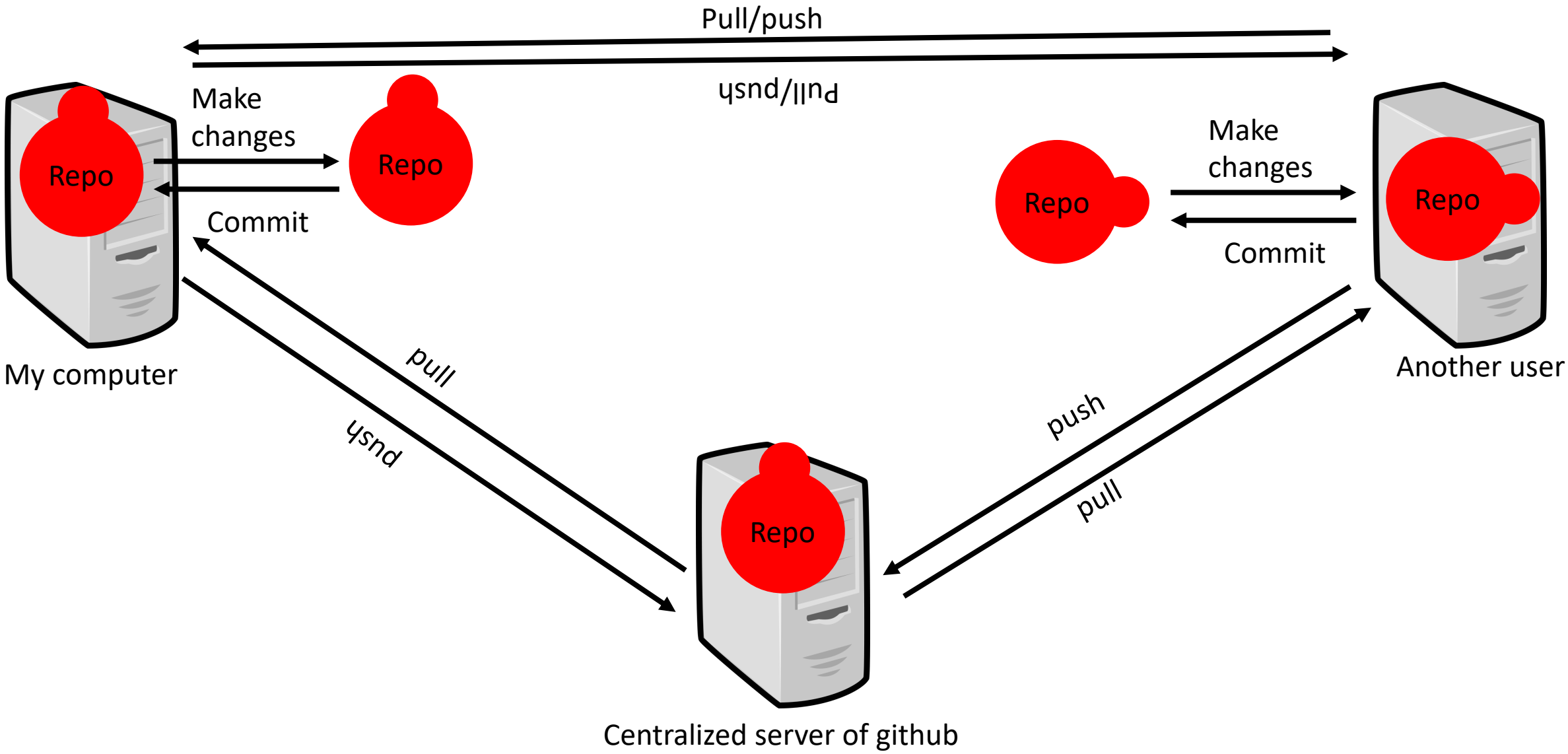
PHY604 Lecture 3

August 31, 2021

Review: Distributed version control with Git



Review: Common Git commands

```
/Users/cdreyer % git --help
usage: git [--version] [--help] [-C <path>] [-c <name>=<value>]
           [--exec-path[=<path>]] [--html-path] [--man-path] [--info-path]
           [-p | --paginate | -P | --no-pager] [--no-replace-objects] [--bare]
           [--git-dir=<path>] [--work-tree=<path>] [--namespace=<name>]
           <command> [<args>]

These are common Git commands used in various situations:

start a working area (see also: git help tutorial)
   clone      Clone a repository into a new directory
   init       Create an empty Git repository or reinitialize an existing one

work on the current change (see also: git help everyday)
   add        Add file contents to the index
   mv         Move or rename a file, a directory, or a symlink
   reset      Reset current HEAD to the specified state
   rm         Remove files from the working tree and from the index

examine the history and state (see also: git help revisions)
   bisect     Use binary search to find the commit that introduced a bug
   grep       Print lines matching a pattern
   log        Show commit logs
   show       Show various types of objects
   status     Show the working tree status

grow, mark and tweak your common history
   branch     List, create, or delete branches
   checkout   Switch branches or restore working tree files
   commit     Record changes to the repository
   diff       Show changes between commits, commit and working tree, etc
   merge      Join two or more development histories together
   rebase     Reapply commits on top of another base tip
   tag        Create, list, delete or verify a tag object signed with GPG

collaborate (see also: git help workflows)
   fetch      Download objects and refs from another repository
   pull       Fetch from and integrate with another repository or a local branch
   push       Update remote refs along with associated objects
```

Review: Unit testing

- Unit testing is the practice in which each smallest, self-contained unit of the code is tested independently of the others

- There are unit testing frameworks out there that help automate the procedure for different codes
  - E.g., **`unittest`** for python

Review: Regression testing

- Simplest requirements:
  - You just need a tool to compare the current output to benchmark
  - You can build up a more complex system from here with simple scripting

- Big codes need a bunch of tests to exercise all possible options for the code
  - If you spend a lot of time hunting down a bug, once you fix it, put a test case in your suite to check that case
  - If someone implements a new functionality, ask them to submit a test
  - You'll never have complete coverage, but your number of tests will grow with time, experience, and code complexity

Today's lecture:

- Finish discussing good programming practices:
    - Misc. good practices
- Numerical differentiation
- Numerical Integration

Comments and Documentation

- Many in computer science will say that “good code documents itself”
  - **Do not believe it.**
  - Remember, we are often writing code for programming novices (both the developers and users)
  - The better people can understand your code, the more productive science will be done with it

- No hard-and-fast rules. Comments should explain the basic idea of what a block of code does
  - Only comment “single lines” if there is something special or unusual about them
  - Keep comments up to date with the code
  - Think about what information will be useful for you in the future, and other developers of your code

- Can often use tools to turn comments in the source into external documentation
  - Robodoc: https://rfsber.home.xs4all.nl/Robo/
  - FORD: http://fortranwiki.org/fortran/show/FORD
  - Pydoc: https://docs.python.org/3/library/pydoc.html
  - Others for python: https://wiki.python.org/moin/DocumentationTools

Debugging tools

- Simplest debugging: print out information at intermediate points in code execution

- Running with appropriate compiler flags (e.g., **`-g`** for gnu compilers) can provide debugging information
  - Can make code run slower, but useful for test purposes

- Interactive debuggers let you step through your code line-by-line, inspect the values of variables as they are set, etc.
  - gdb is the version that works with the GNU compilers. Some graphical frontends exist.
  - Lots of examples online
  - Not very useful for parallel code.

- Particularly difficult errors to find often involve memory management
  - **Valgrind** is an automated tool for finding memory leaks. No source code modifications are necessary.

Building your code with, e.g., Makefiles

- It is good style to separate your subroutines/functions into files, grouped together by purpose
  - Makes a project easier to manage (for you and version control)
  - Reduces compiler memory needs (although, can prevent inlining across files)
  - Reduces compile time—you only need to recompile the code that changed (and anything that might depend on it)
- Makefiles automate the process of building your code
  - No ambiguity of whether your executable is up-to-date with your changes
  - Only recompiles the code that changed (looks at dates)
  - Very flexible: lots of rules allow you to customize how to build, etc.
  - Written to take into account dependencies

We have not really discussed general coding style

- Depends very much on the language, and is often a matter of opinion (google it)
- Some general rules:
  - 1. Use a consistent programming style
  - 2. Use brief but descriptive variable and function names
  - 3. Avoid “magic numbers”
    - Name your constants, specify your flags
  - 4. Use functions and/or subroutines for repetitive tasks
  - 5. Check return values for errors before proceeding
  - 6. Share information effectively (e.g., using modules or namespaces)
  - 7. Limit the scope of your variables, methods, etc.
  - 8. Think carefully about the most effective way to input and output data
  - 9. Be careful about memory, i.e., allocating and deallocating
  - 10. Make your code readable and portable, you will thank yourself (or your collaborators will thank you) later.

Today’s lecture:

- Finish discussing good programming practices:
    - Misc. good practices
- Numerical differentiation
- Numerical Integration

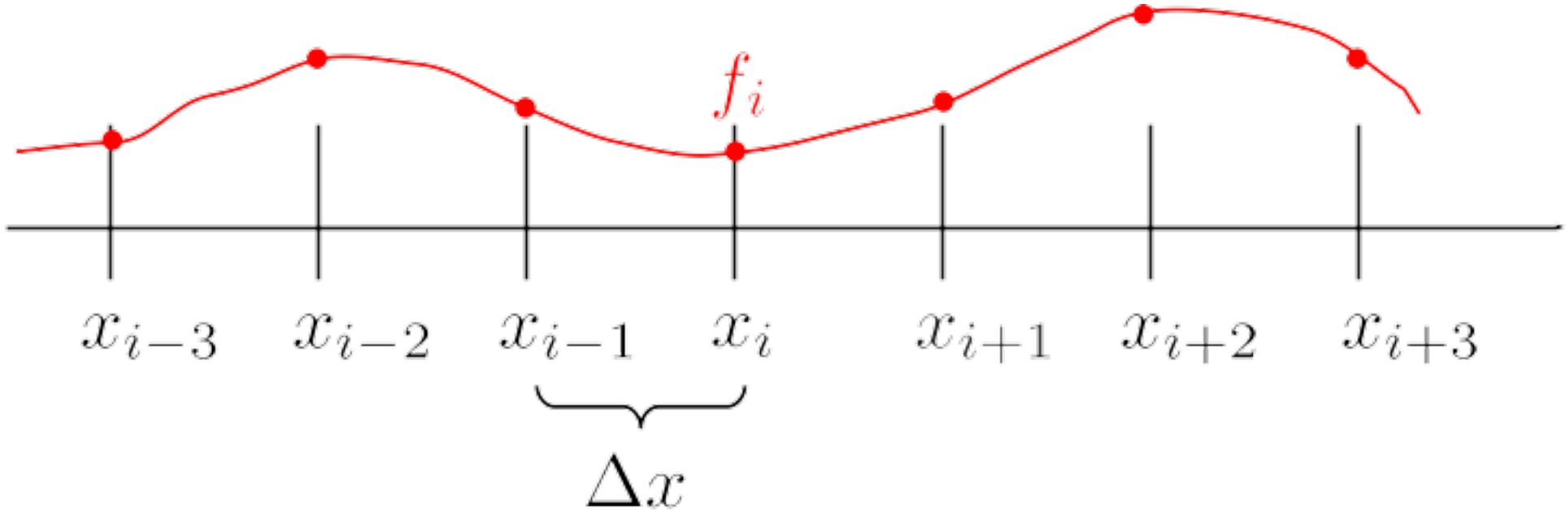
Numerical differentiation, Two situations:

- We have data defined only at a set of (possibly regularly spaced) points
  - Generally speaking, asking for greater accuracy for the derivative involves using more of the discrete points

- We have an analytic expression for f(x) and want to compute the derivative numerically
  - If possible, 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)

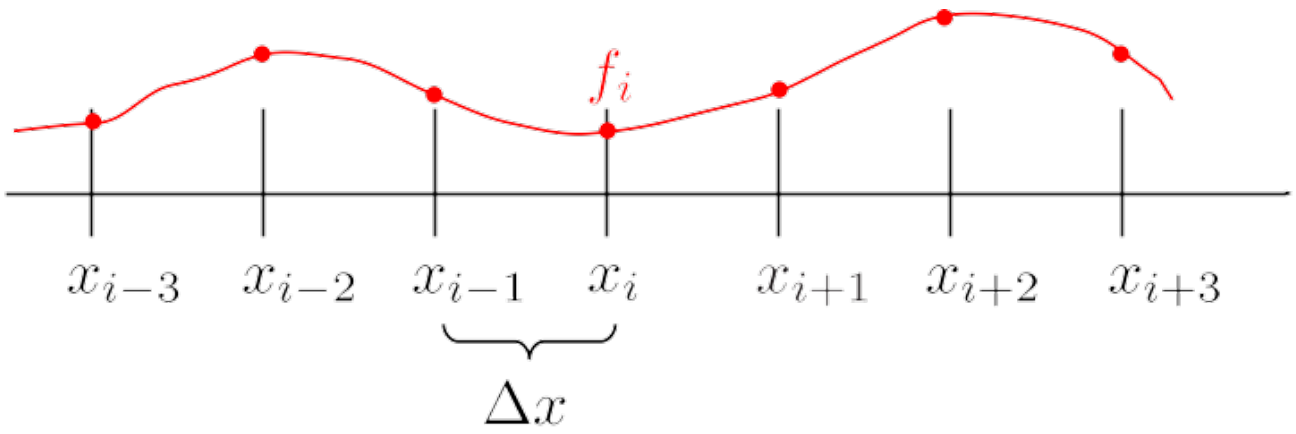
Gridded data

- 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



- Taylor expansion:

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

- Solve for the first derivative:

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

Discrete approx. of *f'*

Leading term in the truncation error

Order of accuracy

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

- The accuracy of the finite difference approximation is determined by size of Δx
- So this finite difference expression is accurate to "order" Δx: $\mathcal{O}(\Delta x)$

- However: Making Δx small means that we are subtracting numbers that are very close to each other, which can result in significant rounding errors

Maximizing the accuracy

- Say we can evaluate the function to accuracy $C\,f(x)$ [also $C\,f(x+\Delta x)$]
  - For double precision: $C \simeq 10^{-16}$
- Worst-case rounding error on derivative is $2C|f(x)|/\,\Delta x$
  - Also need to worry about associative errors: $(x+\Delta x) - x \stackrel{?}{=} \Delta x$
- So total error is: $$\left| \left.\frac{df}{dx}\right|_{x_i} - \frac{f_{i+1}-f_i}{\Delta x} \right| \leq \left.\frac{1}{2}\frac{d^2 f}{dx^2}\right|_{x_i} \Delta x + \frac{2C|f_i|}{\Delta x}$$
- We can minimize to find: $$\Delta x = \sqrt{4C\left|\frac{f_i}{f_i''}\right|} \sim 10^{-8}$$
- So "minimum" error: $$\epsilon = \sqrt{4C\,|f_i f_i''|} \sim 10^{-8}$$

Increasing accuracy with more points in the "stencil"

- First-order "forward" or "backward":

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

2-point stencil

- Second-order "central":

$$f' = \frac{-\frac{1}{2} f_{i-1} + 0 f_i + \frac{1}{2} f_{i+1}}{\Delta x}$$

3-point stencil

Second-order central

- Consider two Taylor expansions:

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

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

- We see that:

$$\left.\frac{df}{dx}\right|_{x_i} = \frac{f_{i+1} - f_{i-1}}{2\Delta x} + \mathcal{O}(\Delta x^2) + ...$$

Error in Second order central

$$\left| \left. \frac{df}{dx} \right|_{x_i} - \frac{f_{i+1} - f_{i-1}}{2\Delta x} \right| \leq \left. \frac{1}{6} \frac{d^3 f}{dx^3} \right|_{x_i} \Delta x^2 + \frac{C|f_i|}{\Delta x}$$

- Minimize WRT Δx: $\Delta x = \sqrt[3]{6C \left| \frac{f(x_i)}{f'''(x_i)} \right|} \sim 10^{-5}$

Assuming double prec.

- Minimum error: $\epsilon \propto \sqrt[3]{C^2 f(x_i)^2 |f'''(x_i)|} \sim 10^{-11}$

Assuming double prec.

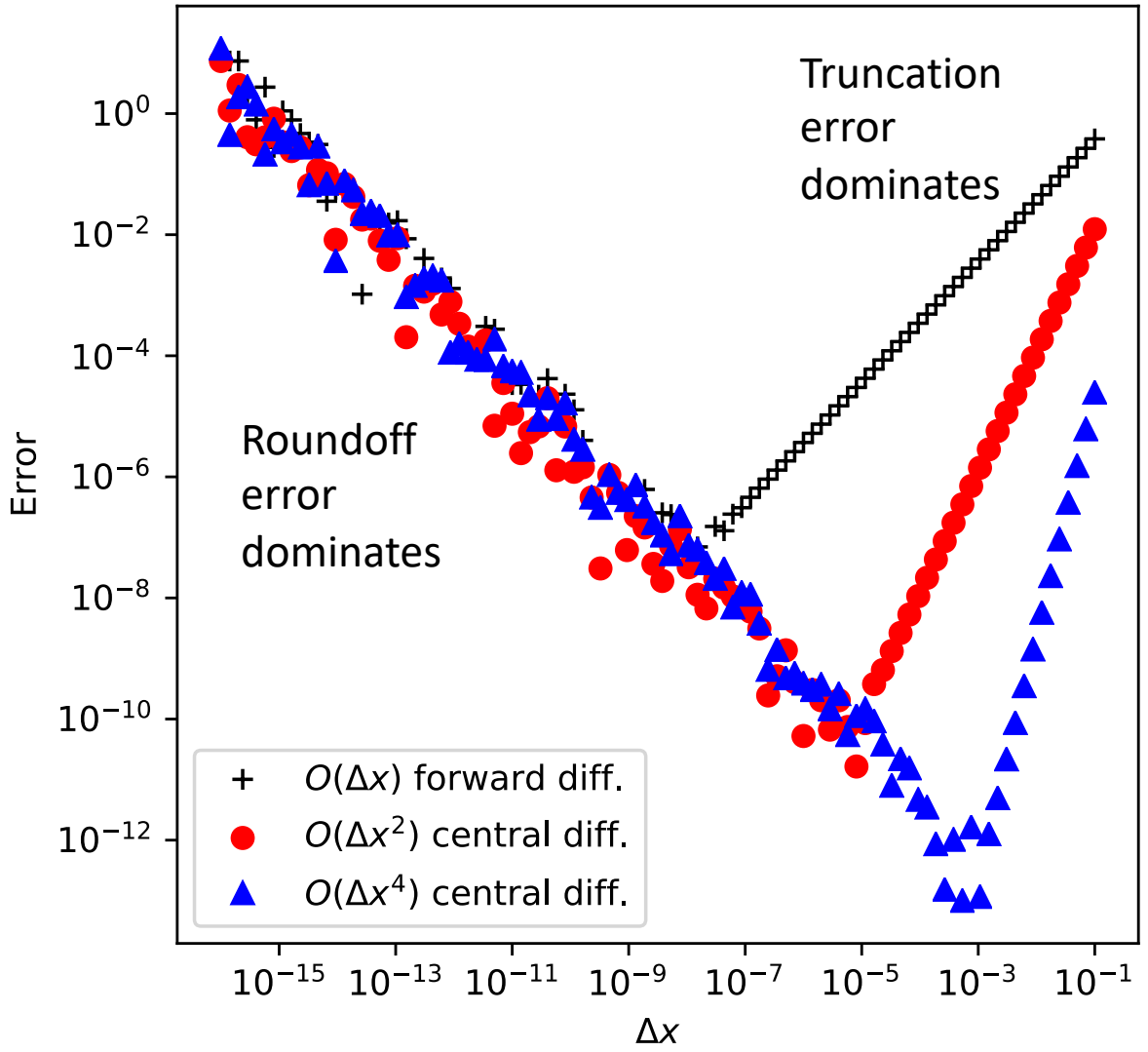
Higher order first derivatives

- To get accuracy to order *n* [i.e., $\mathcal{O}(\Delta x^n)$] follow a similar strategy:
  - 1. Write down Taylor expansion for *n+1* finite difference points up to order *n*+1
  - 2. Solve set of polynomial equation in Δx for *f'*
  - 3. Obtain an expression involving weighted sum of function evaluated at *n+1* points (some weights may be zero)
- Note: may be central, forward, or backward
- For example, for central:

Derivative	Accuracy	–5	–4	–3	–2	–1	0	1	2	3	4	5
1	2					–1/2	0	1/2				
	4				1/12	–2/3	0	2/3	–1/12			
	6			–1/60	3/20	–3/4	0	3/4	–3/20	1/60		
	8		1/280	–4/105	1/5	–4/5	0	4/5	–1/5	4/105	–1/280	

https://en.wikipedia.org/wiki/Finite_difference_coefficient

Example: Derivative of exp(x)



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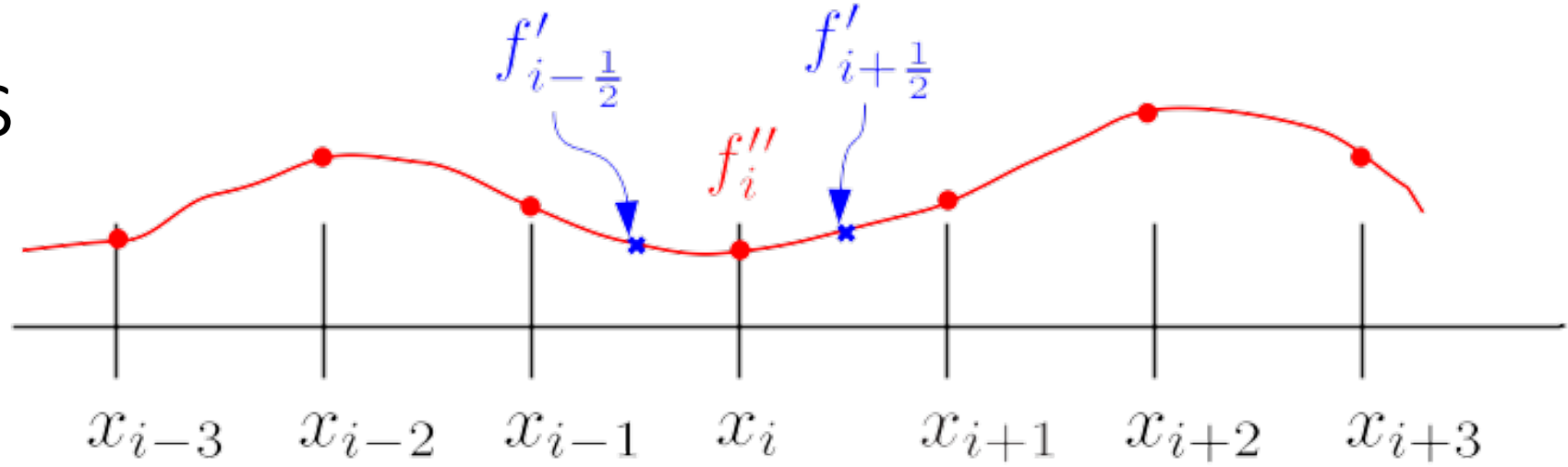
Higher derivatives



- Write second derivative as: $$f''_i = \frac{f'_{i+1/2} - f'_{i-1/2}}{\Delta x}$$
- Insert central difference first derivatives, e.g.: $f'_i = \frac{f_{i+1} - f_i}{\Delta x}$
- So we get: $$f''_i = \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2}$$

Higher derivatives and error

- We can also use the Taylor expansion strategy:

$$f_{i+1} = f_i + \Delta x f_i' + \frac{1}{2}\Delta x^2 f_i'' + \frac{1}{6}\Delta x^3 f_i''' + \frac{1}{24}\Delta x^4 f_i'''' + \ldots$$

$$f_{i-1} = f_i - \Delta x f_i' + \frac{1}{2}\Delta x^2 f_i'' - \frac{1}{6}\Delta x^3 f_i''' + \frac{1}{24}\Delta x^4 f_i'''' + \ldots$$

- Add together and rearrange: $f_i'' = \dfrac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} - \dfrac{1}{12}\Delta x^2 f_i''''$

- Error: $\epsilon = \sqrt{\dfrac{4}{3} C |f_i f_i''''|} \sim 10^{-8}$

Assuming double prec.

Partial and mixed derivatives

- Partial derivatives are a simple generalization
- E.g., central differences for function of two variables *f*(*x*,*y*)

$$\frac{\partial f}{\partial x} = \frac{f(x+\Delta x, y) - f(x-\Delta x, y)}{2\Delta x} \qquad \frac{\partial f}{\partial y} = \frac{f(x, y+\Delta y) - f(x, y-\Delta y)}{2\Delta y}$$

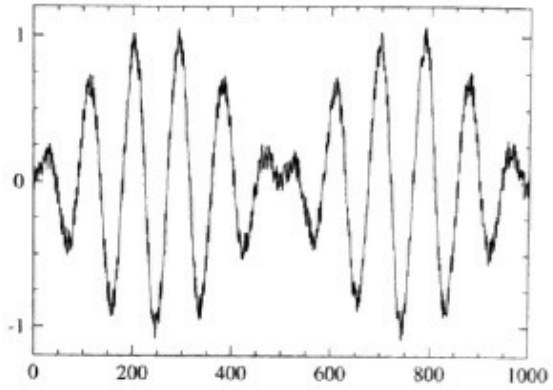
- Mixed second derivative:

$$\frac{\partial^2 f}{\partial y \partial x} = \frac{f(x+\Delta x, y+\Delta y) - f(x-\Delta x, y+\Delta y) - f(x+\Delta x, y-\Delta y) + f(x-\Delta x, y-\Delta y)}{4\Delta x \Delta y}$$

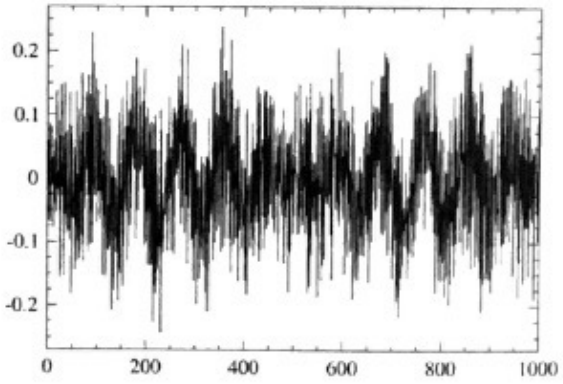
Some final comments on numerical integration

- Taking derivatives of noisy data makes the noise much worse!
  - Fit to a smooth curve and take the derivative of that
  - Smooth the data, e.g., with a Fourier transform
- We can treat data on uneven grids with the same strategy as before, taking into account the different Δx's between points

Noisy data



Derivative



(Newman)

Today’s lecture:

- Finish discussing good programming practices:
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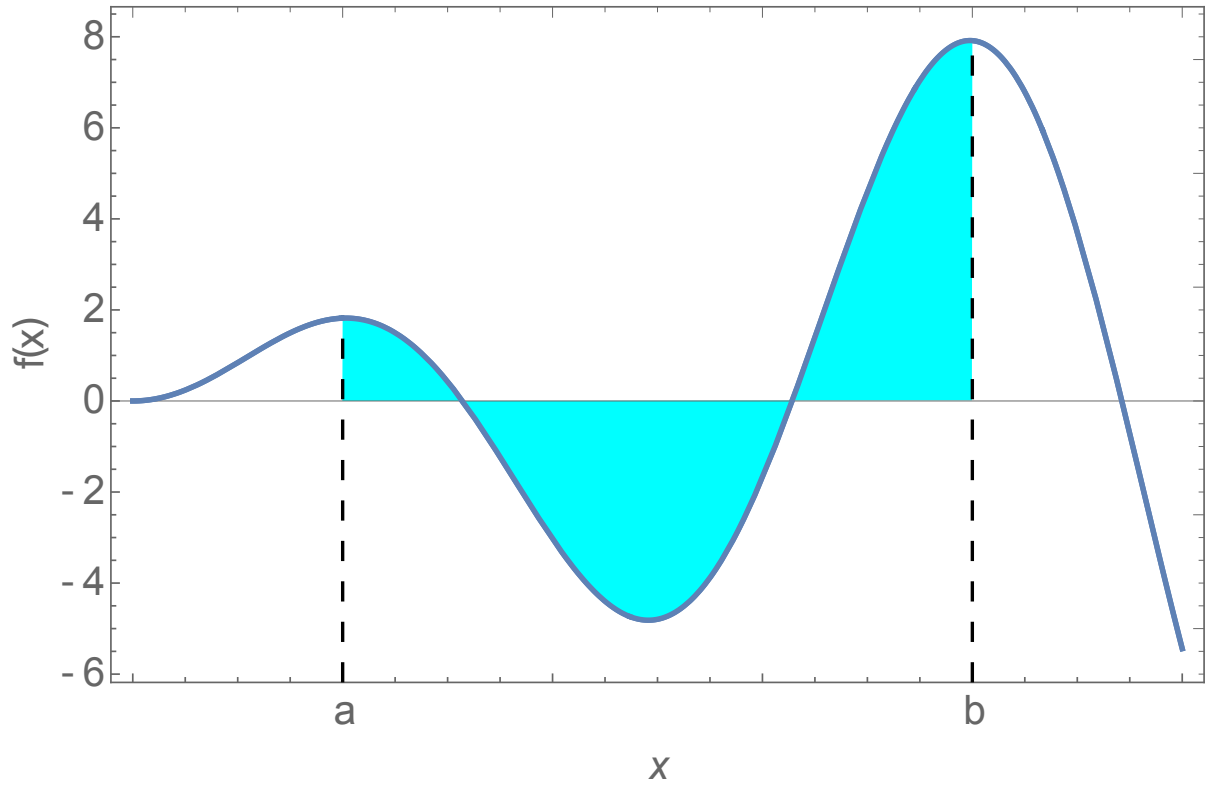
Numerical integration

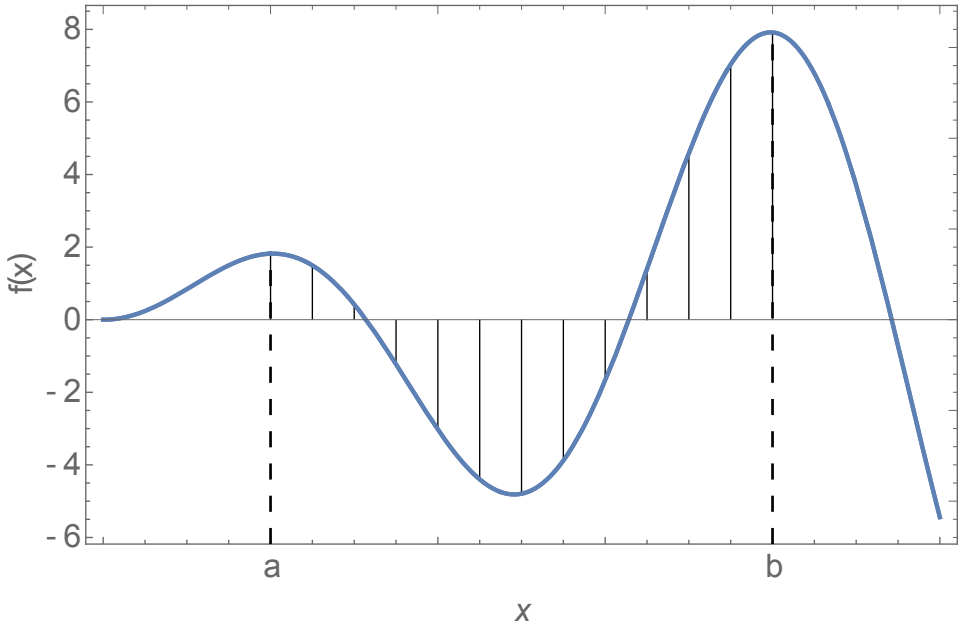
$$\int_a^b f(x)dx$$



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

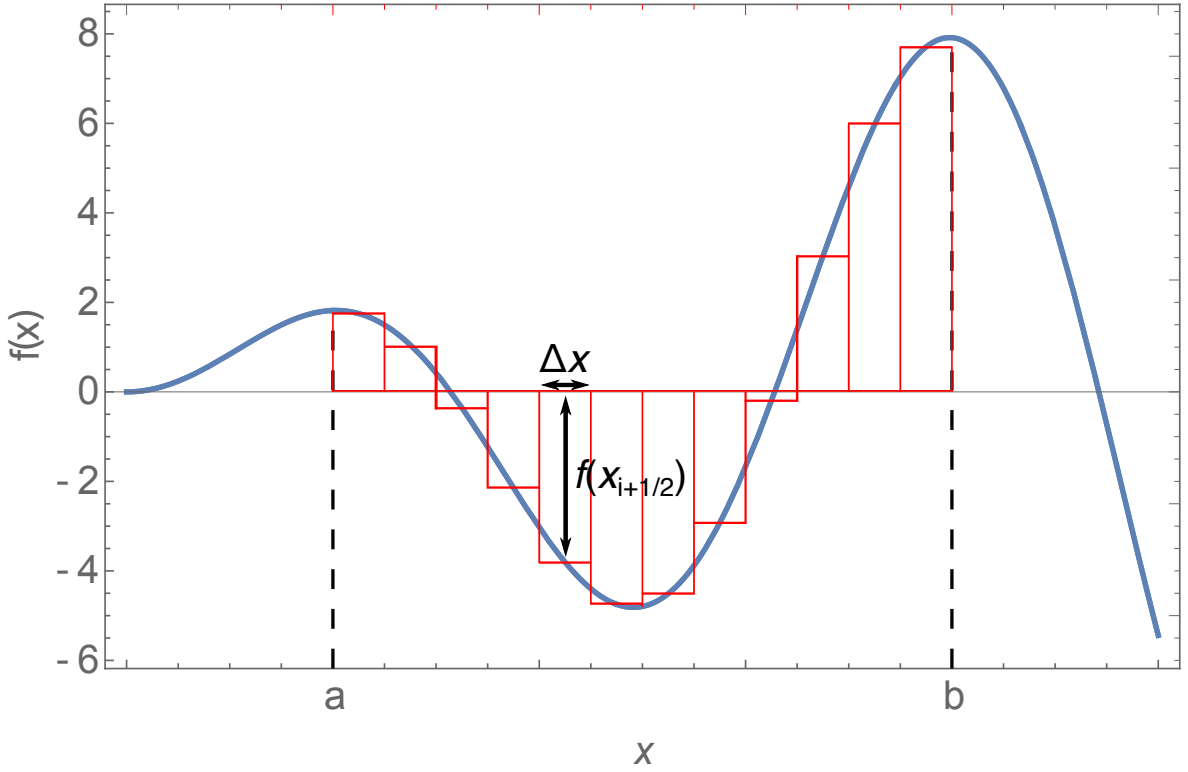
$$\int_a^b f(x)dx = \lim_{N\to\infty} \sum_{i=0}^{N-1} A_i$$



Approach 1: Midpoint rule

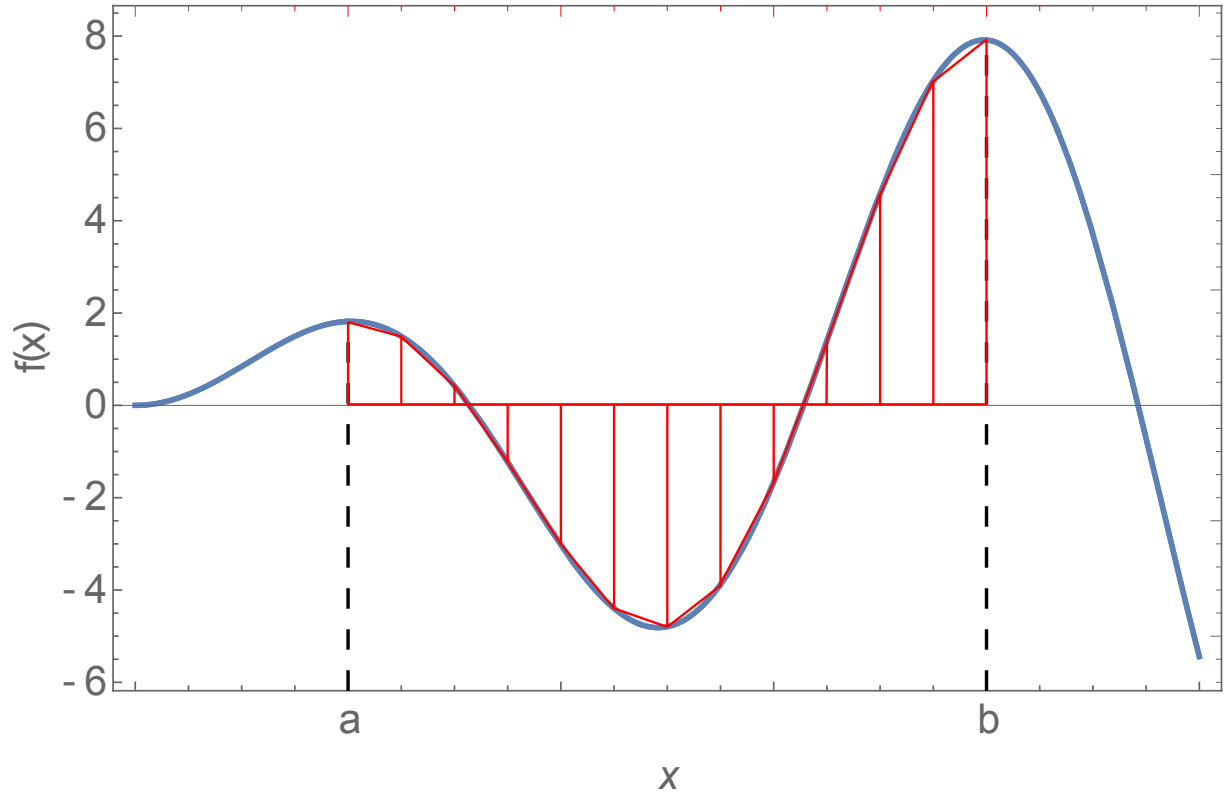
- Approximate area as rectangle with height equal to the midpoint of the subinterval $f(x_{i+1/2})$ and width Δx:

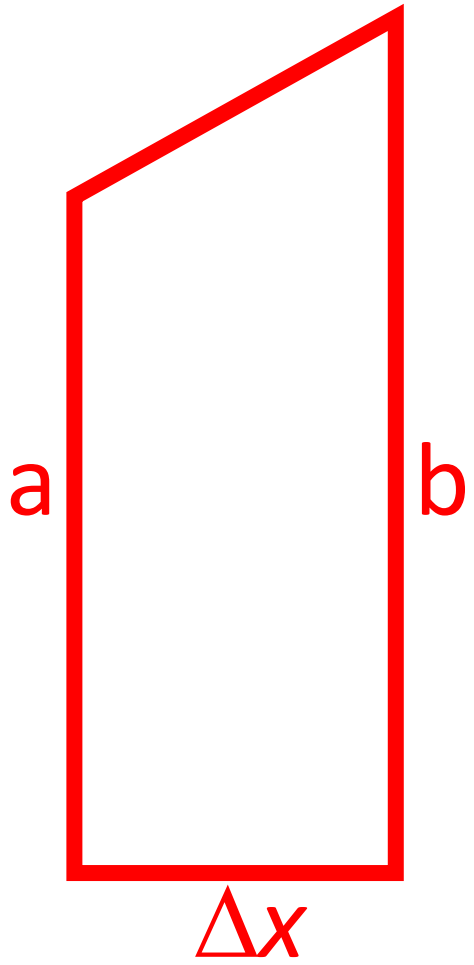
$$\int_a^b f(x)dx \simeq \lim_{N\to\infty} \sum_{i=0}^{N-1} \Delta x f(x_{i+\frac{1}{2}})$$



Approach 2: Trapezoid rule

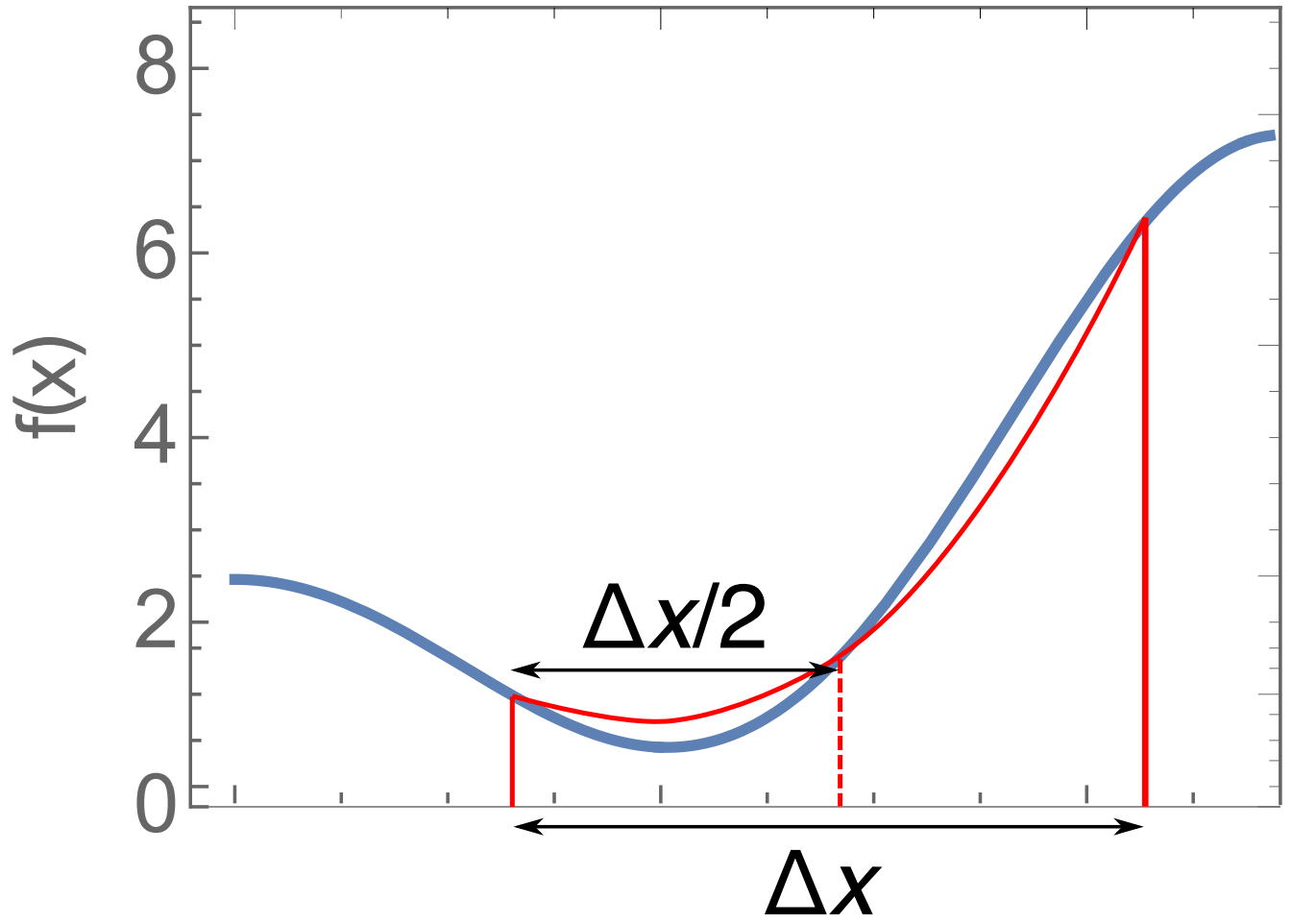
- Area of subintervals approximated as a trapezoid with subinterval endpoints on the curve
- Area of trapezoid: $\Delta x(a+b)/2$





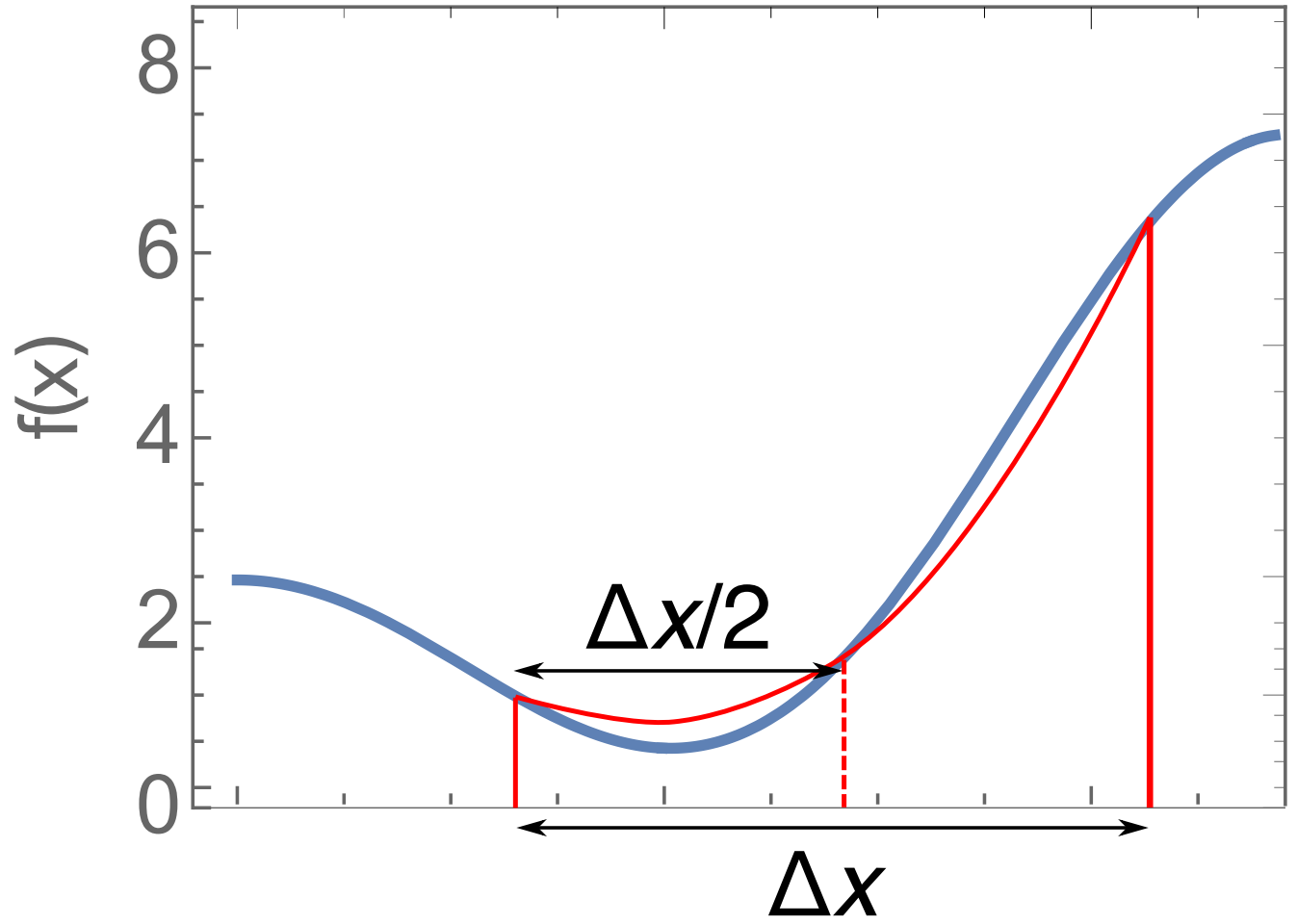
A more accurate technique: Simpson's Rule

- 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?

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

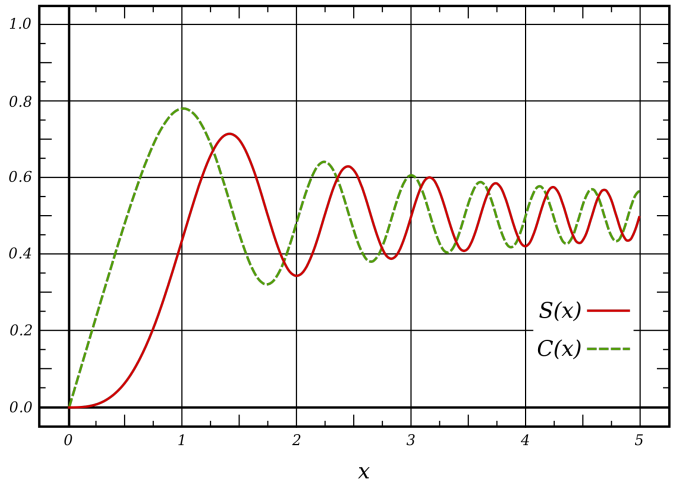
- Now we integrate over the subinterval:

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

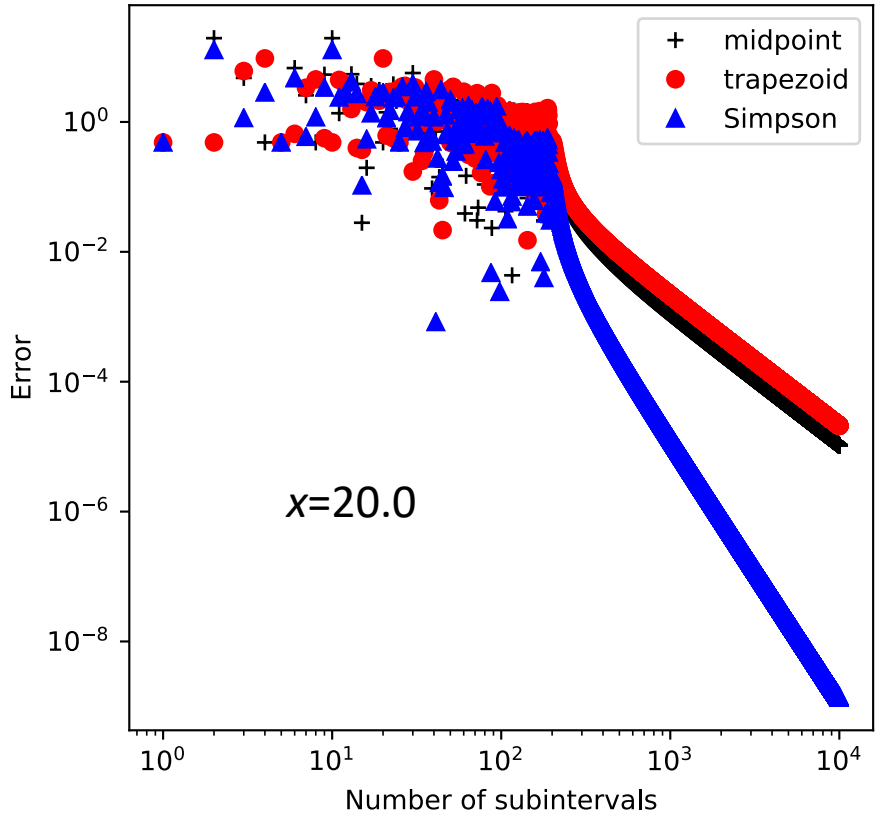
Example: Evaluating the Fresnel integral

- 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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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

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=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,…,N-1 and $\rho(x)$ is a specified weight function
  - Choose x_1, x_2,…,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 ***< 2N (!!!)***
  - 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: $w_1 = \frac{5}{9}, \quad w_2 = \frac{8}{9}, \quad w_3 = \frac{5}{9}$

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: 0.842700792949714 8
3-point Trapezoid: 0.8252629555967492 , Error: -0.017437837352965557
3-point Simpsons: 0.843102830042981 , Error: 0.0004020370932662498
3-point Gauss-Legendre: 0.842690018484510 7 , 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: 0.2843750000000027
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:

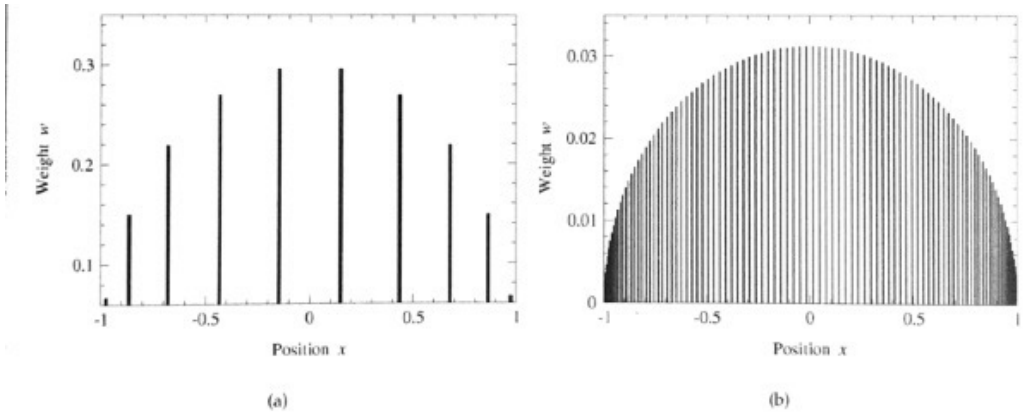

Figure 5.4: Sample points and weights for Gaussian quadrature. The positions and heights of the bars represent the sample points and their associated weights for Gaussian quadrature with (a) $N = 10$ and (b) $N = 100$.

- 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/

- Readings:
  - Wikipedia artical on makefiles
  - Fortran best practices
  - Good Enough Practices in Scientific Computing
  - Blog on numerical differentiation
  - Wikipedia page of finite difference coefficients
  - Newman Chapter 5
  - Garcia Section 10.2