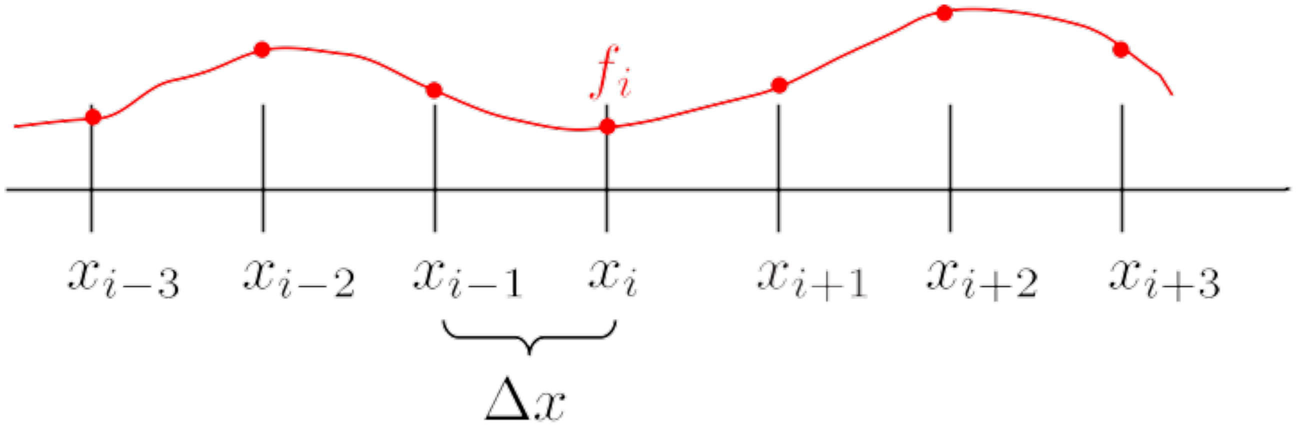
PHY604 Lecture 4

September 2, 2021

Review: Numerical differentiation with "stencils"



- 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

Review: Error in Second order central

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

- 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.

Review: 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

Today's lecture:

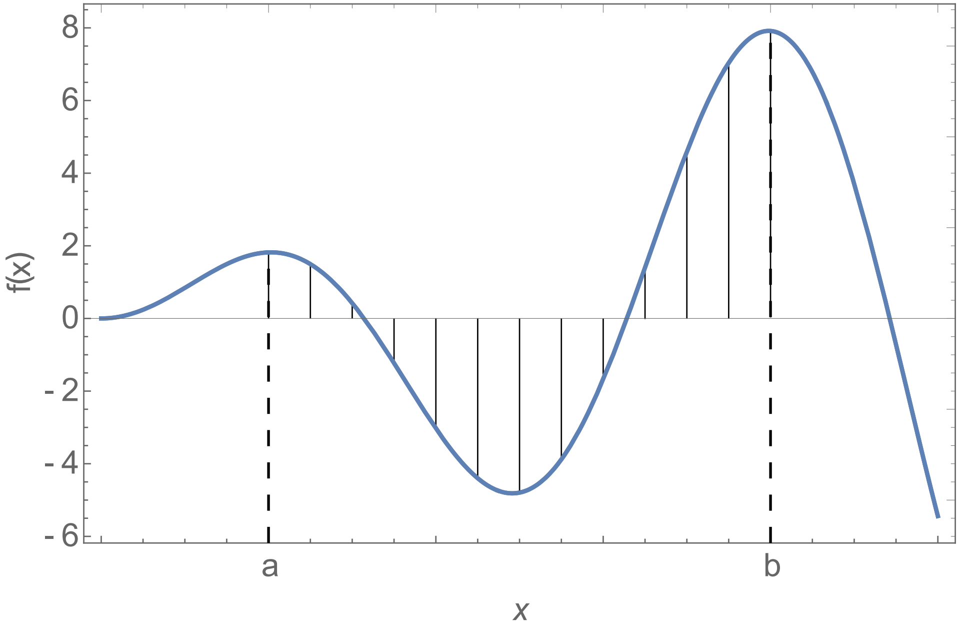
- Finish discussing Numerical Integration

- Begin discussing interpolation
  - Lagrange Interpolation

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

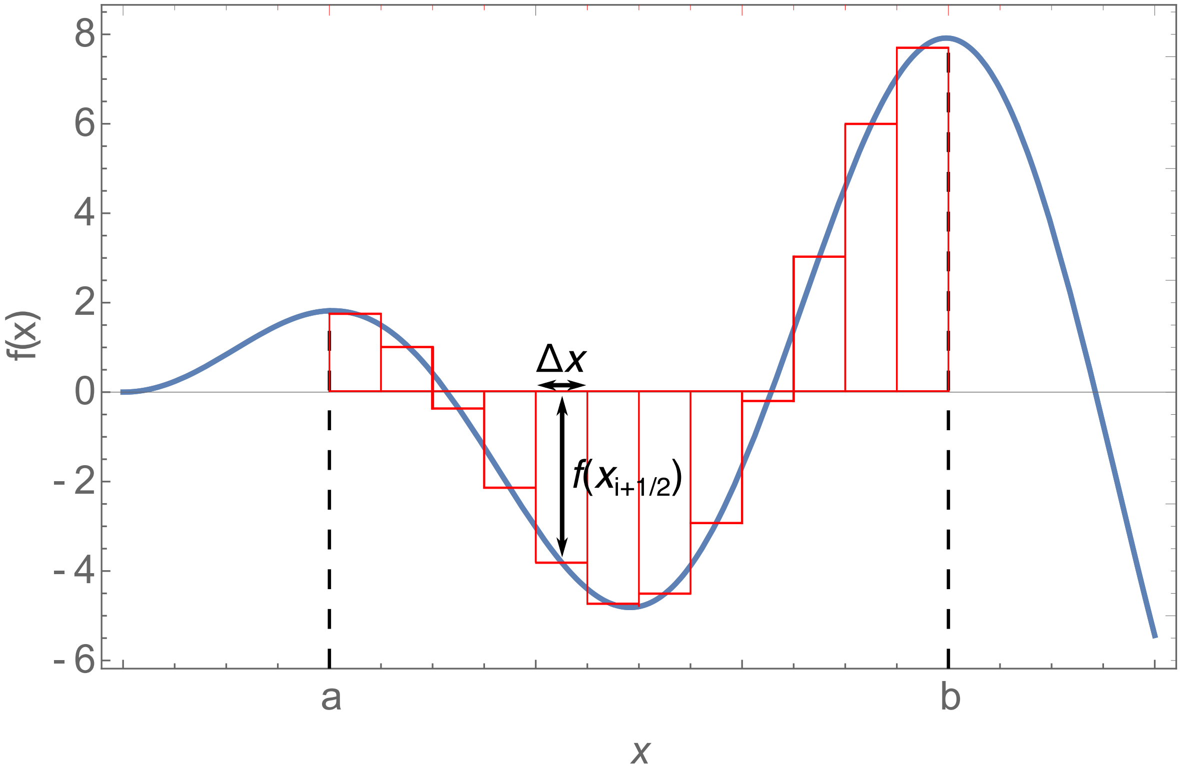
$$\int_a^b f(x)dx = \lim_{N\to\infty} \sum_{i=0}^{N-1} A_i$$



Approach 1: Midpoint rule

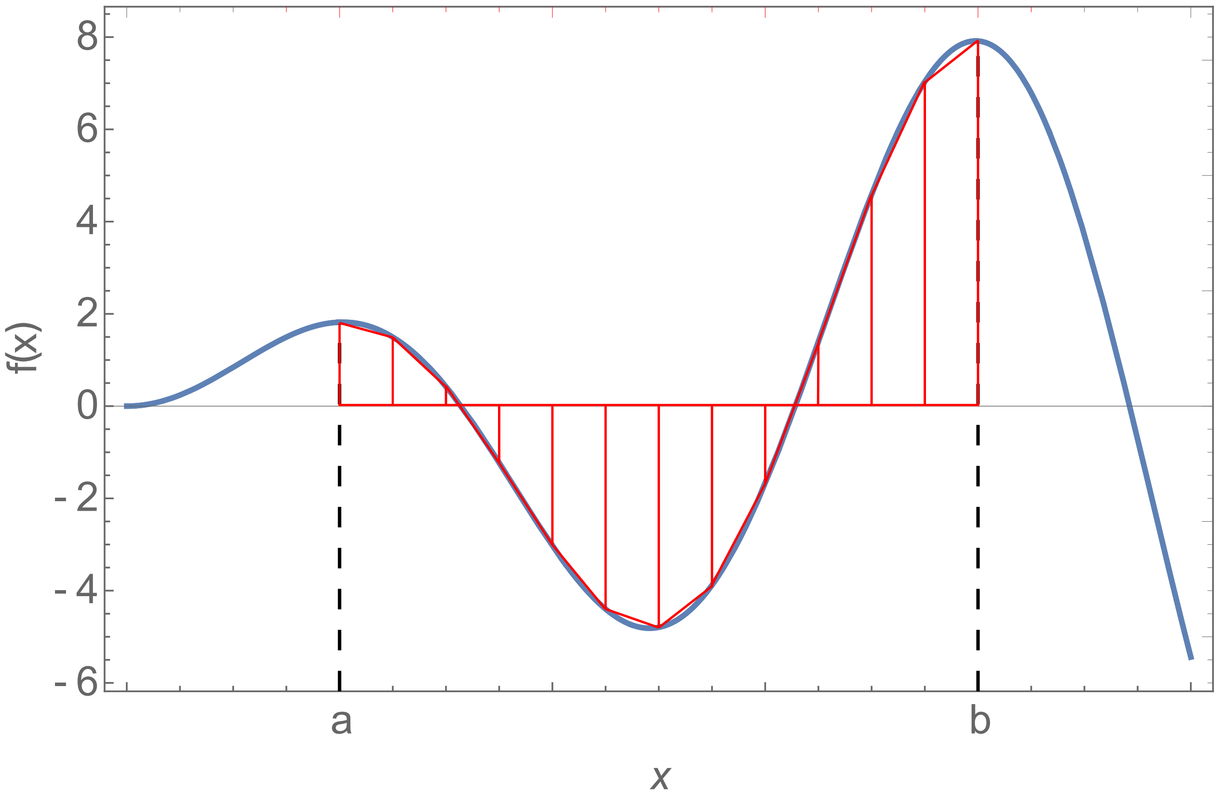
- Approximate area as rectangle with height equal to the midpoint of the subinterval $f(x_{i+1/2})$ and width Δx:

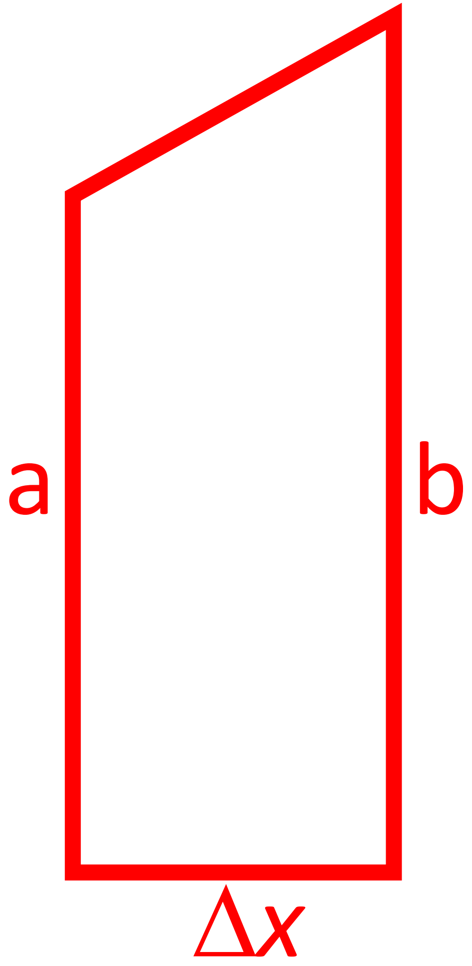
$$\int_a^b f(x)dx \simeq \lim_{N\to\infty} \sum_{i=0}^{N-1} \Delta x f(x_{i+\frac{1}{2}})$$



Approach 2: Trapezoid rule

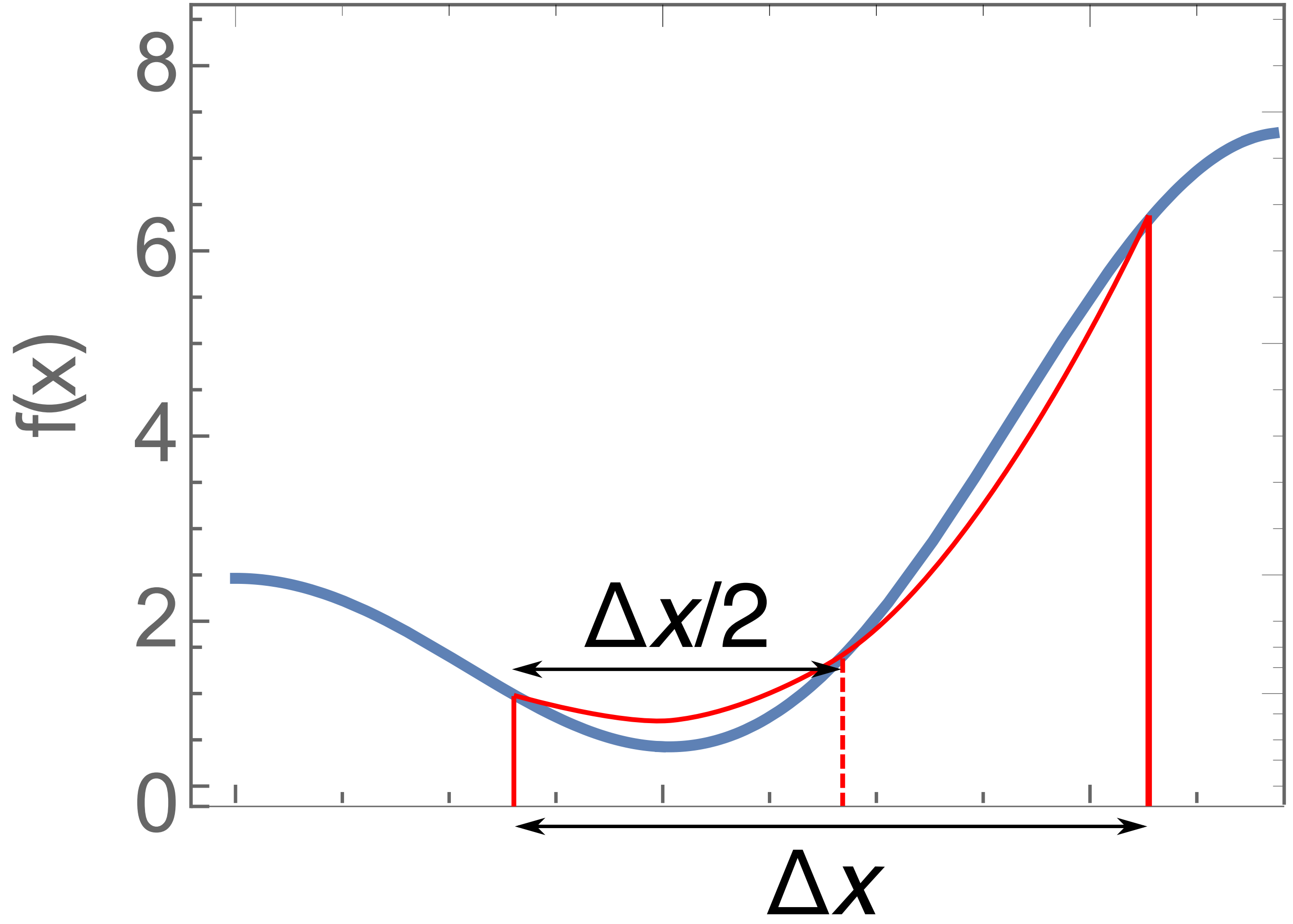
- Area of subintervals approximated as a trapezoid with subinterval endpoints on the curve
- Area of trapezoid: $\Delta x(a+b)/2$





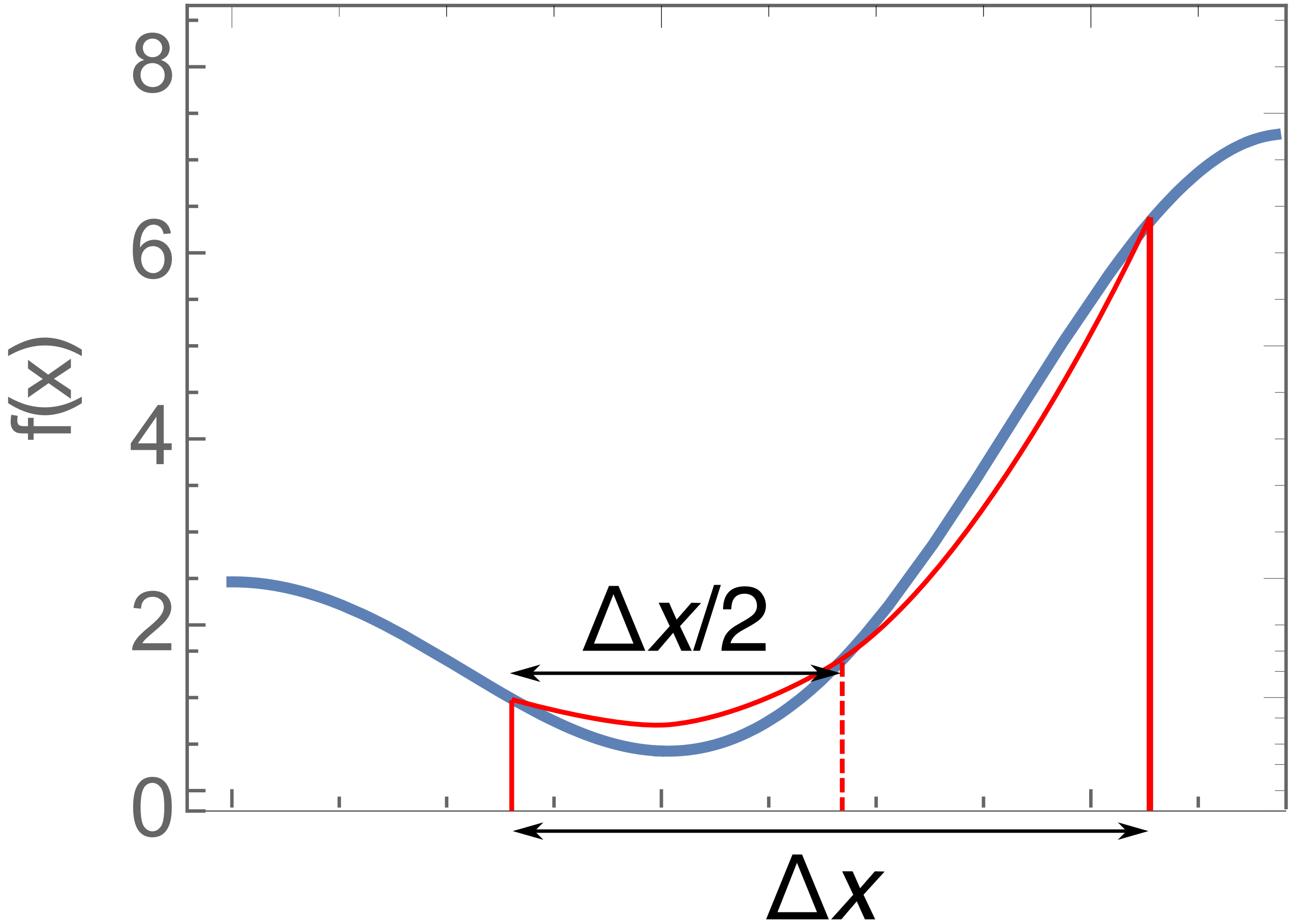
A more accurate technique: Simpson's Rule

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



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?

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

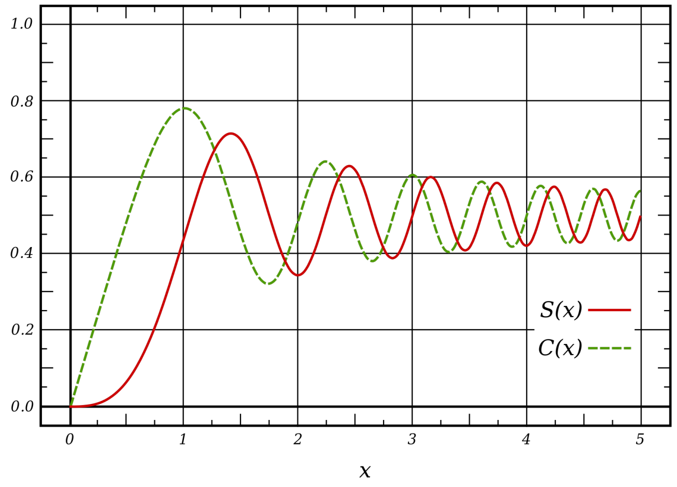
- Now we integrate over the subinterval:

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

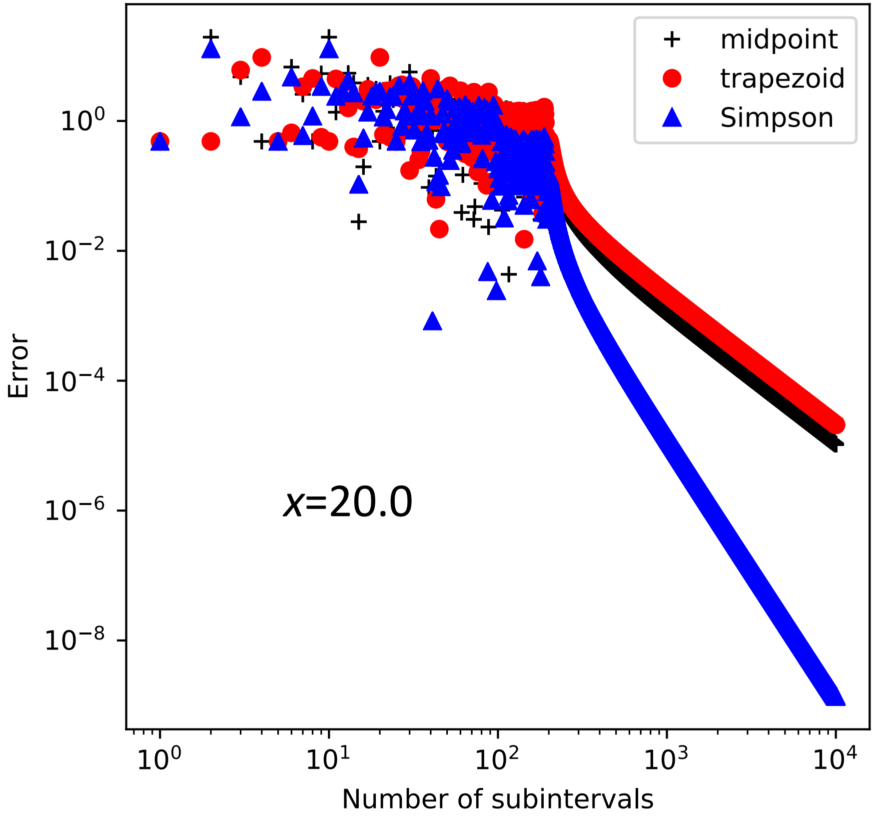
Example: Evaluating the Fresnel integral

- 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 **< 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, *ρ(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:

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

<u>General Solution</u>:

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

- *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: 0.00040203709326662498
3-point Gauss-Legendre: 0.8426900184845107 , Error: -1.0774465204033135e-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:

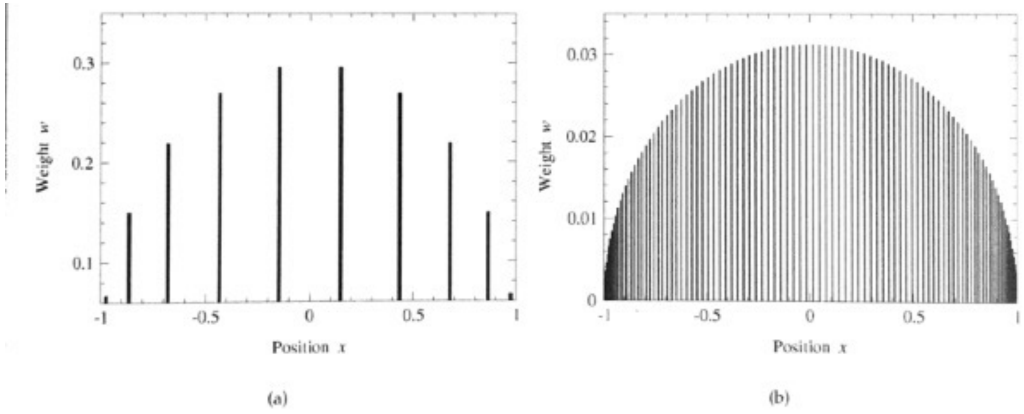


Figure 5.4: Sample points and weights for Gaussian quadrature. The positions and heights of the bars represent the sample points and their associated weights for Gaussian quadrature with (a) $N = 10$ and (b) $N = 100$.

- 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	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)

- 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

Today’s lecture:

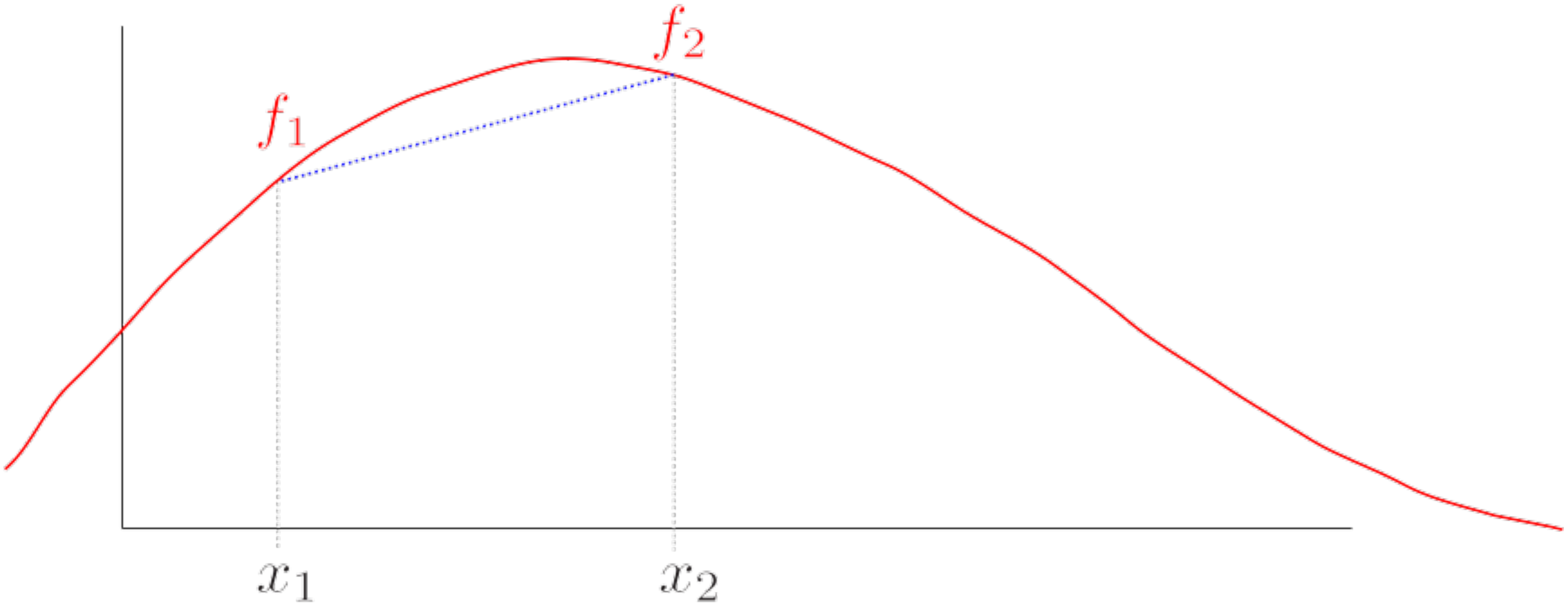
- Finish discussing Numerical Integration

- Begin discussing interpolation
  - Lagrange Interpolation

Interpolation (see Pang Ch. 2)

- Interpolation is needed when we want to infer some local information from a set of incomplete or discrete data
  - E.g., experimental data or from computational simulations
- Many different types of interpolation based on assumptions about and requirements for the data
  - Some ensure no new extrema are introduced
  - Some match derivatives at end points
  - Need to balance number of points used against pathologies (e.g., oscillations)
- Interpolations and fitting are different!
  - *Interpolation* seeks to fill in missing information in some small region of the whole dataset
  - *Fitting* a function to the data seeks to produce a model (guided by physical intuition) so you can learn more about the global behavior of your data

Linear interpolation:
Draw a line between two points



$$f(x) = \frac{f_2 - f_1}{x_2 - x_1}(x - x_1) + f_1$$

Errors in linear interpolation

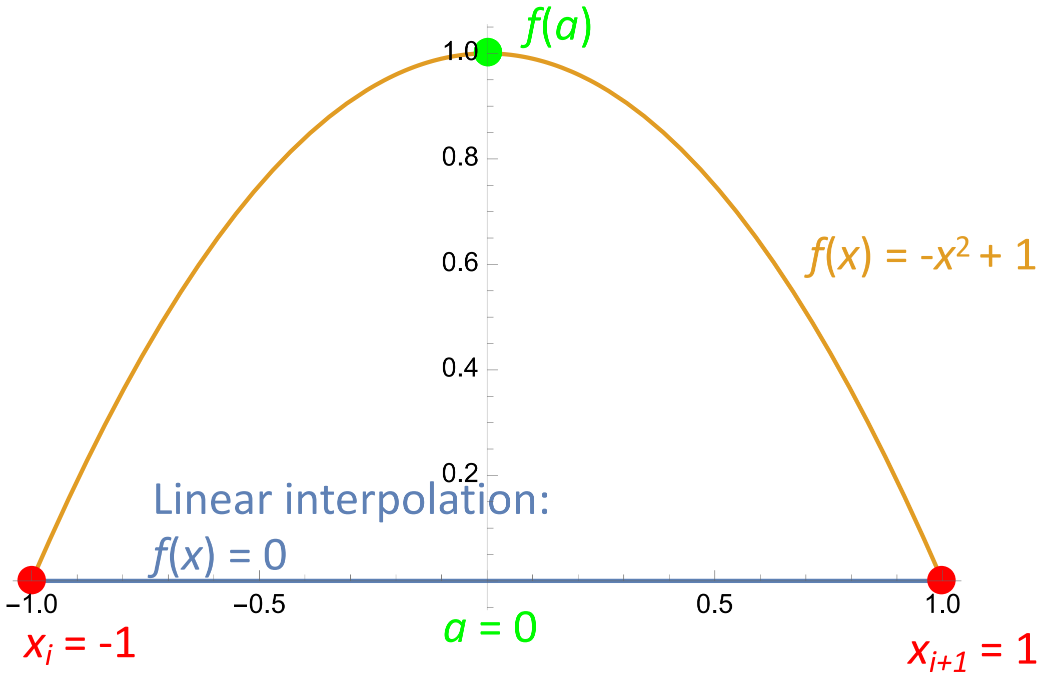
- Exact value at *x*: $f(x) = \underbrace{f_i + \frac{x - x_i}{x_{i+1} - x_i}(f_{i+1} - f_i)}_{\text{Linear interpolant}} + \Delta f(x)$

- What is $\Delta f(x)$?
  - Consider point x = *a* where *a* is in $[x_i, x_{i+1}]$
  - Fit a quadratic to the function at x_i, *a*, x_{i+1}

$$\Delta f(x) = \frac{f''(x)}{2}(x - x_i)(x - x_{i+1})\bigg|_{x=a}$$

- As long as *f* is smooth in the region $[x_i, x_{i+1}]$
- Error of order: $\mathcal{O}(\Delta x^2)$
- Max error: $|\Delta f(x)| \leq \frac{\max[|\Delta f''(x)|]}{8}(x_{i+1} - x_i)^2$

Simple example of errors in linear interpolation:



$$\Delta f(a) = \frac{-2}{2}(-1)(1) = 1$$

- General case: Fit a parabola as we did for Simpson's rule

General approach for interpolation schemes

- Continuous curve is constructed from given discrete set of data
- Interpolated value is read off the curve
- The more points, the higher order the curve can be
- One way to achieve higher-order interpolation is through Lagrange interpolation

Lagrange interpolation

- General method for building a single polynomial that goes through all the points (alternate formulations exist)

- Given n points: $x_0, x_1, \ldots, x_{n-1}$, with associated function values: $f_0, f_1, \ldots, f_{n-1}$
  - Construct basis functions: $$l_i(x) = \prod_{j=0, i \neq j}^{n-1} \frac{x - x_j}{x_i - x_j}$$
  - Note basis function l_i is 0 at all x_j except for x_i (where it is one)

  - Function value at x is: $$f(x) = \sum_{i=0}^{n-1} l_i(x) f_i$$

Example: Quadratic Lagrange polynomial

- Three points: (x_0,f_0), (x_1,f_1), (x_2,f_2)
- Three basis functions:

$$l_0 = \frac{x - x_1}{x_0 - x_1}\frac{x - x_2}{x_0 - x_2} = \frac{(x - x_1)(x - x_2)}{2\Delta x^2}$$

$$l_1 = \frac{x - x_0}{x_1 - x_0}\frac{x - x_2}{x_1 - x_2} = -\frac{(x - x_0)(x - x_2)}{\Delta x^2}$$

$$l_2 = \frac{x - x_0}{x_2 - x_0}\frac{x - x_1}{x_2 - x_1} = \frac{(x - x_0)(x - x_1)}{2\Delta x^2}$$

- Polynomial:

$$f(x) = f_0\frac{(x - x_1)(x - x_2)}{2\Delta x^2} - f_1\frac{(x - x_0)(x - x_2)}{\Delta x^2} + f_2\frac{(x - x_0)(x - x_1)}{2\Delta x^2}$$

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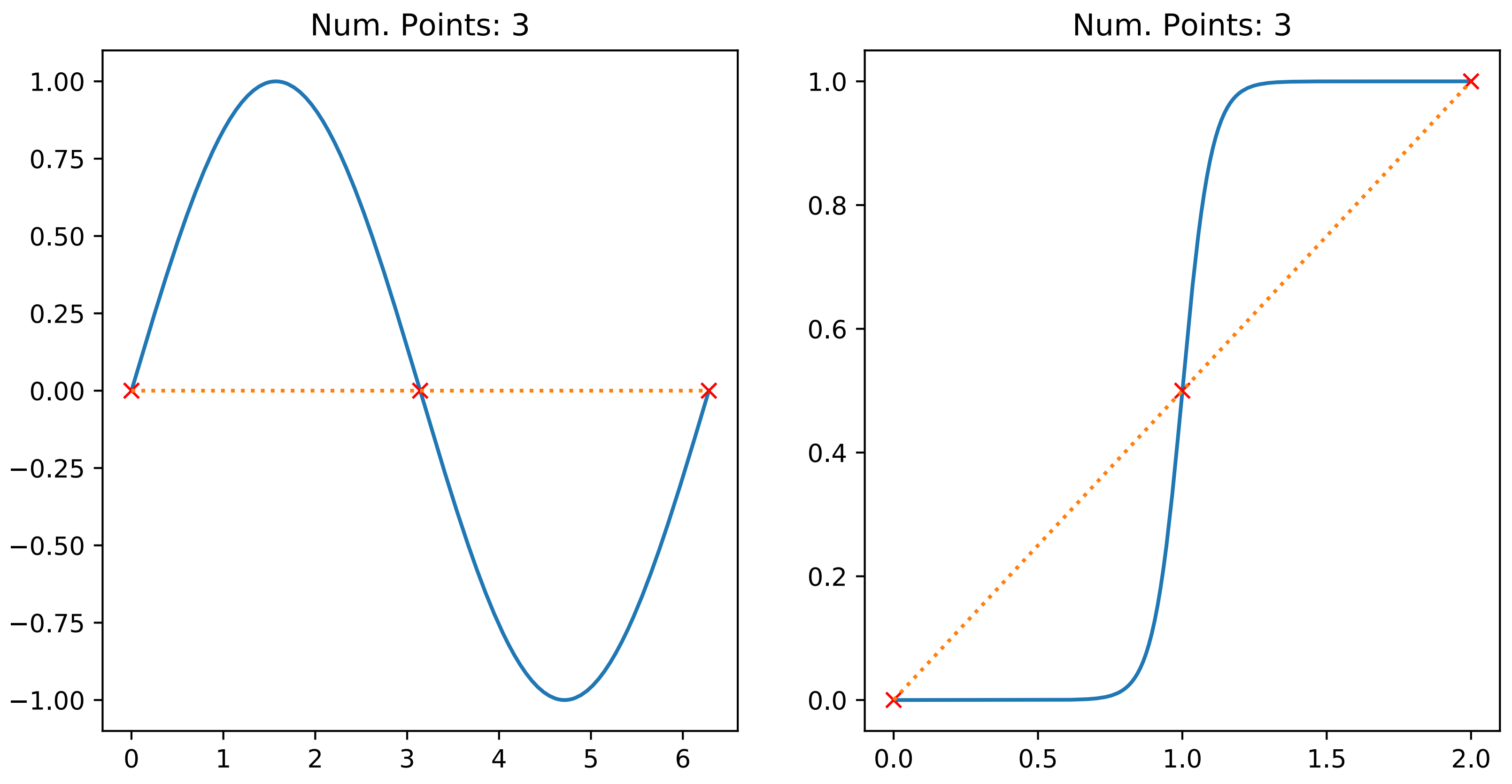
Example: Lagrange Interpolation of two functions



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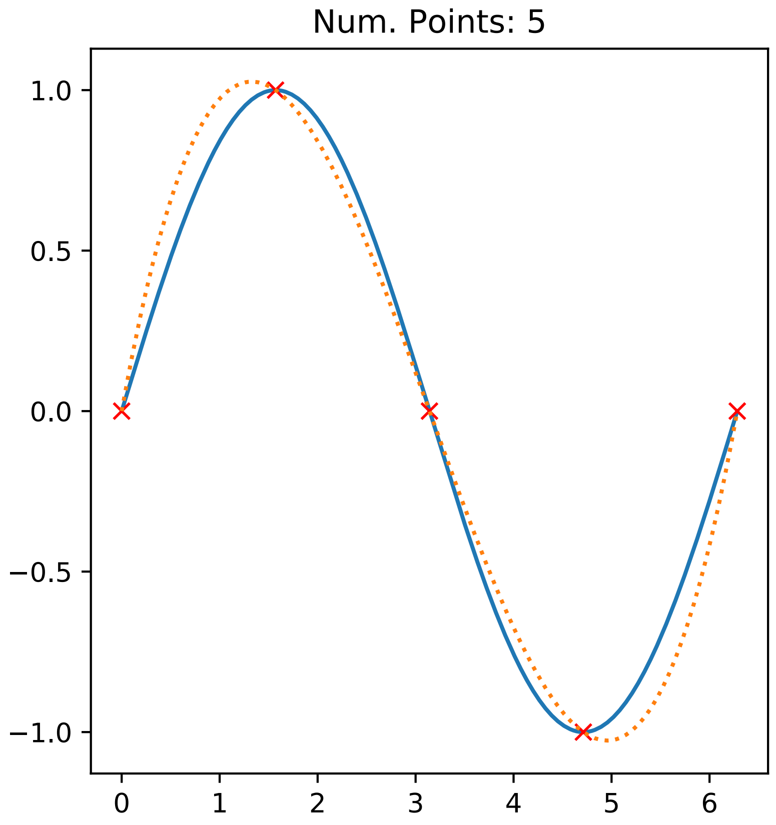

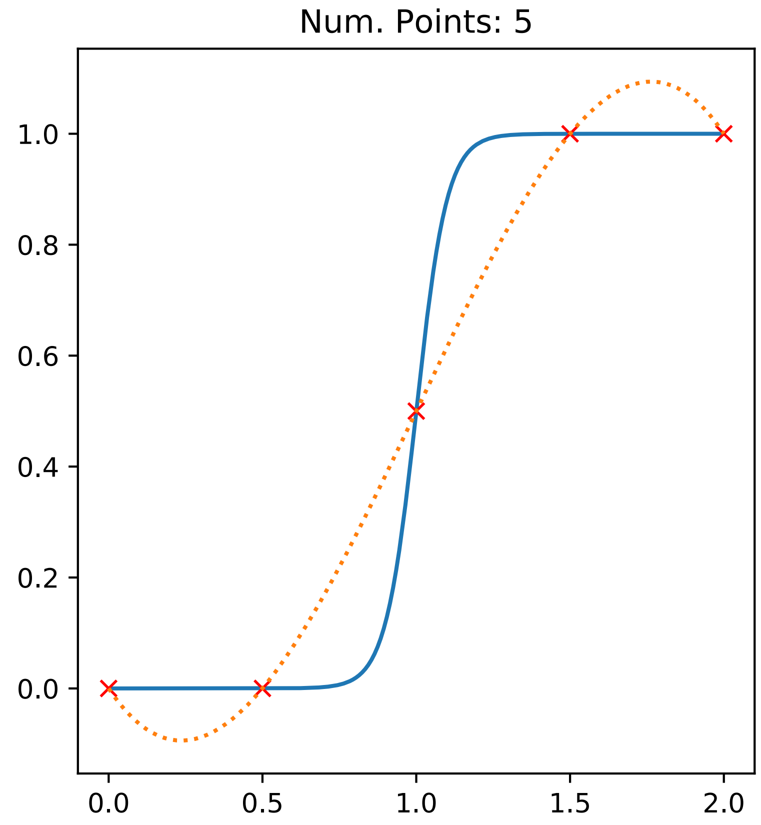

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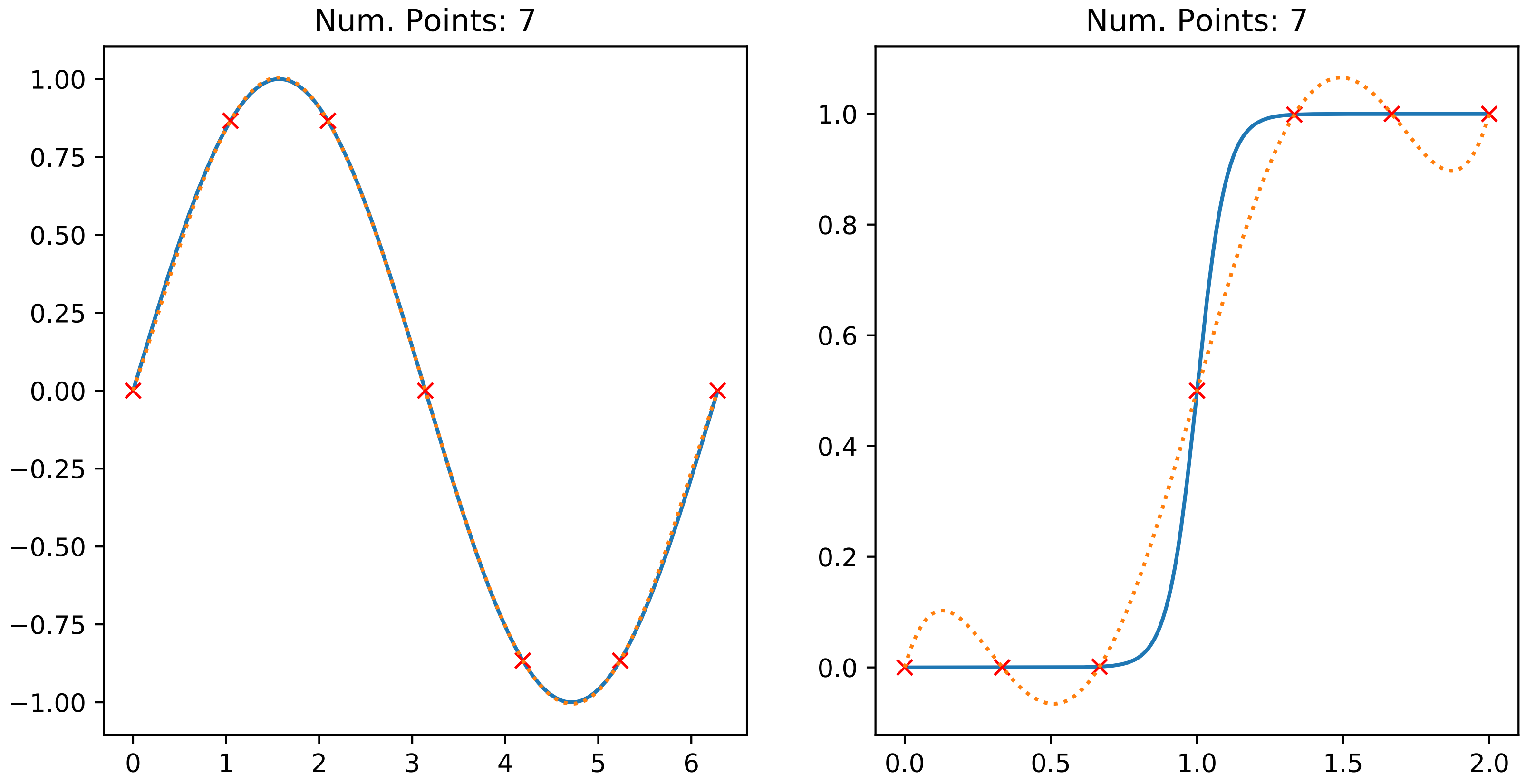

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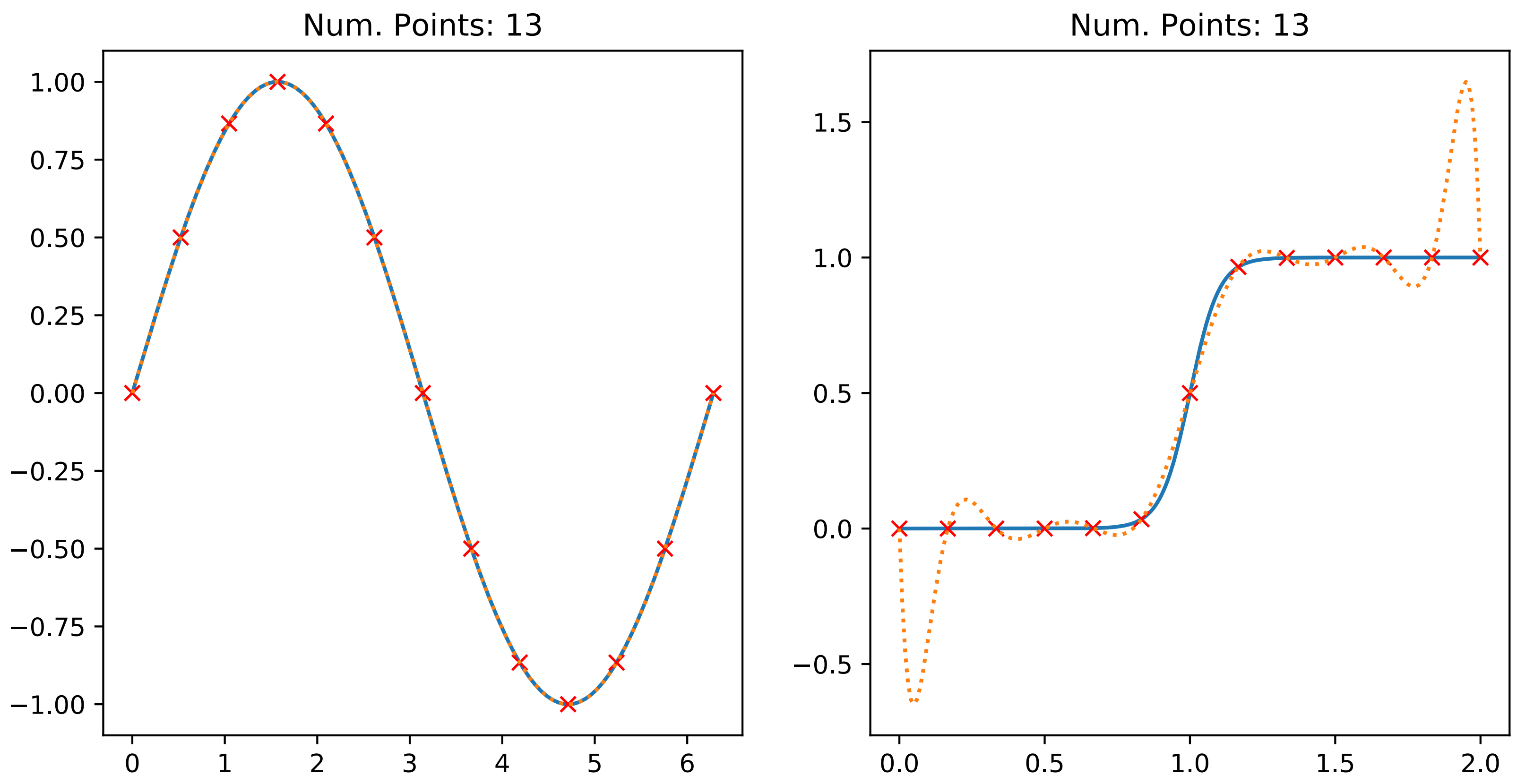
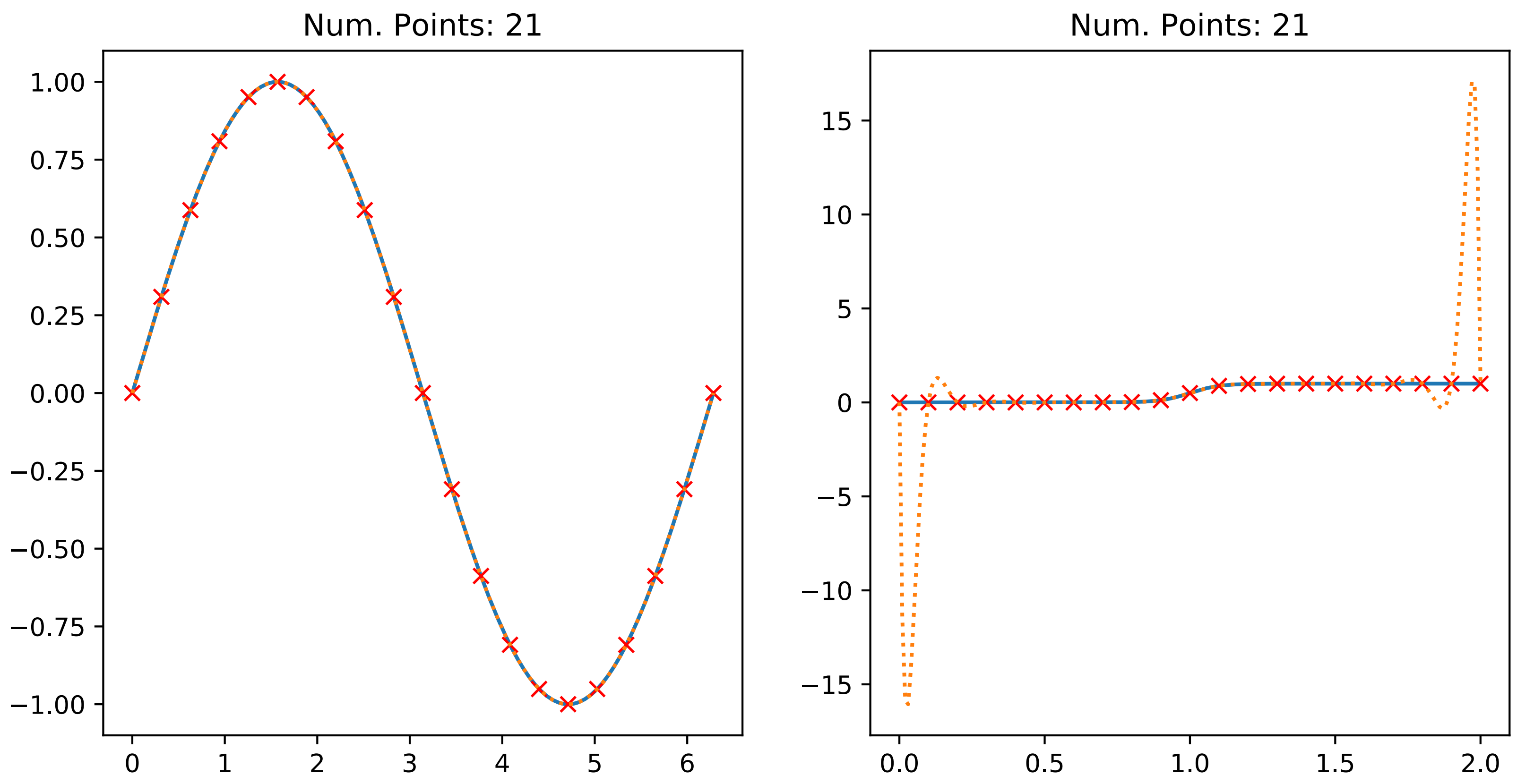


Example: Lagrange Interpolation of two functions



Example: Lagrange Interpolation of two functions

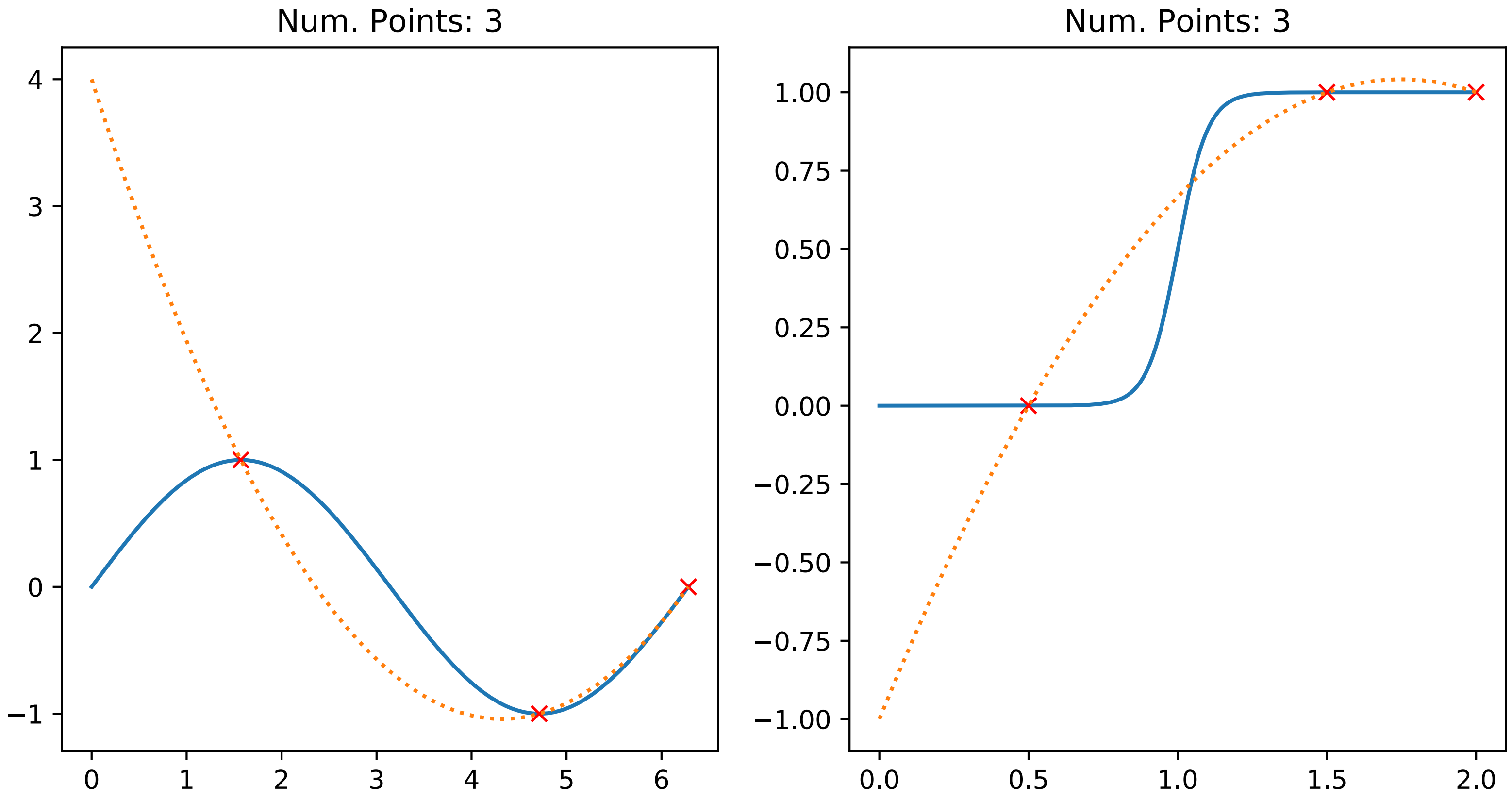
- For the hyperbolic tangent case, increasing the number of points beyond a certain limit increases the error
  - Runge phenomena: Oscillations at the edges of the interval
  - Increasing the number of points causes a divergence in the error
- Can do better by varying the spacing of the interpolating points
  - e.g., Chebyshev polynomial roots are concentrated toward the end of the interval
  - Chebyshev polynomial spacing is usually (almost always) convergent with the number of interpolating points

$$x_k = \frac{1}{2}(a+b) + \frac{1}{2}(b-a)\cos\left(\frac{2k-1}{2n}\pi\right), \quad k = 1, \ldots, n$$

DEMO

- lagrange_poly.ipynb

Example: Lagrange Interpolation of two functions with Chebyshev nodes



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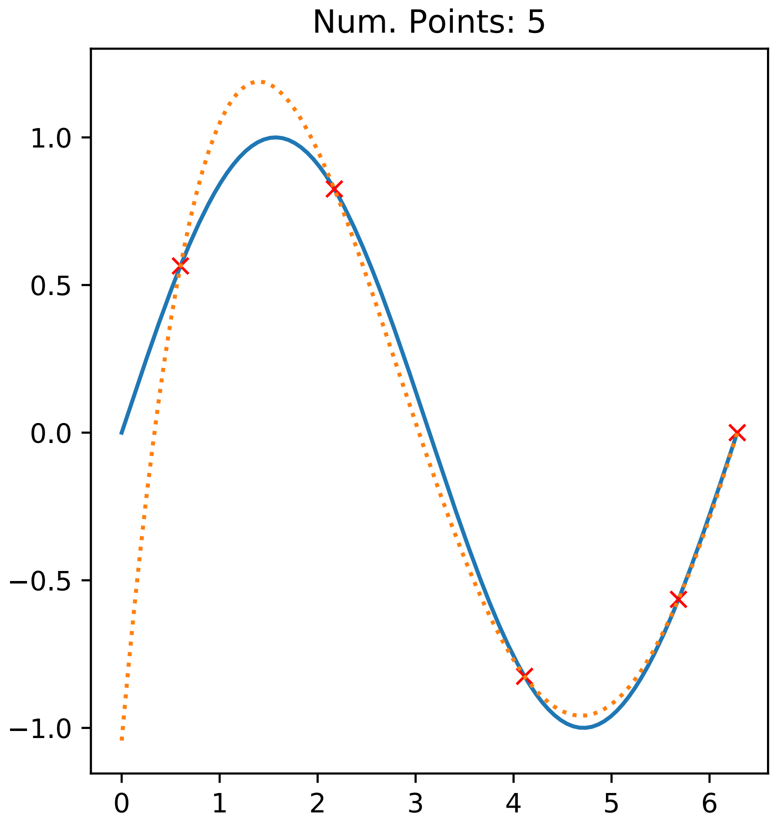

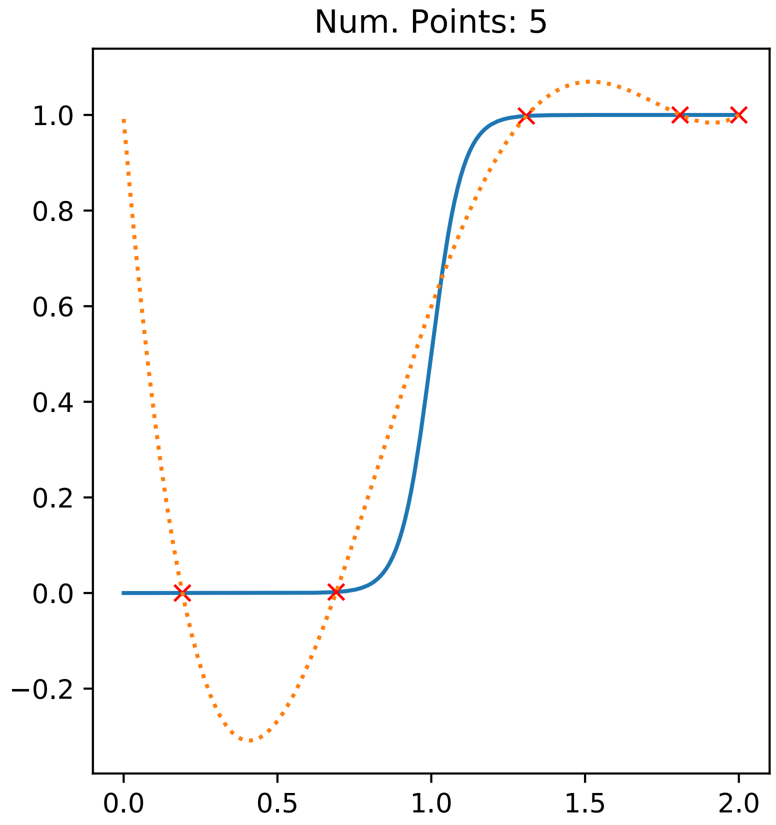

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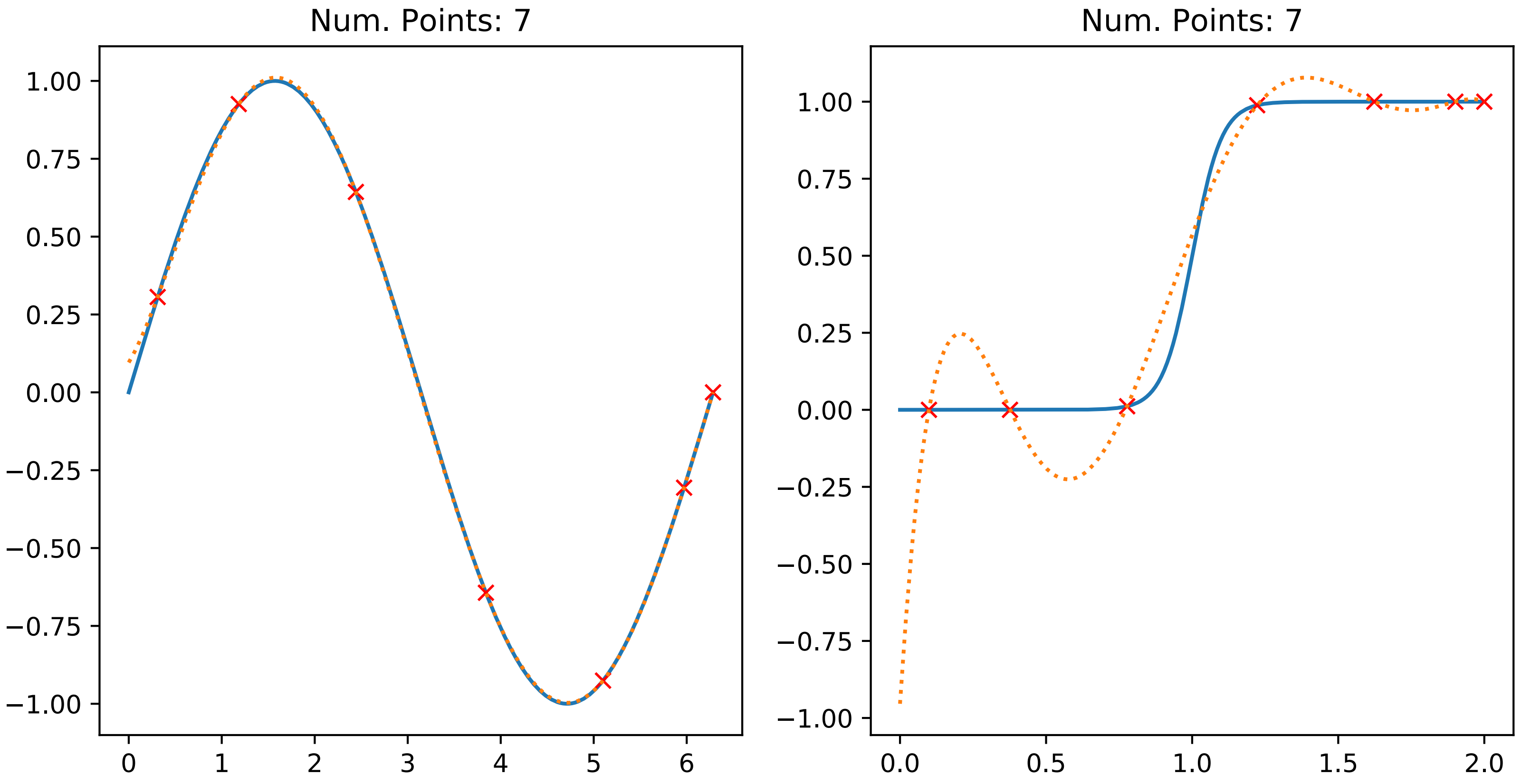

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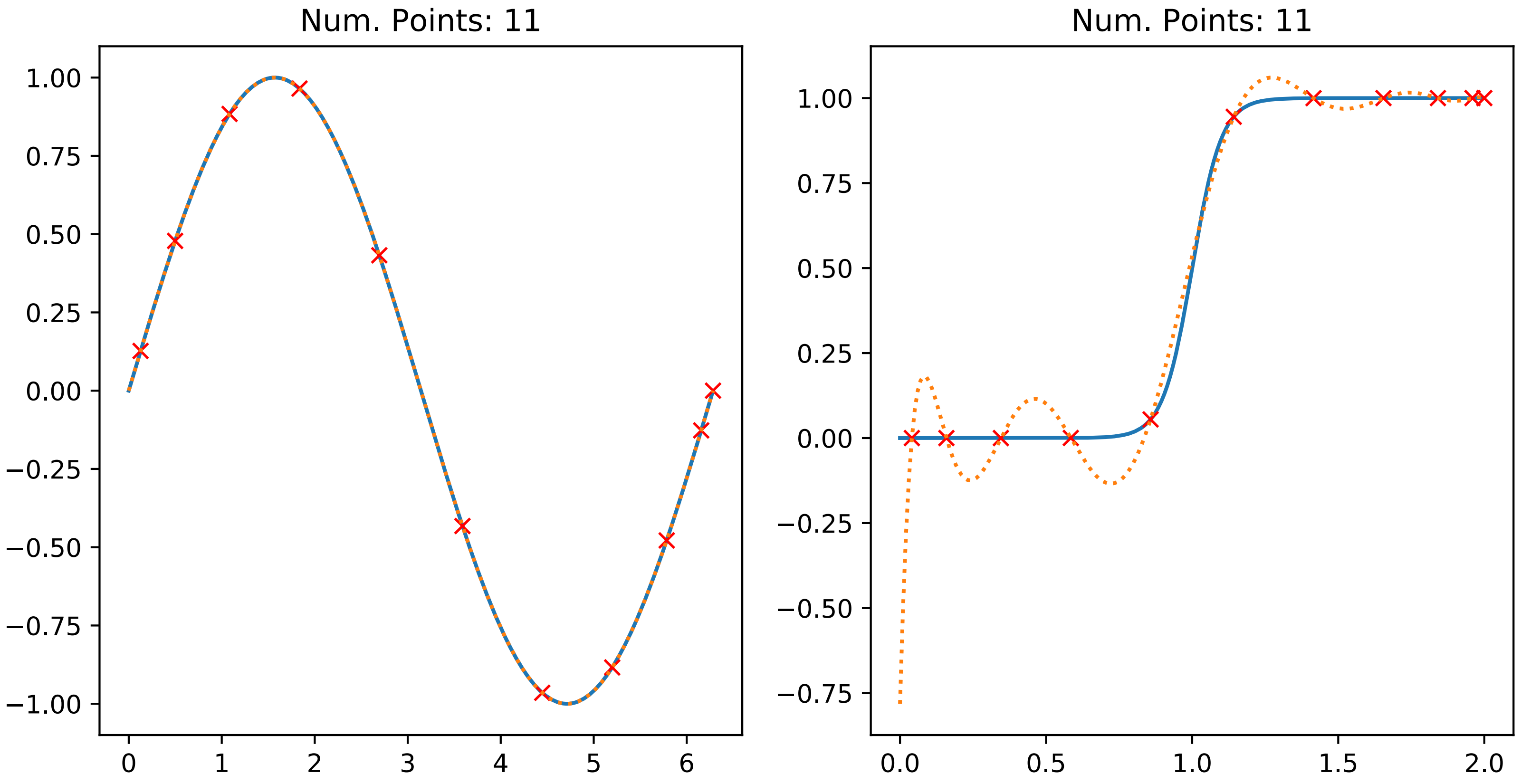

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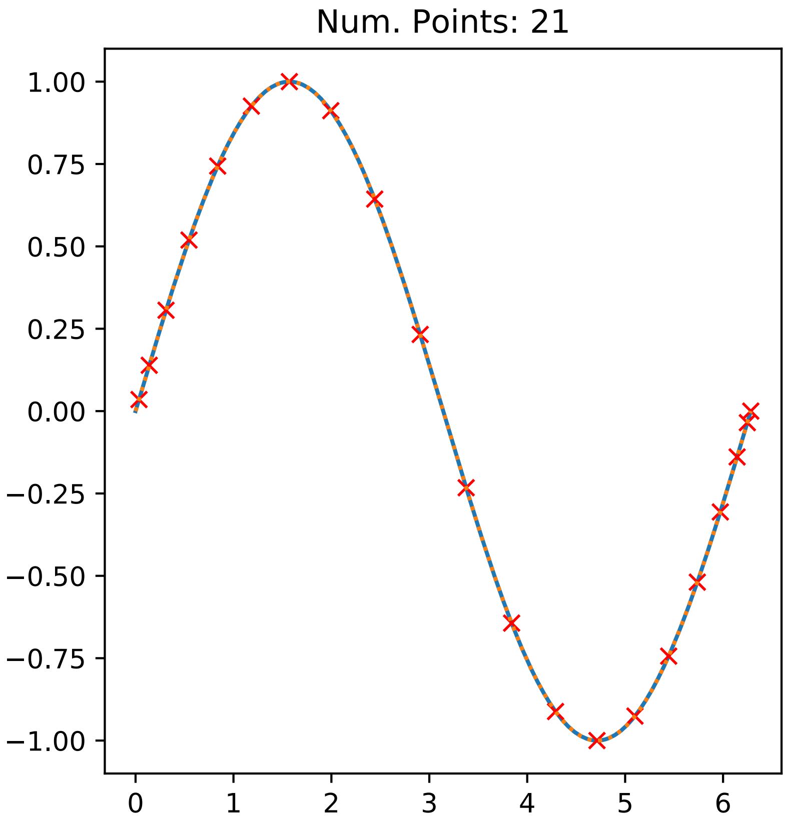

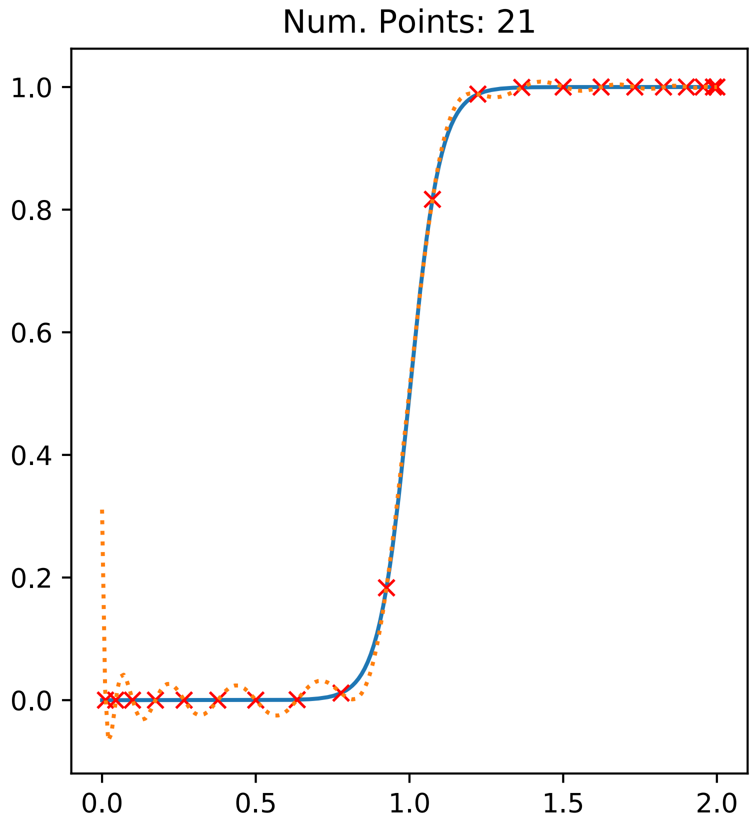

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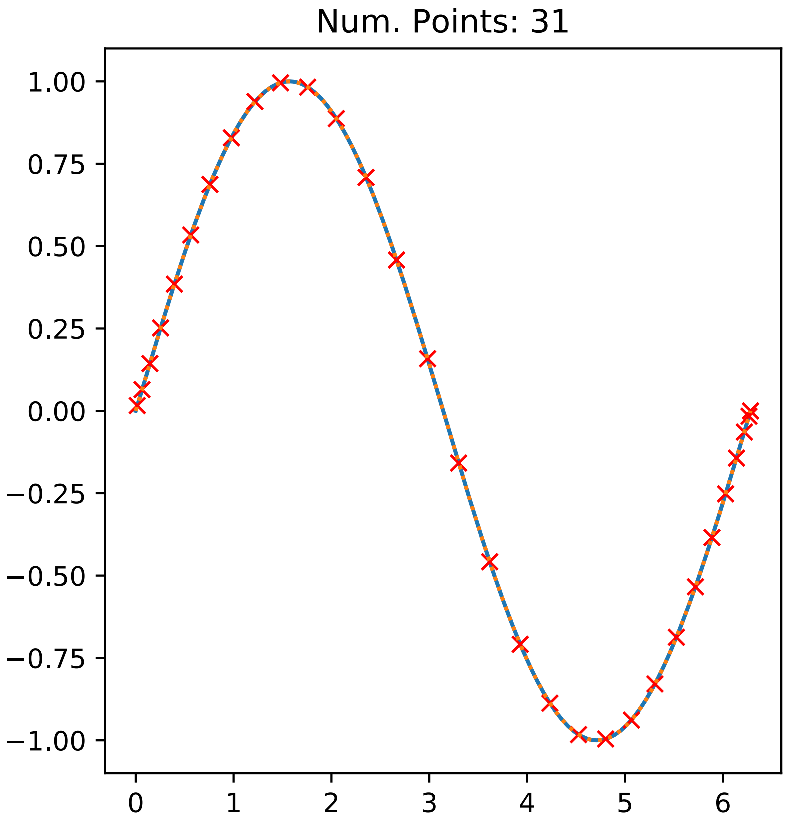
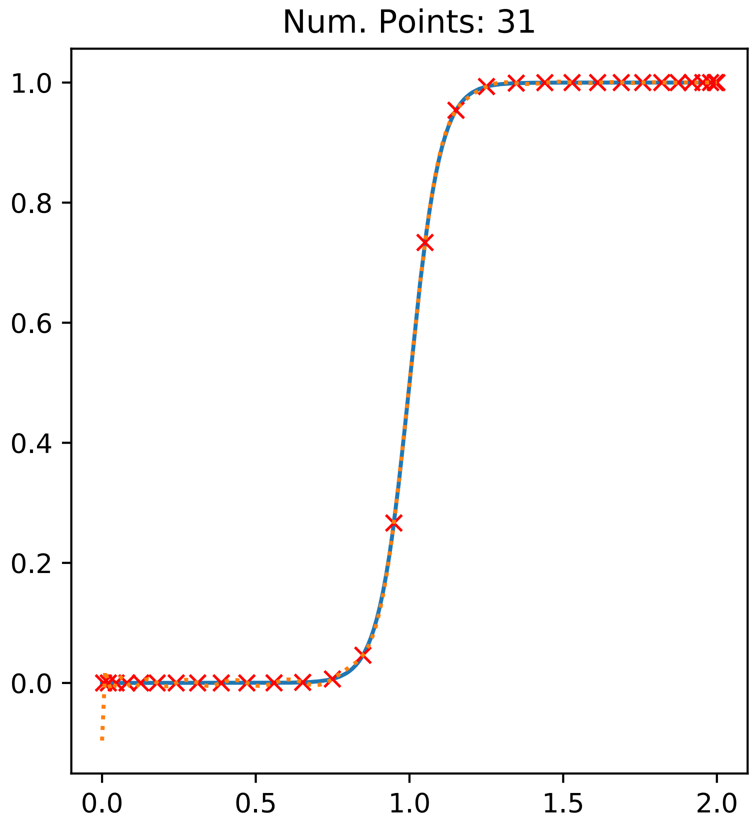
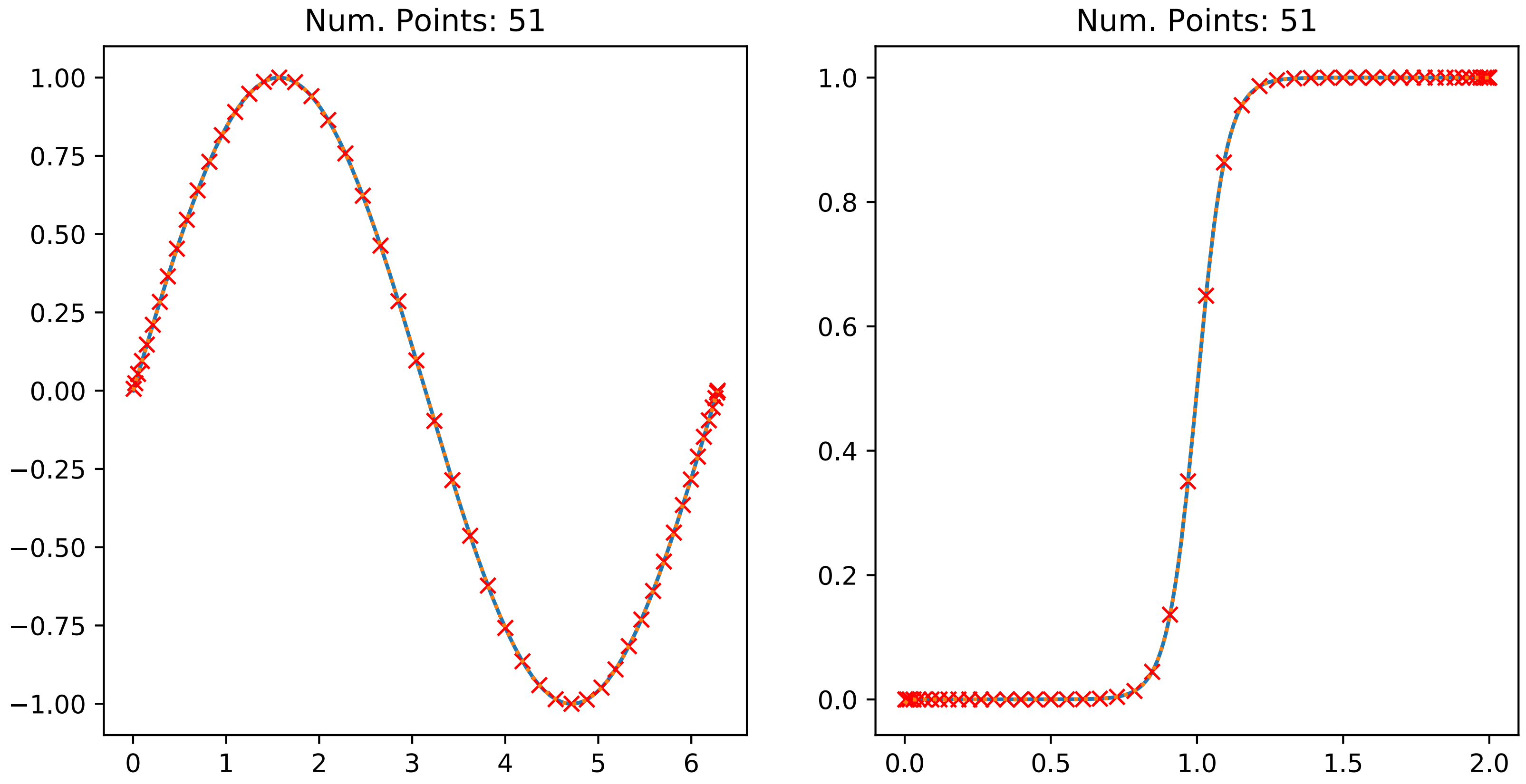




Example: Lagrange Interpolation of two functions with Chebyshev nodes



After class tasks

- Homework and instructions for turning it in will be posted later today
- Readings:
  - Newman Chapter 5
  - Garcia Section 10.2
  - Pang Section 2.1
  - Wikipedia article on Chebyshev nodes
  - Myths about polynomial interpolation