# PHY604 Lecture 7

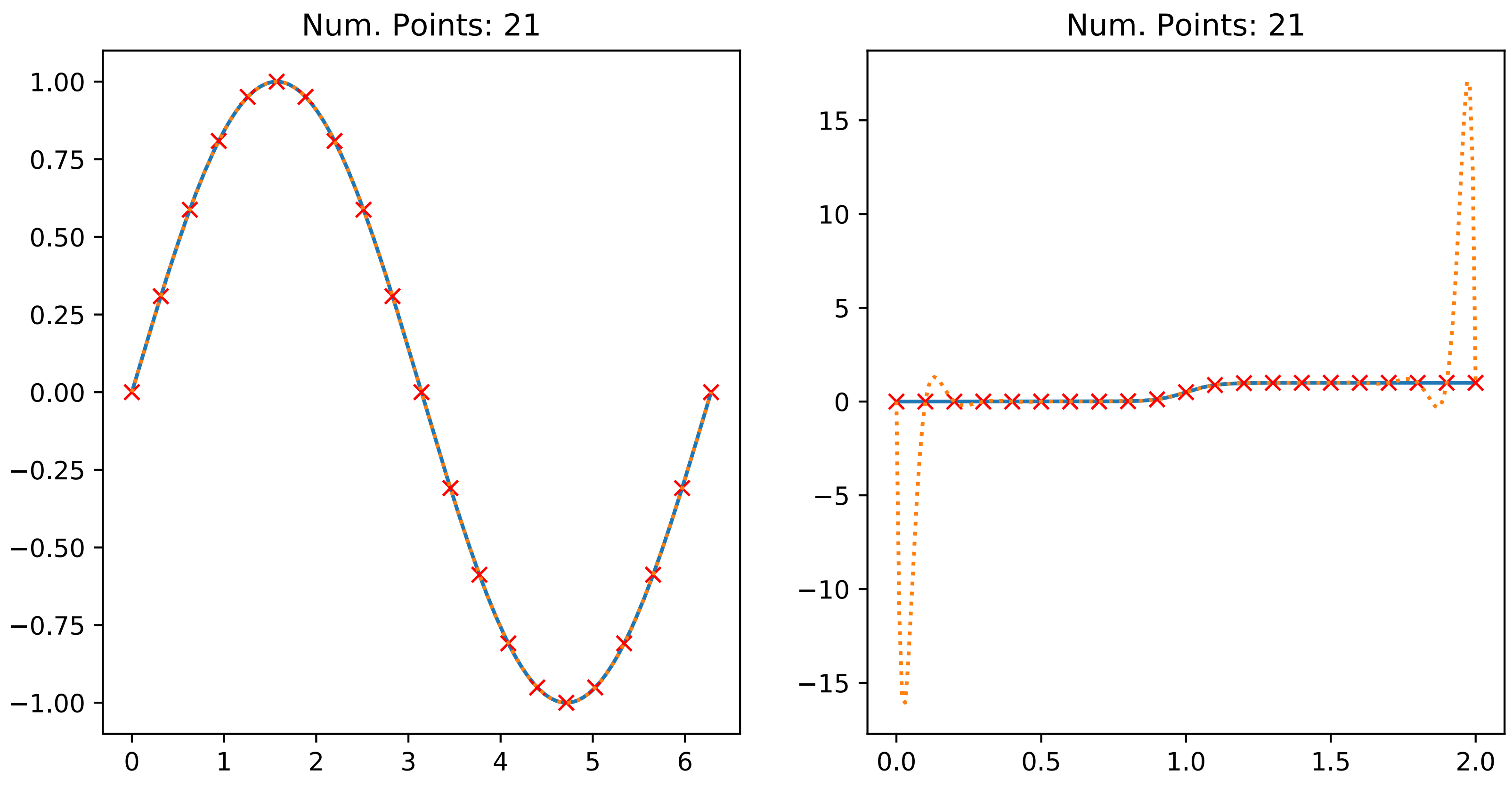
September 21, 2023

# Review: Lagrange interpolation

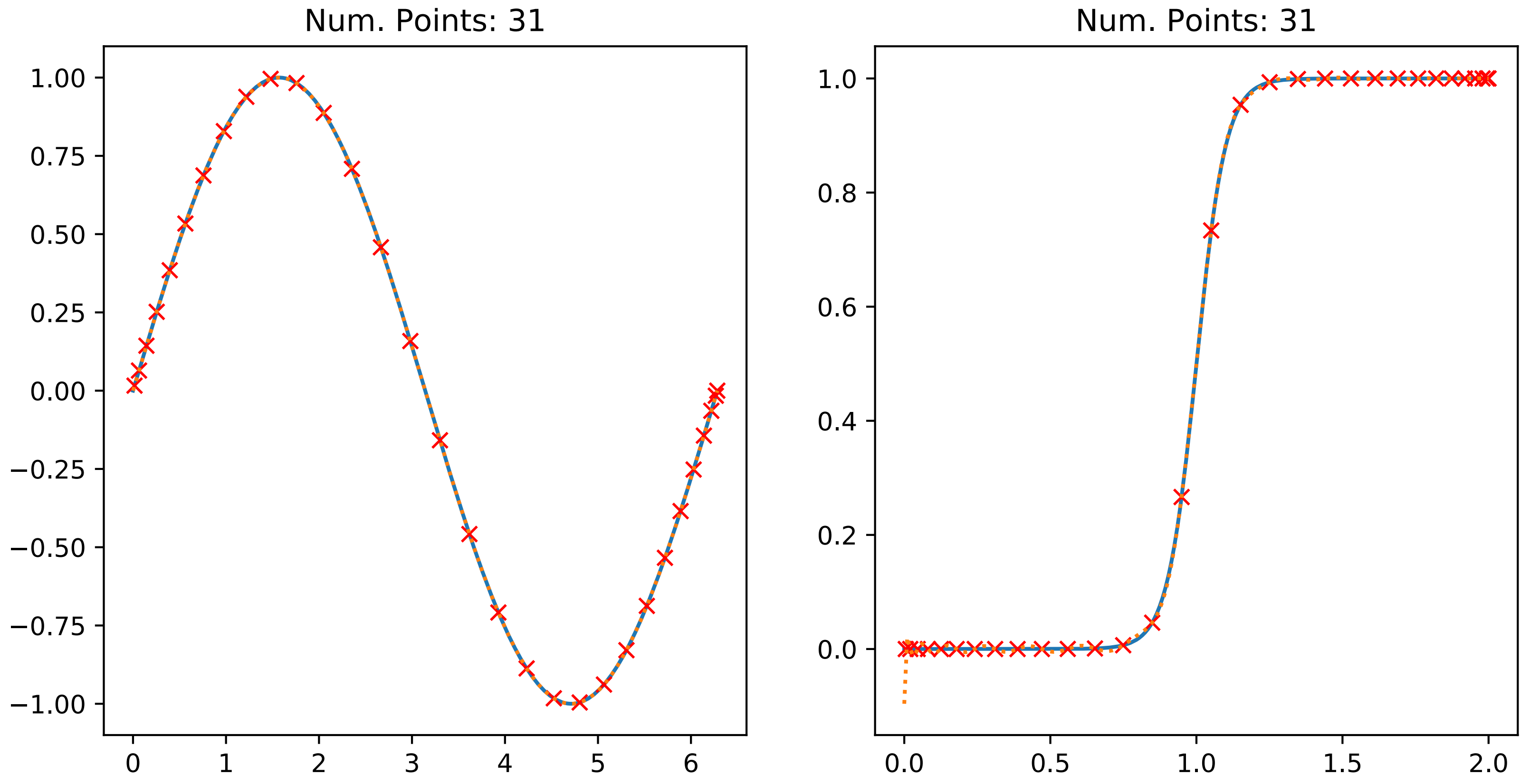
- General method for building a single polynomial that goes through all the points (alternate formulations exist)

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

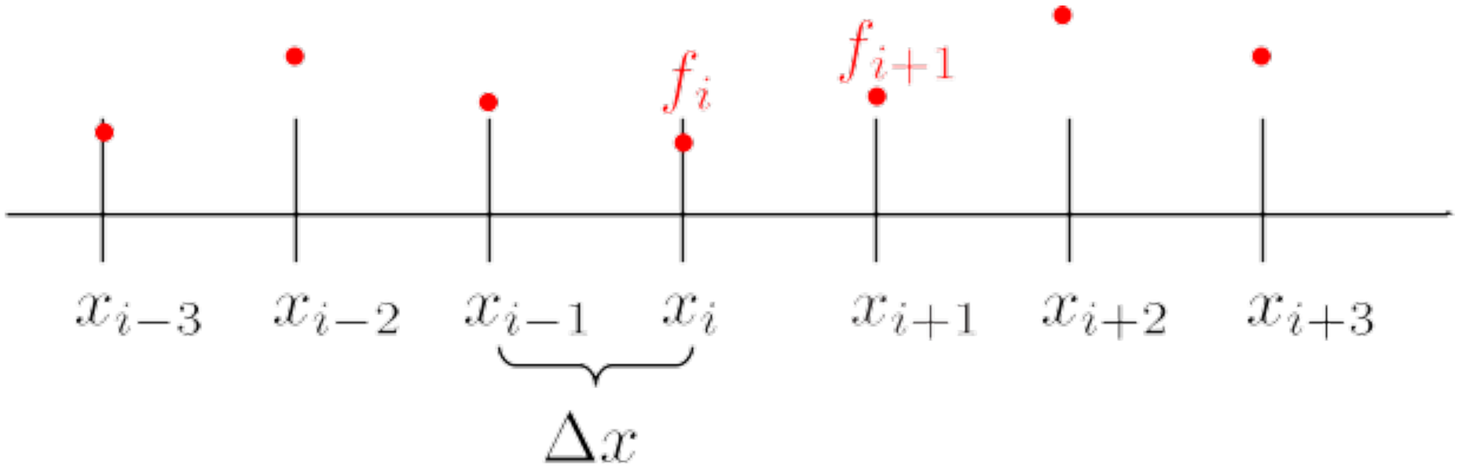
# Review: Lagrange Interpolation of two functions on even grid



# Review: Lagrange Interpolation of two functions with Chebyshev nodes



# Review: Splines




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

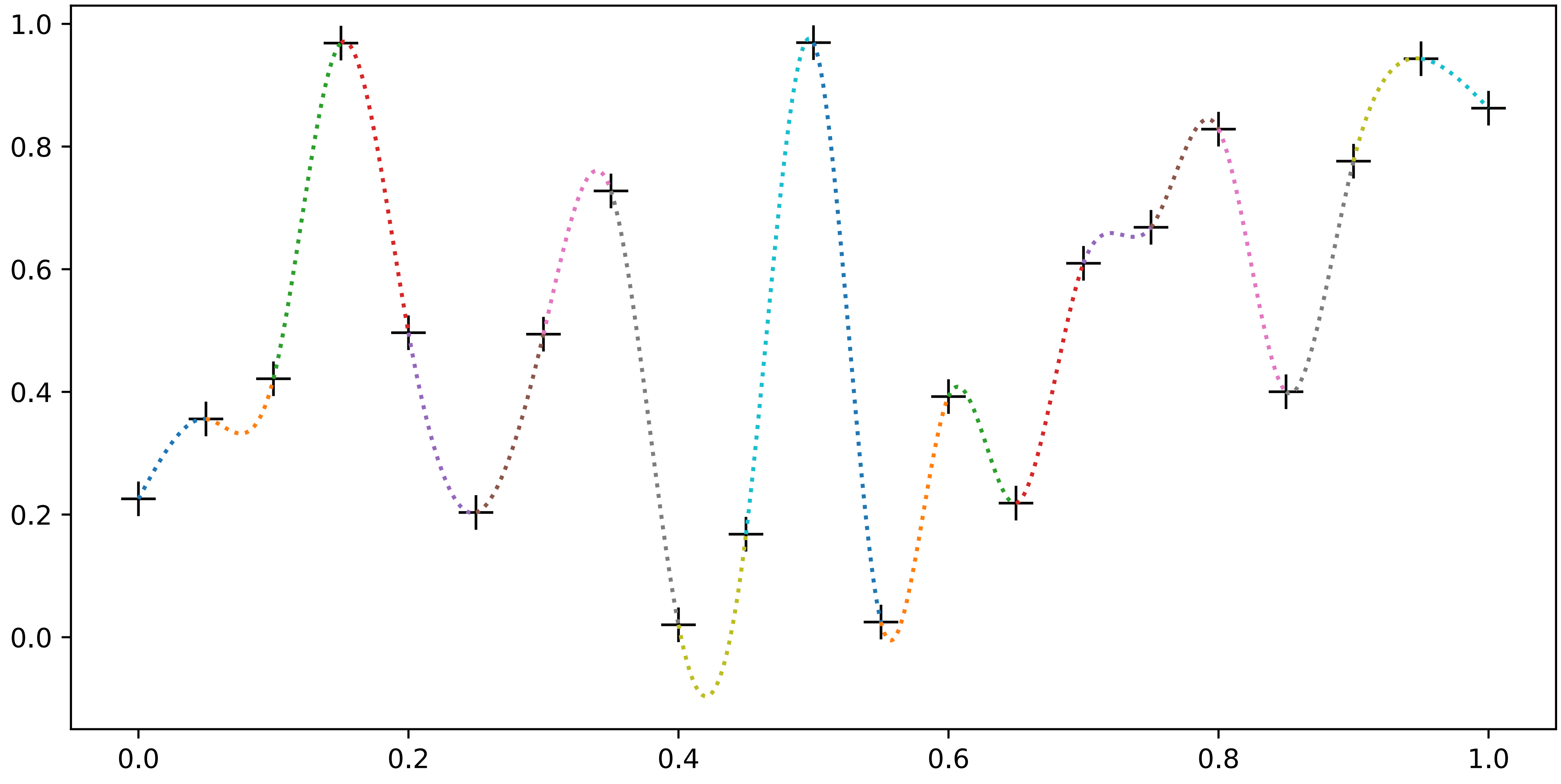
$$p_i(x) = \sum_{k=0}^{m} c_{ik} x^k$$

- 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

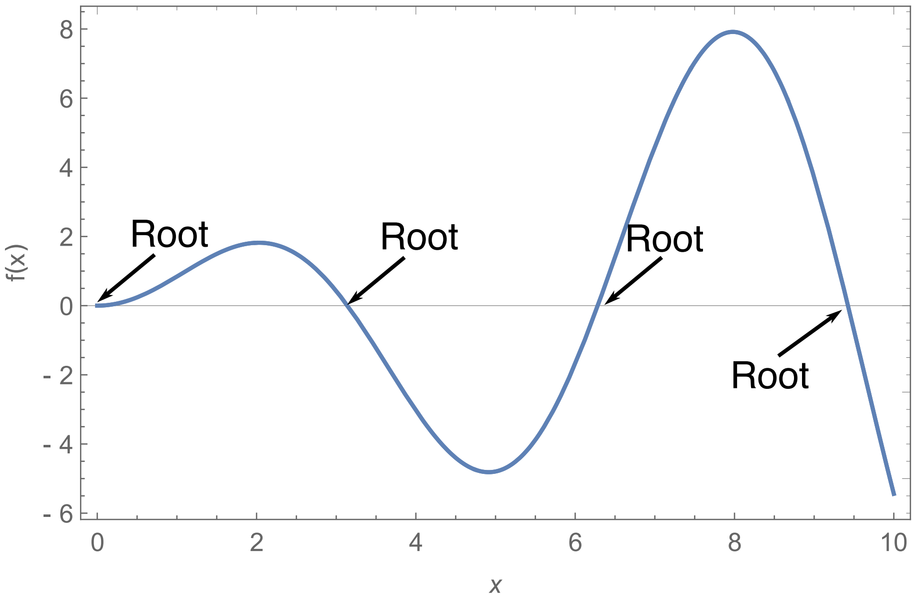
# Review: Cubic spline for random numbers



# Review: 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.:



# Review: 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

# Today's lecture

- Finish discussing roots of functions:
  - Newton Raphson method
  - Secant method
- Begin discussing ordinary differential equations

# 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

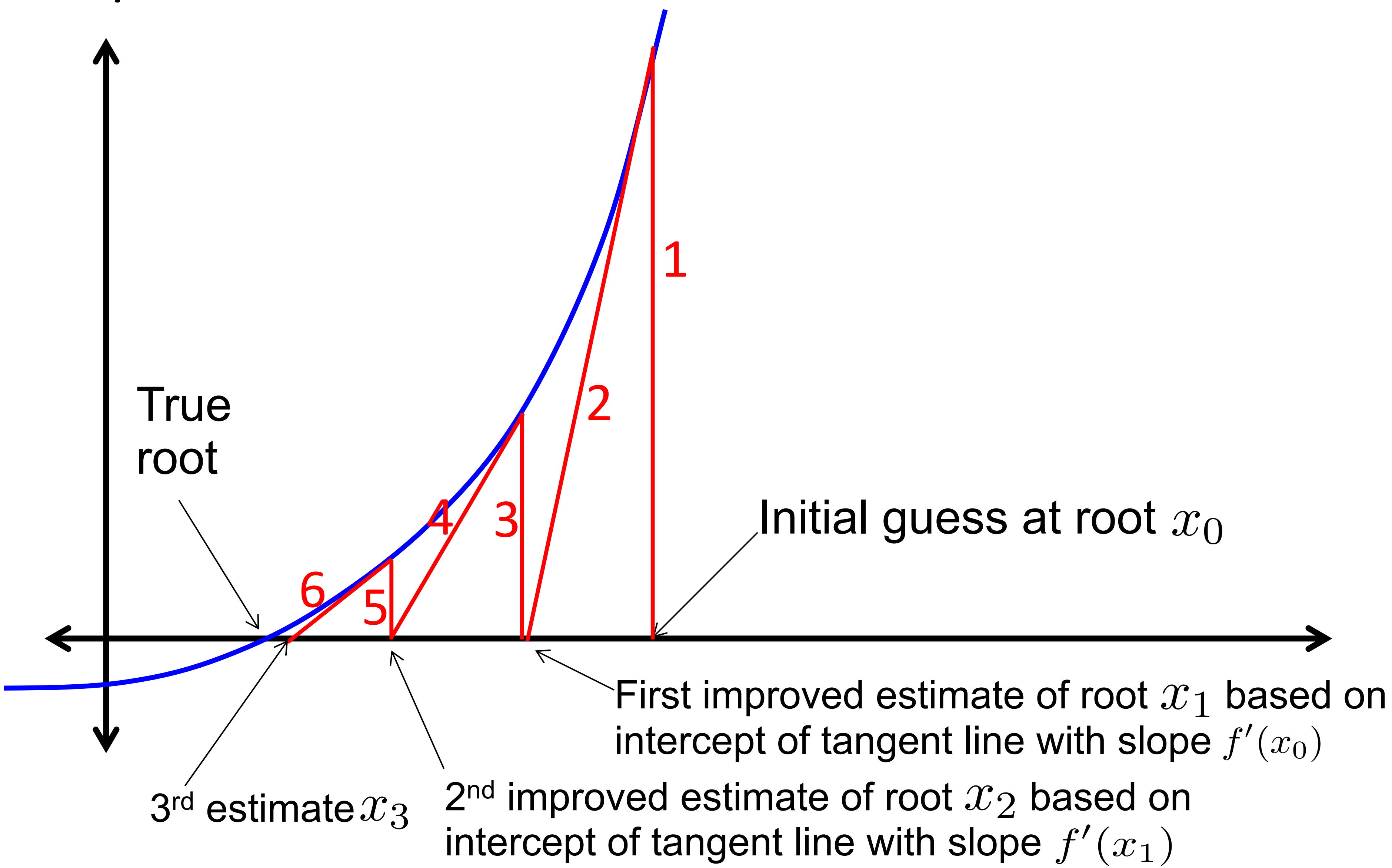
- 1. Make an **initial guess** for the root: $x_0$
- 2. Use the Taylor series expansion to **find a better estimate** of the root:

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

- 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:

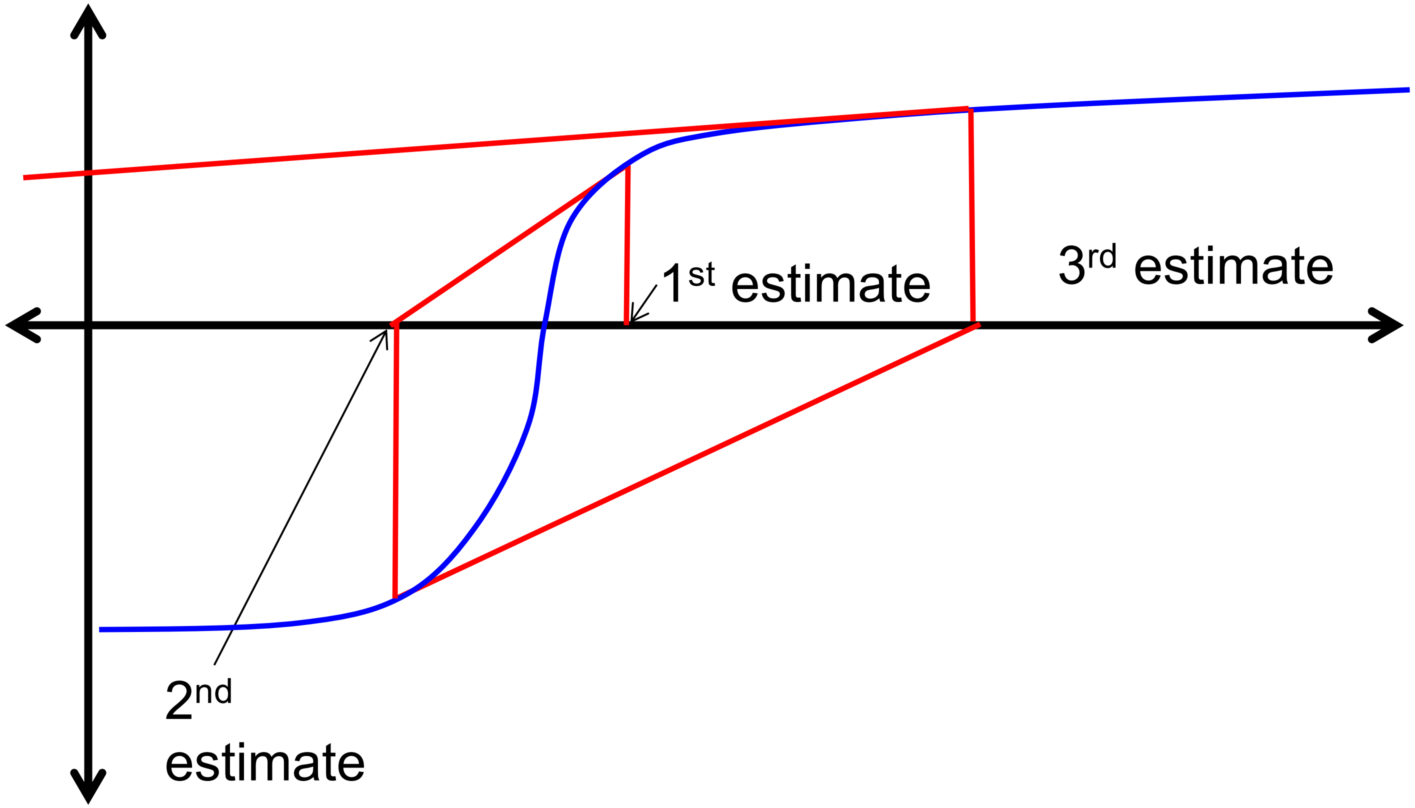
$$x_n \simeq x_{n-1} - \frac{f(x_{n-1})}{f'(x_{n-1})}$$

# Geometrical Interpretation of Newton-Raphson Iteration



# Failure of Newton-Raphson

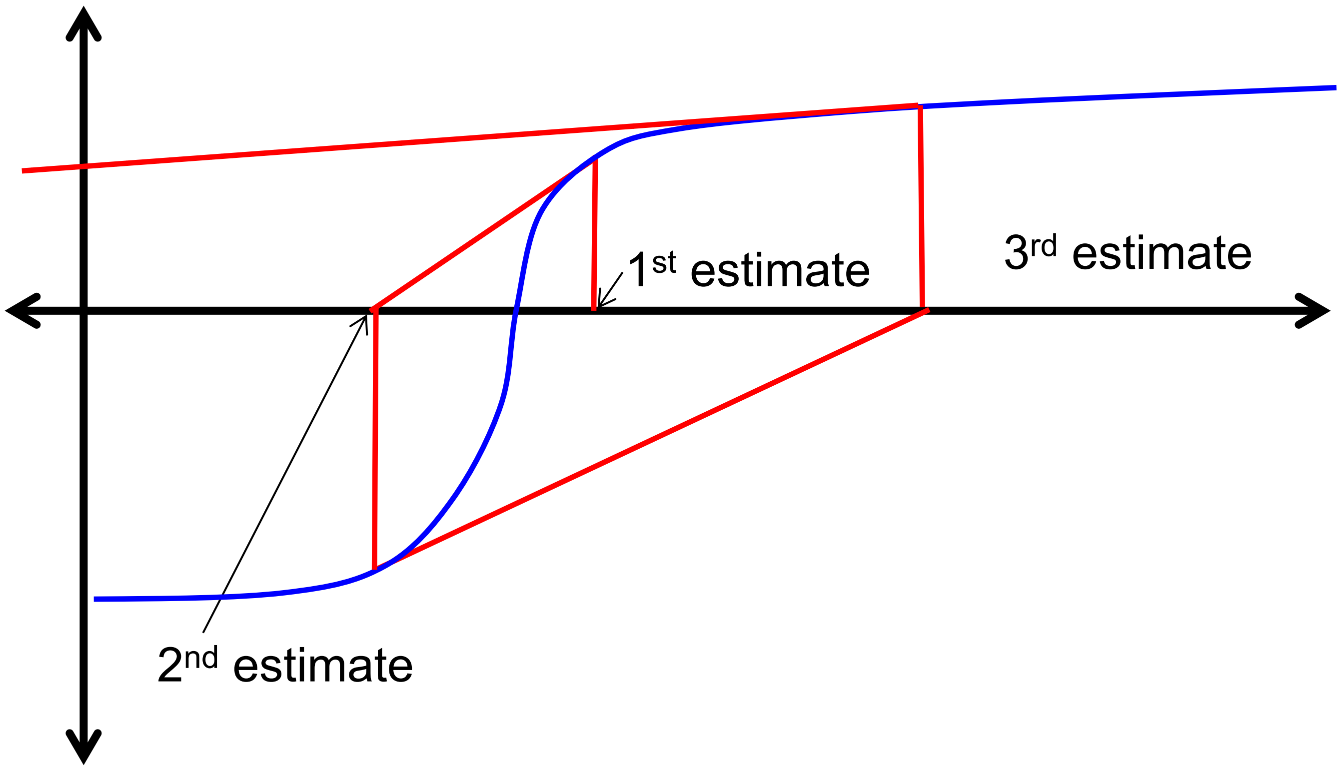
- Example of a simple function that will defeat Newton-Raphson Iteration:




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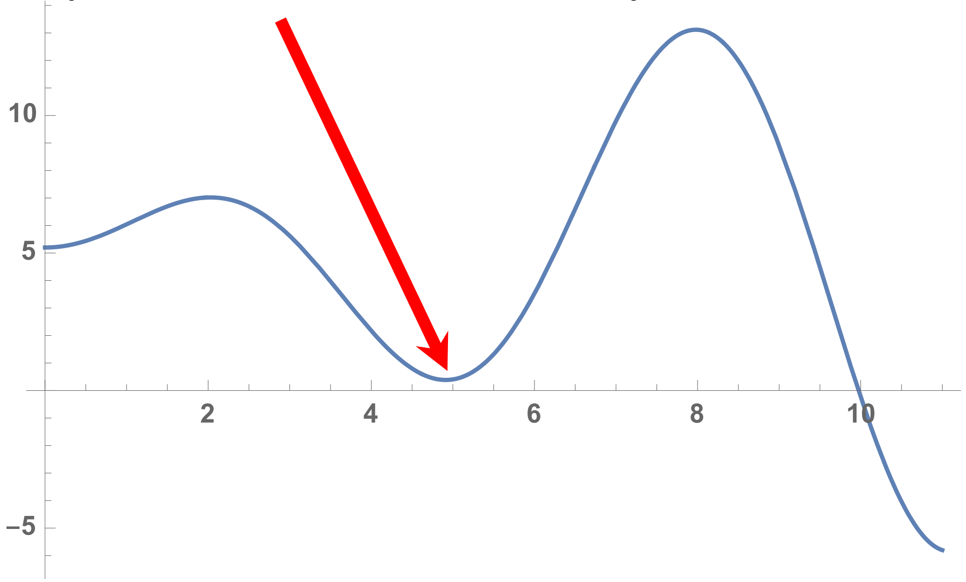
- Could stop when value of the function evaluated at the *n*th estimate less than small number : $|f(x_n)| < \epsilon$
  - But this can be deceptive; final estimate may not be near the root, might just be close to zero



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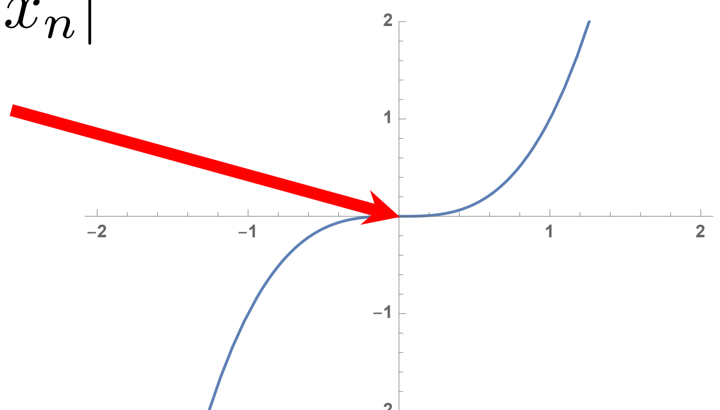
- Could stop when change between estimates becomes small relative to the current (*n*th) estimate: $|x_{n+1} - x_n| < \epsilon |x_n|$
  - Better, but still fails when root is located at zero



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- 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
- So let's use:

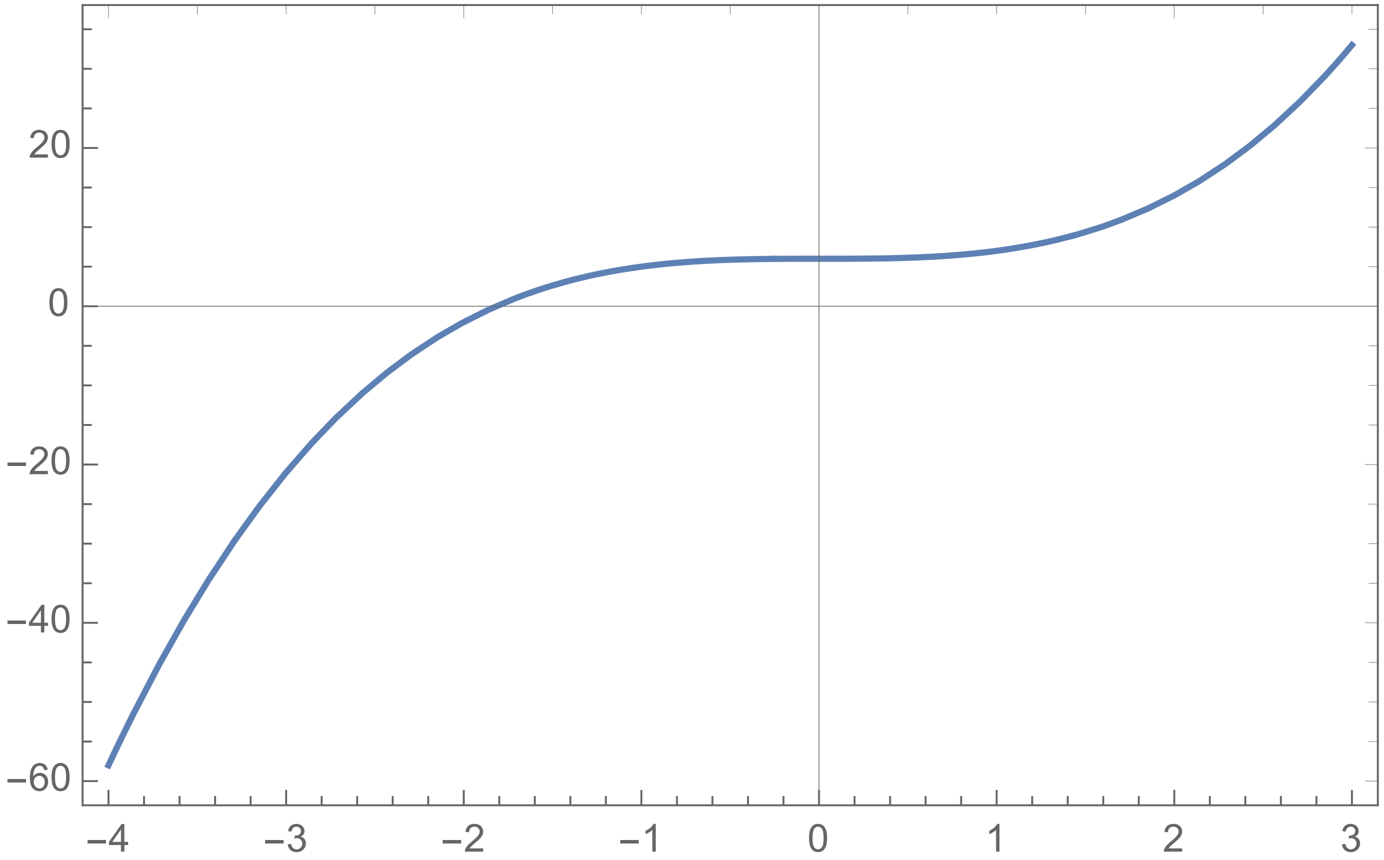
$$|x_{n+1} - x_n| < \begin{cases} \epsilon |x_n|, & \text{when } |x_n| \neq 0 \\ \epsilon, & \text{when } |x_n| = 0 \end{cases}$$

# Pseudocode of Newton-Raphson Algorithm

- 1. Choose initial guess at the root ($x_0$), and the convergence tolerance ($\varepsilon$).
- 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

# Today’s lecture

- Finish discussing roots of functions:
    - Newton Raphson method
    - Secant method
- Begin discussing ordinary differential equations

# Differential equations (Newman Ch. 8)

- One of the major applications of computation to science and engineering is solving differential equations
  - Even for very simple-looking equations if they are "nonlinear," they are difficult or imposible to solve analytically
- Classifications:
  - Initial value problems
  - Boundary value problems
  - Eigenvalue problems
- Often problems are described by systems of coupled differential equations
- As with the other topics, there are many different methods
  - We just want to see the basic ideas and popular methods

# Example of system of differential equations: Equations of motion

- We know that the equations of motion for a point particle with mass are given by:

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}(t), \qquad \frac{d\mathbf{v}}{dt} = \mathbf{a}(\mathbf{x}, \mathbf{v}, t)$$

- In order to fully describe the trajectory of this particle, we need to specify initial conditions, i.e., the position and velocity, of the particle at the initial time $t = 0$:

$$\mathbf{x}(0) = \mathbf{x}_0, \qquad \mathbf{v}(0) = \mathbf{v}_0$$

# Approximating the Equations of Motion

- If we consider a time interval that is sufficiently short, we can approximate the differential by

$$dt \simeq \Delta t$$

- We can then approximate the time derivative of the position by:

$$\frac{d\mathbf{x}}{dt} \simeq \frac{\mathbf{x}(t + \Delta t) - \mathbf{x}(t)}{\Delta t}$$

- Similarly, the time derivative of the velocity can be approximated by

$$\frac{d\mathbf{v}}{dt} \simeq \frac{\mathbf{v}(t + \Delta t) - \mathbf{v}(t)}{\Delta t}$$

# Euler’s method for integrating the equations of motion

- We can then substitute the approximate derivatives into the equations of motion to obtain:

$$\frac{\mathbf{x}(t+\Delta t)-\mathbf{x}(t)}{\Delta t} \simeq \mathbf{v}(t), \quad \frac{\mathbf{v}(t+\Delta t)-\mathbf{v}(t)}{\Delta t} \simeq \mathbf{a}(\mathbf{x},\mathbf{v},t)$$

- We can then solve for the new values of the position and velocity

$$\mathbf{v}(t+\Delta t) \simeq \mathbf{v}(t) + \mathbf{a}(\mathbf{x},\mathbf{v},t)\Delta t$$

$$\mathbf{x}(t+\Delta t) \simeq \mathbf{x}(t) + \mathbf{v}(t)\Delta t$$

- This algorithm for “integrating” the equations of motion forward in time in known as Euler’s method

# Aside: Notation for coupled systems of ordinary differential equations

- The equations we were solving with Euler's method were of the form:

$$\frac{dy_1}{dt} = f_1(y_1, y_2, \ldots, y_N, t)$$
$$\frac{dy_2}{dt} = f_2(y_1, y_2, \ldots, y_N, t)$$
$$\vdots$$
$$\frac{dy_N}{dt} = f_N(y_1, y_2, \ldots, y_N, t)$$

- This is a set of coupled first-order ordinary differential equations (ODEs)

# Aside: Euler's Method for Coupled Systems of ODEs

- Use shorthand notation for the time at the *n*th step: $t^n$, and denote $y_i(t^n)$ as $y_i^n$
- Then approximate the derivatives are written:

$$\frac{dy_i}{dt} \simeq \frac{y_i^{n+1} - y_i^n}{\Delta t}$$

- And Euler's method for a set of coupled ODEs is:

$$\begin{aligned}
y_1^{n+1} &= y_1^n + \Delta t f_1(y_1, y_2, \ldots, y_N, t) \\
y_2^{n+1} &= y_2^n + \Delta t f_2(y_1, y_2, \ldots, y_N, t) \\
&\vdots \\
y_N^{n+1} &= y_N^n + \Delta t f_N(y_1, y_2, \ldots, y_N, t)
\end{aligned}$$

# Aside: Coupled systems of ODEs in vector notation

- In order to simplify the description of the second order Runge-Kutta algorithm we use the following vector notation to simplify the equations:

$$\mathbf{y} \equiv (y_1, y_2, y_3, \ldots, y_N)$$

$$\mathbf{f} \equiv (f_1, f_2, f_3, \ldots, f_N)$$

- Using this notation, the original set of ODEs is:

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(\mathbf{y}, t)$$

- In this notation Euler's method is:

$$\mathbf{y}^{n+1} = \mathbf{y}^n + \Delta t \mathbf{f}(\mathbf{y}^n, t^n)$$

# Example: A body orbiting the sun

- We consider the Sun's location to be at the origin and the plane of the orbit to be the x-y plane

- In this case we have: $\mathbf{a}(\mathbf{x}) = \frac{-GM_{\text{sun}}}{r^2}\hat{\mathbf{x}}$

- Where: $\hat{\mathbf{x}} = \frac{\mathbf{x}}{r} = \frac{\mathbf{x}}{x^2 + y^2}$

- The components of the acceleration are then given by:

$$a_x(x, y) = \frac{-GM_{\text{sun}}x}{r^3}, \quad a_y(x, y) = \frac{-GM_{\text{sun}}y}{r^3}$$

# Euler's method for body orbiting the sun

- Now we discretize in time and apply Euler's method:

$$v_x(t+\Delta t) = v_x(t) - \frac{GM_{\text{sun}}x(t)\Delta t}{\left(x(t)^2 + y(t)^2\right)^{3/2}}$$

$$v_y(t+\Delta t) = v_y(t) - \frac{GM_{\text{sun}}y(t)\Delta t}{\left(x(t)^2 + y(t)^2\right)^{3/2}}$$

$$x(t+\Delta t) = x(t) + v_x(t)\Delta t$$

$$y(t+\Delta t) = y(t) + v_y(t)\Delta t$$

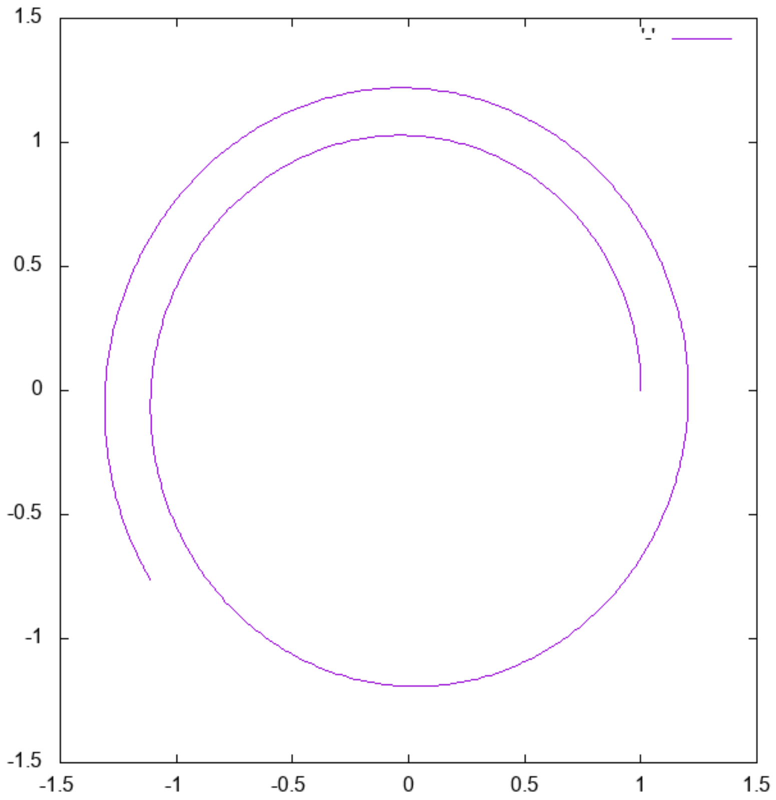
# Parameters for orbit problem

- We'll use units of solar masses, and Astronomical Units (AU) for distance
  - In these units, $M_{sun}$=1 and $G$ = 39.47 $AU^3 M_{sun}^{-1} yr^{-2}$

- Initial conditions:
  - At $t$ = 0 we'll place the body along the $x$-axis at a distance of 1 AU from the sun and give it the Earth's velocity in the $y$-direction:
    - $x(0)$ = 1, $y(0)$ =0
    - $v_y$ (0) = 6.283185 AU/yr
  - We will try a time step of 1 day: $\Delta t$ = 1/365 yr

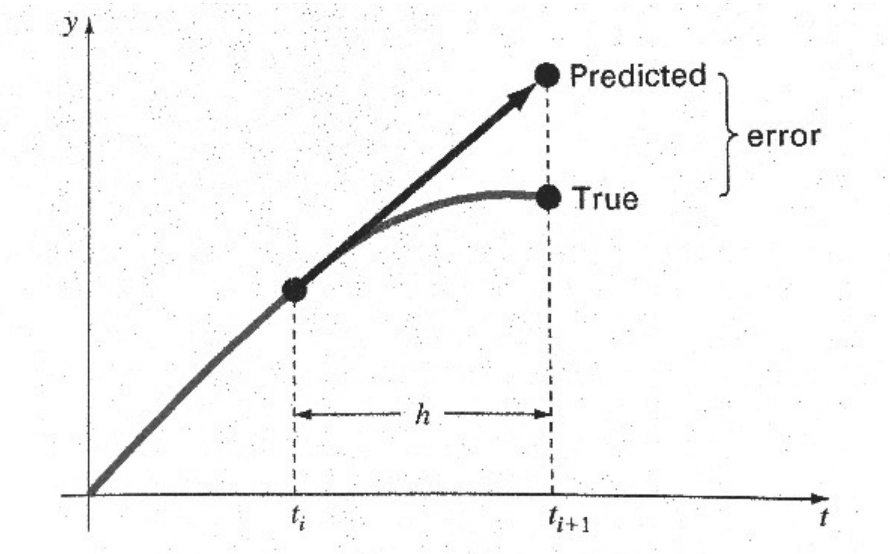
# Example program for Euler orbit problem

- See **`orbit_examples.ipynb`**

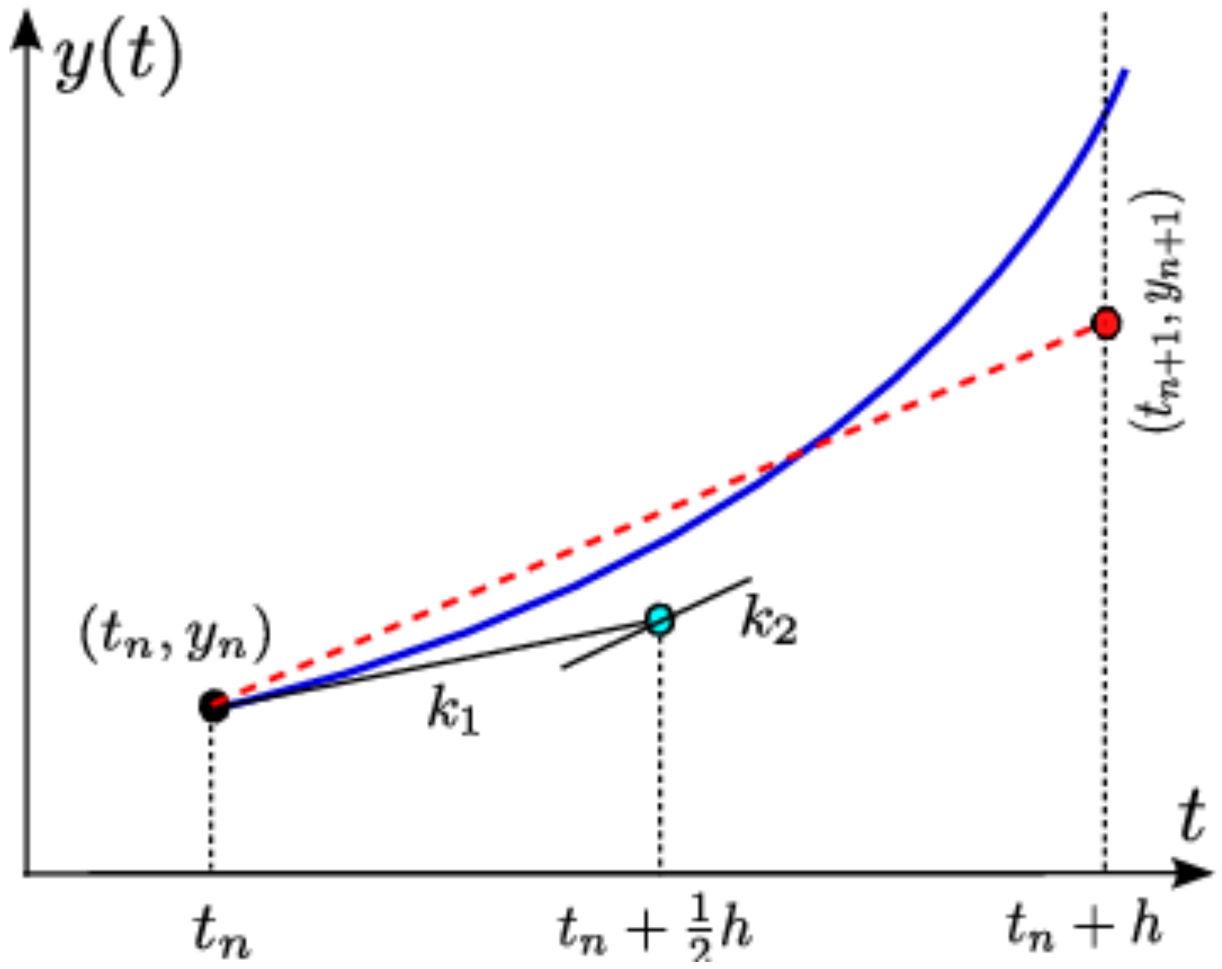


# More accurate ODE numerical methods

- The problem with Euler's method is that the right-hand-side of the equations is evaluated at the beginning of the timestep
- The right-hand-side usually changes over the course of each timestep and we may be getting an inaccurate answer as a result
  - It would be better if we could evaluate the right-hand-side in the middle of the timestep.
  - However, we can't do that unless we know the solution in advance
- We could use higher-order finite differences, however this is not a common approach
- **Strategy:** Use Euler's method to estimate the solution at the midpoint of the timestep. And then use this estimate to evaluate the right-hand-side
- This is called a second order Runge-Kutta method



# Second-order Runge-Kutta method




Fadlisyah, Muhammad thesis (2014)

# Second-order Runge-Kutta method

- Taylor expand around *t* + 1/2 Δ*t* :

$$y(t+\Delta t) = y(t+\frac{1}{2}\Delta t) + \frac{1}{2}\Delta t \frac{dy}{dt}\bigg|_{t+\frac{1}{2}\Delta t} + \frac{1}{8}\Delta t^2 \frac{d^2 y}{dt^2}\bigg|_{t+\frac{1}{2}\Delta t} + \mathcal{O}(\Delta t^3)$$

$$y(t) = y(t+\frac{1}{2}\Delta t) - \frac{1}{2}\Delta t \frac{dy}{dt}\bigg|_{t+\frac{1}{2}\Delta t} + \frac{1}{8}\Delta t^2 \frac{d^2 y}{dt^2}\bigg|_{t+\frac{1}{2}\Delta t} - \mathcal{O}(\Delta t^3)$$

- Subtract the two expressions

$$y(t+\Delta t) = y(t) + \Delta t \frac{dy}{dt}\bigg|_{t+\frac{1}{2}\Delta t} + \mathcal{O}(\Delta t^3)$$

Need *f* evaluated at midpoint

$$= y(t) + \Delta t f(y(t+\frac{1}{2}\Delta t), t+\frac{1}{2}\Delta t) + \mathcal{O}(\Delta t^3)$$

# Second-order Runge-Kutta method

- **Step 1:** Estimate change due of the right-hand side using Euler's method:

$$\mathbf{k}_1 = \Delta t \mathbf{f}(\mathbf{y}^n, t^n)$$

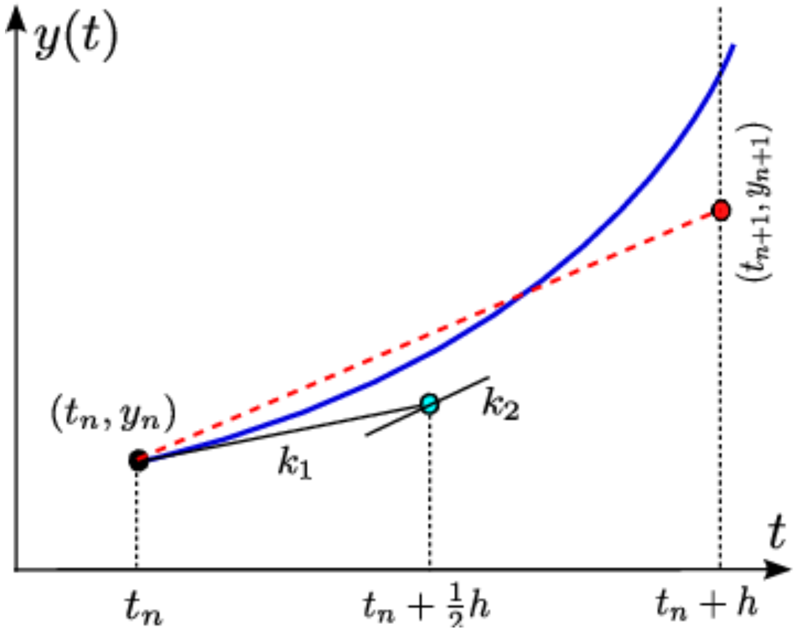
- **Step 2:** Use estimate to predict value of solution at midpoint of the timestep. Evaluate right hand side at midpoint:

$$\mathbf{y}^{n+1} = \mathbf{y}^n + \Delta t \mathbf{f}(\mathbf{y}^n + \frac{1}{2}\mathbf{k}_1, t^n + \frac{1}{2}\Delta t)$$

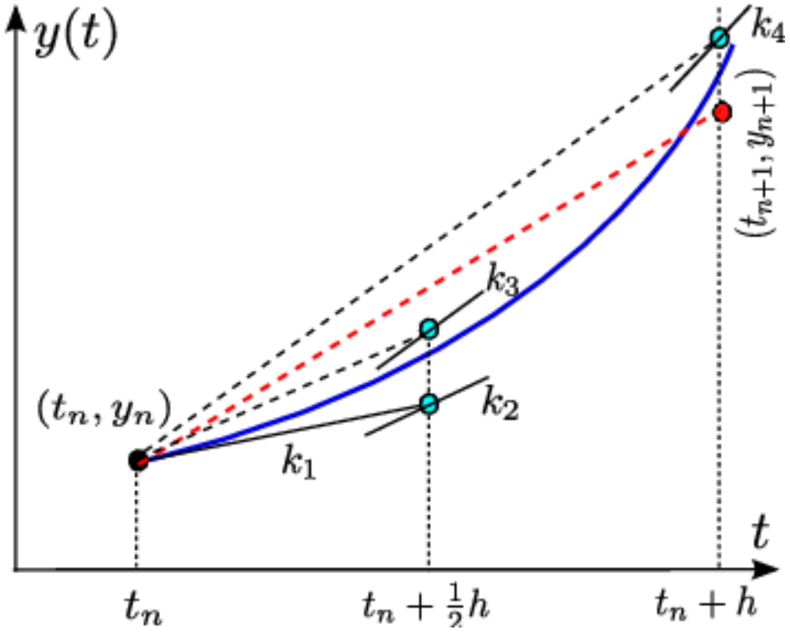
- See **`rk2_orbit.f08`**

# Second and fourth-order Runge-Kutta methods

2nd order




4th order

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# The fourth-order Runge-Kutta method

- In practice, the workhorse algorithm for first-order sets of ODEs is the fourth-order Runge-Kutta algorithm which (we state here without derivation)
- Step 1: $$\mathbf{k}_1 = \Delta t\ \mathbf{f}(\mathbf{y}^n, t^n)$$
- Step 2: $$\mathbf{k}_2 = \Delta t\ \mathbf{f}(\mathbf{y}^n + \frac{1}{2}\mathbf{k}_1, t^n + \frac{1}{2}\Delta t)$$
- Step 3: $$\mathbf{k}_3 = \Delta t\ \mathbf{f}(\mathbf{y}^n + \frac{1}{2}\mathbf{k}_2, t^n + \frac{1}{2}\Delta t)$$
- Step 4: $$\mathbf{k}_4 = \Delta t\ \mathbf{f}(\mathbf{y}^n + \mathbf{k}_3, t^n + \Delta t)$$
- Step 5: $$\mathbf{y}^{n+1} = \mathbf{y}^n + \frac{1}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4)$$

# Runge-Kutta methods

- Euler method can be thought of as the first-order RK method
  - Accurate to first order in $\Delta t$, i.e., error is order $\Delta t^2$

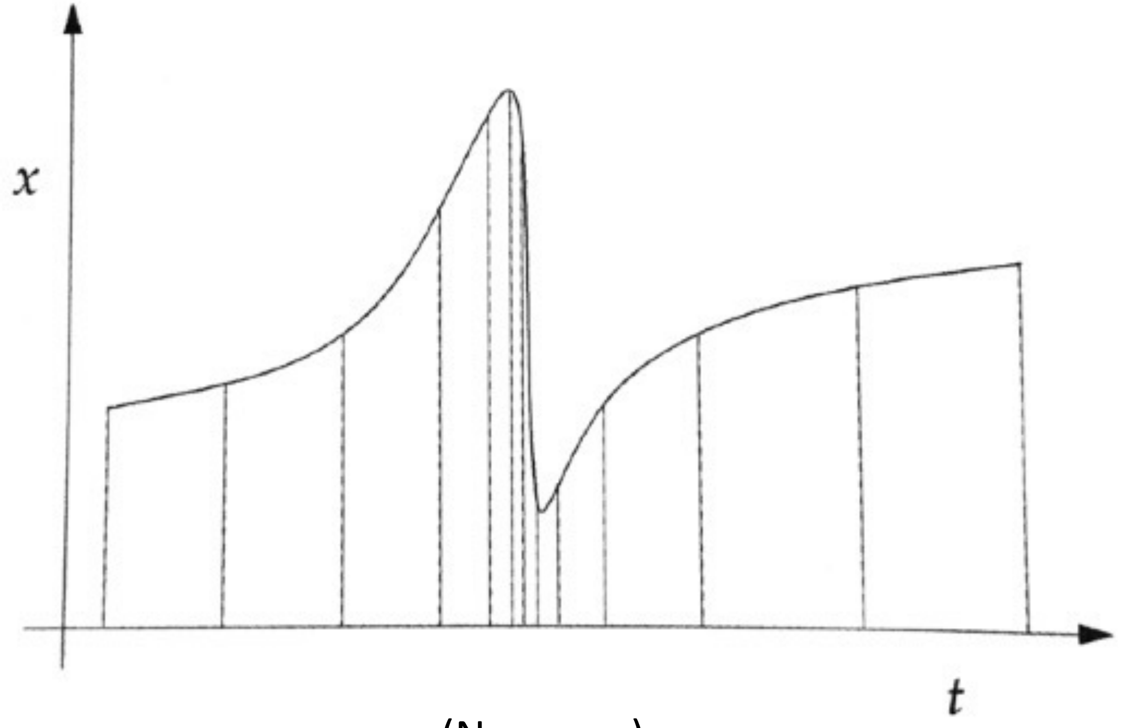
- Second-order RK method accurate to $\Delta t^2$, so error $\Delta t^3$

- Fourth-order RK method accurate to $\Delta t^4$, so error $\Delta t^5$
  - By far the most common method for the numerical solution of ODEs
  - Balances accuracy and complexity

- Quoted accuracies are for one step, errors accumulate over the number of steps needed in the calculation, usually loose an order of accuracy (see Newman)

# Adaptive step size

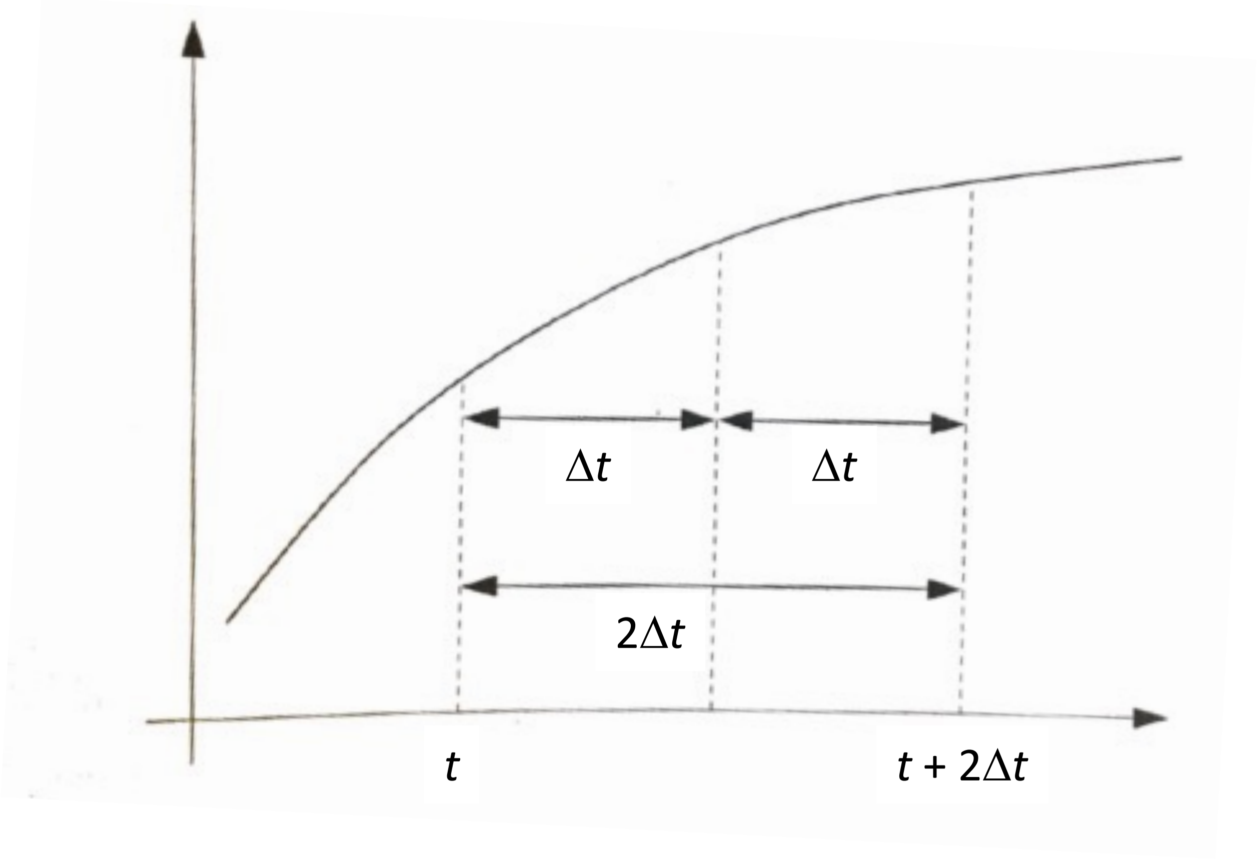
- So far, we have set by hand a constant step size $\Delta t$
- Often, we can get better results by varying the step size
  - Increase in regions where function varies rapidly, decrease where it varies slowly
- Approach: vary $\Delta t$ so the error introduced per unit interval is roughly constant
  - First we need to estimate the error in the steps




(Newman)

# Adaptive step size: Estimating the error

- 1. Choose initial (small) $\Delta t$
- 2. Use RK method to do two $\Delta t$ steps of the solution
- 3. Go back to initial $t$ and do an RK step with $2\Delta t$
- 4. Compare the results to estimate the error



# Adaptive step size: Estimating the error

- True value of function related to estimate $y_{\Delta t}$ :

$$y(t + 2\Delta t) = y_{\Delta t} + 2c\Delta t^5$$

- For doubled step size $y_{2\Delta t}$ :

$$y(t + 2\Delta t) = y_{2\Delta t} + 32c\Delta t^5$$

- So per step error is:

$$\epsilon = c\Delta t^5 = \frac{1}{30}(y_{\Delta t} - y_{2\Delta t})$$

- Take $\delta$ to be the target accuracy per step. Then the step size necessary to get that accuracy is:

$$\Delta t' = \Delta t \sqrt[5]{\frac{30\delta}{|y_{\Delta t} - y_{2\Delta t}|}}$$

# Adaptive step size: Complete approach

- 1. Choose initial $\Delta t$
- 2. Use RK method to do two $\Delta t$ steps of the solution
- 3. Go back to initial $t$ and do an RK step with $2\Delta t$
- 4. Compare the results to estimate the error
- 5. Calculate ideal step size $\Delta t'$
  - If $\varepsilon > \delta$, then redo the calculation with $\Delta t'$
  - If $\varepsilon < \delta$, take the results obtained using $\Delta t$ and move on to time $t + \Delta t$. In the next iteration use $\Delta t'$ as the timestep

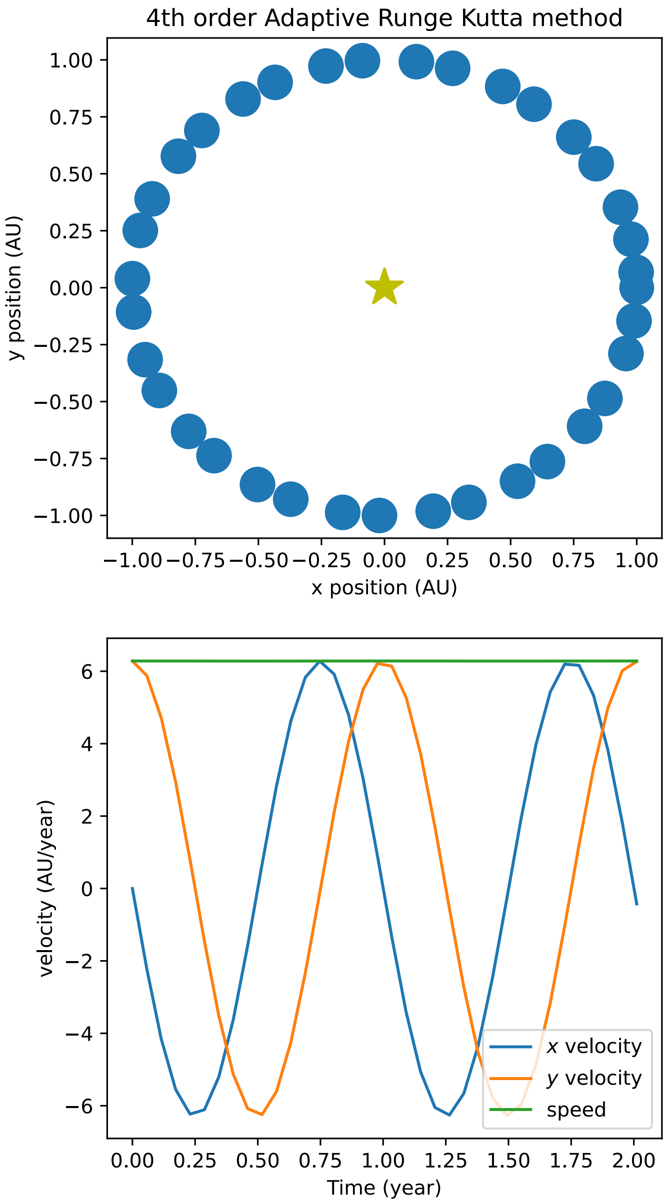
- Requires at least 3 RK steps for every two actually used, but usually results in an overall speedup for a given accuracy
- Usually limit how much $\Delta t'$ can differ from $\Delta t$ (e.g., by less than a factor of two) in case the denominator happens to diverge

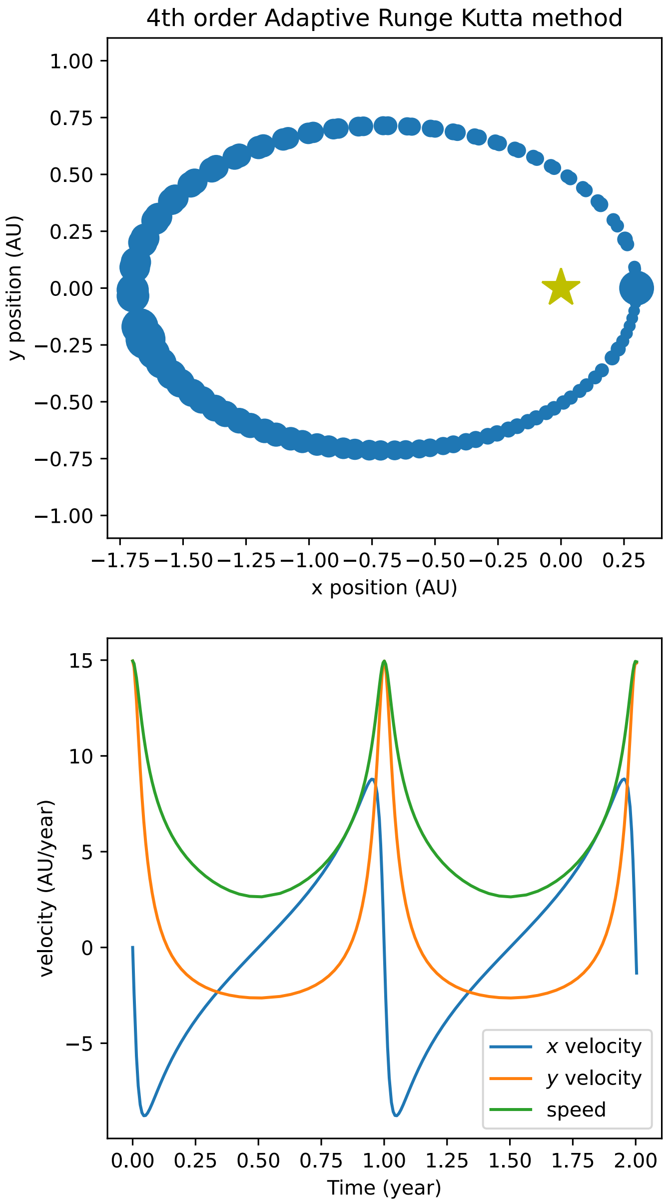
# Example: Elliptical orbit with adaptive 4th-order RK

<u>Circular</u>:

$x_0$= 1 AU

$v_{y0}$ =6.283185 AU/year




<u>Elliptical</u>:

$x_0$= 0.3 AU

$v_{y0}$ =14.955378 AU/year

# After class tasks

- Homework 1 due Today by 11:59pm
  - Let me know if you have HW questions or questions/issues on github classroom
  - Office hours: Mondays, 3:00pm to 4:00pm; Thursdays, 9:50am 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:
  - Newman Ch. 8
  - Wikipedia page on root finding