# PHY604 Lecture 4

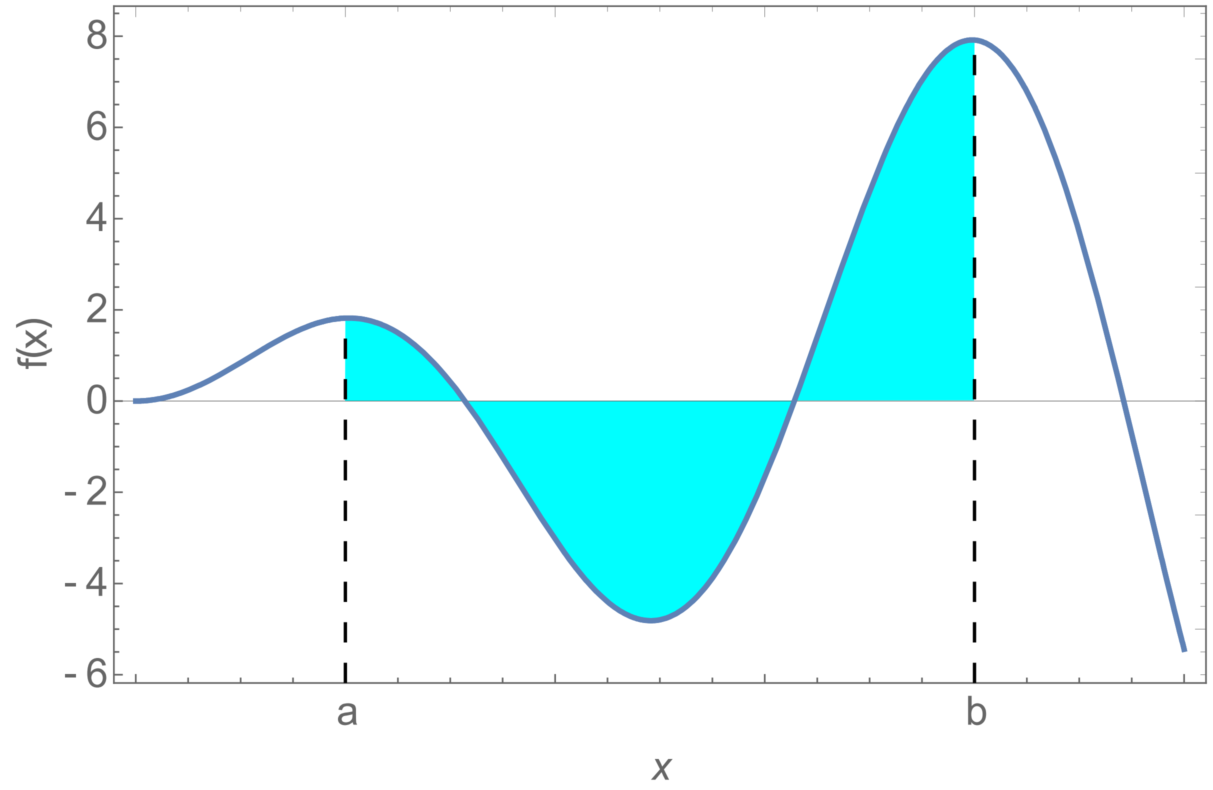
September 4, 2025

# Today’s lecture:

- Numerical integration

# Numerical integration

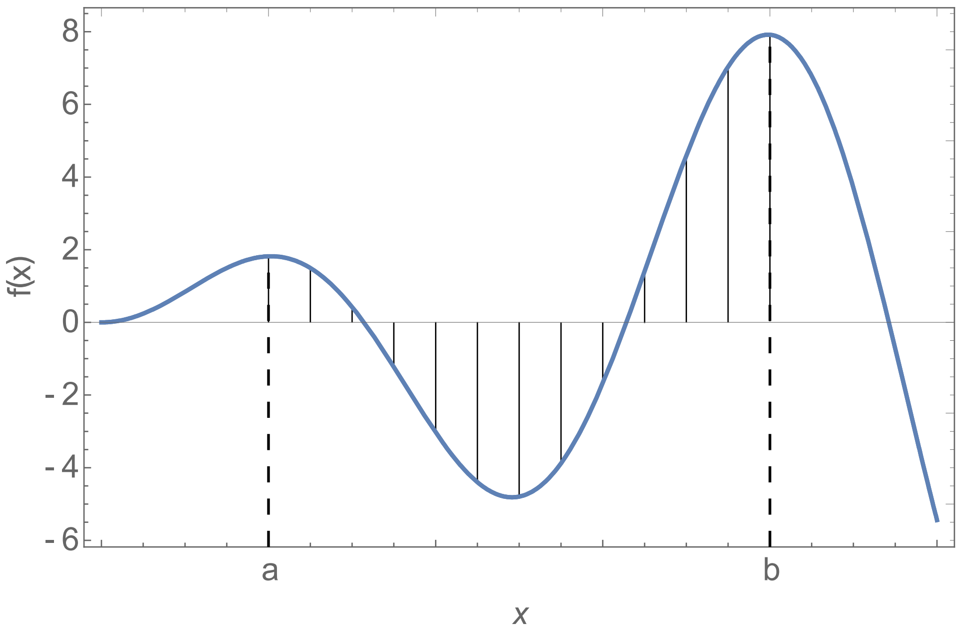
$$\int_a^b f(x)dx$$



# Strategy for numerical integration:

- Quadrature rule: method that represents the integral as a (weighted) sum at a discrete number of points
  - Newton-Cotes quadrature: Fixed spacing between points
- 1. Discretize: Break up the interval into sub-intervals
- 2. Approximate the area under the curve in a subinterval by a simple polygon (rectangle, trapezoid) or a simple function (polynomial)
- 3. Sum the areas of the subintervals
- 4. Converge the integral by making more and more subintervals or using a more sophisticated weighting method

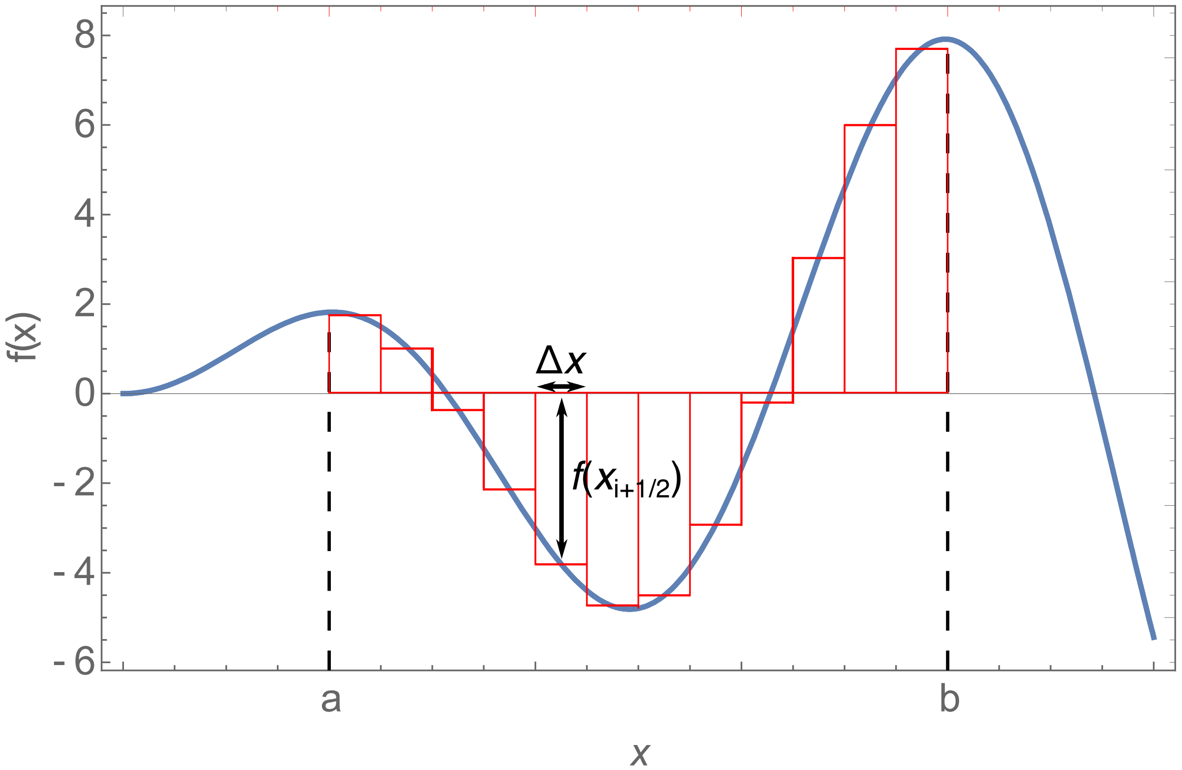
$$\int_a^b f(x)dx = \lim_{N\to\infty} \sum_{i=0}^{N-1} A_i$$



# Approach 1: Midpoint rule

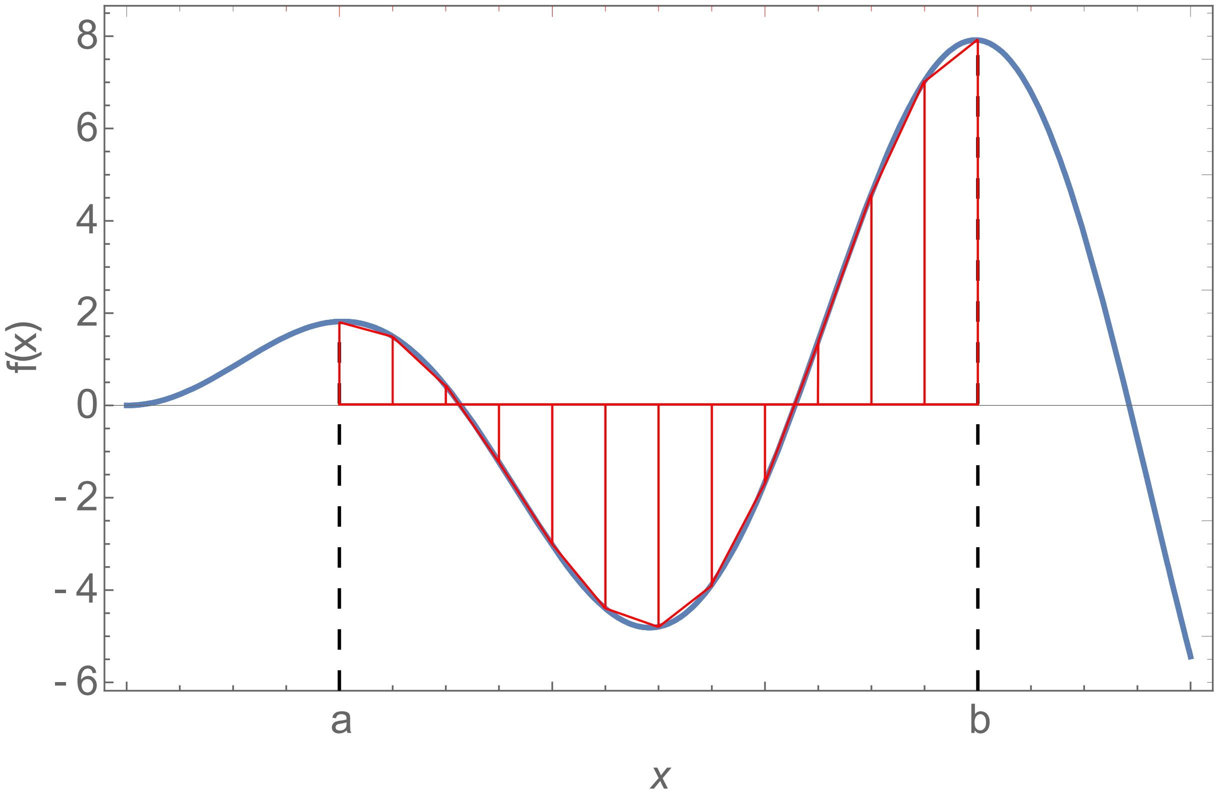
- Approximate area as rectangle with height equal to the midpoint of the subinterval $f(x_{i+1/2})$ and width $\Delta x$:

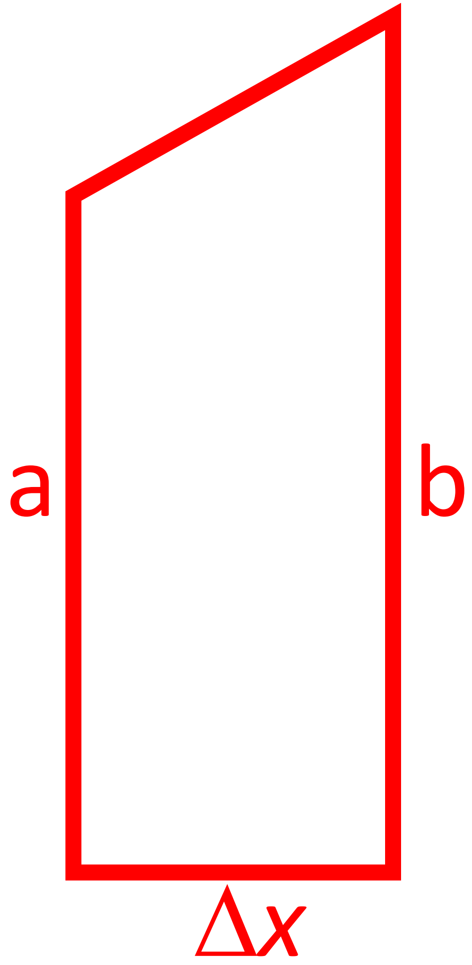
$$\int_a^b f(x)dx \simeq \lim_{N\to\infty} \sum_{i=0}^{N-1} \Delta x f(x_{i+\frac{1}{2}})$$



# Approach 2: Trapezoid rule

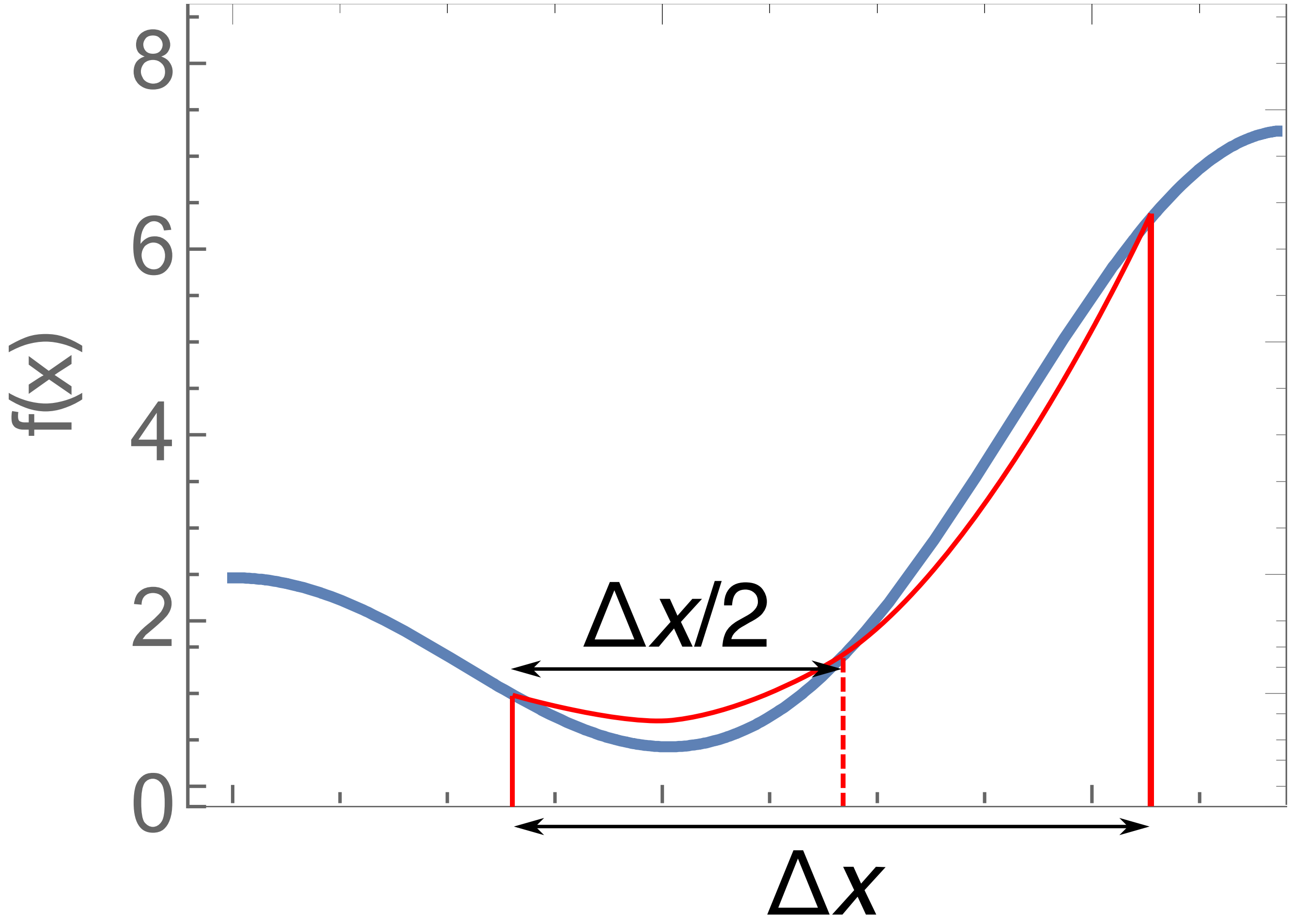
- Area of subintervals approximated as a trapezoid with subinterval endpoints on the curve
- Area of trapezoid: $\Delta x(a+b)/2$



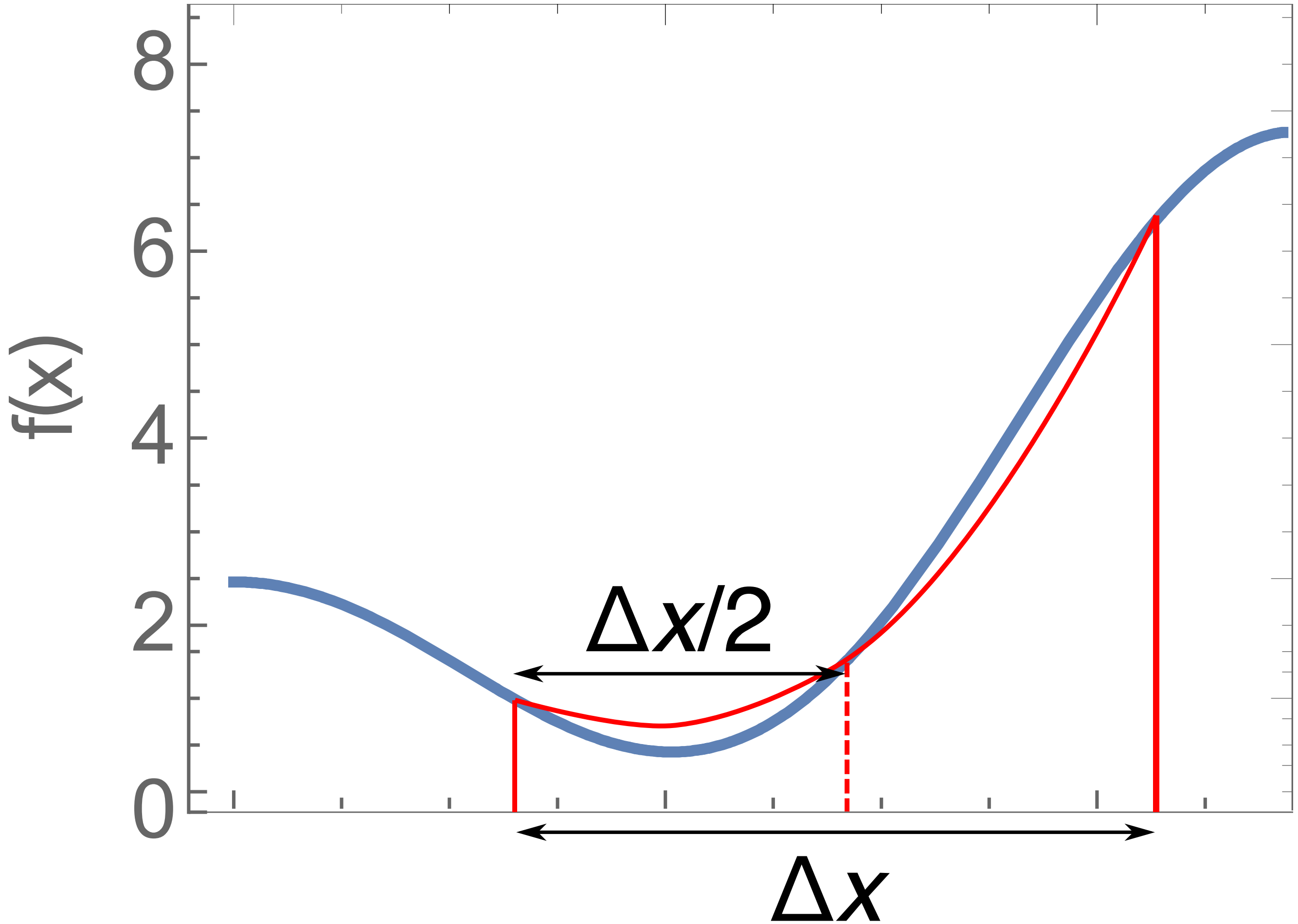
# A more accurate technique: Simpson's Rule

- Approximate area of each subinterval by area under a parabola passing through points $f(x_i)$, $f(x_{i+1/2})$,$f(x_{i+1})$



# A more accurate technique: Simpson's Rule

$$\int_a^b f(x)dx \simeq \lim_{N\to\infty} \sum_{i=0}^{N-1} \Delta x \frac{f(x_i) + 4f(x_{i+\frac{1}{2}}) + f(x_{i+1})}{6}$$



# Where does Simpson's rule come from?

- Consider the parabolic curve:

$$g(x) = Ax^2 + Bx + C$$

- We require it passes through the endpoints and midpoint of our function *f*(*x*):

$$g(x_i) = Ax_i^2 + Bx_i + C = f(x_i)$$

$$g(x_{i+\frac{1}{2}}) = Ax_{i+\frac{1}{2}}^2 + Bx_{i+\frac{1}{2}} + C = f(x_{i+\frac{1}{2}})$$

$$g(x_{i+1}) = Ax_{i+1}^2 + Bx_{i+1} + C = f(x_{i+1})$$

- Solve for *A*,*B*,*C*

$$g(x) = f(x_i)\frac{(x - x_{i+\frac{1}{2}})(x - x_{i+1})}{(x_i - x_{i+\frac{1}{2}})(x_i - x_{i+1})} + f(x_{i+\frac{1}{2}})\frac{(x - x_i)(x - x_{i+1})}{(x_{i+\frac{1}{2}} - x_i)(x_{i+\frac{1}{2}} - x_{i+1})} + f(x_{i+1})\frac{(x - x_i)(x - x_{i+\frac{1}{2}})}{(x_{i+1} - x_i)(x_{i+1} - x_{i+\frac{1}{2}})}$$

# Where does Simpson's rule come from?

$$g(x) = f(x_i)\frac{(x - x_{i+\frac{1}{2}})(x - x_{i+1})}{(x_i - x_{i+\frac{1}{2}})(x_i - x_{i+1})} + f(x_{i+\frac{1}{2}})\frac{(x - x_i)(x - x_{i+1})}{(x_{i+\frac{1}{2}} - x_i)(x_{i+\frac{1}{2}} - x_{i+1})} + f(x_{i+1})\frac{(x - x_i)(x - x_{i+\frac{1}{2}})}{(x_{i+1} - x_i)(x_{i+1} - x_{i+\frac{1}{2}})}$$

- Now we integrate over the subinterval:

$$\int_{x_i}^{x_{i+1}} g(x)dx = \frac{x_i - x_{i+1}}{6}\left[f(x_i) + 4f(x_{i+\frac{1}{2}}) + f(x_{i+1})\right]$$

# Errors in NC quadrature integration

- Error can be reduced by increasing the order of the polynomial or increasing the number of subintervals
- We can estimate errors in a similar way as we did for numerical differentiation (Taylor expand around points and take integrals), see, e.g., Newman Section 5.2.
  - For example, for the trapezoid rule:

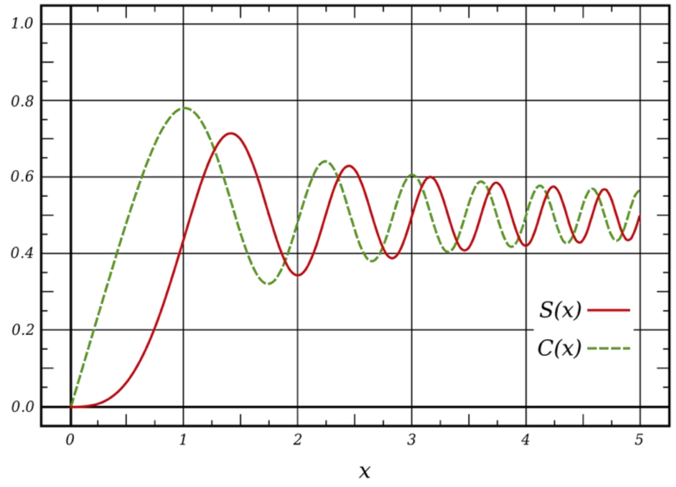
$$\epsilon = \frac{1}{12}\Delta x^2[f'(a) - f'(b)]$$

  - First term in Euler-Maclaurin formula
  - Simpson's rule is $O(\Delta x^4)$
  - If we know the derivatives at the endpoints, we can calculate the error

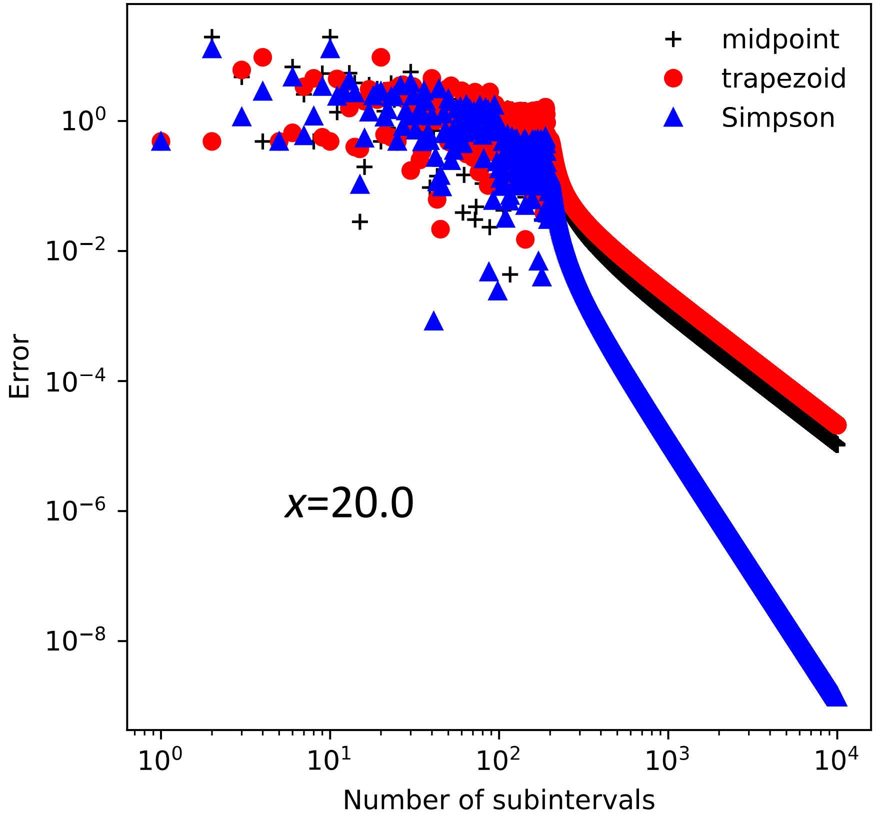
# Example: Evaluating the Fresnel integral

- Fresnel functions are used in optics to describe near-field diffraction
- They can be written as an integral (or infinite sum):

$$S(x) = \int_0^x \sin(\pi t^2/2)dt$$



(Wikipedia)

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# Adaptive integration

- If we do not know $f'(x)$, we can still estimate the error:
  - 1. Perform the integration with $N_1$ and $N_2=2*N_1$ subintervals
  - 2. For, e.g., the trapezoid rule, the error using $N_1$ will be four times that using $N_2$
  - 3. The "exact" result, $I$ is: $I = I_1 + c\Delta x_1^2 = I_2 + c\Delta x_2^2$
  - 4. Then the error on the second estimate is:

$$\epsilon_2 = c\Delta x_2^2 = \frac{1}{3}(I_2 - I_1)$$

- We can use this approach to decide when our integral is converged to our satisfaction
  - Keep doubling the number of subintervals until the error is small enough
  - Can use the results from previous function evaluations (See Newman Sec. 5.3 and 5.4 or Garcia Sec. 10.2)

# Romberg Integration

- If *i* indicates a step in the procedure on the previous slide (i.e., doubling the number of subintervals), then we can write the integral as:

$$I = I_i + \frac{1}{3}(I_i - I_{i-1}) + \mathcal{O}(\Delta x^4)$$

- Equivalent to Simpson's rule!
- For every additional step (doubling of subintervals), we can build more and more accurate estimates
- See Newman Sec. 5.4 or Garcia Sec. 10.2 for more details

# Dealing with infinity as a limit (Newman Sec. 5.8)

- Say we need to integrate over half of the number line:

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

- It is impractical to simply increase the upper bound until convergence
- Instead, make a change of variables:

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

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

- So the integral is:

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

# Beyond Newton-Cotes: Gaussian Quadrature

- As an extra degree of freedom, lets vary the space between integration points
- We must first determine integration rules for unequal spacing
  - How do we determine weights?

$$\int_a^b f(x)dx \simeq w_1 f(x_1) + ... + w_N f(x_N)$$

- Then, we choose a particular optimal choice of nonuniform points
- Many types of Gaussian quadrature

# Theorem behind Gaussian integration

- Lt $q(x)$ be a polynomial of degree $N$ such that:

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

  - $k=0,\ldots,N-1$ and $\rho(x)$ is a specified weight function
  - Choose $x_1, x_2,\ldots,x_N$ as the roots of the polynomial $q(x)$, and use them as grid points:

$$\int_a^b f(x)\rho(x)dx \simeq w_1 f(x_1) + w_2 f(x_2) + \ldots + w_N f(x_N)$$

  - There exists a set of $w$'s where this formula is exact if $f(x)$ is a polynomial of degree **< 2*N* *(!!!)***
  - Note that with $N$ values, we can fit an $N$-1 degree polynomial and derive an integration formula exact for polynomials of order $<N$
    - Very accurate for curves well approximated as high-degree polynomials
  - Many choices of weighting function, $\rho(x)$, leading to different $q$'s and $x$'s and $w$'s

# Example from Garcia Sec. 10.3: Three-point Gauss-Legendre rule

- Three-point: Three grid points in the interval [-1,1]
  - $q(x)$ is cubic
- Take as the weight function $\rho(x)=1$ (Gauss-Legendre)
- We can convert an arbitrary interval [$a$,$b$] to [1,-1]:

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

$$dx = \frac{1}{2}(b-a)dz$$

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

# Step 1: Find polynomial *q*(*x*)

$$q(x) = c_0 + c_1 x + c_2 x^2 + c_3 x^3$$

- Apply the theorem to get three equations for the coefficients:

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

General Solution:

$$c_0 = 0, \quad c_1 = -a, \quad c_2 = 0, \quad c_3 = 5a/3$$

- *a* is an arbitrary constant, if we take it to be 3/2, we get the Legendre polynomial $P_3(x)$:

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

# Step 2: Find the roots

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

- Easily factors to:

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

- So out quadrature becomes:

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

# Step 3: Find the weights

- The theorem tells us that this quadrature is exact for polynomials up to degree 2*N*-1
- Start with *f*(*x*)=1: $$\int_{-1}^{1} dx = 2 = w_1 + w_2 + w_3$$
- Now f(*x*)=*x*: $$\int_{-1}^{1} x dx = 0 = -\sqrt{3/5} w_1 + \sqrt{3/5} w_3$$
- Finally *f*(*x*)=*x*²: $$\int_{-1}^{1} x^2 dx = \frac{2}{3} = \frac{3}{5} w_1 + \frac{3}{5} w_3$$
- Solve to get: $$w_1 = \frac{5}{9}, \;\; w_2 = \frac{8}{9}, \;\; w_3 = \frac{5}{9}$$

# Put it together:
# 3 point Gauss-Legendre quadrature

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

# Example: Error function

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

- Evaluate erf(1):

```
Exact: 0.8427007929497148
3-point Trapezoid: 0.8252629555967492 , Error: -0.017437837352965557
3-point Simpsons: 0.843102830042981 , Error: 0.00040203709326624 98
3-point Gauss-Legendre: 0.8426900184845107 , Error: -1.077446520403313 5e-05
```

# Example: 5th degree polynomial

$$I = \int_0^1 (1 + x^2 + x^3 + x^4 + x^5) dx$$

```
Exact: 2.4499999999999997
3-point Trapezoid: 2.734375 , Error: 0.28437500000000027
3-point Simpsons: 2.4791666666666665 , Error: 0.029166666666666785
3-point Gauss-Legendre: 2.45 , Error: 4.440892098500626e-16
```

# Weights and positions have been tabulated

- From Newman Sec. 5.6:

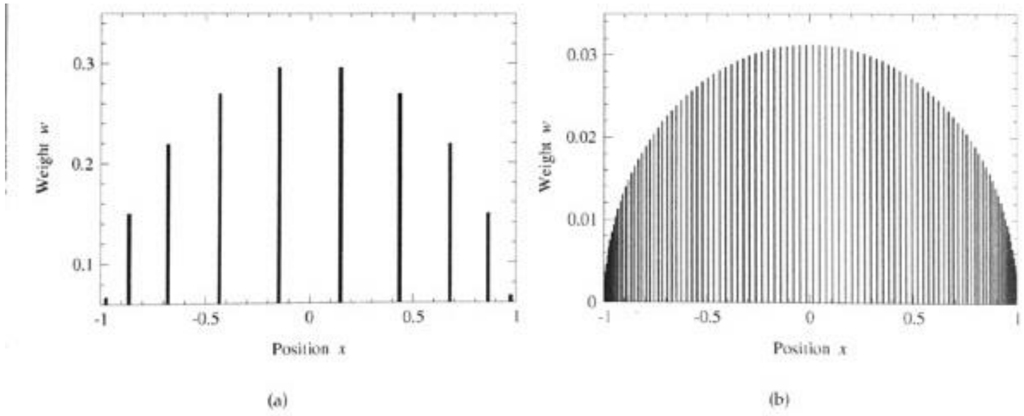


**Figure 5.4: Sample points and weights for Gaussian quadrature.** The positions and heights of the bars represent the sample points and their associated weights for Gaussian quadrature with (a) $N = 10$ and (b) $N = 100$.

- From Garcia 10.3:

Table 10.7: Grid points and weights for Gauss-Legendre integration.

| $\pm x_i$ | $w_i$ | $\pm x_i$ | $w_i$ |
|---|---|---|---|
| $N = 2$ | | $N = 8$ | |
| 0.5773502692 | 1.0000000000 | 0.1834346425 | 0.3626837834 |
| $N = 3$ | | 0.5255324099 | 0.3137066459 |
| 0.0000000000 | 0.8888888889 | 0.7966664774 | 0.2223810345 |
| 0.7745966692 | 0.5555555556 | 0.9602898565 | 0.1012285363 |
| $N = 4$ | | $N = 12$ | |
| 0.3399810436 | 0.6521451549 | 0.1252334085 | 0.2491470458 |
| 0.8611363116 | 0.3478548451 | 0.3678314990 | 0.2334925365 |
| $N = 5$ | | 0.5873179543 | 0.2031674267 |
| 0.0000000000 | 0.5688888889 | 0.7699026742 | 0.1600783285 |
| 0.5384693101 | 0.4786286705 | 0.9041172564 | 0.1069393260 |
| 0.9061798459 | 0.2369268850 | 0.9815606342 | 0.0471753364 |

# Types of Gaussian Quadrature

| Interval | $\omega(x)$ | 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)

- Roots and weights are tabulated, so no need to compute them

# Choosing an integration method (Newman Sec. 5.7)

- Trapezoid method:
  - Trivial to program
  - Equally spaced points, often true of experimental data
  - Good choice for poorly behaved data (noisy, singularities)
  - Adaptive method gives guaranteed accuracy level
  - Not very accurate for given number of points
- Romberg integration:
  - Equally spaced points, often true of experimental data
  - Guaranteed accuracy level
  - Potentially high accuracy for small number of points
  - Will not work well for noisy of pathological data/integrands
- Gaussian Quadrature
  - Potentially high accuracy for small number of points
  - Simple to program (weights and roots tabulated)
  - Will not work well for noisy of pathological data/integrands
  - Need to have data on specific, unequally-spaced grid

# After class tasks

- If you do not already have one, make an account on github: https://github.com/
- Let me know if you having issues with github classroom!

- Readings:
  - Newman Chapter 5
  - Garcia Section 10.2