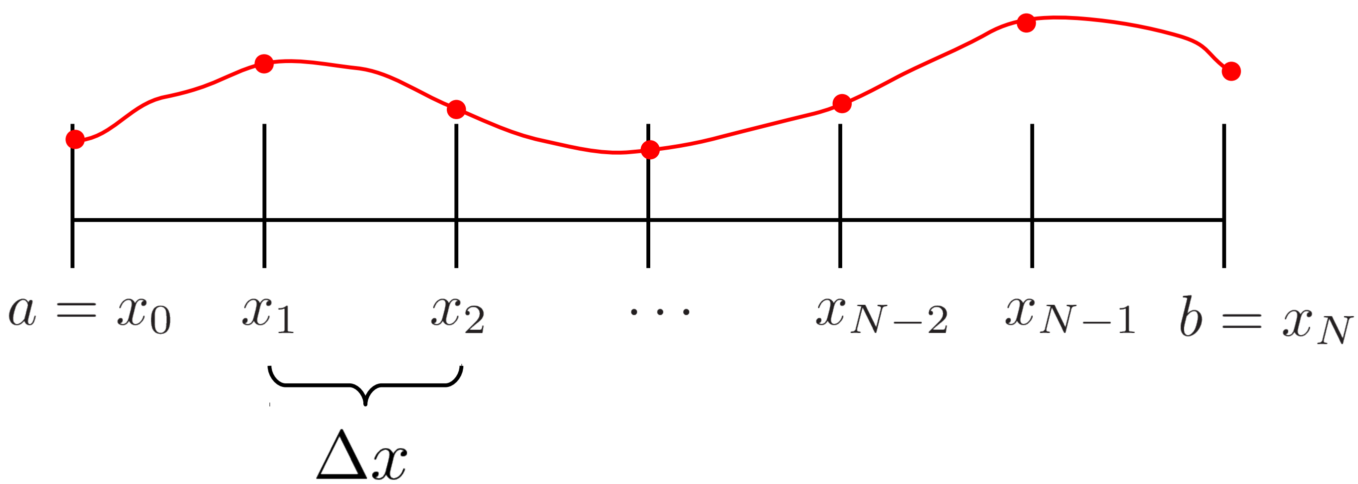
- Forms of these exist where the end-points of the interval are not used—these are open integration rules
  - Usually not very desirable
  - See, for example, Numerical Recipes

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

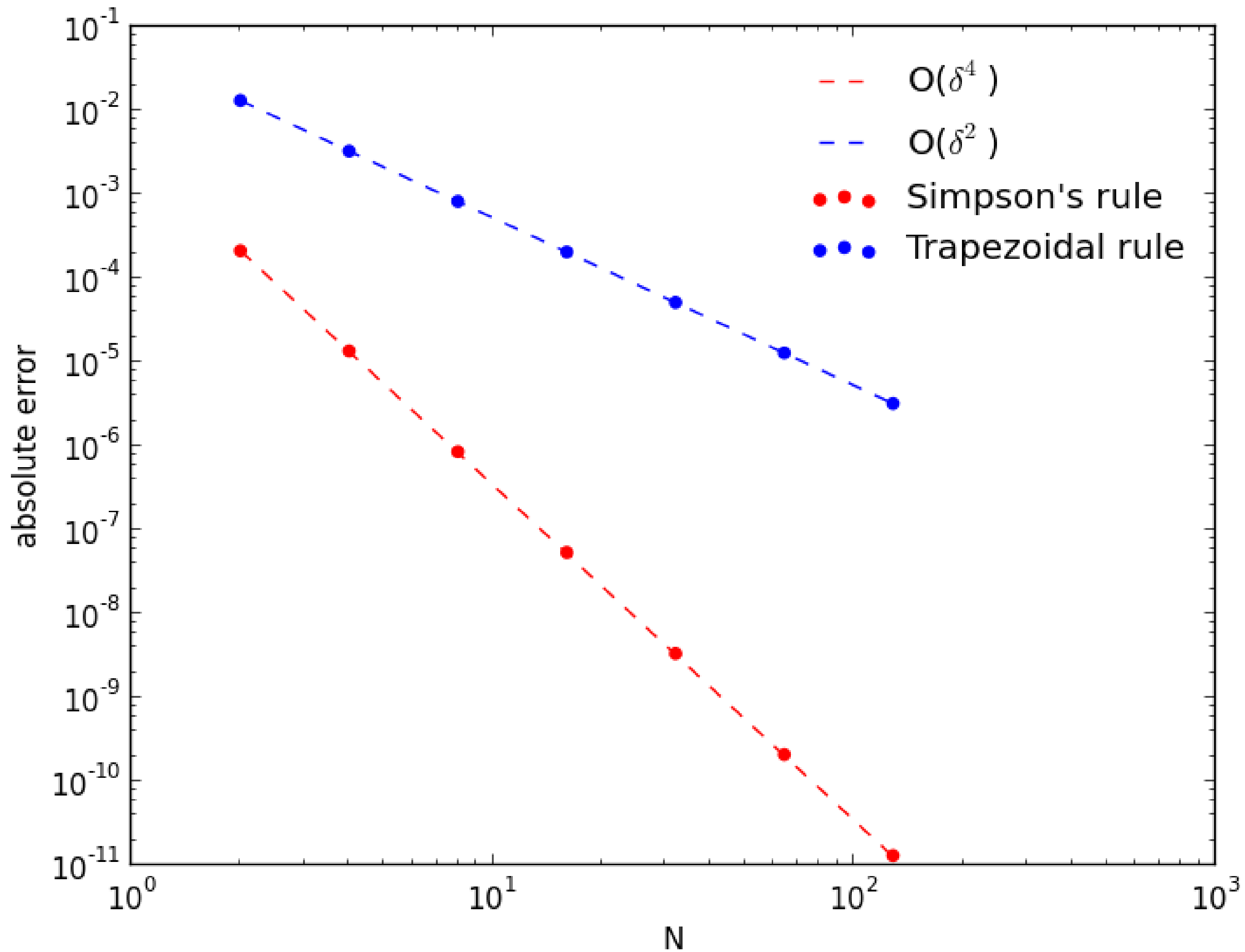
$$\int_a^b f(x)dx = \frac{\Delta x}{2} \sum_{i=0}^{N-1} (f_i + f_{i+1}) + \mathcal{O}(\Delta x^2)$$

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

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

Notice that the order of accuracy here appears different than the case when we just had a single interval. This is because the error in each subinterval adds, and there are N = (b-a)/Δx intervals, so we lose an order.

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)

Infinity?

- Integration over the whole (or half) number line to infinity requires a change of variables.
  - Consider:

$$I = \int_0^\infty f(x)dx$$

  - Make a change of variables:

$$z \equiv \frac{x}{1+x} \quad \Longleftrightarrow \quad x = \frac{z}{1-z}$$

$$dx = \frac{dz}{(1-z)^2}$$

  - Our integral becomes

$$I = \int_0^1 f\left(\frac{z}{1-z}\right)\frac{dz}{(1-z)^2}$$

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

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

  - $k = 0, \ldots, N\text{-}1$ and $\rho(x)$ is a specified weight function.
  - Choose $x_1, x_2, \ldots x_N$ 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, $\rho(x)$, 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.

Integration Summary

(based on Neumann 5.7, Garcia Ch. 10)

- When you are free to pick the evaluation points:
  - Trapezoid rule is pretty robust
    - Works even for functions that may be noisy or rapidly change or have singularities (these can cause problems for other methods)
    - Can be done adaptively to get error estimate
  - Simpson's rule is more accurate than trapezoid
    - Can have troubles with singularities
  - Gaussian quadrature
    - Highly accurate with few points
    - No error estimation or ability to do iteration
    - Need to first compute integration points

Multi-dimensional Integration

- For multi-dimensional integration, Monte Carlo methods may be faster (less function evaluations)
  - We'll look at this later in the semester