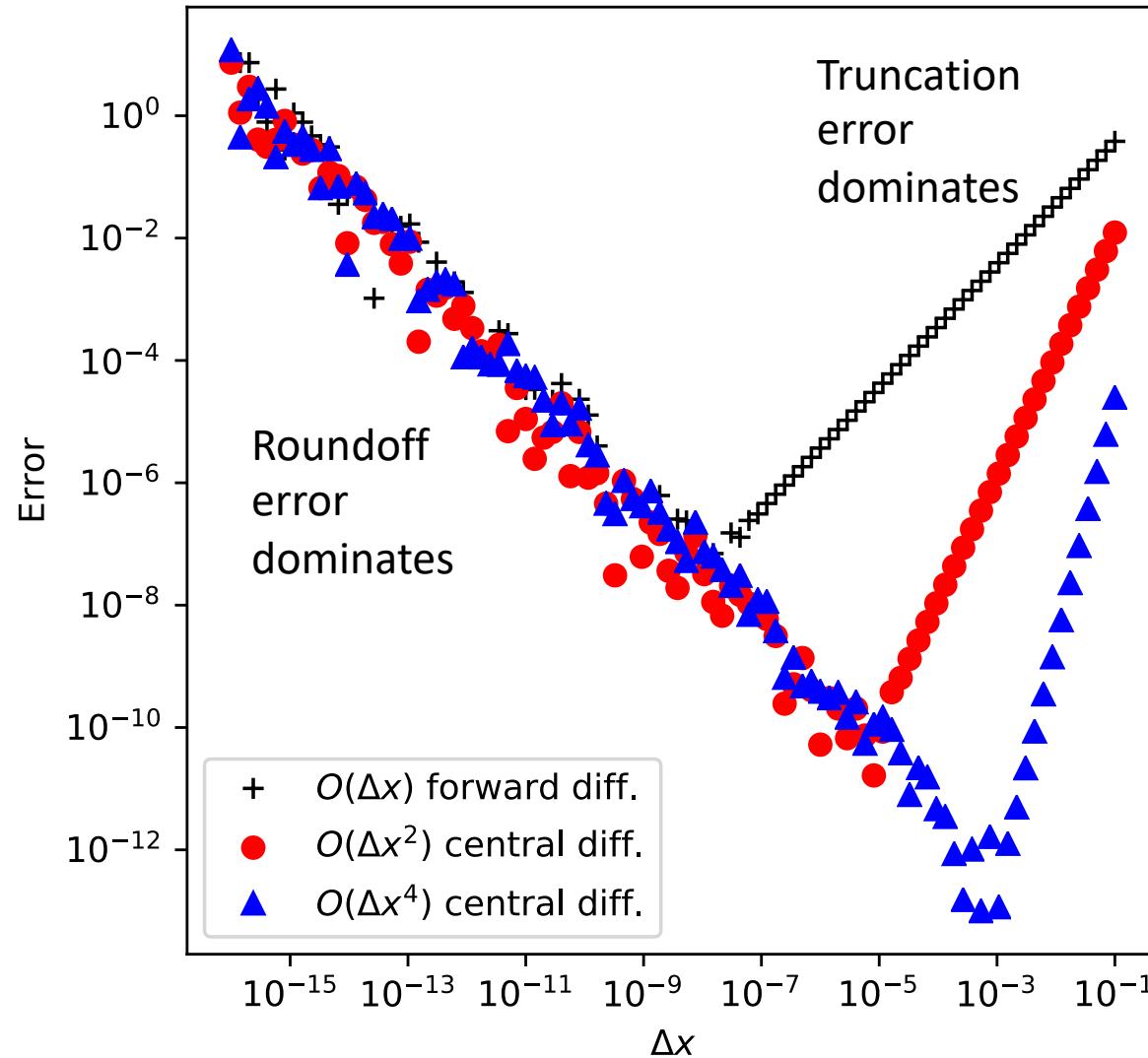


PHY604 Lecture 4

September 14, 2023

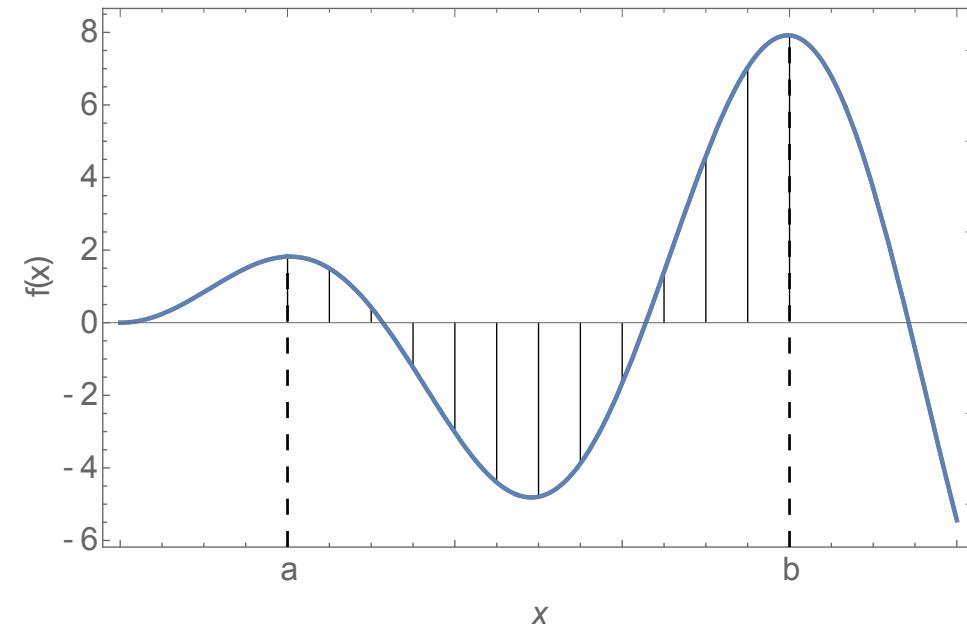
Review: Derivative of $\exp(x)$



Review: 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

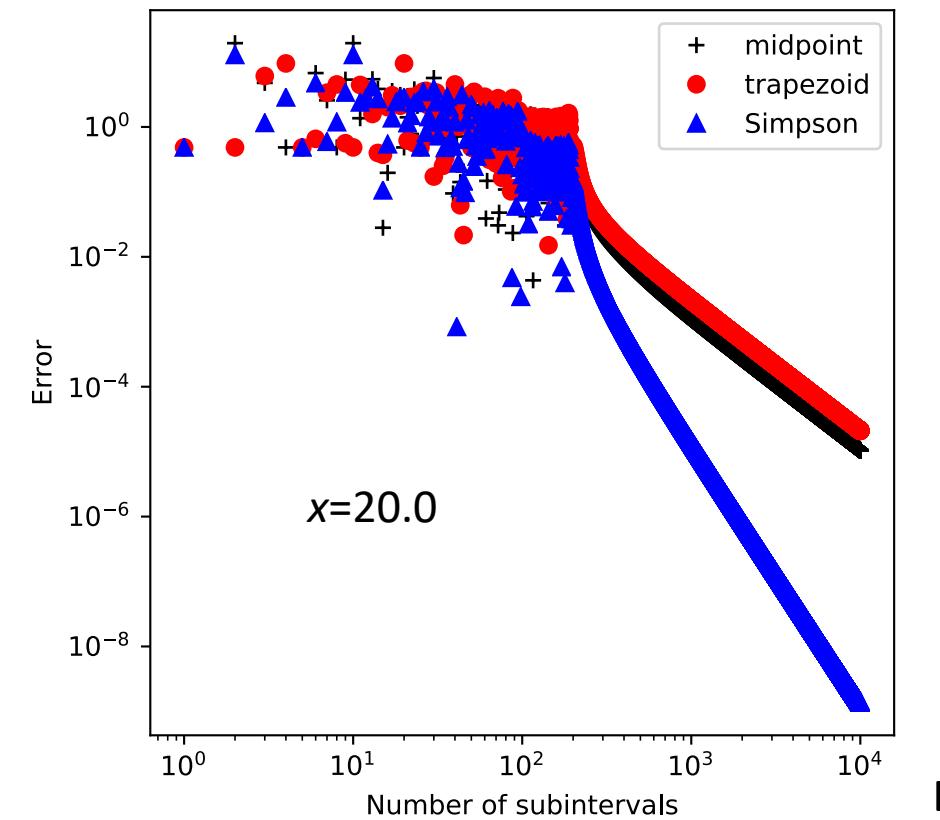
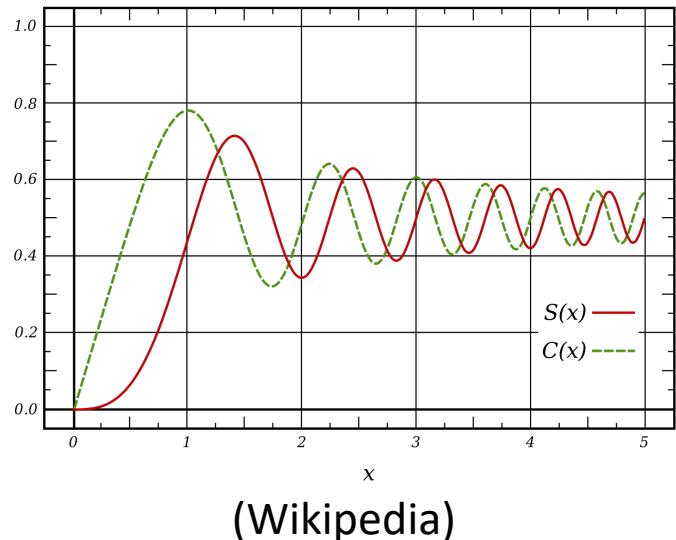
$$\int_a^b f(x)dx = \lim_{N \rightarrow \infty} \sum_{i=0}^{N-1} A_i$$



Review: 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):

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



Review: 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)

Today's lecture:

- Finish discussing Numerical Integration
- Begin discussing interpolation
 - Lagrange Interpolation

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:

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

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

- 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?

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

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

Theorem behind Gaussian integration

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

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

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

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

- 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 $[1,-1]$:

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

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

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

Step 1: Find polynomial $q(x)$

$$q(x) = c_0 + c_1x + c_2x^2 + c_3x^3$$

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

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

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 our 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 $2N-1$

- Start with $f(x)=1$:
$$\int_{-1}^1 dx = 2 = w_1 + w_2 + w_3$$

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

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

- 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

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

- Evaluate $\operatorname{erf}(1)$:

Exact: 0.8427007929497148

3-point Trapezoid: 0.8252629555967492 , Error: -0.017437837352965557

3-point Simpsons: 0.843102830042981 , Error: 0.0004020370932662498

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: 2.449999999999997

3-point Trapezoid: 2.734375 , Error: 0.28437500000000027

3-point Simpsons: 2.4791666666666665 , Error: 0.0291666666666785

3-point Gauss-Legendre: 2.45 , Error: 4.440892098500626e-16

Weights and positions have been tabulated

- From Newman Sec. 5.6:

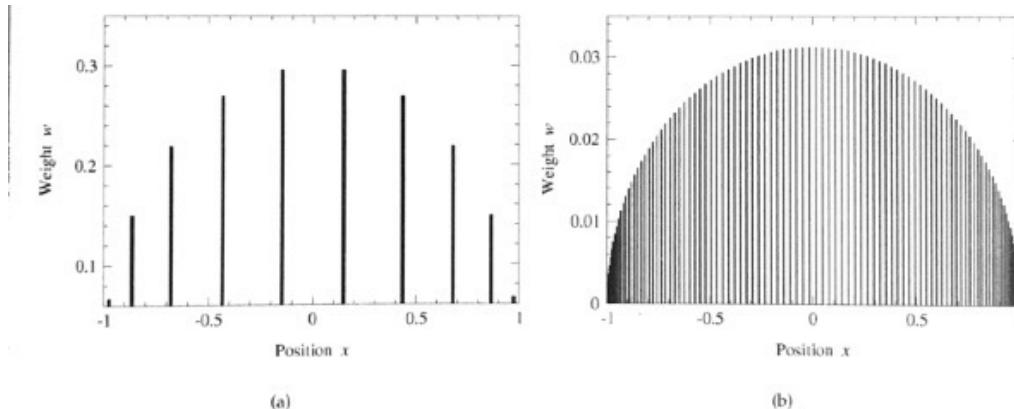


Figure 5.4: Sample points and weights for Gaussian quadrature. The positions and heights of the bars represent the sample points and their associated weights for Gaussian quadrature with (a) $N = 10$ and (b) $N = 100$.

- 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
$[0, \infty)$	e^{-x}	Laguerre polynomials	25.4.45	Gauss–Laguerre quadrature
$[0, \infty)$	$x^\alpha e^{-x}$	Generalized Laguerre polynomials		Gauss–Laguerre quadrature
$(-\infty, \infty)$	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 or 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 or pathological data/integrands
 - Need to have data on specific, unequally-spaced grid

Today's lecture:

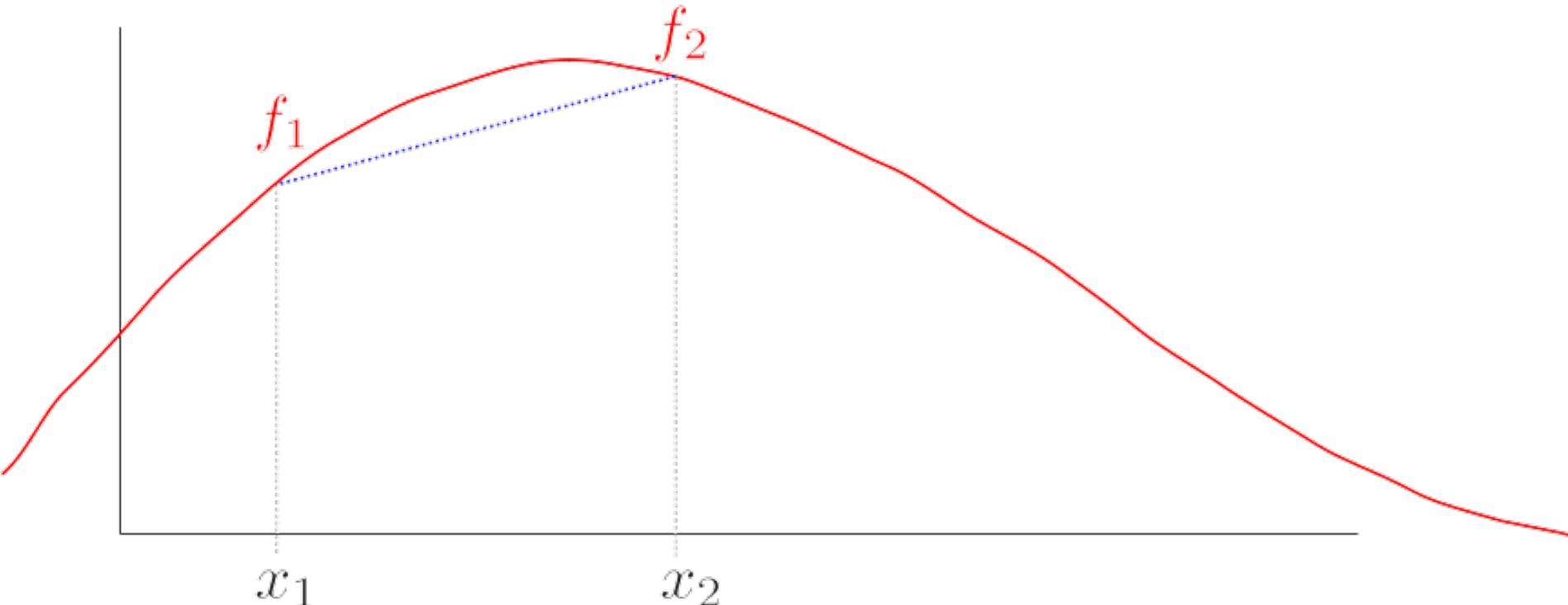
- Finish discussing Numerical Integration
- Begin discussing interpolation
 - Lagrange Interpolation

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



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

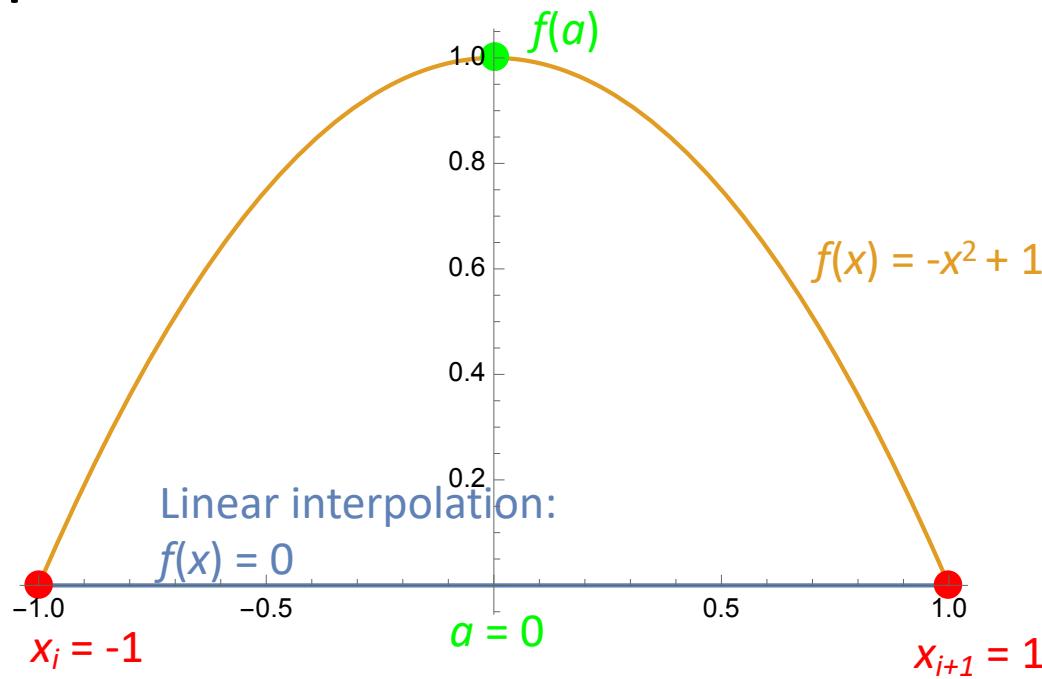
Errors in linear interpolation

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

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

- 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, \dots, x_{n-1} , with associated function values: f_0, f_1, \dots, f_{n-1}

- Construct basis functions:
$$l_i(x) = \prod_{j=0, j \neq i}^{n-1} \frac{x - x_j}{x_i - x_j}$$

- 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:

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

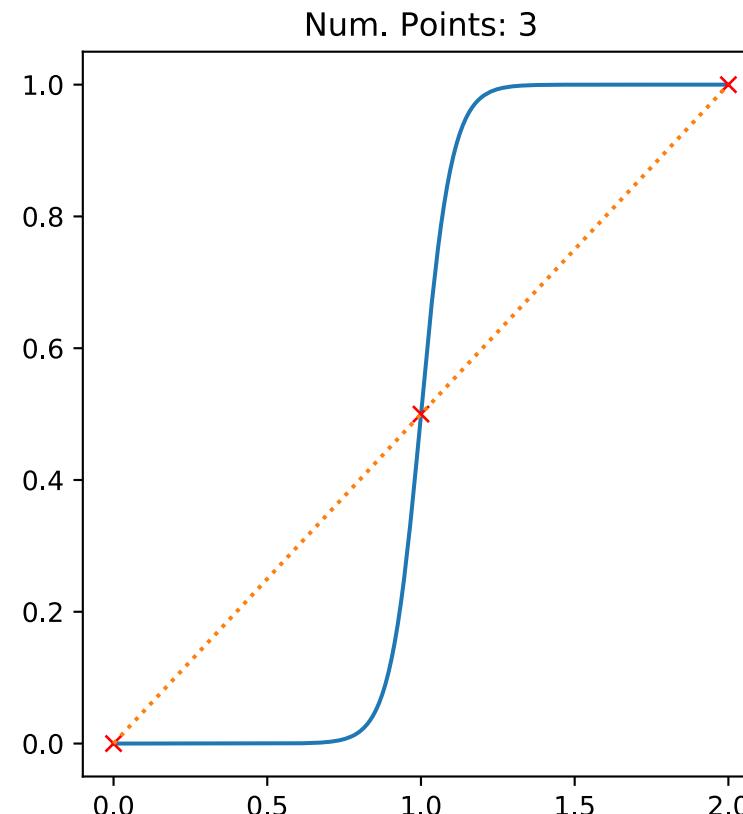
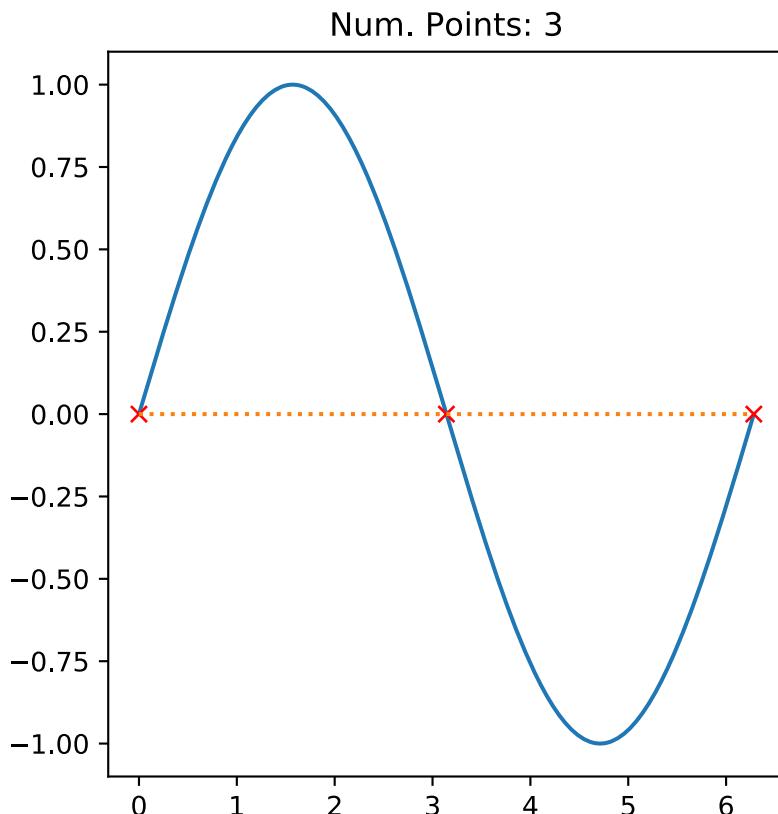
$$l_1 = \frac{x - x_0}{x_1 - x_0} \frac{x - x_2}{x_1 - x_2} = -\frac{(x - x_0)(x - x_2)}{\Delta x^2}$$

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

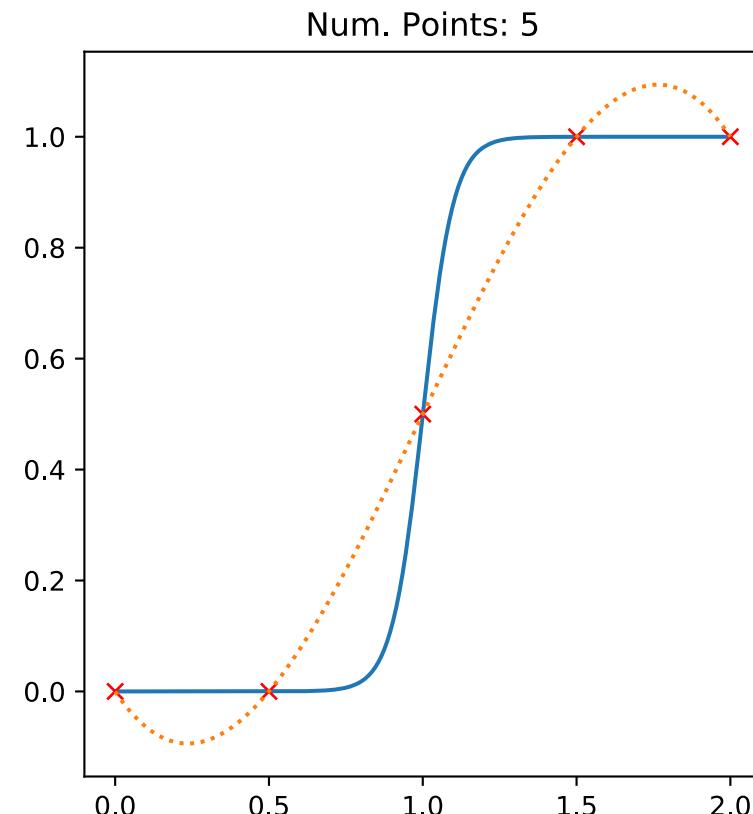
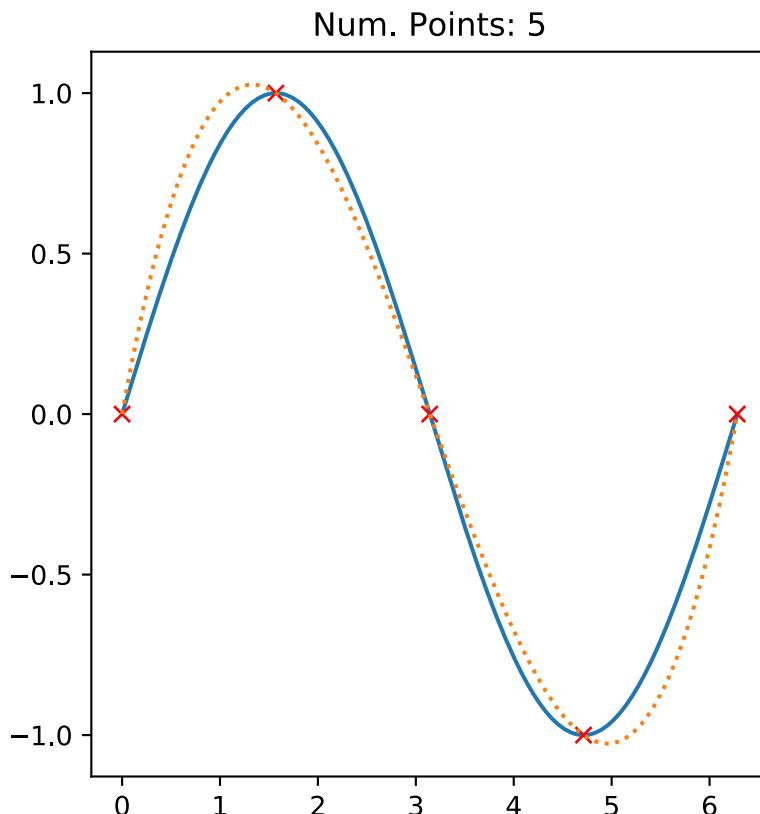
- Polynomial:

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

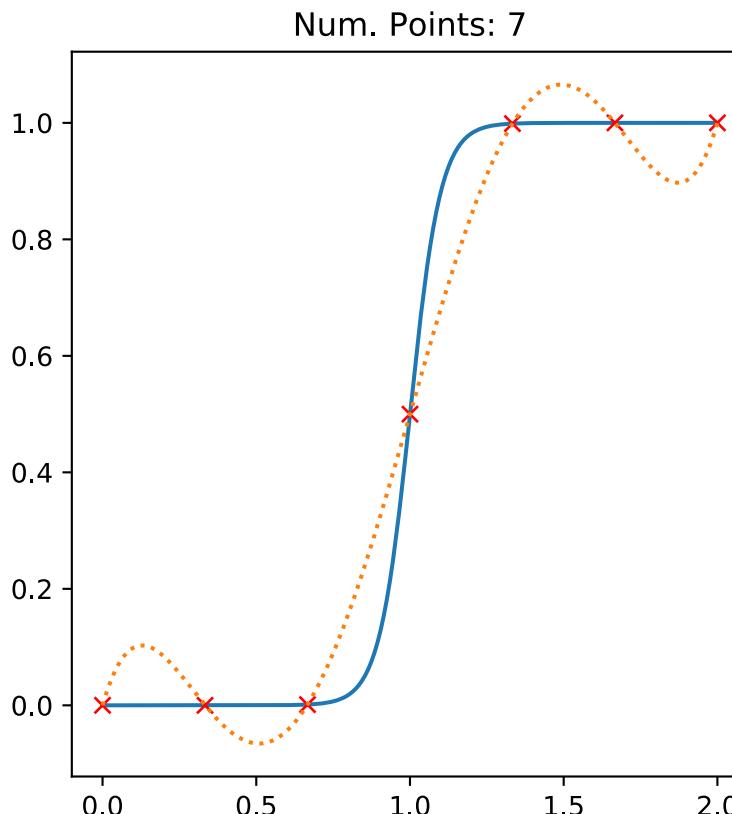
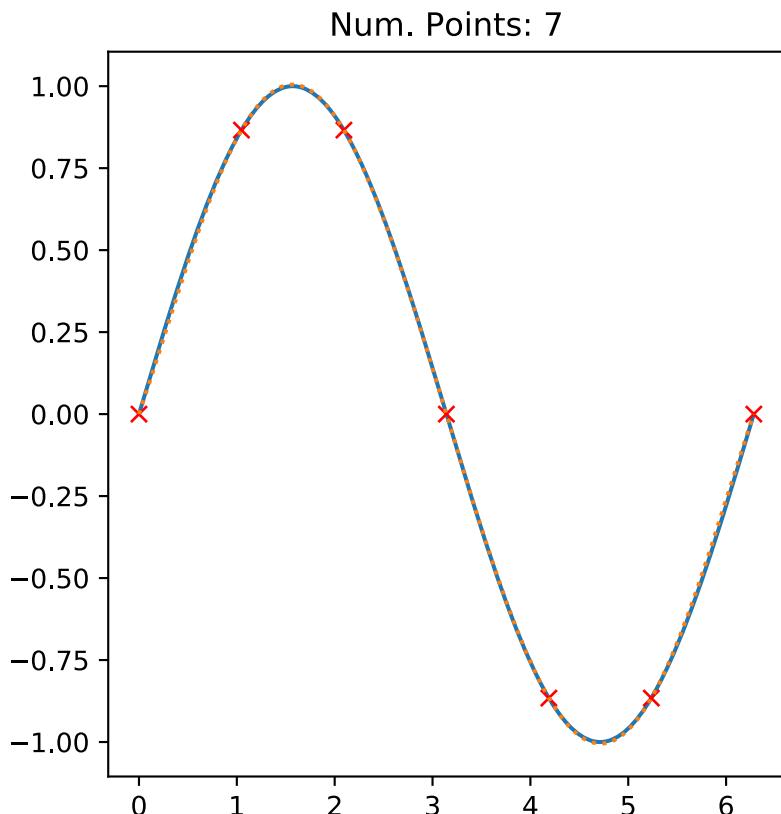
Example: Lagrange Interpolation of two functions



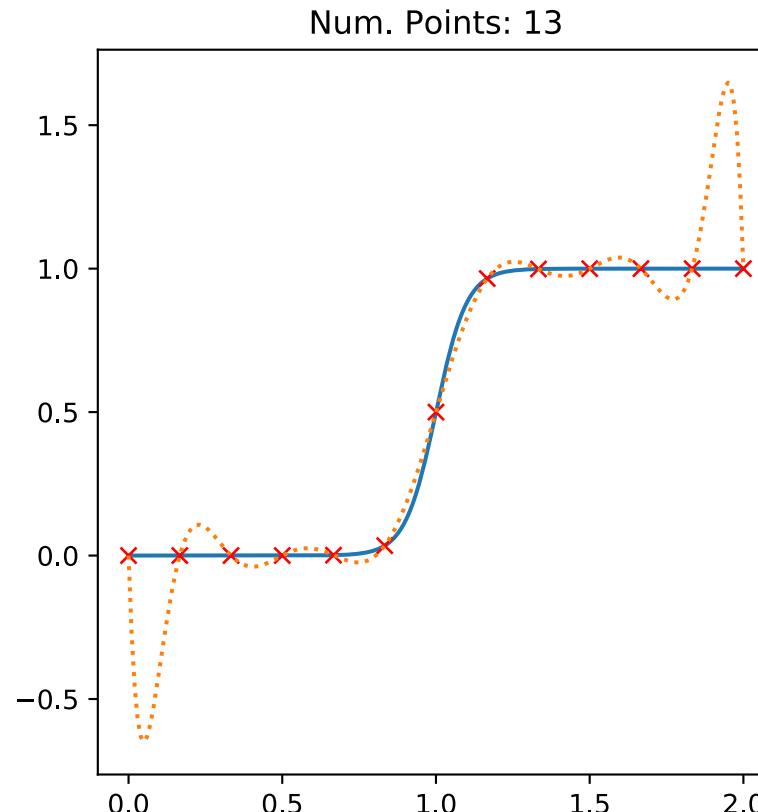
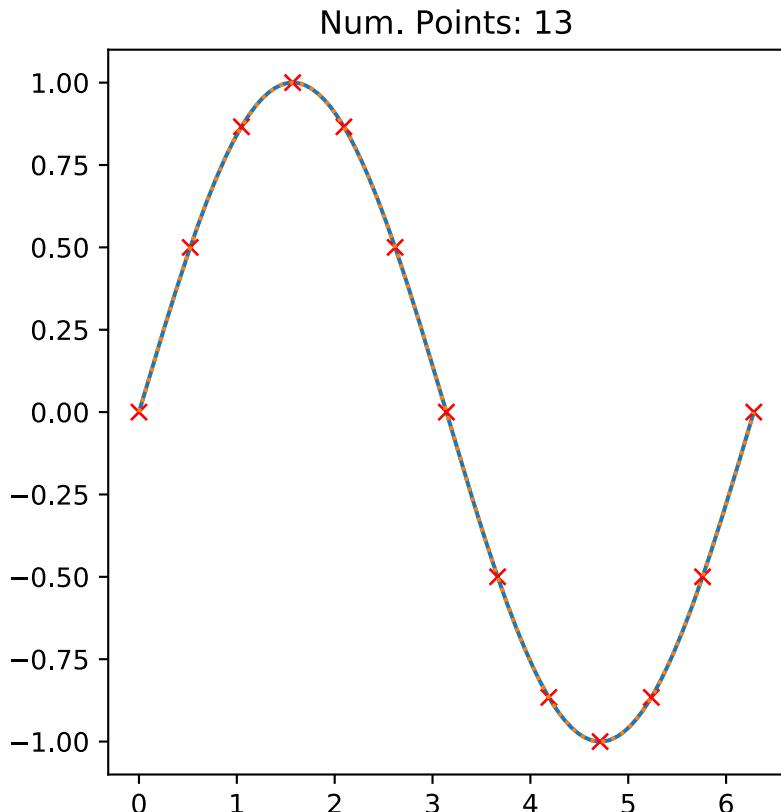
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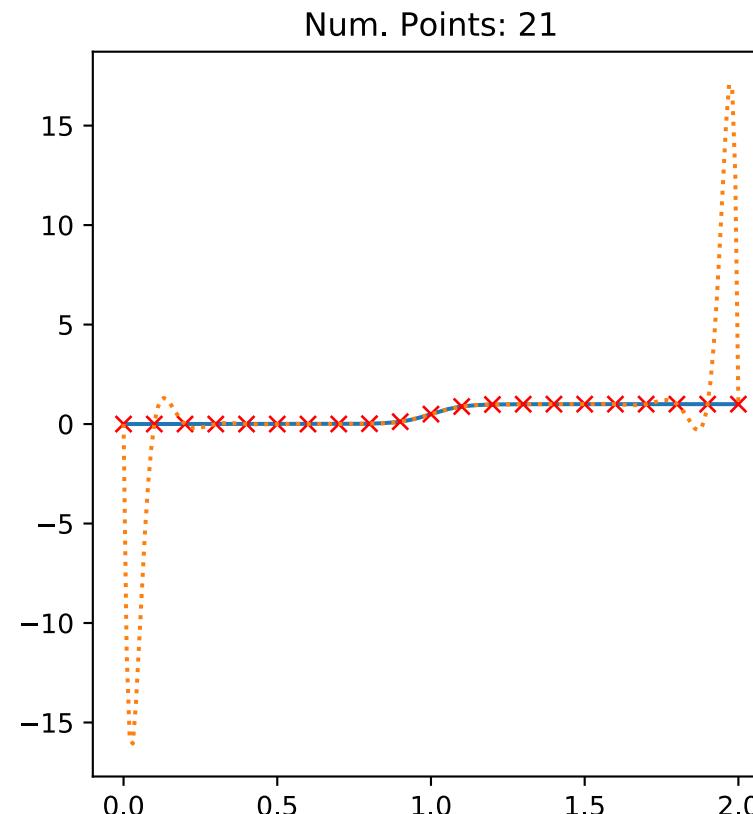
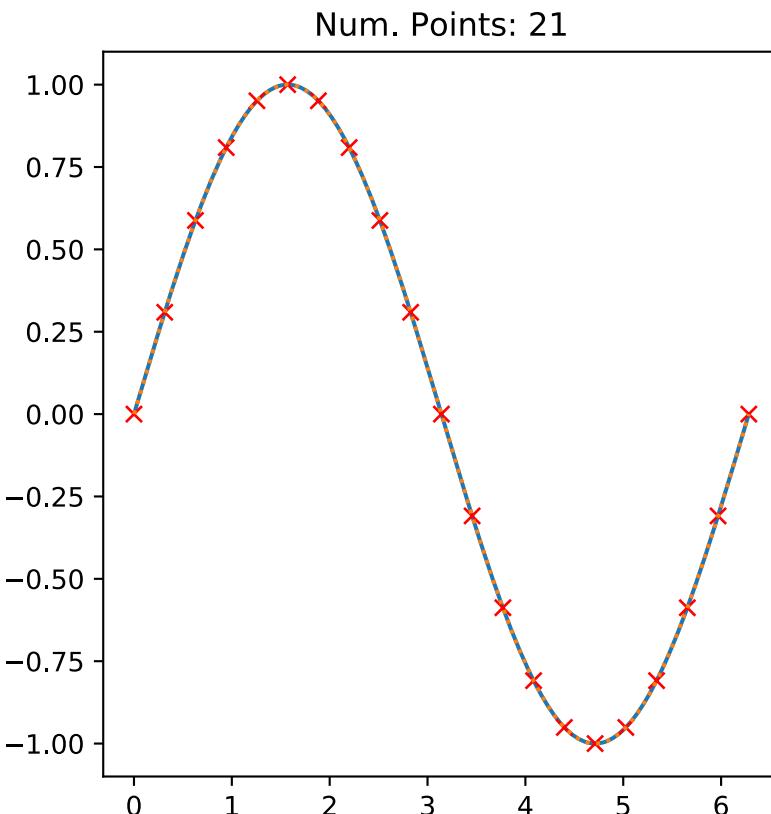
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Example: Lagrange Interpolation of two functions



Example: Lagrange Interpolation of two functions

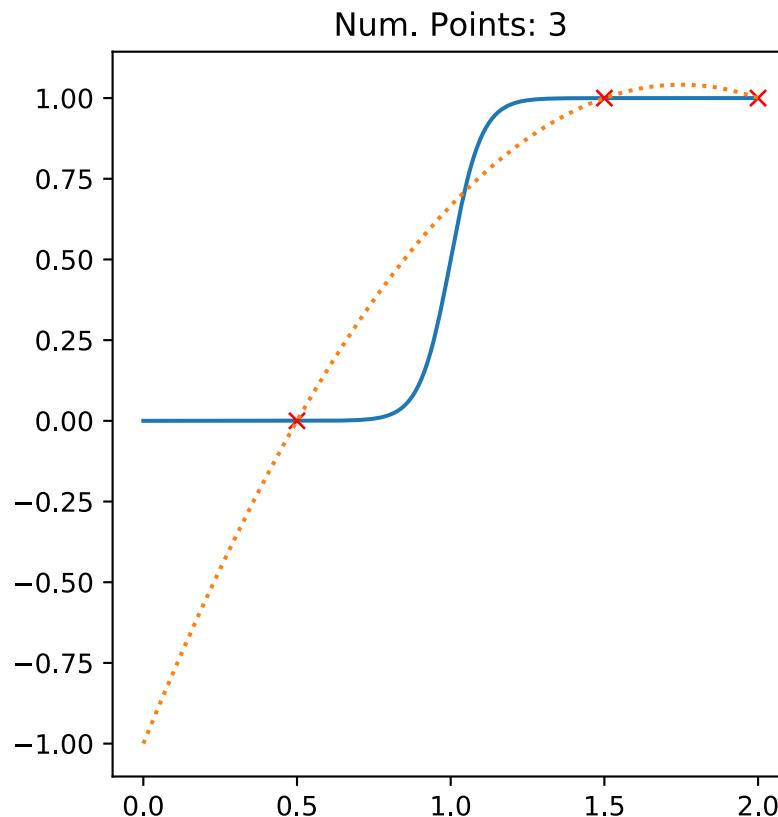
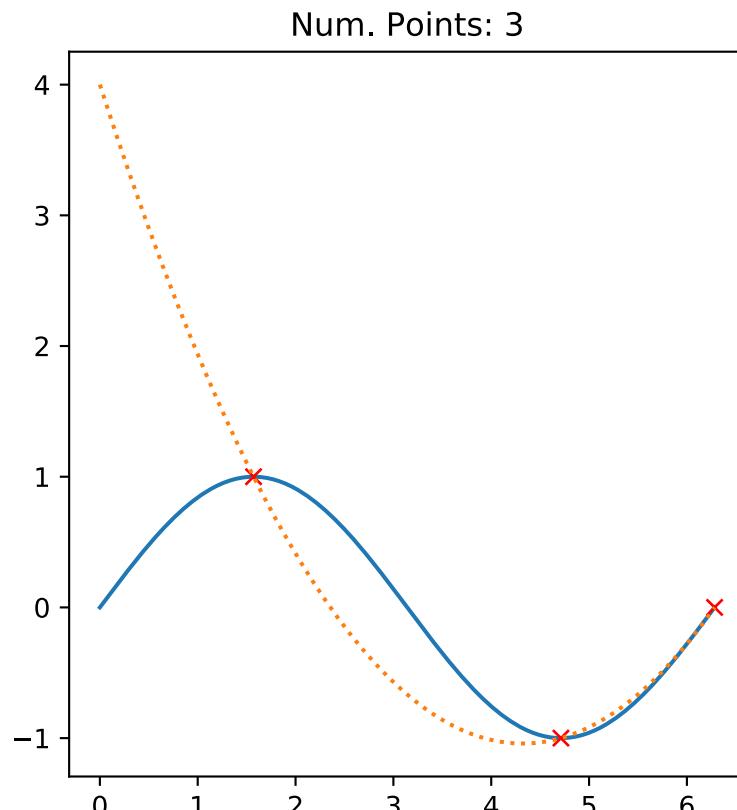


Example: Lagrange Interpolation of two functions

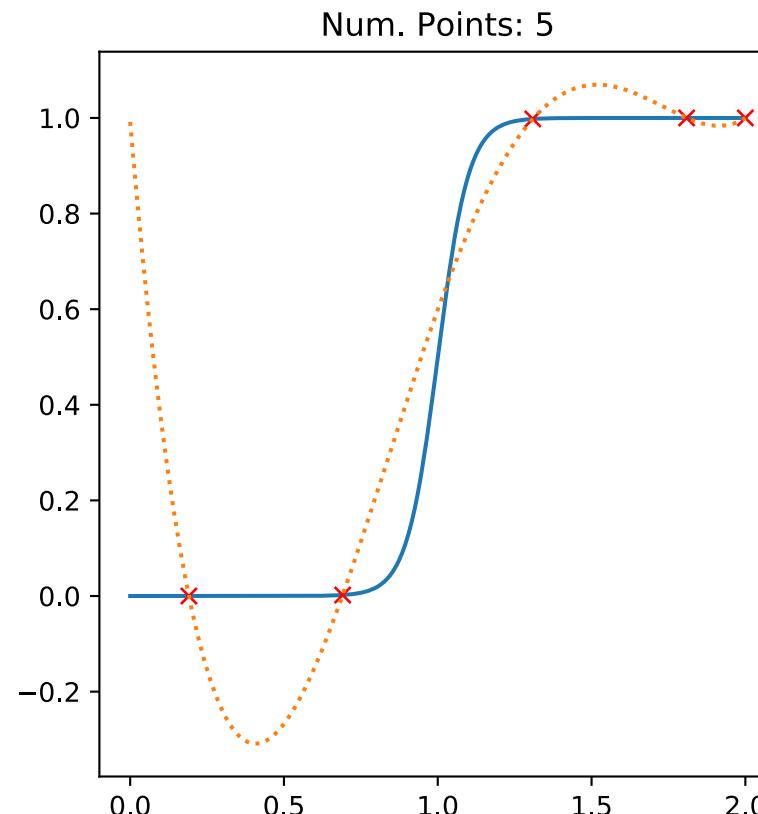
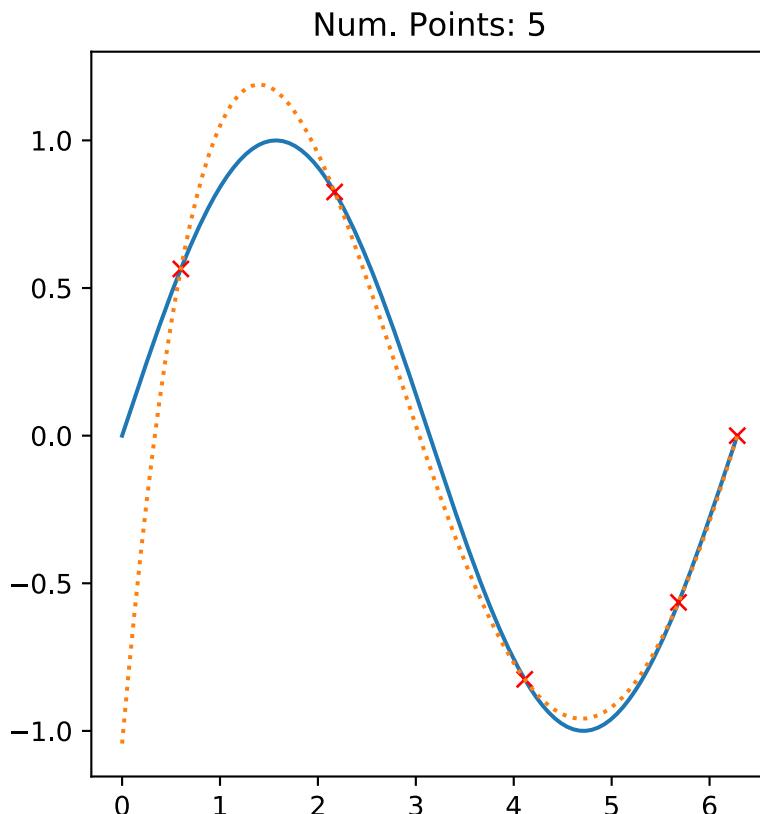
- For the hyperbolic tangent case, increasing the number of points beyond a certain limit increases the error
 - Runge phenomena: Oscillations at the edges of the interval
 - Increasing the number of points causes a divergence in the error
- Can do better by varying the spacing of the interpolating points
 - 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

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

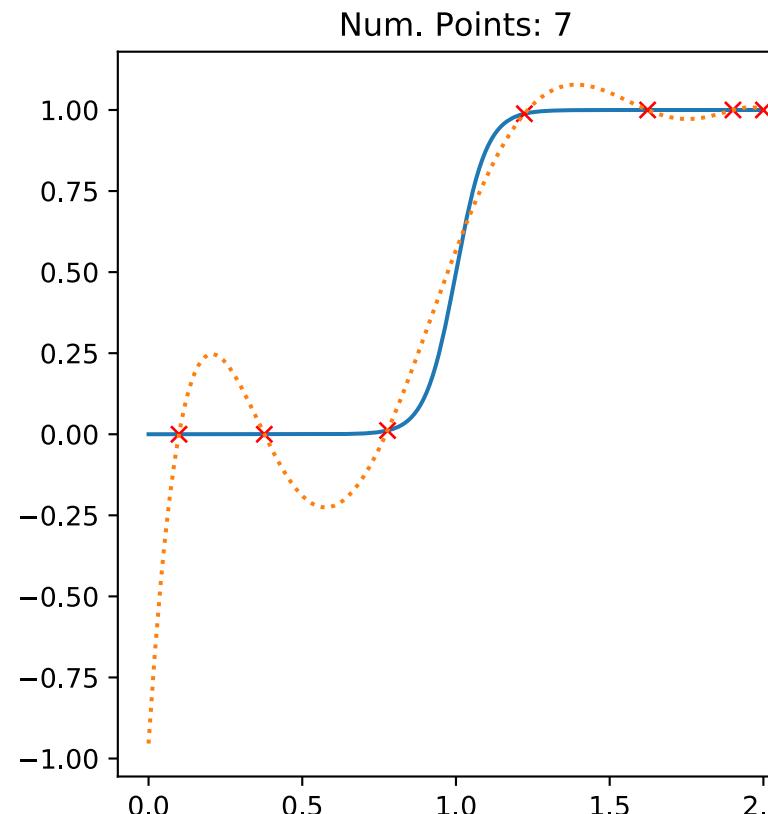
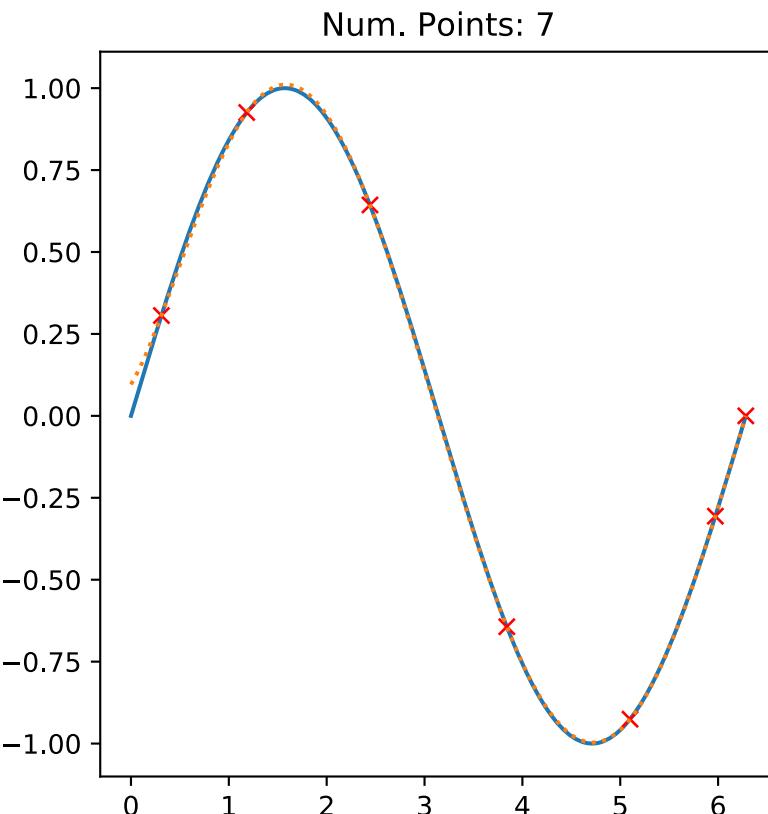
Example: Lagrange Interpolation of two functions with Chebyshev nodes



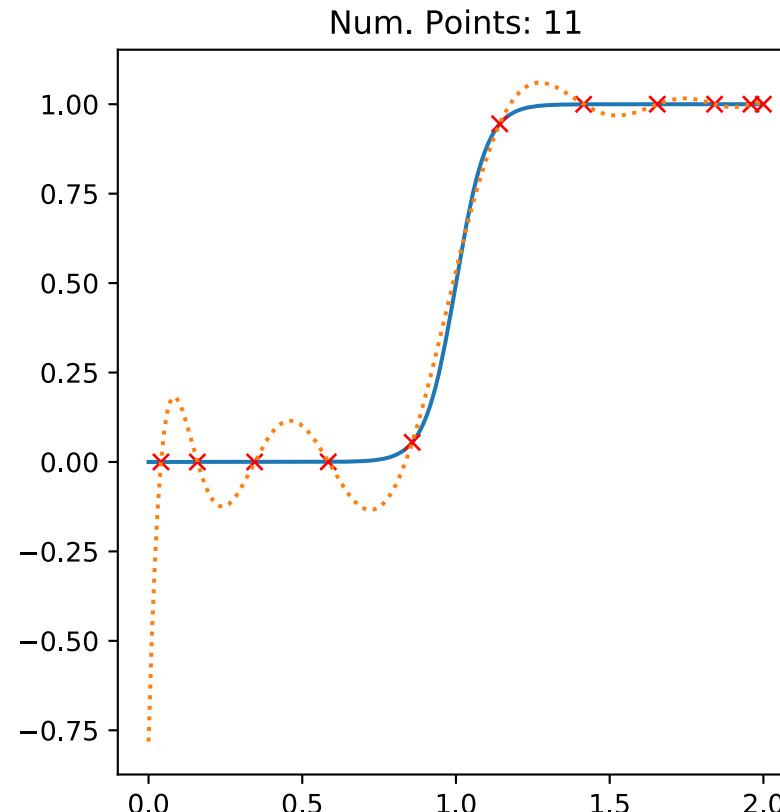
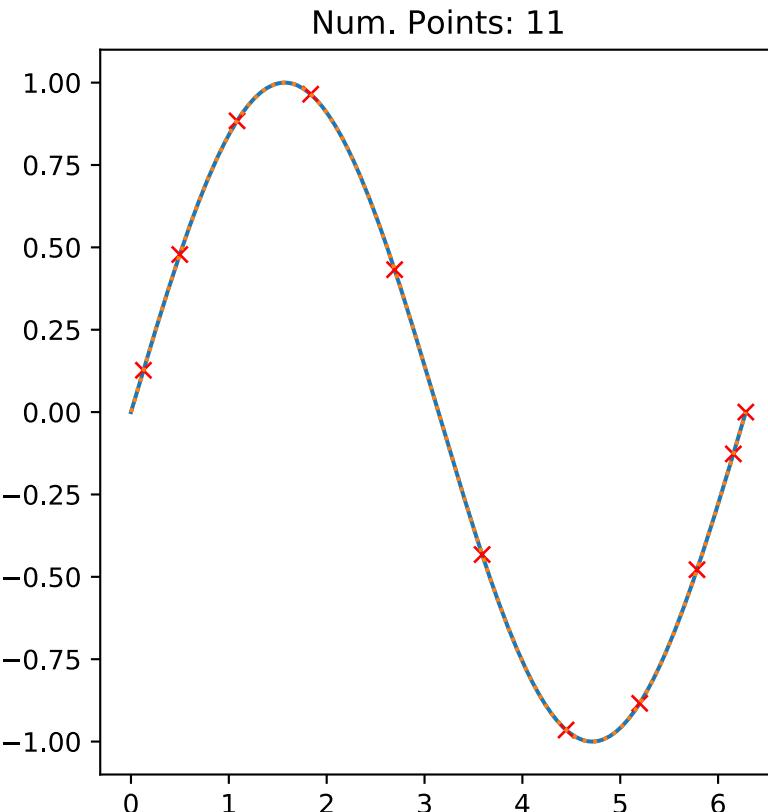
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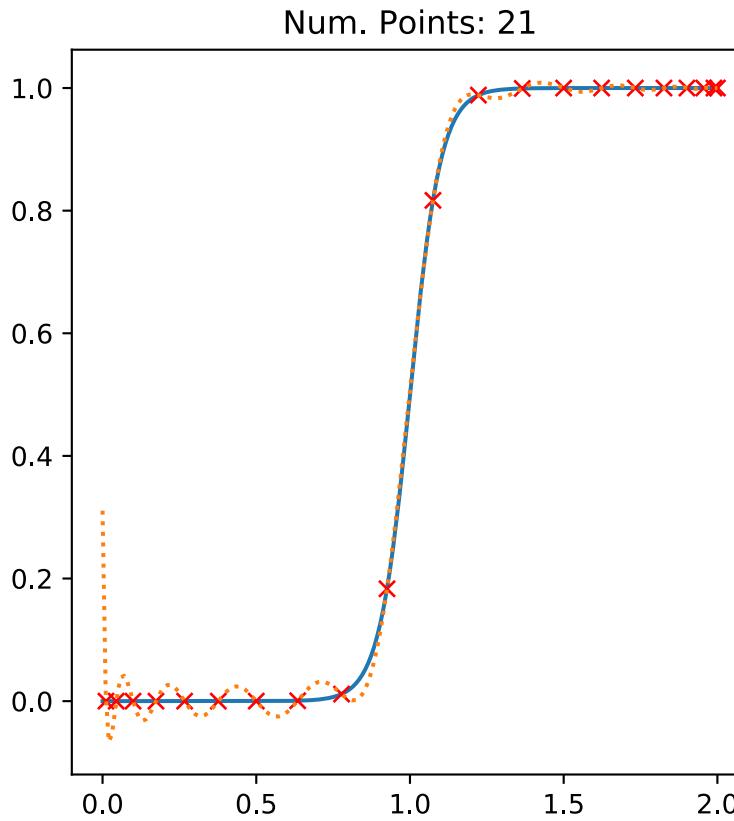
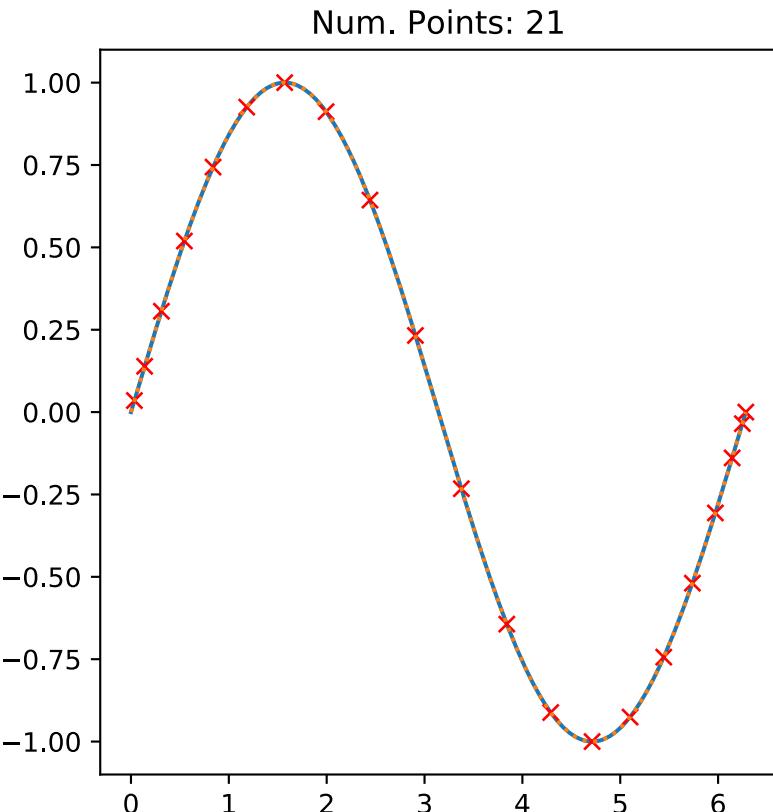
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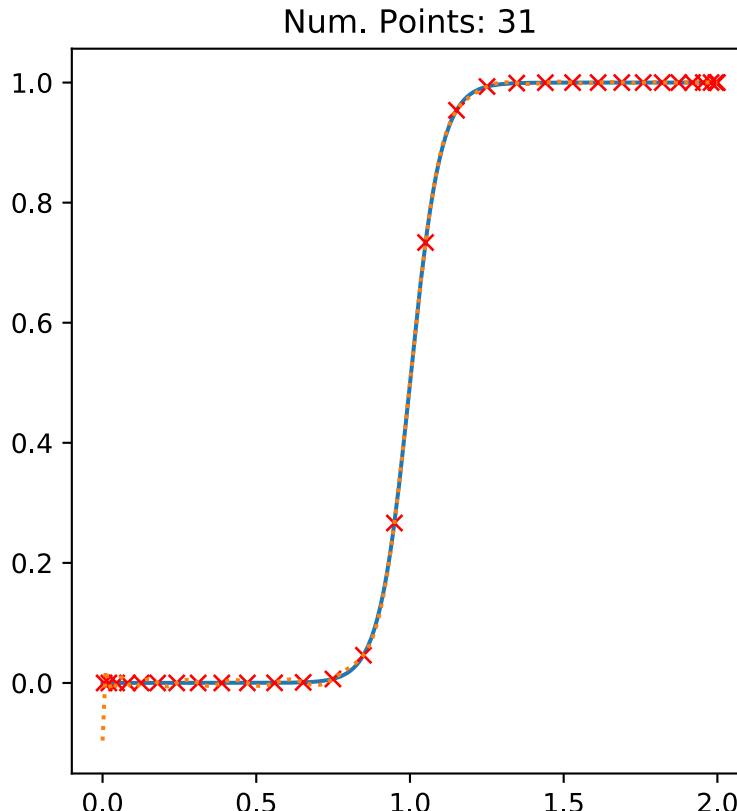
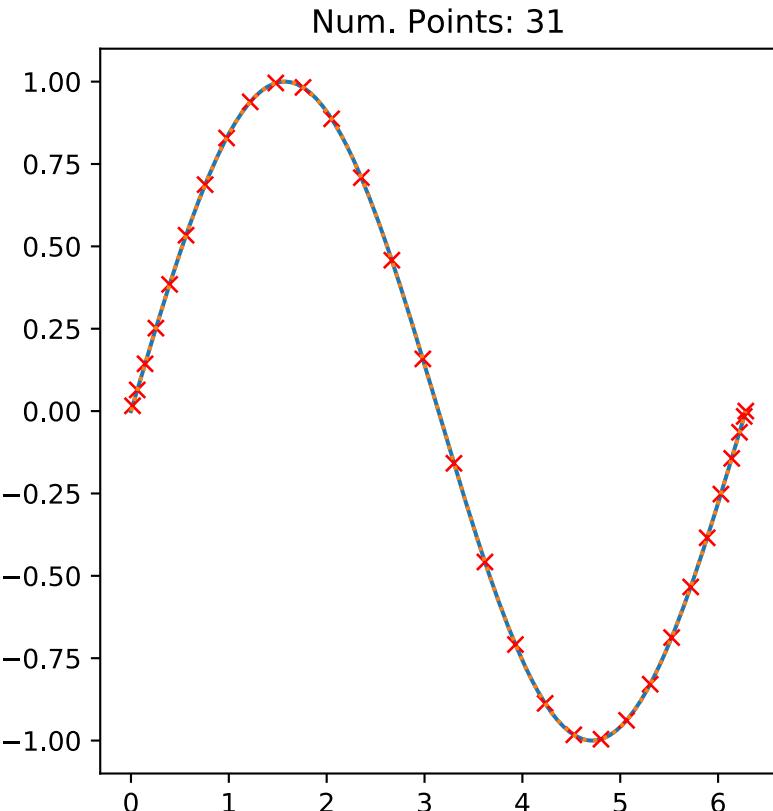
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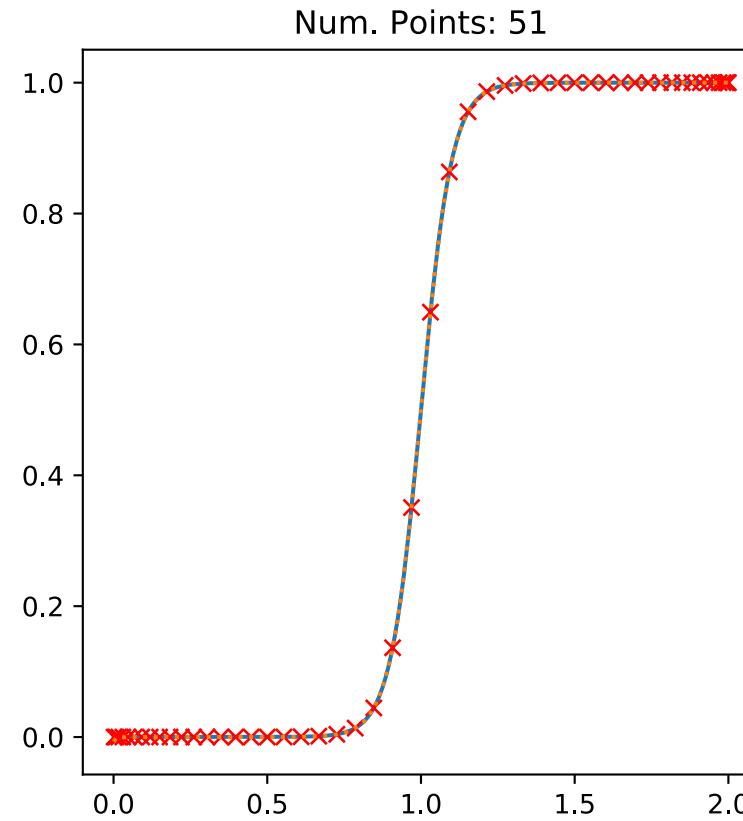
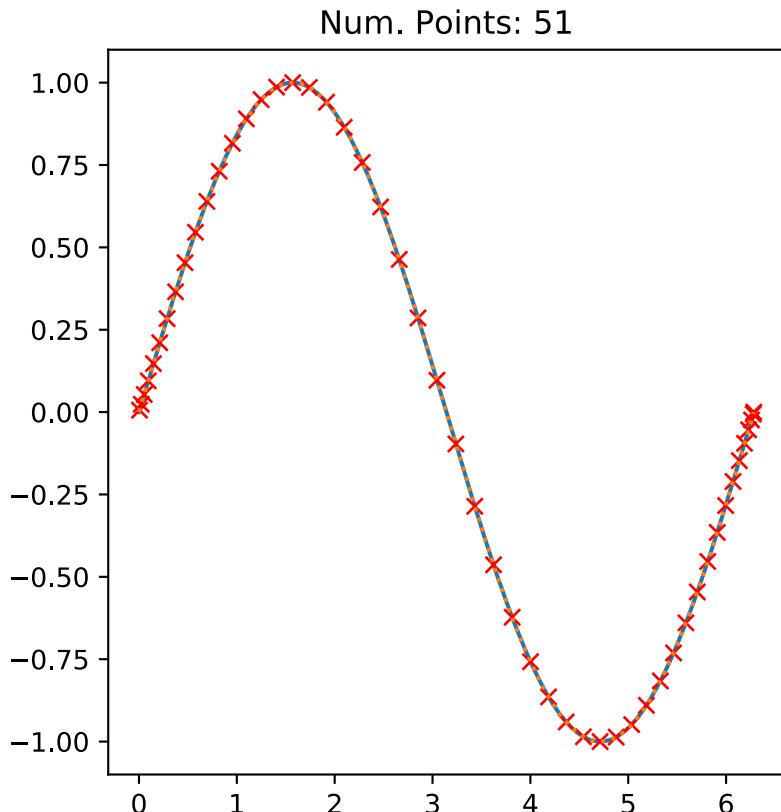
Example: Lagrange Interpolation of two functions with Chebyshev nodes



Example: Lagrange Interpolation of two functions with Chebyshev nodes



Example: Lagrange Interpolation of two functions with Chebyshev nodes



After class tasks

- Homework and instructions for turning it in are posted
 - Due **Sept. 21, 2023**
- Readings:
 - Newman Chapter 5
 - Garcia Section 10.2
 - Pang Section 2.1
 - [Wikipedia article on Chebyshev nodes](#)
 - [Myths about polynomial interpolation](#)