PHY604 Lecture 6

September 19, 2023

Review:
3 point Gauss-Legendre quadrature

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

Review: Gauss-Legendre quadrature

- From Newman Sec. 5.6:

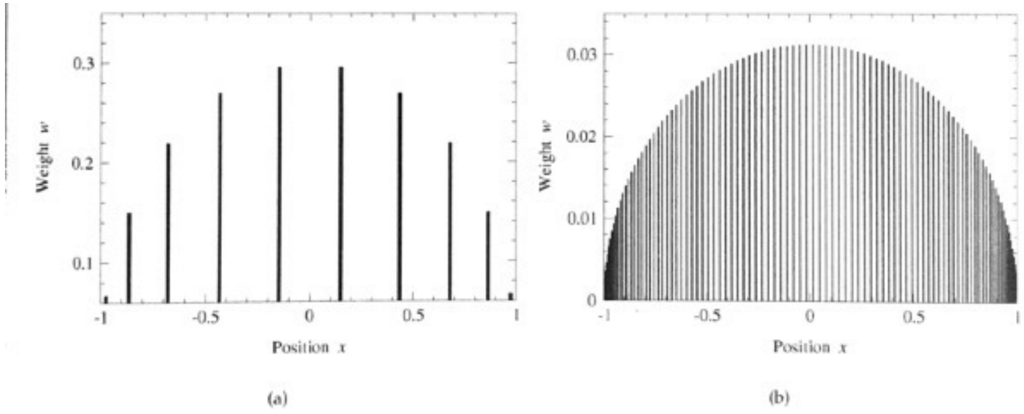


Figure 5.4: Sample points and weights for Gaussian quadrature. The positions and heights of the bars represent the sample points and their associated weights for Gaussian quadrature with (a) $N = 10$ and (b) $N = 100$.

- 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

Review: 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

Review: 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, ... , x_{n-1}, with associated function values: f_0, f_1, ..., 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: $$f(x) = \sum_{i=0}^{n-1} l_i(x) f_i$$

Review: 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:

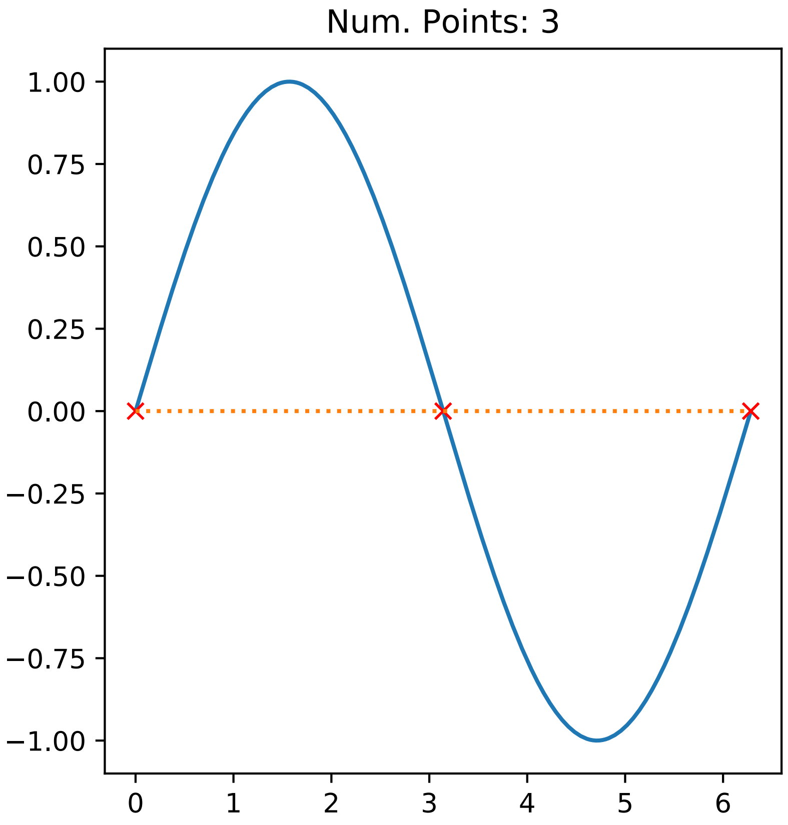
$$f(x) = f_0\frac{(x-x_1)(x-x_2)}{2\Delta x^2} - f_1\frac{(x-x_0)(x-x_2)}{\Delta x^2} + f_2\frac{(x-x_0)(x-x_1)}{2\Delta x^2}$$

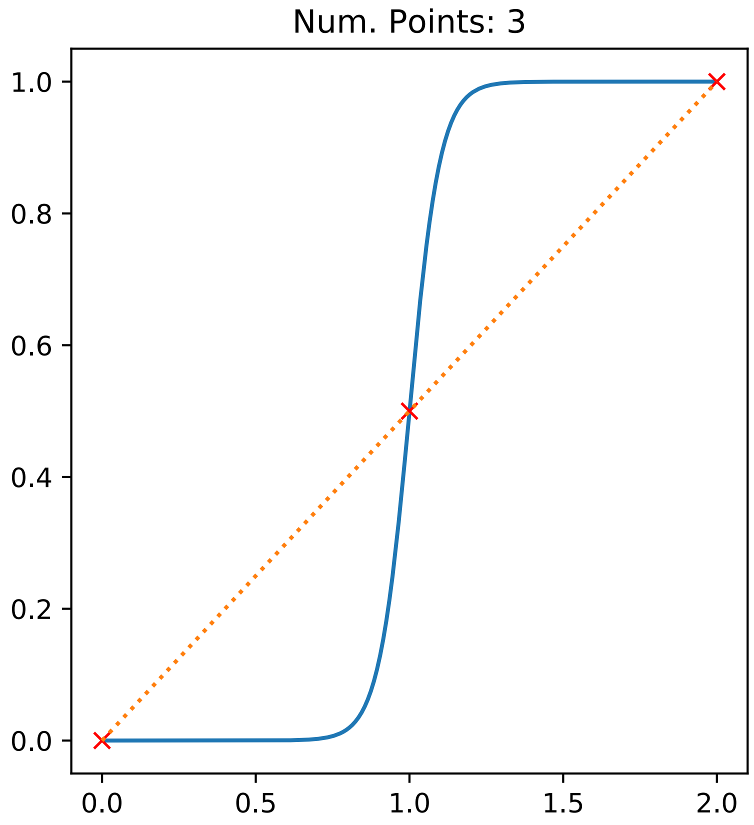
D

Today’s lecture:

- Continue discussing interpolation
    - Lagrange Interpolation
    - Cubic splines
- Begin discussing finding roots of functions
    - Bisection method
    - Newton Raphson method
    - Secant method

Example: Lagrange Interpolation of two functions





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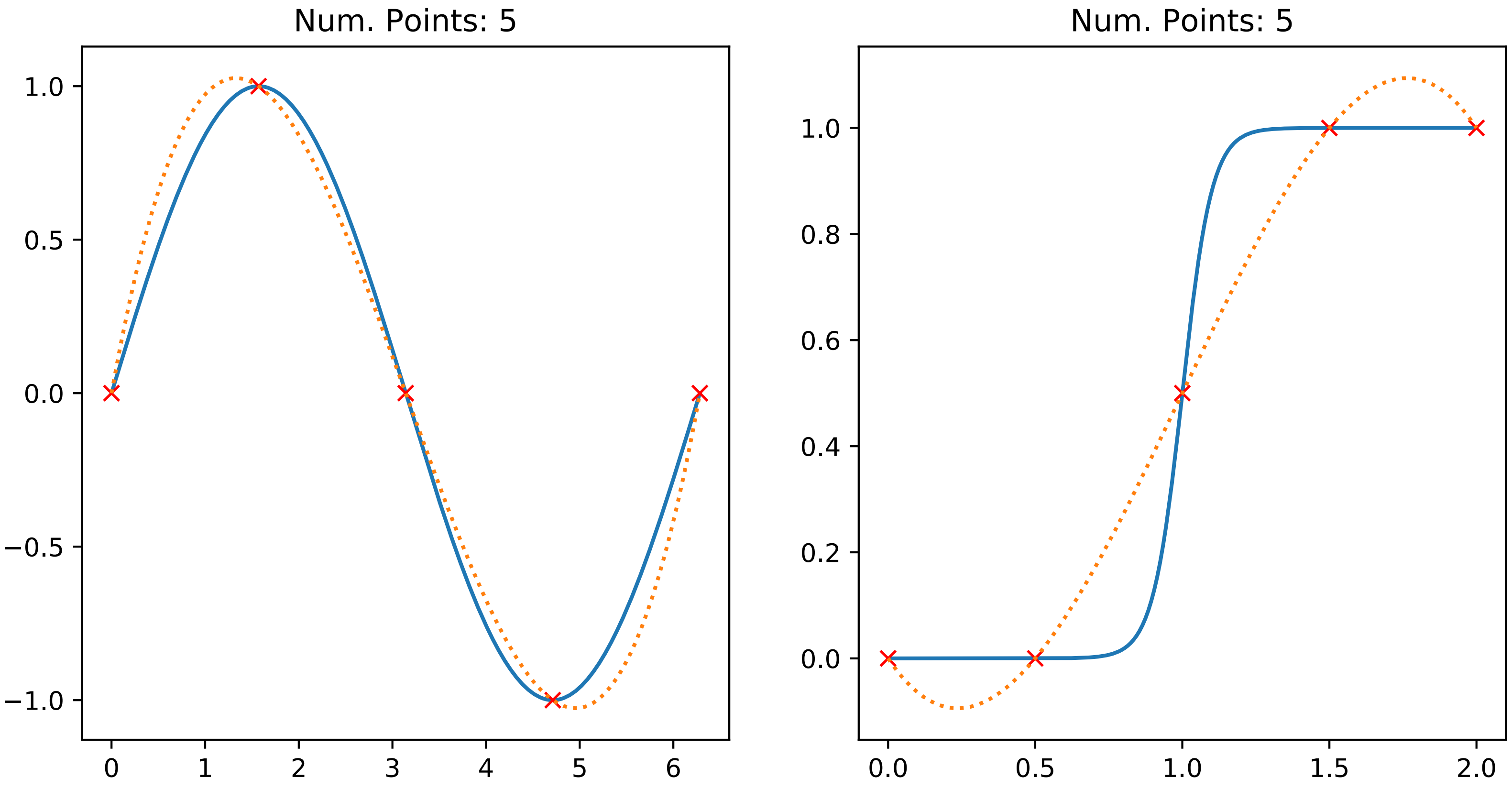

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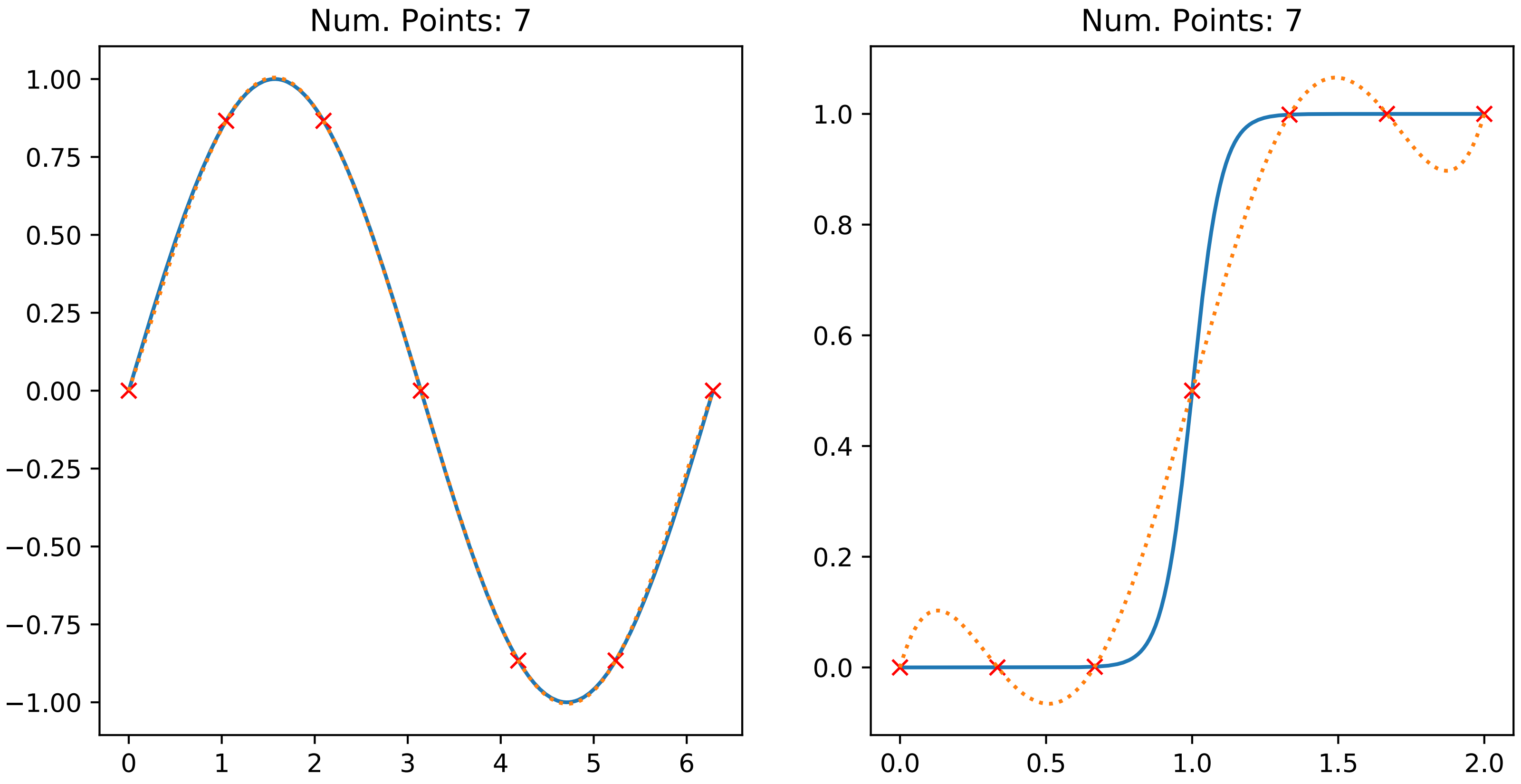

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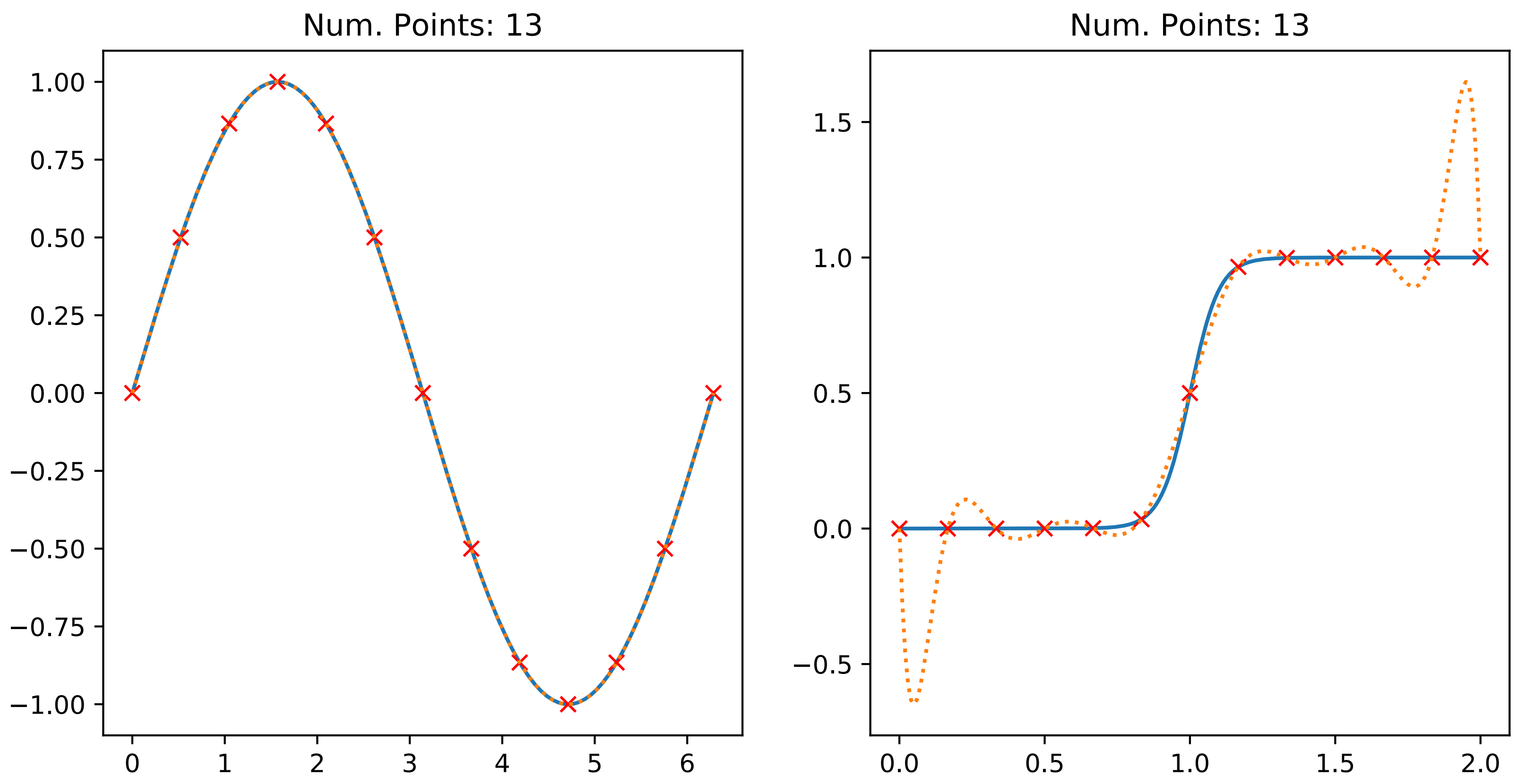

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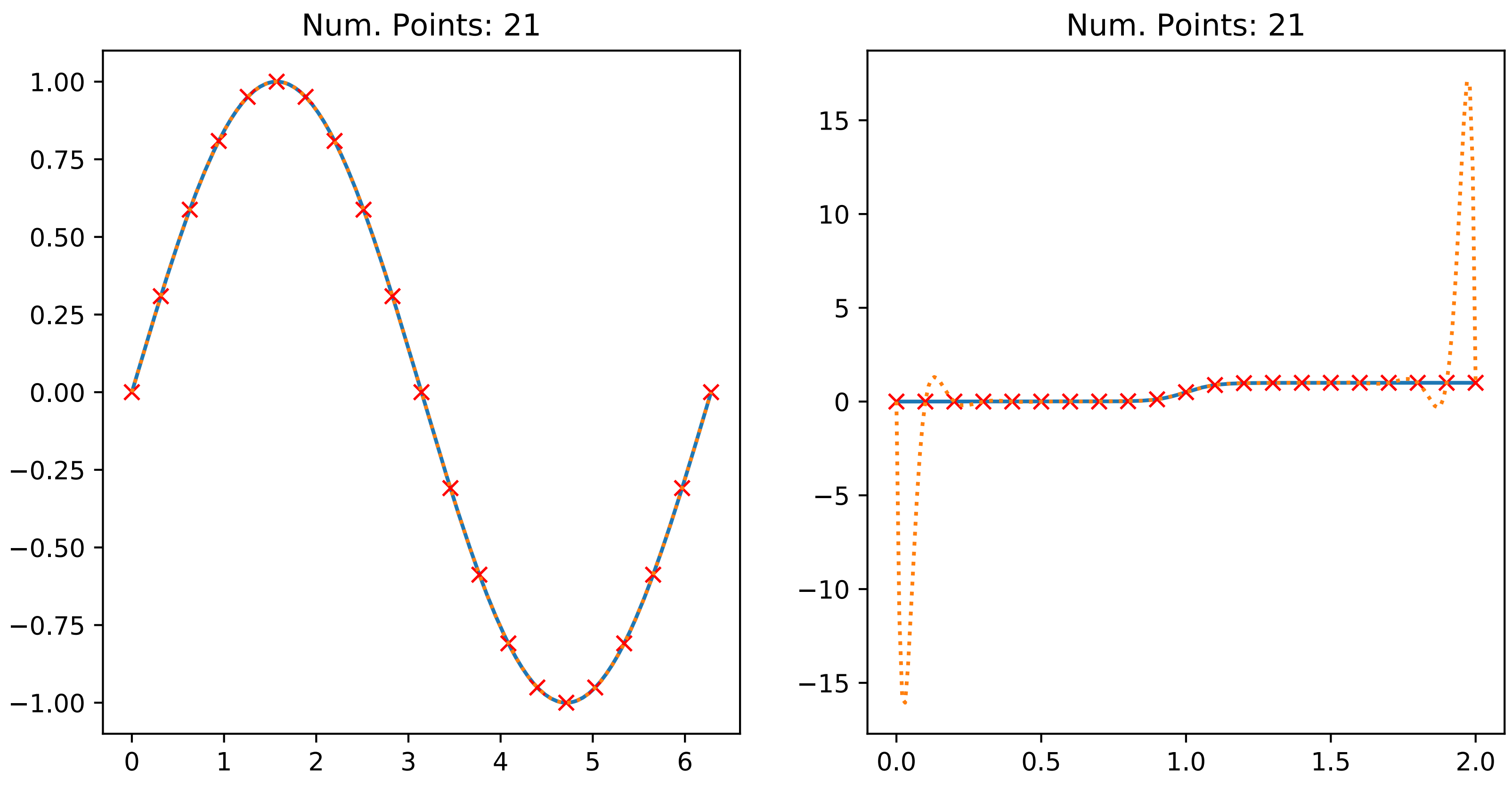
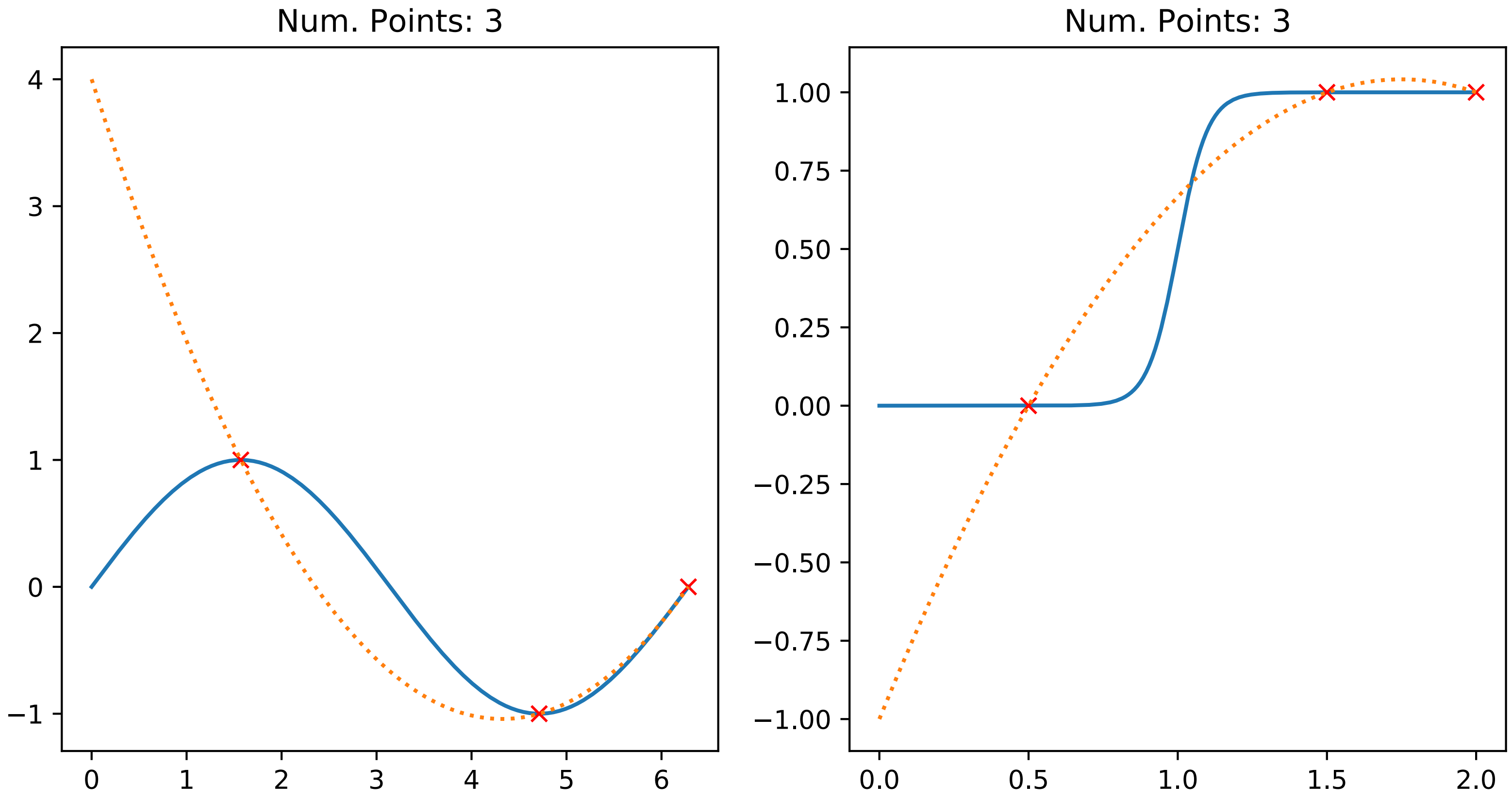


Example: Lagrange Interpolation of two functions with Chebyshev spacing

- 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

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

Example: Lagrange Interpolation of two functions with Chebyshev nodes



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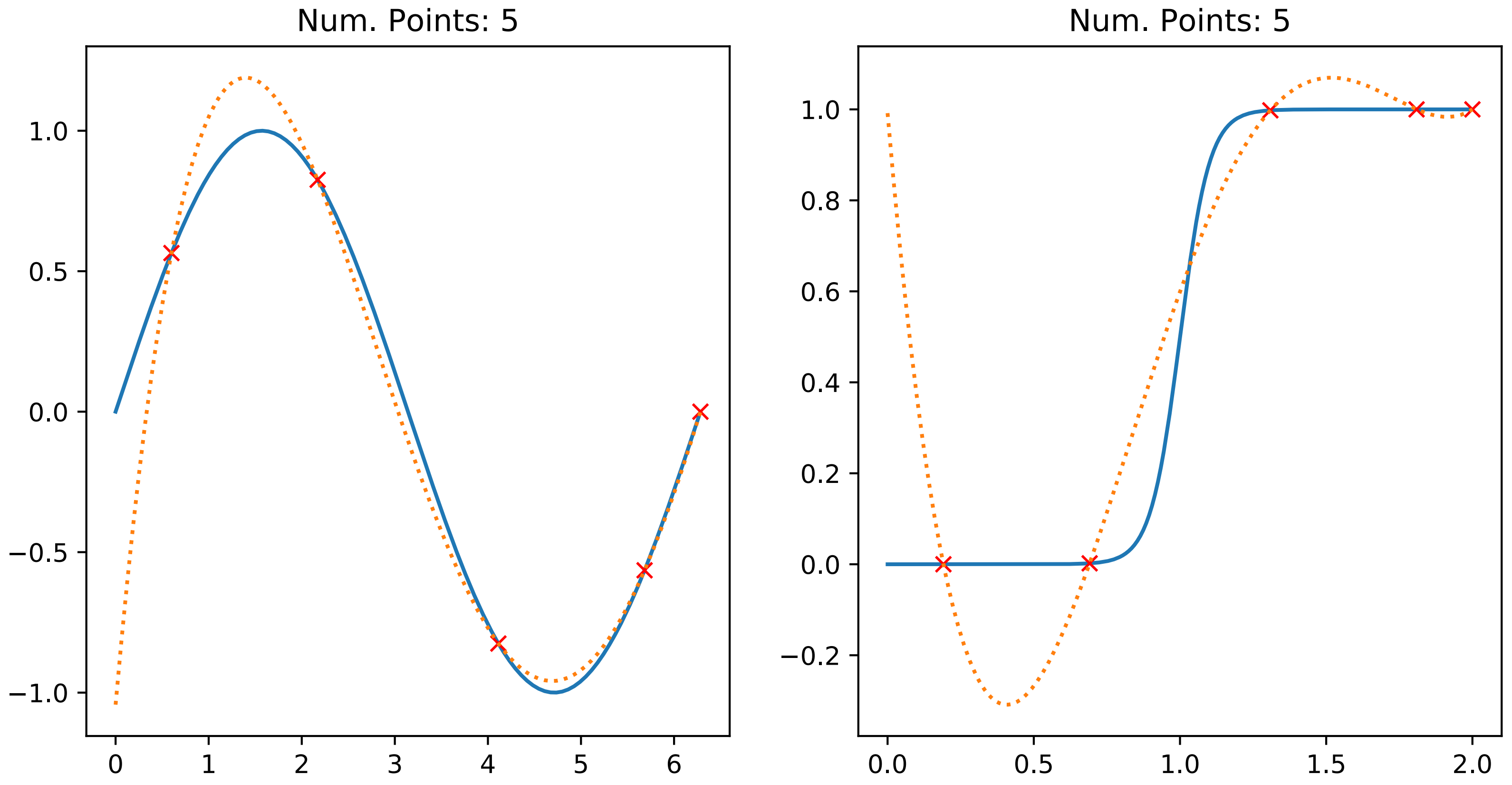

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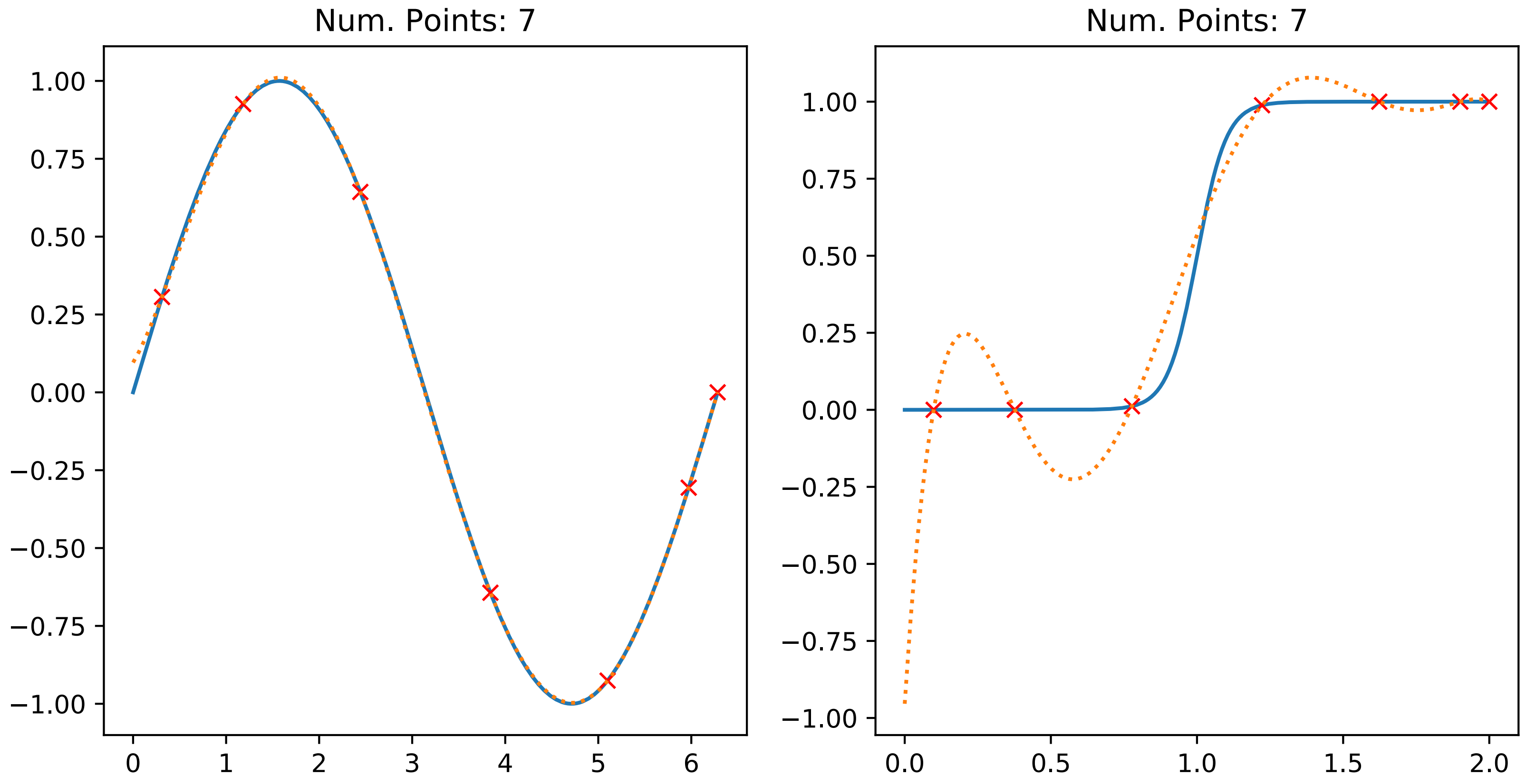

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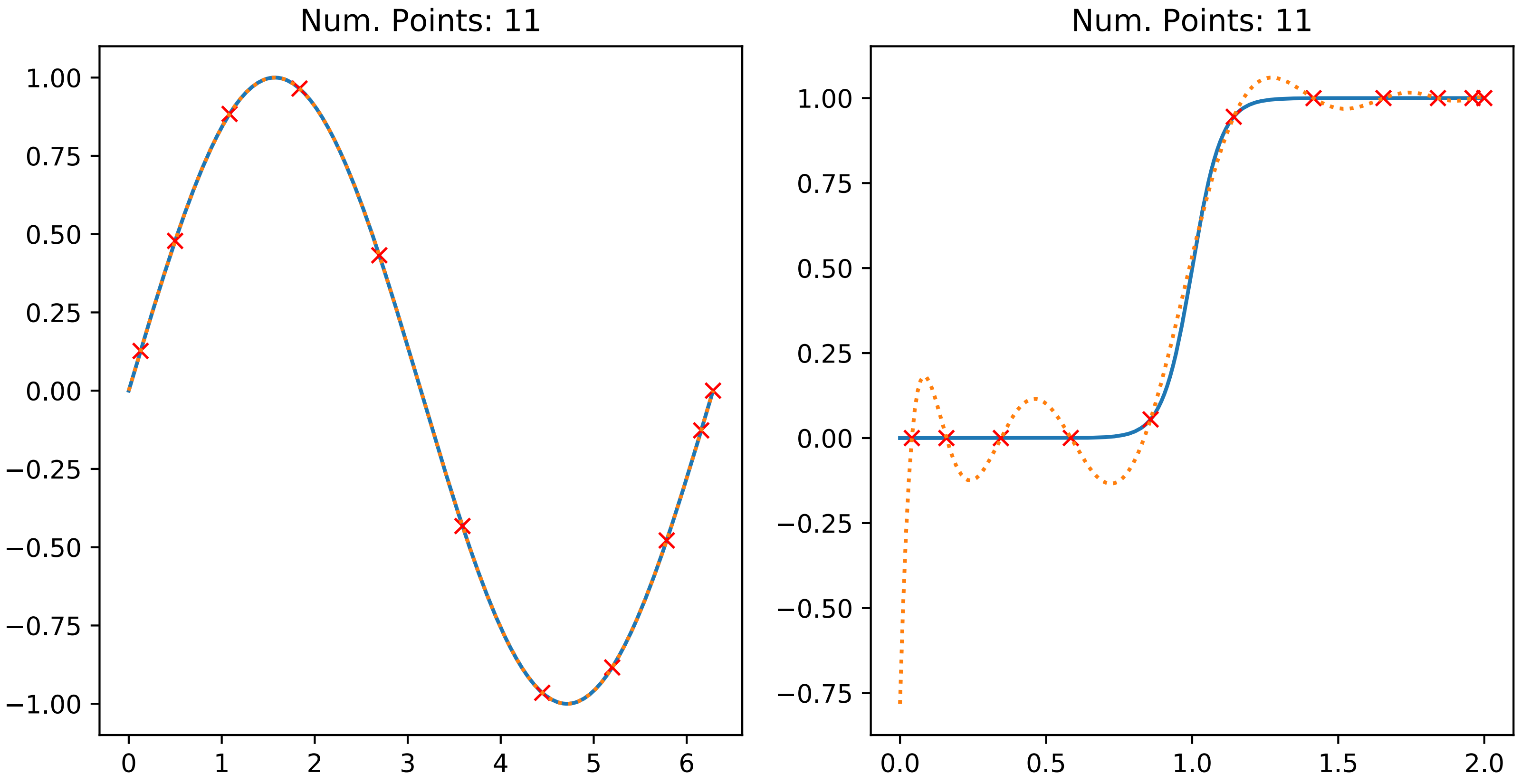

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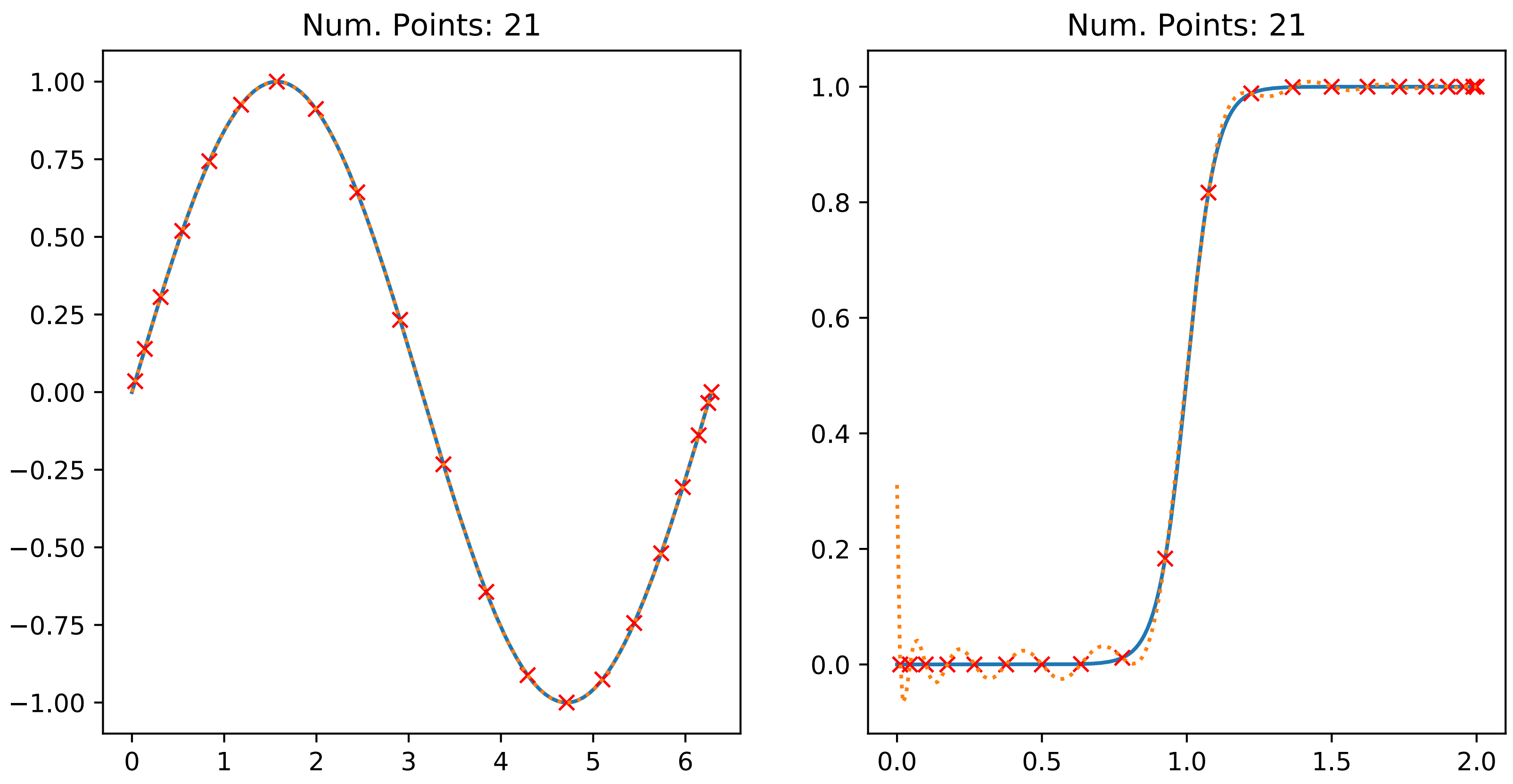

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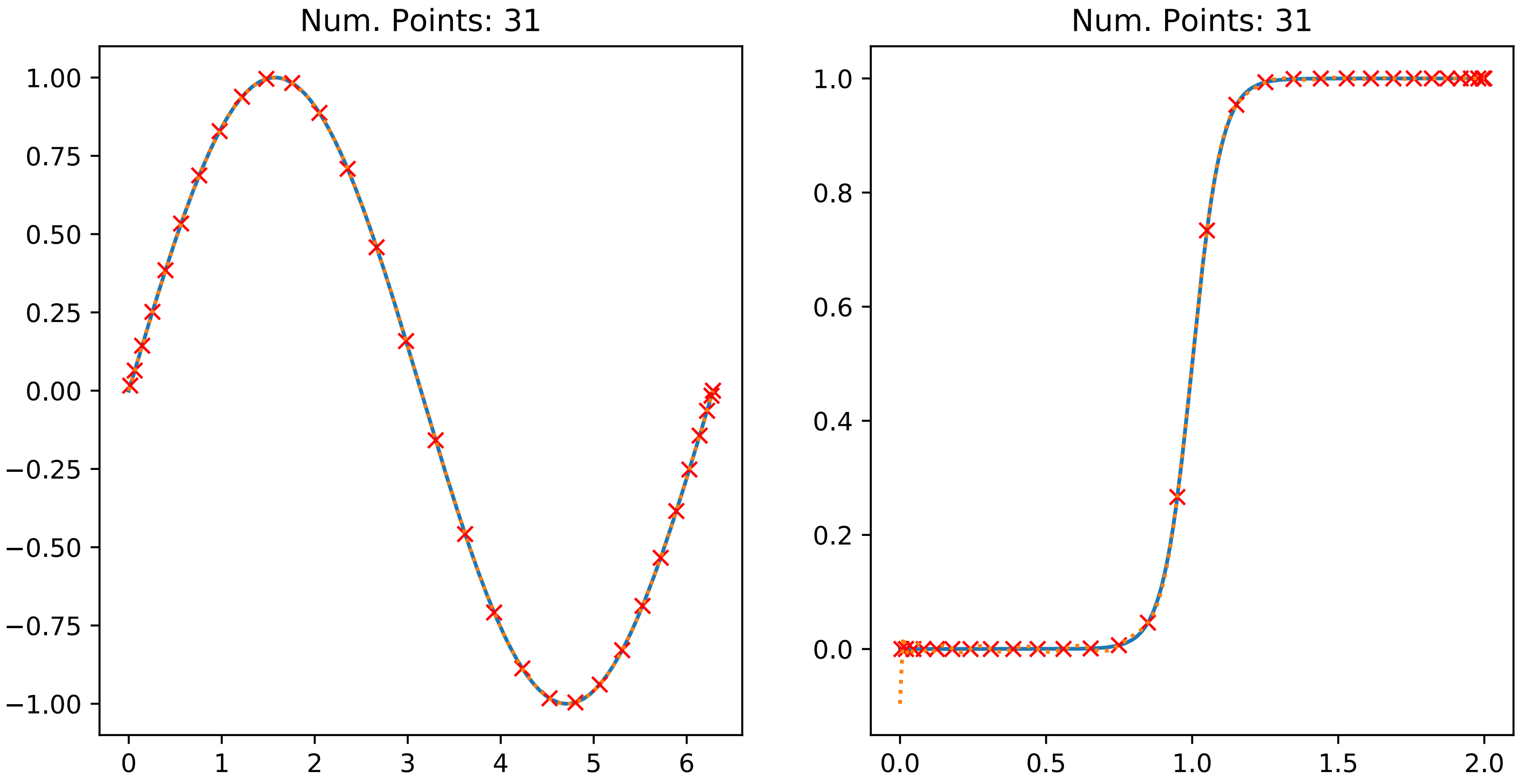

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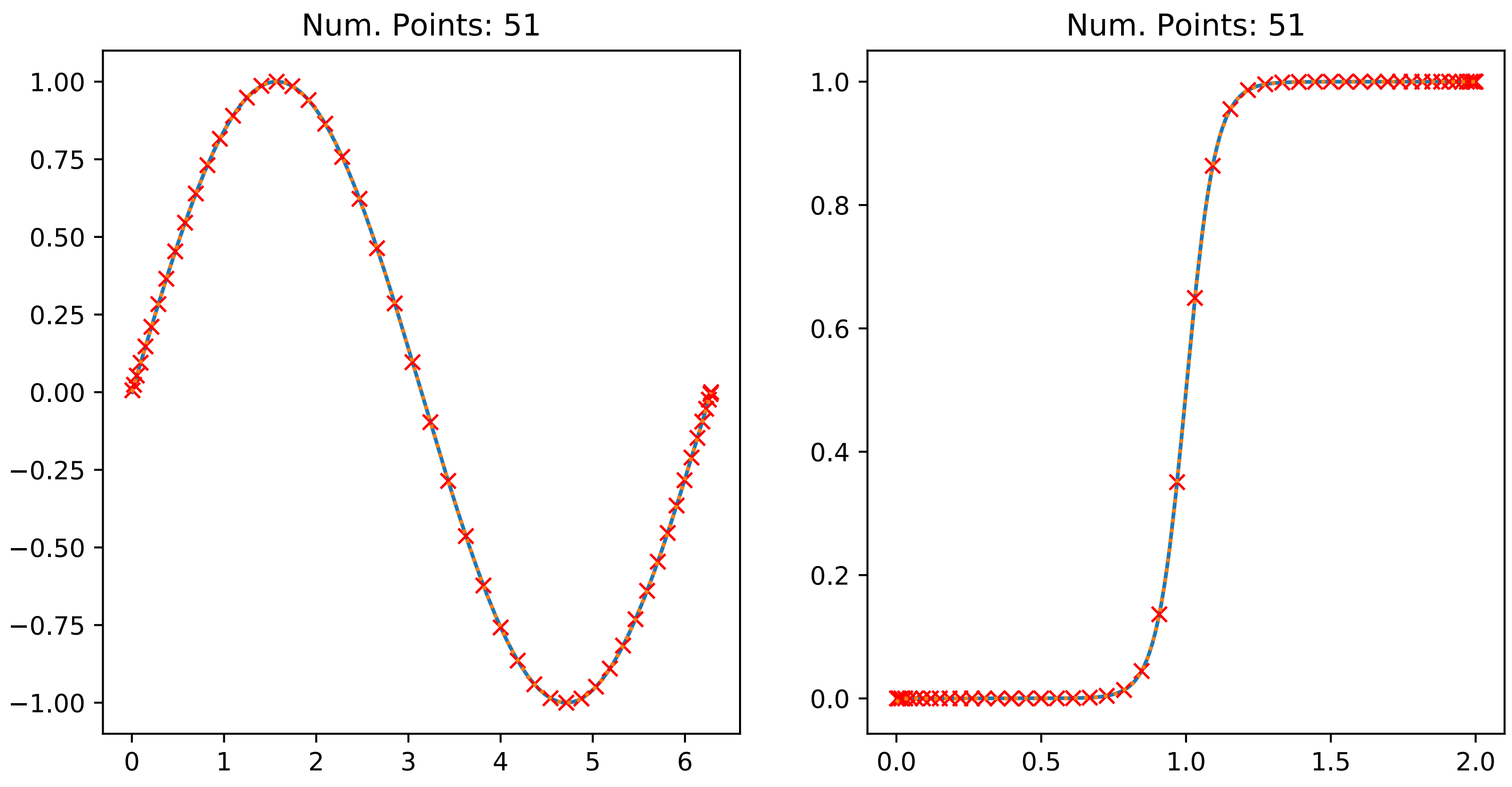


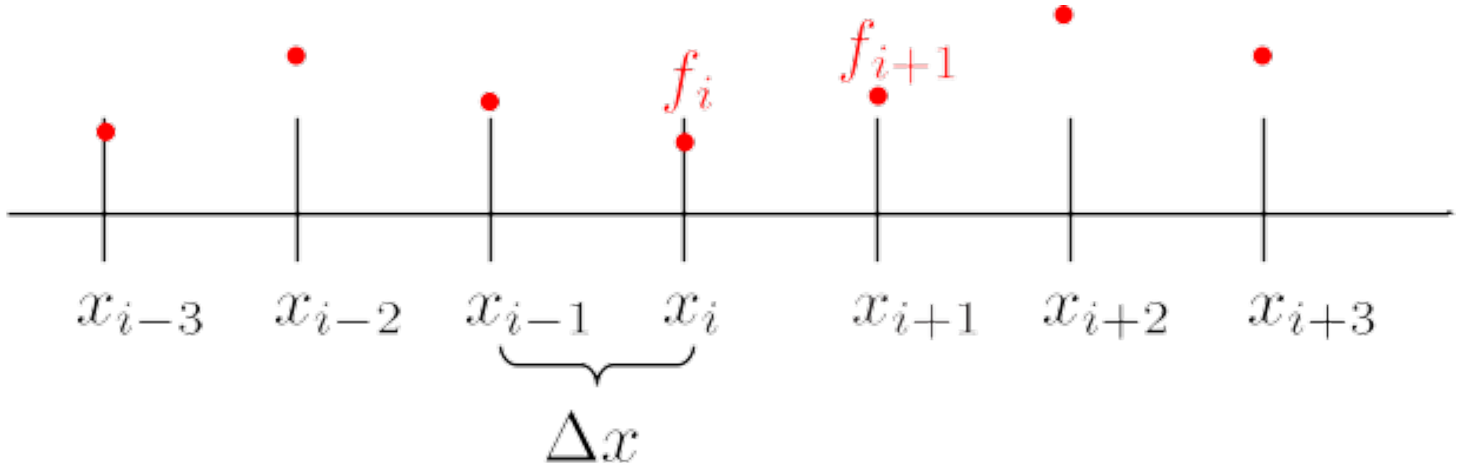
Today’s lecture:

- Continue discussing interpolation
  - Lagrange Interpolation
  - Cubic splines
- Begin discussing finding roots of functions
  - Bisection method
  - Newton Raphson method
  - Secant method

Splines (Pang Sec. 2.4)

- So far, we've only worried about going through the specified points
- Large number of points → two distinct options:
  - Use a single high-order polynomial that passes through them all
  - Fit a (somewhat) high order polynomial to *each interval* and match all derivatives at each point—this is a spline
- Splines match the derivatives at end points of intervals
  - Piecewise splines can give a high-degree of accuracy
- Cubic spline is the most popular
  - Matches first and second derivative at each data point
  - Results in a smooth appearance
  - Avoids severe oscillations of higher-order polynomial

Splines



- We have a set of regular-spaced discrete data: $f_i = f(x_i)$ at $x_0, x_1, x_2, \ldots, x_n$
- m-th order polynomial to approximate $f(x)$ for x in $[x_i, x_{i+1}]$:

$$p_i(x) = \sum_{k=0}^{m} c_{ik} x^k$$

- Coefficients chosen so $p_i(x_i) = f_i$ and from smoothness condition: all derivatives (l) match at the endpoints

$$p_i^{(l)}(x_{i+1}) = p_{i+1}^{(l)}(x_{i+1}), \quad l = 0, 1, \ldots, m-1$$

- Except for points on the boundary of the curve

Splines: Determining the coefficients

- There are n intervals; in each interval: m+1 coefficients for the polynomial

- Total: (m+1)n coefficients:
  - Smoothness condition on interior points: (m)(n-1) equations
  - Curve passing through interior points: (n-1) equations
  - Remaining m+1 equations from imposing conditions on derivatives at end points
    - Natural spline: Setting highest-order derivative to zero at both endpoints

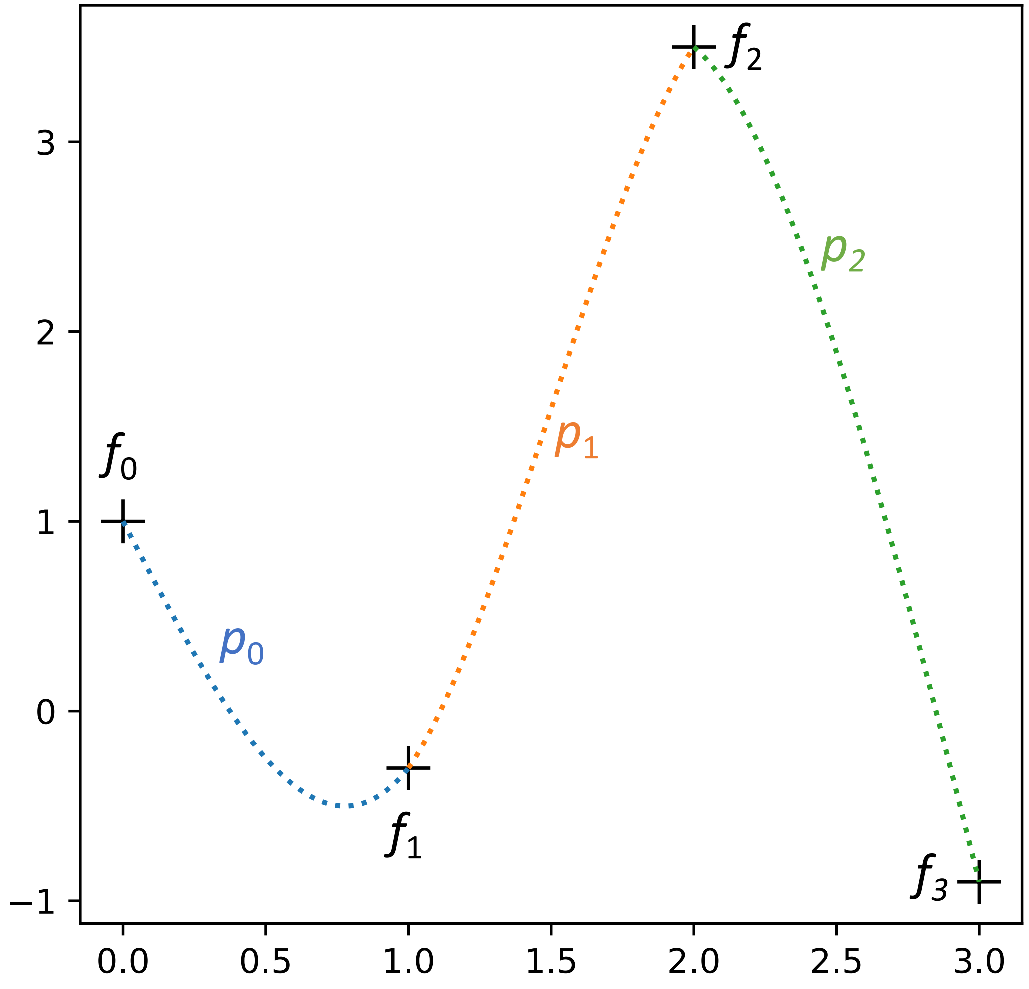
Most popular: Cubic splines, $m = 3$

- Easy to implement
- Produce a curve that appears to be seamless
- Avoids distortions near the edges
- Only piecewise continuous, third derivatives are discontinuous

Cubic spline example: 3 intervals

- Order: m=3, intervals: n=3, points: x = 0, 1, 2, 3
- Constraints: $(m+1)n$ = 12

  - Interior point 1:
  $$p_0(x_1) = f_1$$
  $$p_1(x_1) = f_1$$
  $$p_0'(x_1) = p_1'(x_1)$$
  $$p_0''(x_1) = p_1''(x_1)$$
  - Interior point 2:
  $$p_1(x_2) = f_2$$
  $$p_2(x_2) = f_2$$
  $$p_1'(x_2) = p_2'(x_2)$$
  $$p_1''(x_2) = p_2''(x_2)$$



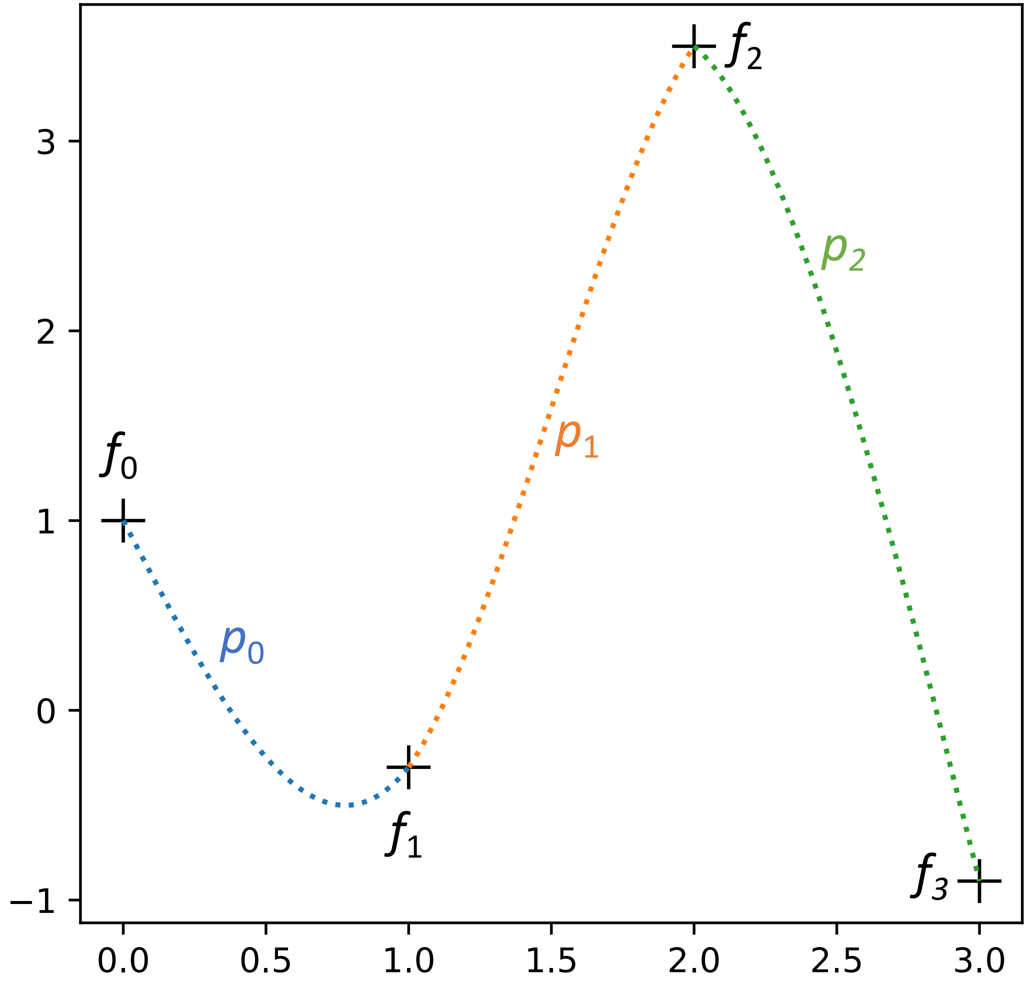
Cubic spline example: 3 intervals

- At the boundaries:

$$p_0(x_0) = f_0$$
$$p_2(x_3) = f_3$$

- Natural spline, second derivatives at the boundary set to zero

$$p_0''(x_0) = 0$$
$$p_2''(x_3) = 0$$



Now solve for the coefficients:

- Linearly interpolate the second derivative:

$$p_i''(x) = \frac{1}{\Delta x}\left[(x - x_i)p_{i+1}'' - (x - x_{i+1})p_i''\right]$$

- Integrate twice:

$$p_i(x) = \frac{1}{6\Delta x}\left\{p_{i+1}''\left[(x - x_i)^3 + 6A(x - x_i)\right] - p_i''\left[(x - x_{i+1})^3 + 6B(x - x_{i+1})\right]\right\}$$

- Impose constraints: $p_i(x_i) = f_i, \;\; p(x_{i+1}) = f_{i+1}$

Now solve for the coefficients:

$$p_i(x) = \alpha_i(x - x_i)^3 + \beta_i(x - x_{i+1})^3 + \gamma_i(x - x_i) + \eta_i(x - x_{i+1})$$

- Results:

$$\alpha_i = \frac{p''_{i+1}}{6\Delta x}, \quad \beta_i = -\frac{p''_i}{6\Delta x}, \quad \gamma_i = \frac{-p''_{i+1}\Delta x^2 + 6f_{i+1}}{6\Delta x}, \quad \eta_i = \frac{p''_i\Delta x^2 - 6f_i}{6\Delta x}$$

- For now, in terms of second derivative

- To get second derivative, use continuity condition

$$p'_{i-1}(x_i) = p'_i(x_i)$$

Now solve for the coefficients:

$$p''_{i-1}\Delta x + 4p''_i\Delta x + p''_{i+1}\Delta x = \frac{6}{\Delta x}(f_{i-1} - 2f_i + f_{i+1})$$

- Applies to all interior points
- Natural boundary conditions:

$$p''_0 = 0,\ p''_n = 0$$

- Results in a system of linear equations

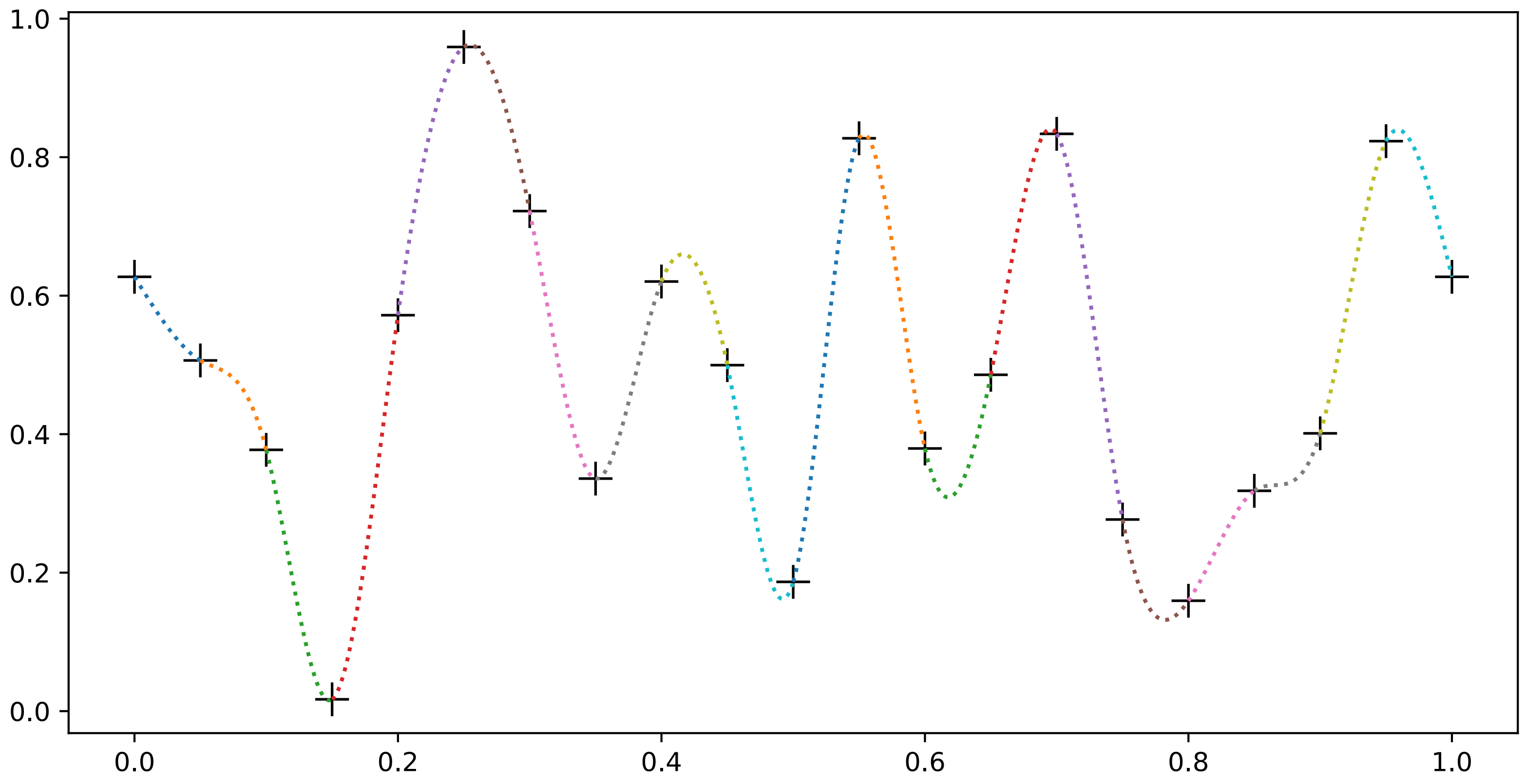
Results in system of linear equations

- Can be written as a tridiagonal matrix:

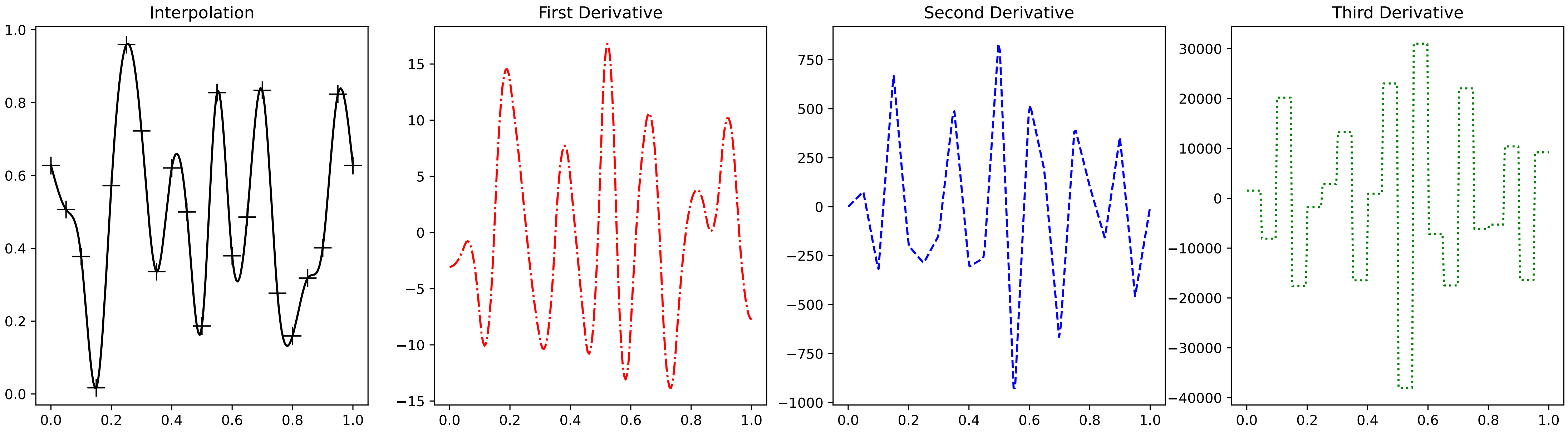
$$\begin{pmatrix} 4\Delta x & \Delta x & & & & \\ \Delta x & 4\Delta x & \Delta x & & & \\ & \Delta x & 4\Delta x & \Delta x & & \\ & & \ddots & \ddots & \ddots & \\ & & & \Delta x & 4\Delta x & \Delta x \\ & & & & \Delta x & 4\Delta x \end{pmatrix} = \begin{pmatrix} p''_1 \\ p''_2 \\ p''_3 \\ \vdots \\ p''_{n-2} \\ p''_{n-1} \end{pmatrix} \frac{6}{\Delta x} \begin{pmatrix} f_0 - 2f_1 + f_2 \\ f_1 - 2f_2 + f_3 \\ f_2 - 2f_3 + f_4 \\ \vdots \\ f_{n-3} - 2f_{n-2} + f_{n-1} \\ f_{n-2} - 2f_{n-1} + f_n \end{pmatrix}$$

- We will discuss linear algebra in a later class

Example: Cubic spline for random numbers



Example: Derivatives of cubic splines



Today’s lecture:

- Continue discussing interpolation
  - Lagrange Interpolation
  - Cubic splines
- Begin discussing finding roots of functions
  - Bisection method
  - Newton Raphson method
  - Secant method

Purpose: Find the root of a function

- Root of a function $f(x)$ is x_r such that: $f(x_r) = 0$
- Why? We can cast more general solutions in the form of finding roots.
  - Example: Suppose I have the following equation for velocity of a free-falling mass m with a coefficient of drag c_d:

$$v(t) = \sqrt{\frac{gm}{c_d}} \tanh\left(\sqrt{\frac{gc_d}{m}} t\right)$$

  - I would like to find the mass that would give me a velocity of 36 m/s after 4s of free fall. We can do this by rewriting the equation as:

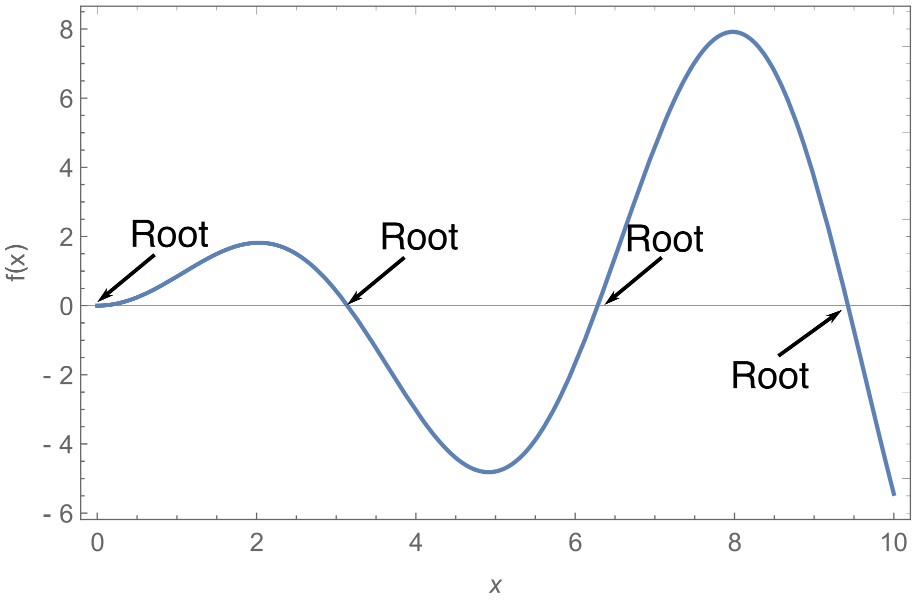
$$f(m) = \sqrt{\frac{gm}{c_d}} \tanh\left(\sqrt{\frac{gc_d}{m}} t\right) - v(t)$$

  - And finding the root of $f(m)$ for t = 4s and v = 36 m/s

Purpose: Find the root of a function

- For very simple functions, we can find the root analytically
  - For more complicated functions, we must do this numerically

- First rule of root finding: If possible, plot the function to get an idea of where roots are, how many, etc.:



Bisection method

- 1. Choose two initial guesses for the root, a lower (x_l) and upper (x_u)
  - Chosen such that the function evaluated at x_l and x_u have different signs
  - This can be checking by ensuring that: $f(x_l)\, f(x_u) < 0$
- 2. An estimate for the root is determined as the midpoint between the guesses

$$x_r = \frac{x_l + x_u}{2}$$

- 3. Make the following evaluations to determine in which subinterval the root lies, and thus obtain a refined guess:
  - If $f(x_l)\, f(x_r) < 0$, set $x_u = x_r$, return to step 2
  - If $f(x_l)\, f(x_r) > 0$, set $x_l = x_r$, return to step 2
  - If $f(x_l)\, f(x_r) = 0$ to some tolerance, x_r is the root and the calculation is complete

Newton-Raphson method

- Let x_r be a root of $f(x)$. Expand $f(x)$ in a Taylor series about around a different point x_0 that is close to x_r :

$$f(x) \simeq f(x_0) + f'(x_0)(x - x_0)$$

- Then:

$$f(x_r) = 0 \simeq f(x_0) + f'(x_0)(x_r - x_0)$$

- So:

$$x_r \simeq x_0 - \frac{f(x_0)}{f'(x_0)}$$

- Of course, this is only accurate if x_0 is close to x_r, but we can use this relation to refine the guess for the root

Newton-Raphson method procedure

- 1. Make an **initial guess** for the root: x_0
- 2. Use the Taylor series expansion to **find a better estimate** of the root:

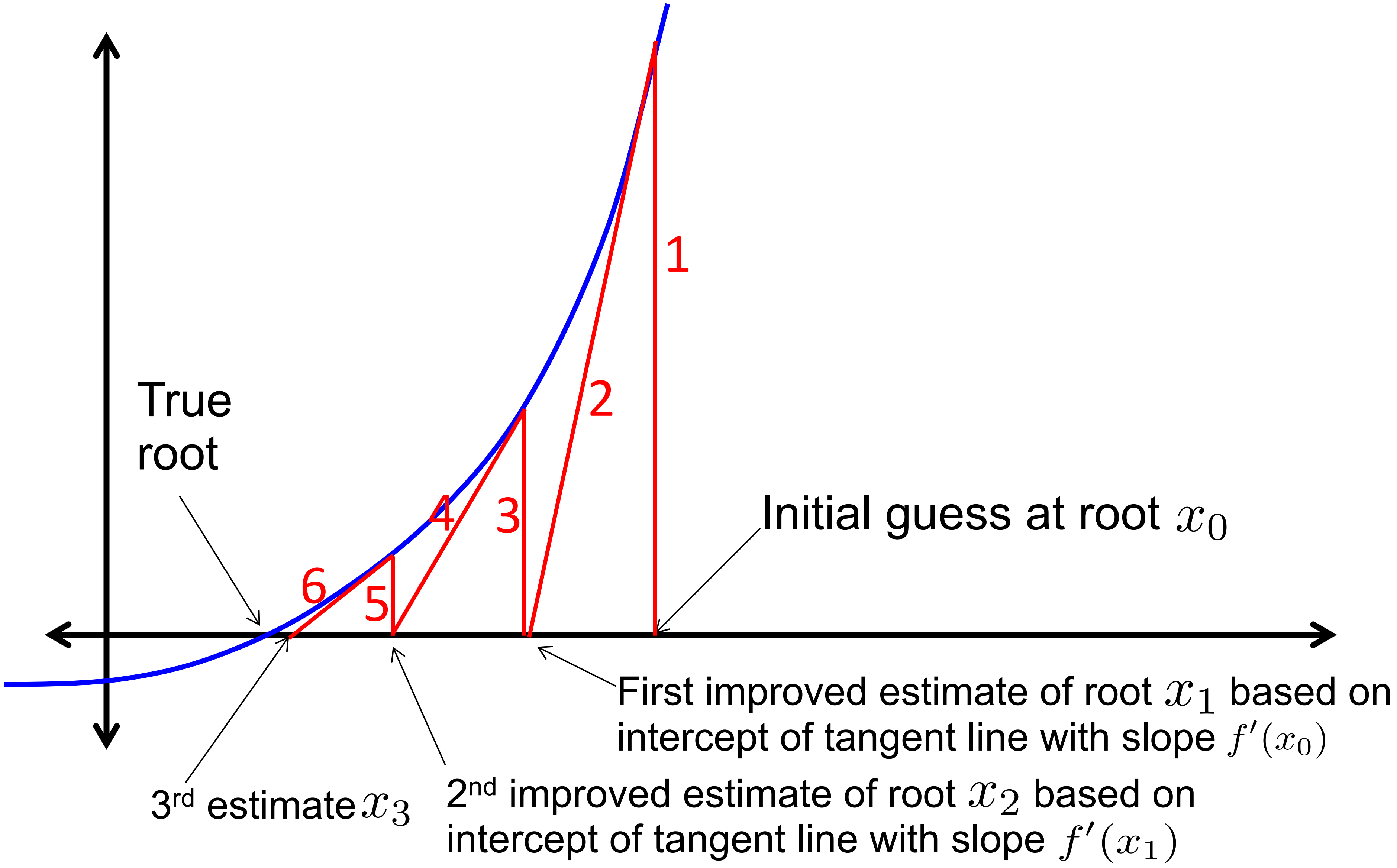
$$x_1 \simeq x_0 - \frac{f(x_0)}{f'(x_0)}$$

- 3. Use x_1 as an improved estimate at the root and employ the Taylor series expansion again to get a better estimate x_2

- Repeat process until the answer is accurate enough at the *n*th estimate:

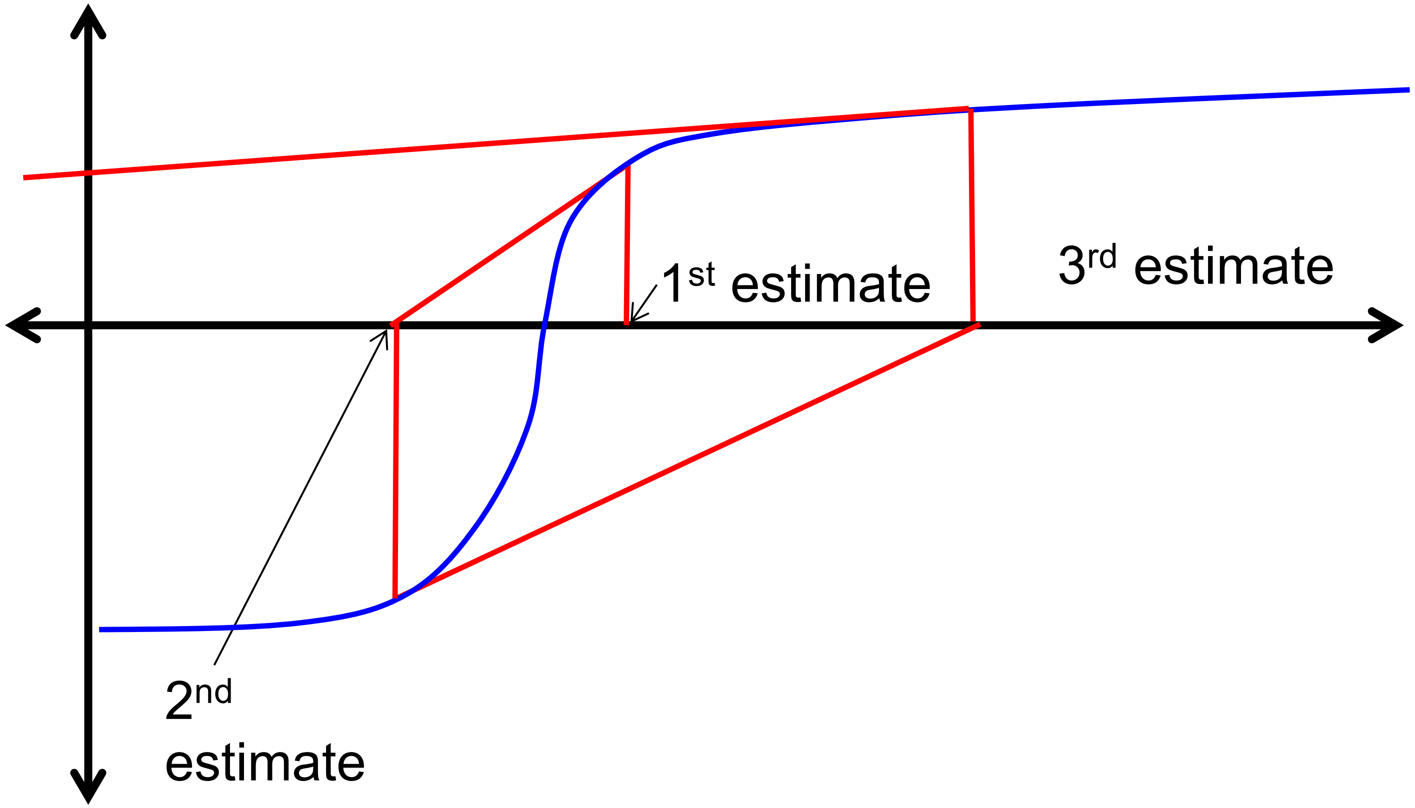
$$x_n \simeq x_{n-1} - \frac{f(x_{n-1})}{f'(x_{n-1})}$$

Geometrical Interpretation of Newton-Raphson Iteration



Failure of Newton-Raphson

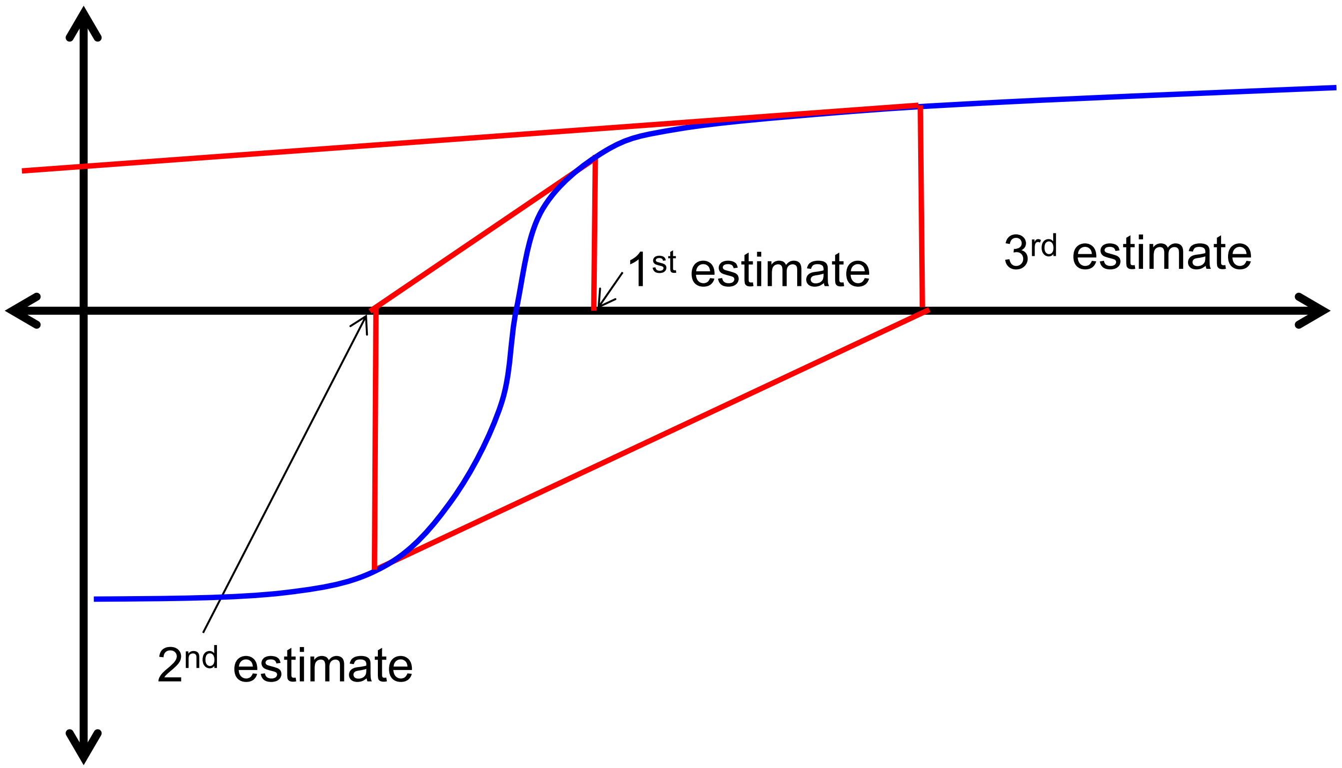
- Example of a simple function that will defeat Newton-Raphson Iteration:



- Each estimate gets further from the true root. Estimates are diverging not converging

Stopping criteria for iterations must be chosen carefully

- Could stop when we reach some maximum number of iterations
  - Estimate may be no where near the root
  - We can consider this case a failure of the method and warn user about it.



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- Could stop when we reach some maximum number of iterations
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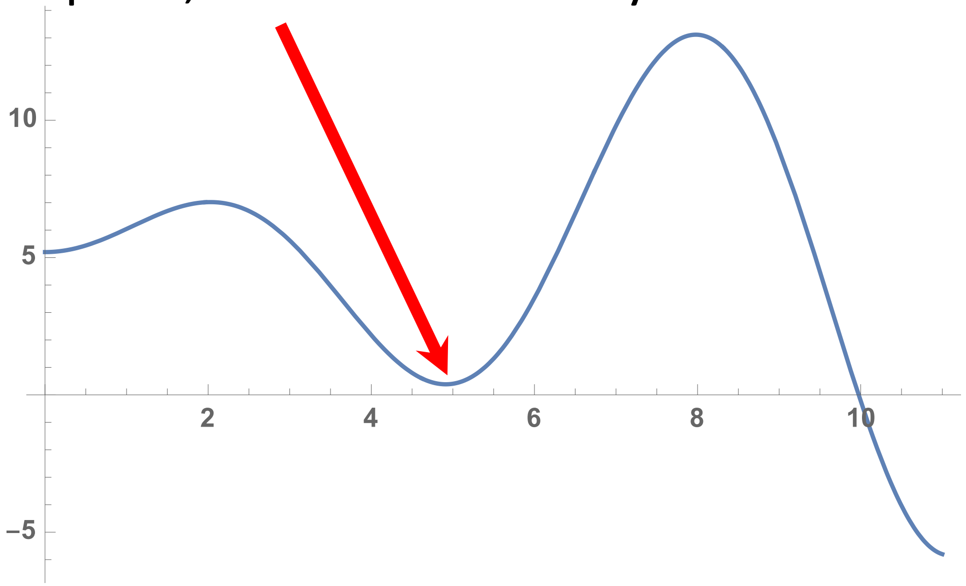
- Could stop when value of the function evaluated at the *n*th estimate less than small number : $|f(x_n)| < \epsilon$
  - But this can be deceptive; final estimate may not be near the root, might just be close to zero



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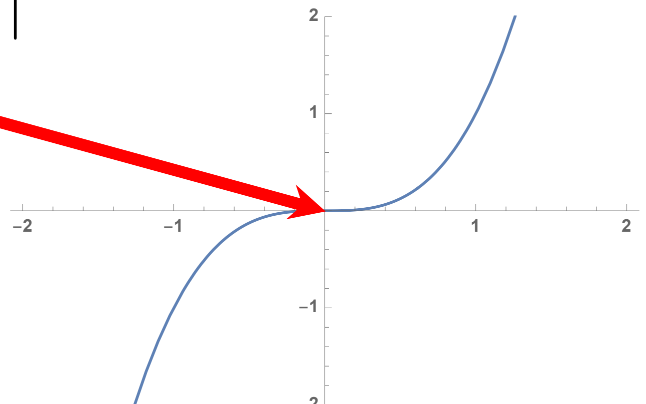
- Could stop when change between estimates becomes small relative to the current (*n*th) estimate: $|x_{n+1} - x_n| < \epsilon |x_n|$
  - Better, but still fails when root is located at zero



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  - Better, but still fails when root is located at zero
- So let's use:

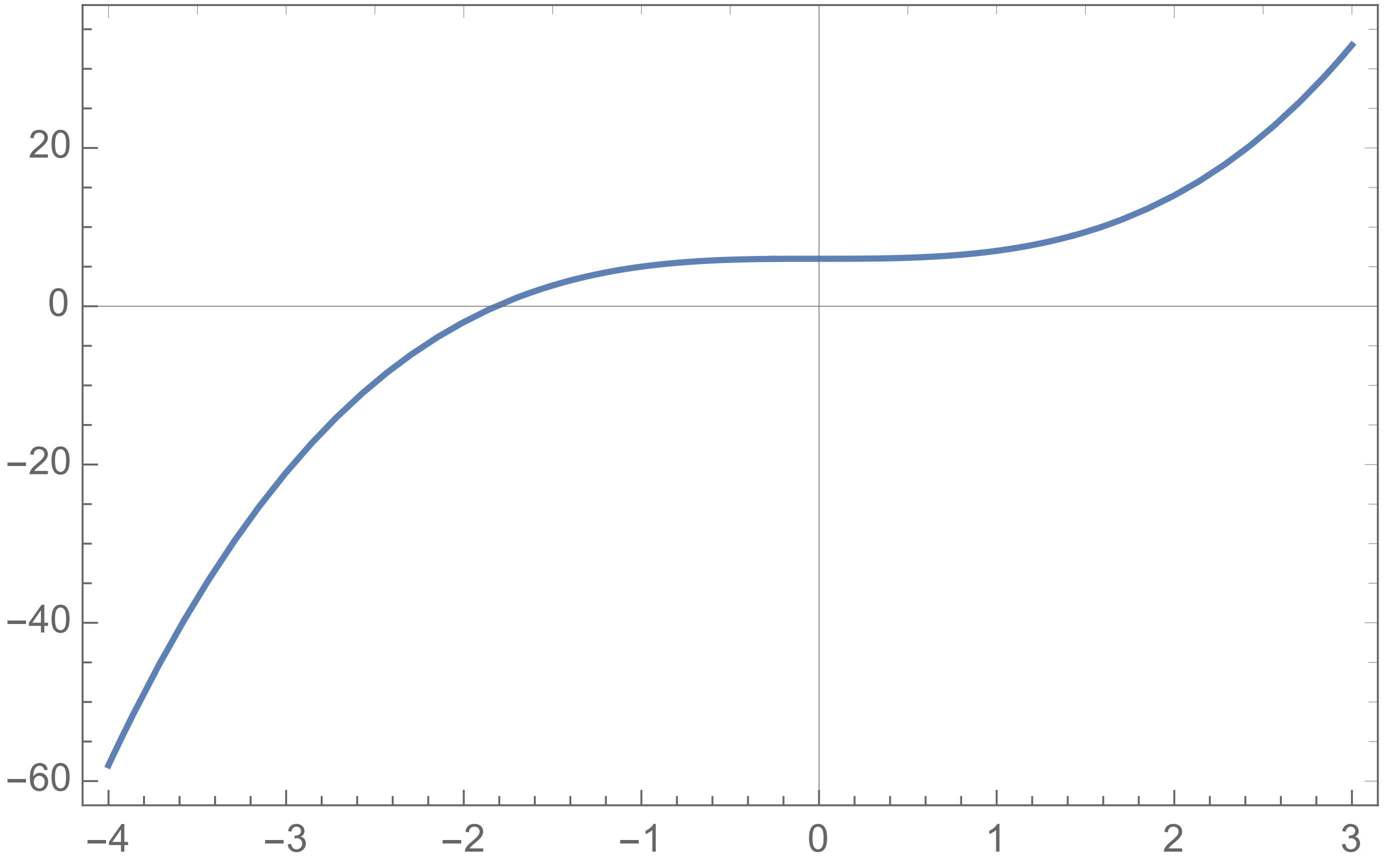
$$|x_{n+1} - x_n| < \begin{cases} \epsilon |x_n|, & \text{when } |x_n| \neq 0 \\ \epsilon, & \text{when } |x_n| = 0 \end{cases}$$

Pseudocode of Newton-Raphson Algorithm

- 1. Choose initial guess at the root (x_0), and the convergence tolerance (ε).
- 2. Loop through n up to a maximum number N_{max} (exit and tell the user that the root finding has failed if it reaches N_{max})
- 3. Make sure $f'(x) \neq 0$
- 4. Compute new estimate of root: $x_n \simeq x_{n-1} - \dfrac{f(x_{n-1})}{f'(x_{n-1})}$
- 5. Check convergence criteria:

$$|x_{n+1} - x_n| < \begin{cases} \epsilon |x_n|, & \text{when } |x_n| \neq 0 \\ \epsilon, & \text{when } |x_n| = 0 \end{cases}$$

Example: $f(x) = x^3 + 6$



- See **NR_root.ipynb**

Secant method

- Similar to the Newton-Raphson method, but does not require calculating the derivative of the function
- Start with two initial guesses, x_{i-1} and x_i
- Use finite difference derivative to get a new guess x_{i+1}

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

- Proceed in the same way as the Newton-Raphson method

Summary of root-finding methods

- Bisection:
  - Robust (with appropriate initial guesses)
  - Slow, each iteration reduces error by a factor of two
  - Need to make sure root is within initial guesses

- Newton-Raphson:
  - Fast: often only takes a few iterations
  - Need to know derivative of function, and they must exist
  - Can diverge, e.g., in cases with small second derivatives

- Secant method
  - Similar convergence speed as NR method
  - Don’t need analytical derivatives
  - Same divergence properties as NR method
  - Numerical derivatives may be noisy

After class tasks

- Homework 1 has been posted
  - Let me know if you have HW questions or questions/issues on github classroom
  - Office hours: Mondays, 3:00pm to 4:00pm; Thursdays, 11:05am to 1:00pm
    - Feel free to send me an email, and remember, if you push your changes, I should be able to see them
- Readings:
  - Pang Section 2.1 and 3.3
  - Wikipedia article on Chebyshev nodes
  - Myths about polynomial interpolation
  - Wikipedia page on root finding