Computational Environments and Toolchains

Topic 02 — Scientific Computing using Python

Lecture 03 — scipy

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Autumn Semester, 2022

Outline

- matplotlib (2D and 3D plotting library)
- numpy (high performance matrix library)
- scipy (scientific computation library)

Outline

Outline

What is SciPy?

SciPy

is a library of algorithms and mathematical tools built to work with NumPy arrays..

- Special functions (`scipy.special`)
- Integration (`scipy.integrate`)
- Optimization (`scipy.optimize`)
- Interpolation (`scipy.interpolate`)
- Fourier Transforms (`scipy.fftpack`)
- Signal Processing (`scipy.signal`)
- Linear Algebra (`scipy.linalg`)
- Sparse Eigenvalue Problems with ARPACK
- Compressed Sparse Graph Routines (`scipy.sparse.csgraph`)
- Spatial data structures and algorithms (`scipy.spatial`)
- Statistics (`scipy.stats`)
- Multidimensional image processing (`scipy.ndimage`)
- File IO (`scipy.io`)
- Weave (`scipy.weave`)

Importing

- The SciPy docs recommend loading the various modules as

scipy.py

```
5 import numpy as np
6 import scipy as sp
7 import matplotlib as mpl
8 import matplotlib.pyplot as plt
```

- Each subpackage must be imported separately

scipy.py

```
10 from scipy import linalg, optimize
```

- In addition to the **help**(), there is a sp.info() function that outputs things without a pager
- Python also has a **dir**() function that lists the names a module defines

Health Warning

Every numerical method has its own strengths, weaknesses, and assumptions

- You should research a bit to understand what these methods are doing under the hood.
- Many of the SciPy methods are wrappers to well-tested implementations of algorithms that were developed many years (decades even) ago.
- But if your problem does not satisfy the assumptions that the algorithm or its implementation assumed then all bets are off regarding the reliability of the generated results.

Outline

Numerical Integration

We want to compute:

$$I = \int_a^b f(x)\ \mathrm{x} \tag{1}$$

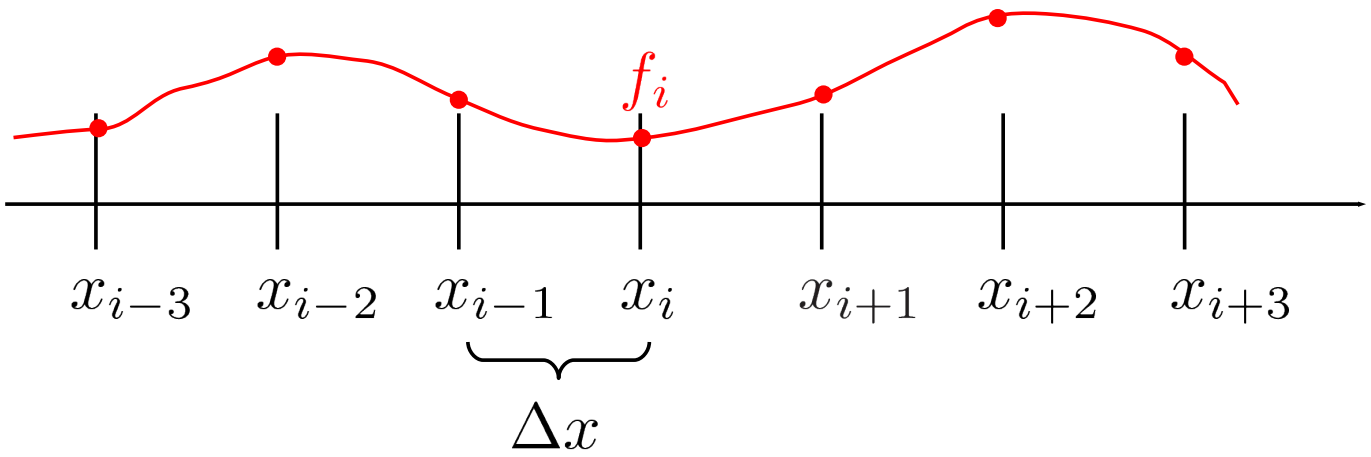
We can imagine 2 situations

1. Our function, $f(x)$ is defined only at a set of (possibly regularly spaced) points.
   - Generally speaking, asking for greater accuracy involves using more of the discrete points in the approximation for I.
2. We have an analytic expression for $f(x)$
   - We have the freedom to pick our integration points, and this can allow us to optimise the calculation of I

- Any numerical integration method that represents the integral as a (weighted) sum at a discrete number of points is called a quadrature rule.
- Fixed spacing between points: Newton-Cotes quadrature

Gridded Data

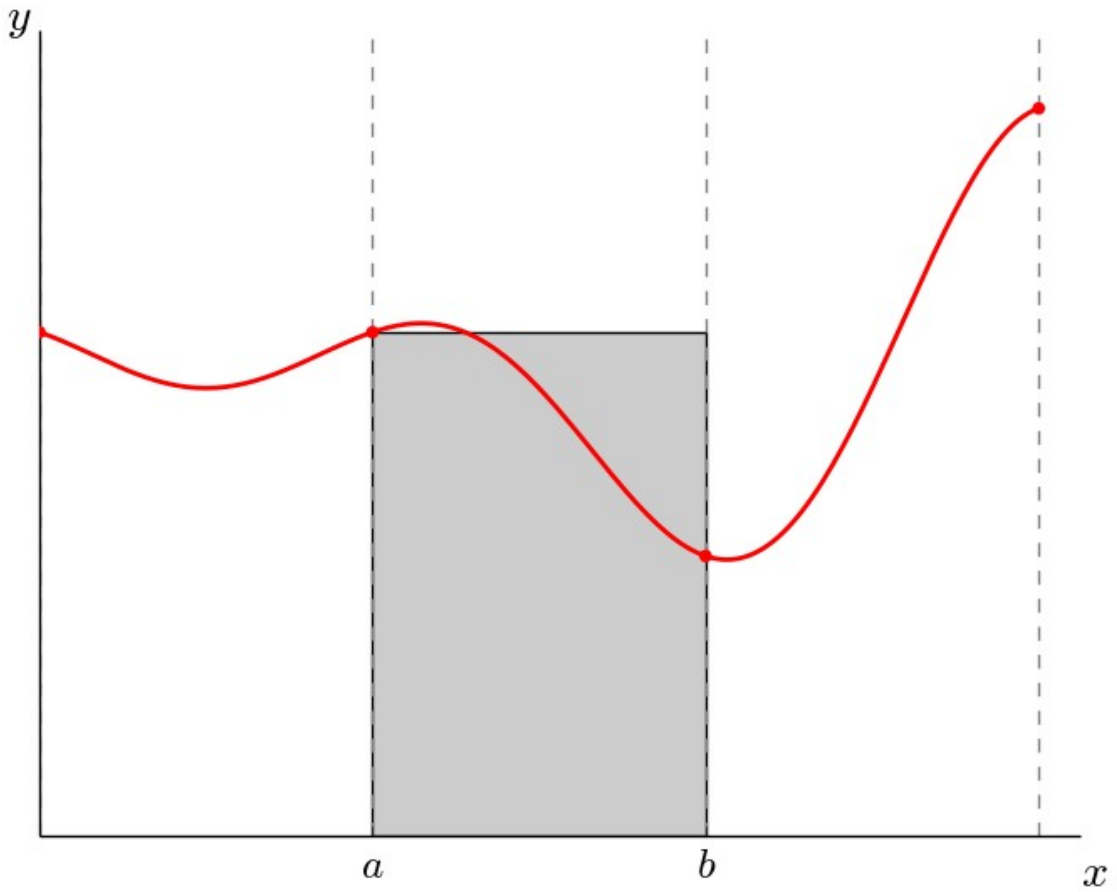
- Discretized data is represented at a finite number of locations
  - Integer subscripts are used to denote the position (index) on the grid
  - Structured/regular: spacing is constant



  - Data is known only at the grid points: $f_i = f(x_i)$

Rectangular Rule

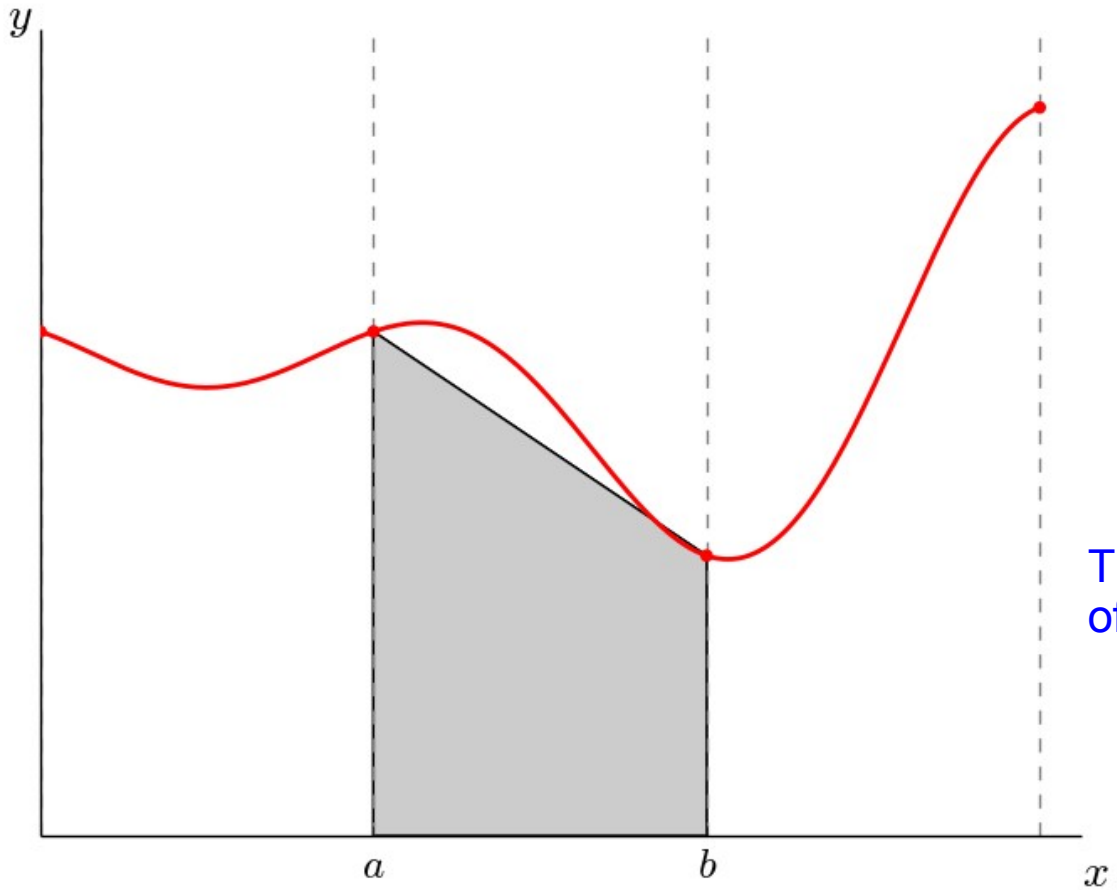
- Simplest case: piecewise constant interpolant (rectangle rule)



$$I \equiv \int_a^b f(x)dx \approx \Delta x f(a)$$

Trapezoidal Rule

- One step up: piecewise linear interpolant (trapezoid rule)



This is just the area of a trapezoid

$$I \equiv \int_a^b f(x)dx \approx \Delta x \frac{f(a) + f(b)}{2}$$

Simpson's Rule

- Piecewise quadratic interpolant (Simpson's rule)
  - 3 unknowns and 3 points

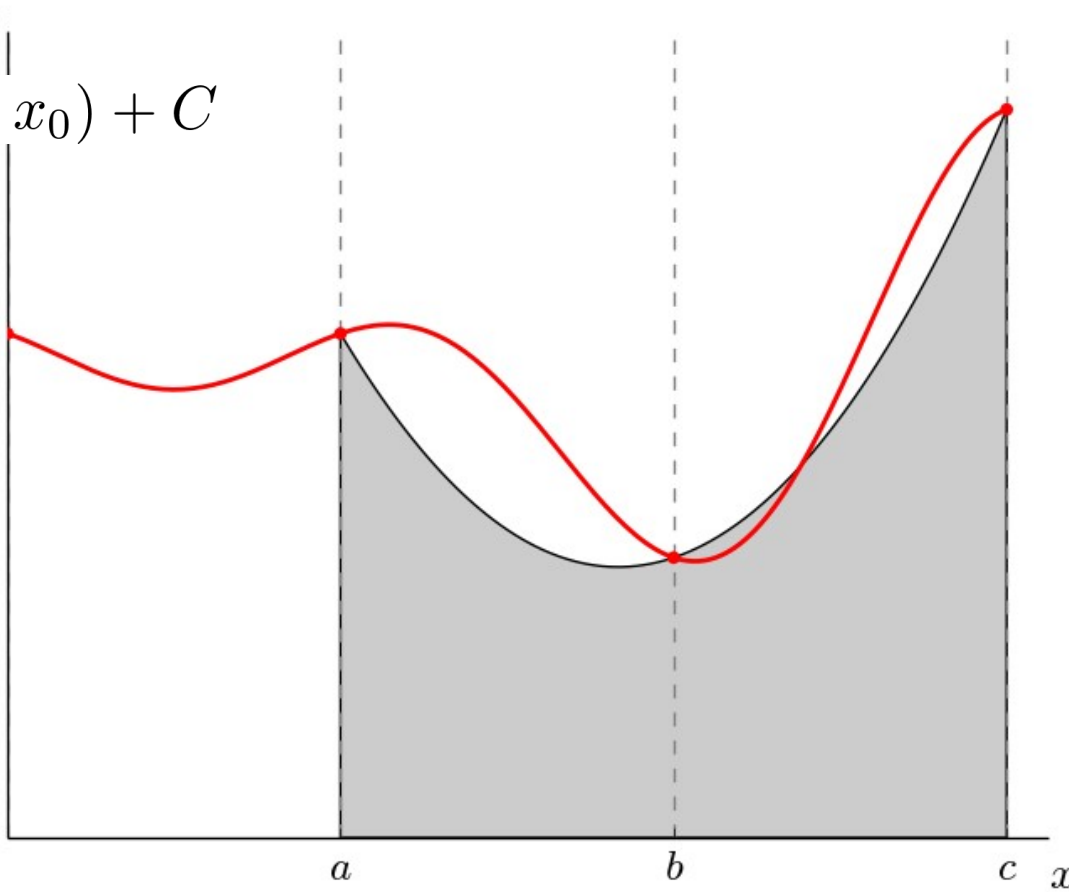
$$f(x) = A(x - x_0)^2 + B(x - x_0) + C$$

  - Solving:

$$A = \frac{f_a - 2f_b + f_c}{2\delta^2}$$

$$B = -\frac{f_c - 4f_b + 3f_a}{2\delta}$$

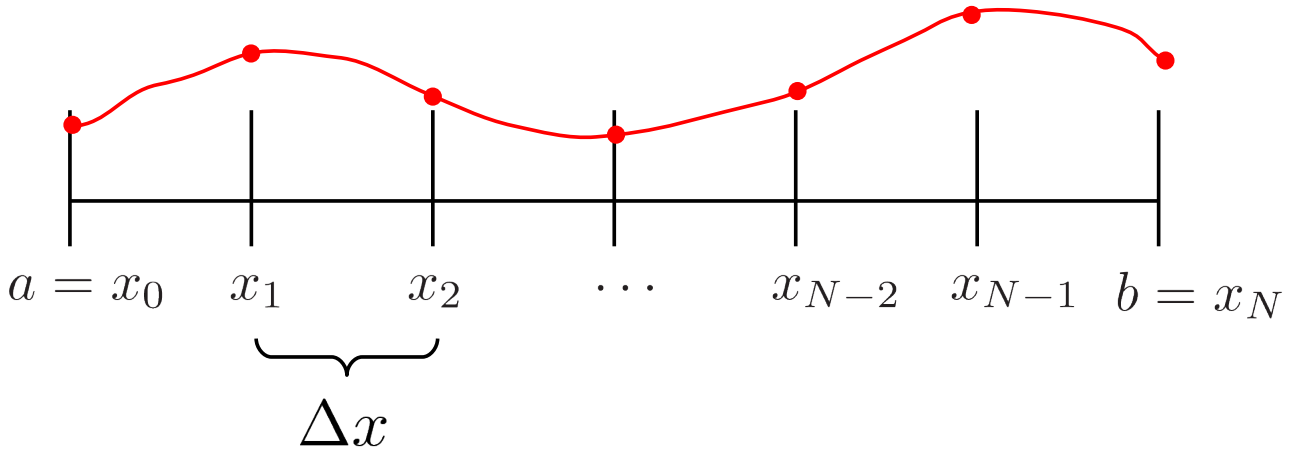
$$C = f_a$$



$$I = \int_{x_0}^{x_2} [A(x - x_0)^2 + B(x - x_0) + C]dx = \frac{c - a}{6}(f_0 + 4f_1 + f_2)$$

Compound Integration

- Break interval into chunks



$$I \equiv \int_a^b f(x)dx = \sum_{i=0}^{N-1} \underbrace{\int_{x_i}^{x_{i+1}} f(x)dx}_{\text{Integral over a single slab}}$$

Compound Integration

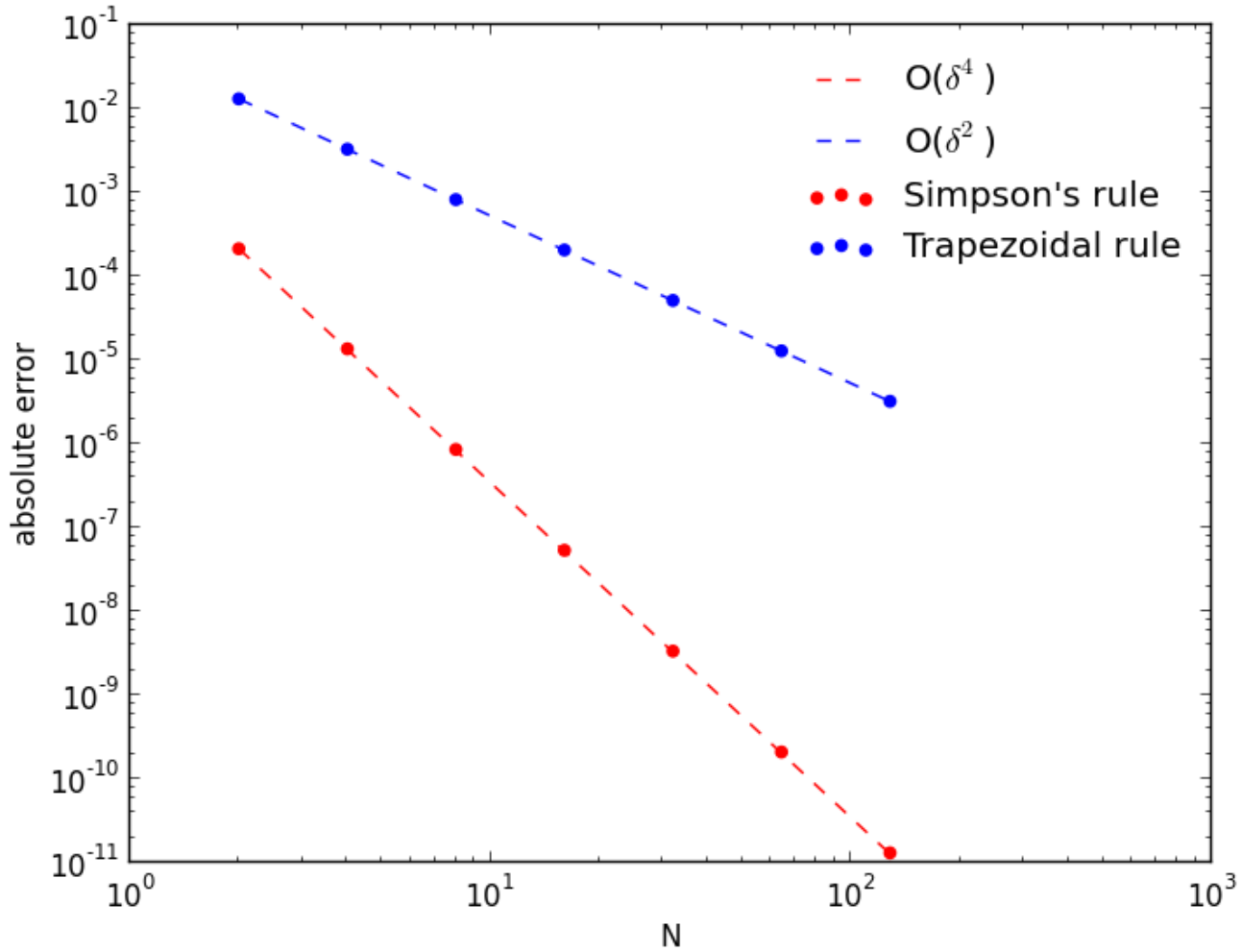
- Compound Trapezoidal

$$\int_a^b f(x)dx = \frac{\Delta x}{2} \sum_{i=0}^{N-1} (f_i + f_{i+1}) + \mathcal{O}(\Delta x^2)$$

- Compound Simpson's
  - Integrate pairs of slabs together (requires even number of slabs)

$$\int_a^b f(x)dx = \frac{\Delta x}{3} \sum_{i=0}^{N/2-1} (f_{2i} + 4f_{2i+1} + f_{2i+2}) + \mathcal{O}(\Delta x^4)$$

Compound Integration



$$\int_0^1 e^{-x} dx$$

Always a good idea to check the convergence rate!

Gaussian Quadrature

- Instead of fixed spacing, what if we strategically pick the spacings?
  - We want to express

$$\int_a^b f(x)dx \approx w_1 f(x_1) + \ldots w_N f(x_N)$$

  - w's are weights. We will choose the location of points x_i

Gaussian Quadrature

- Gaussian quadrature: fundamental theorem
  - q(x) is a polynomial of degree N, such that

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

  - k = 0, ..., N-1 and ρ(x) is a specified weight function.
  - Choose x_1, x_2, ... x_N as the roots of the polynomial q(x)
  - We can write

$$\int_a^b f(x)\rho(x)dx \approx w_1 f(x_1) + \ldots w_N f(x_N)$$

    and there will be a set of w's for which the integral is exact if f(x) is a polynomial of degree < 2N!

Gaussian Quadrature

- Many quadratures exist:

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)

- In practice, the roots and weights are tabulated for these out to many numbers of points, so there is no need to compute them.

Gaussian Quadrature

- Example:

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

```
erf(1) (exact):              0.84270079295
3-point trapezoidal:         0.825262955597 -0.017437837353
3-point Simpson's:           0.843102830043 0.00040203709326 6
3-point Gauss-Legendre:      0.842690018485 -1.0774465204e-05
```

Notice how well the Gauss-Legendre does for this integral.

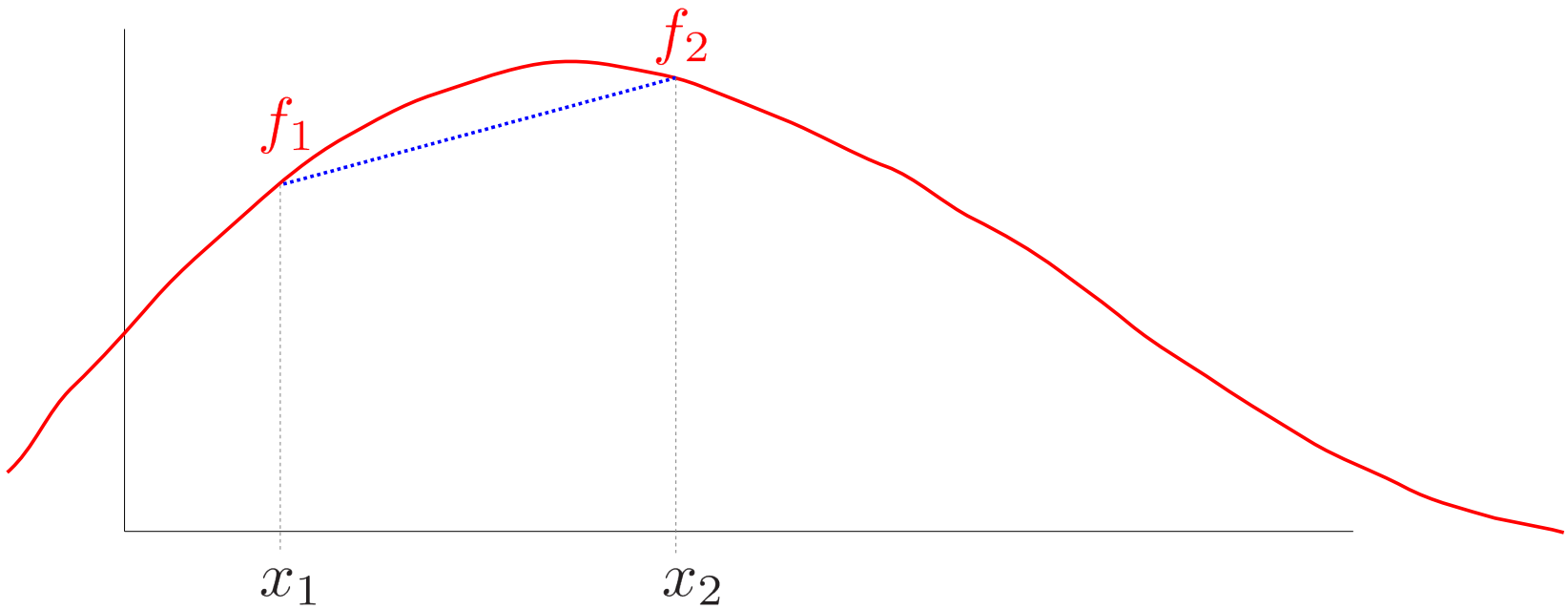
Outline

Interpolation

- We frequently have data only at a discrete number of points
  - Interpolation fills in the gaps by making an assumption about the behavior of the functional form of the data
- Many different types of interpolation exist
  - Some ensure no new extrema are introduced
  - Some match derivatives at end points
  - ...
- Generally speaking: larger number of points used to build the interpolant, the higher the accuracy in a local region
  - Pathological cases exist
  - You may want to enforce some other property on the form of the interpolant

Linear Interpolation

- Simplest idea—draw a line between two points



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

  - Exactly recovers the function values at the end points

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:

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

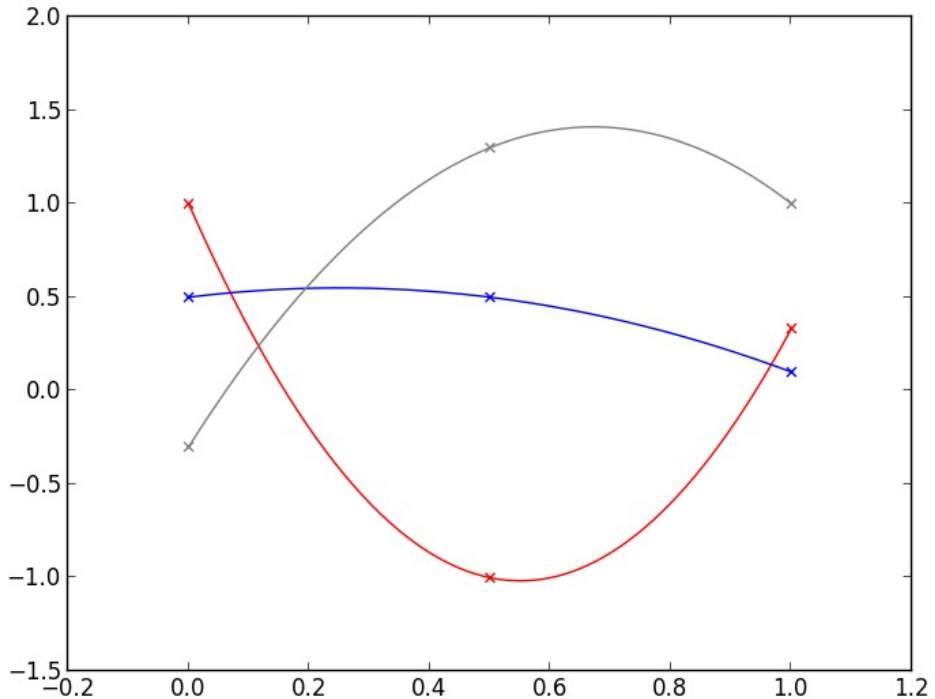
    - Basis function l_i is 0 at all x_j except for x_i (where it is 1)
  - Function value at x is:

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

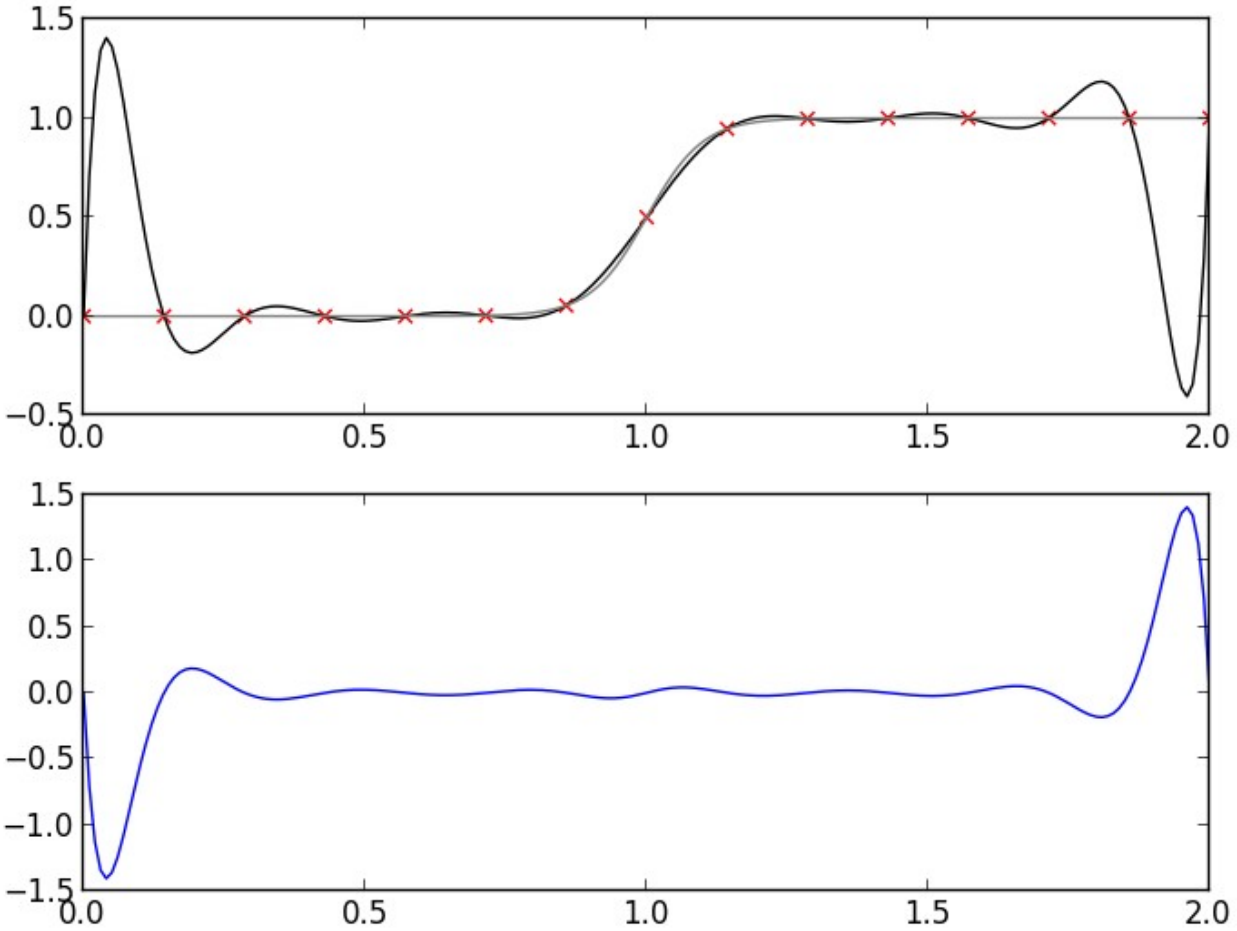
Lagrange Interpolation

- Quadratic Lagrange polynomial:

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



Lagrange Interpolation

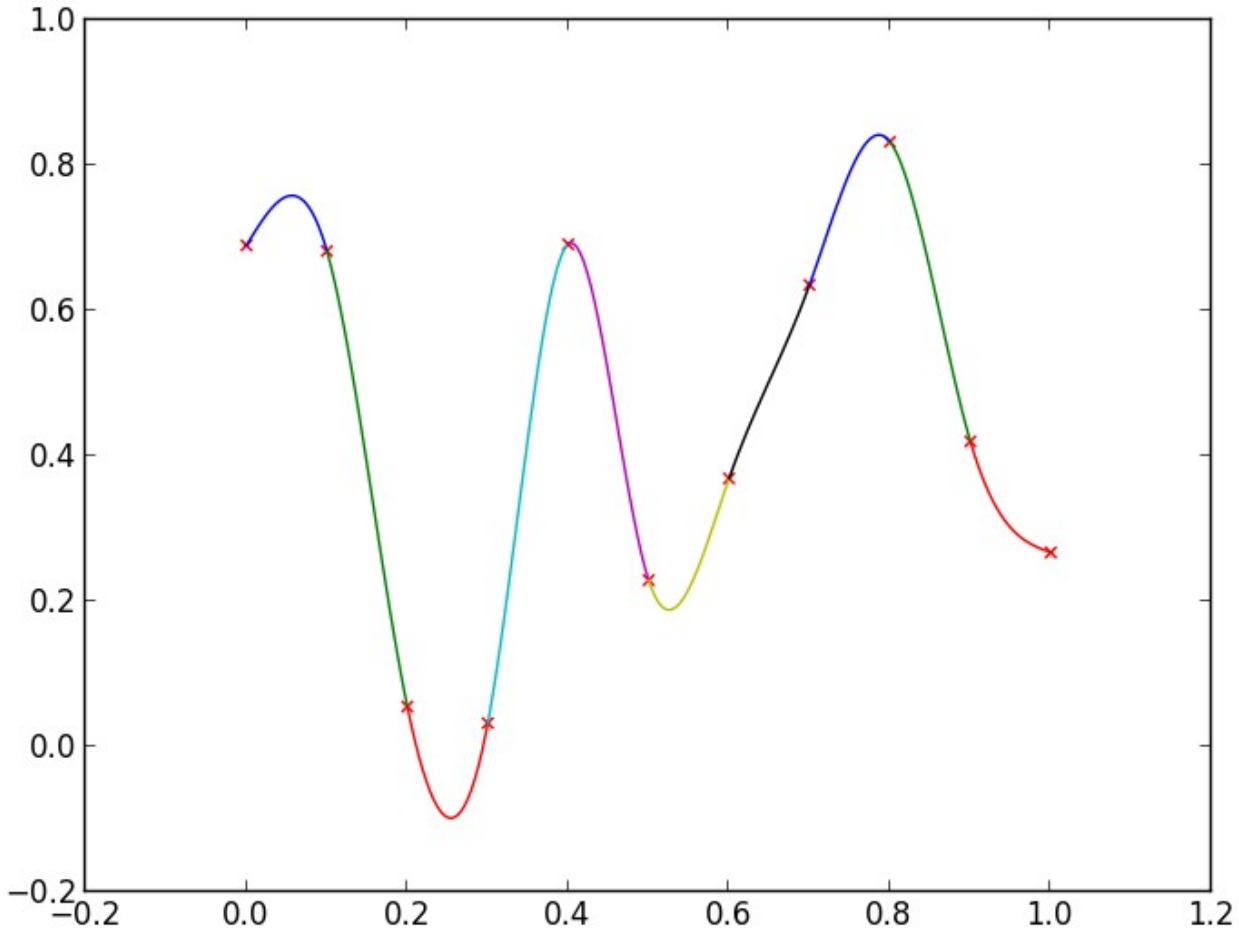


High-order is not always better: Interpolation through 15 points sampled uniformly from tanh(). The error is shown below.

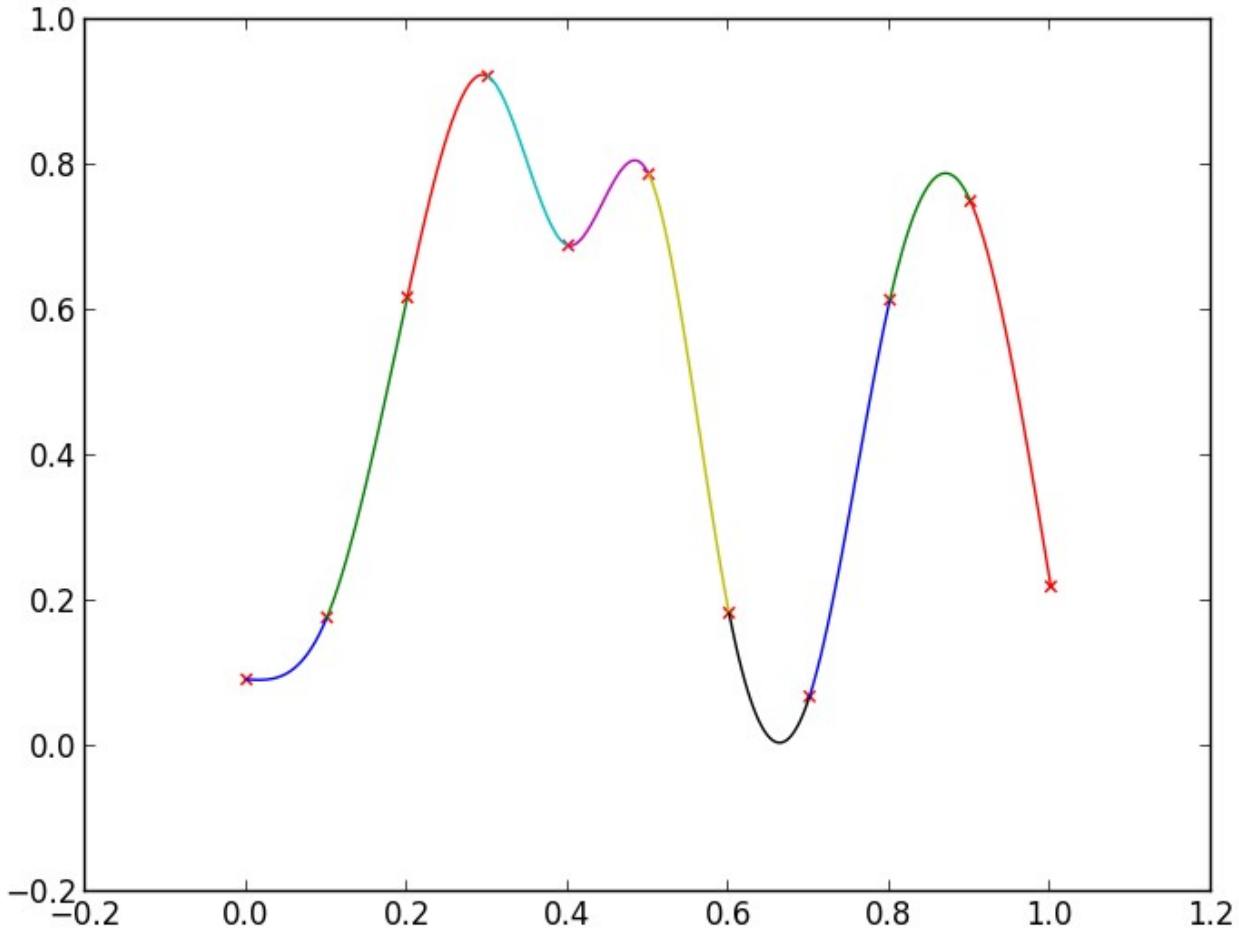
Splines

- 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

Cubic Splines



Cubic Splines



Note that the splines can overshoot the original data values

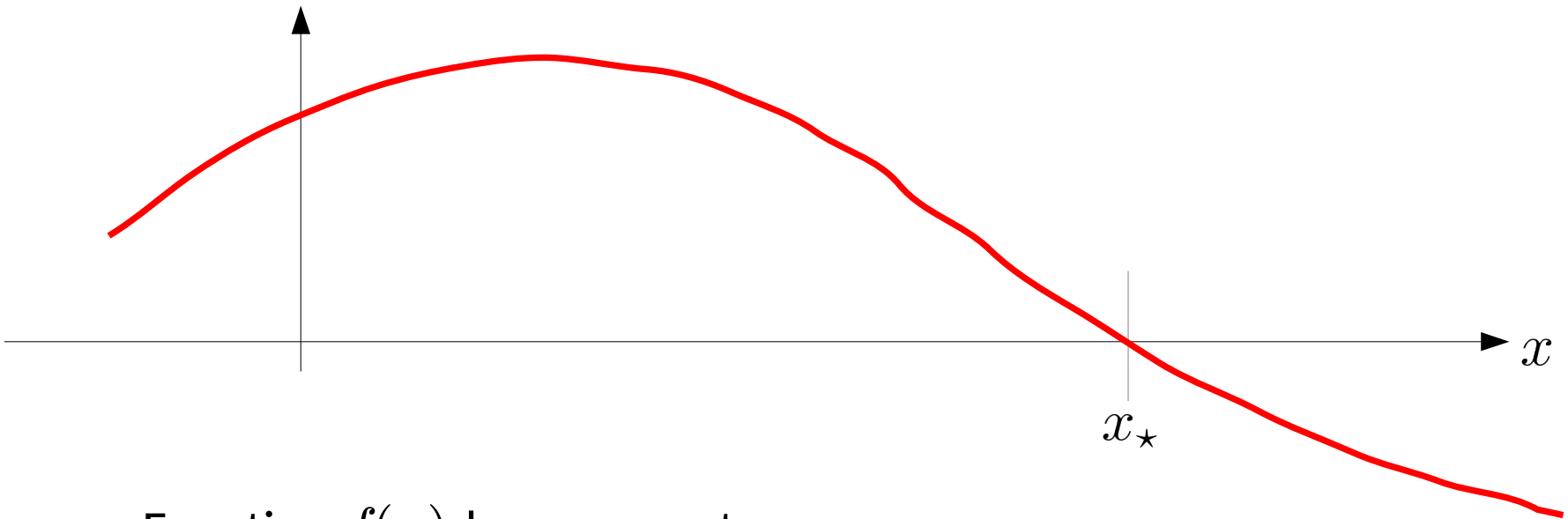
Cubic Splines

- Note: cubic splines are not necessarily the most accurate interpolation scheme (and sometimes far from...)
- But, for plotting/graphics applications, they look right

Outline

Root Finding

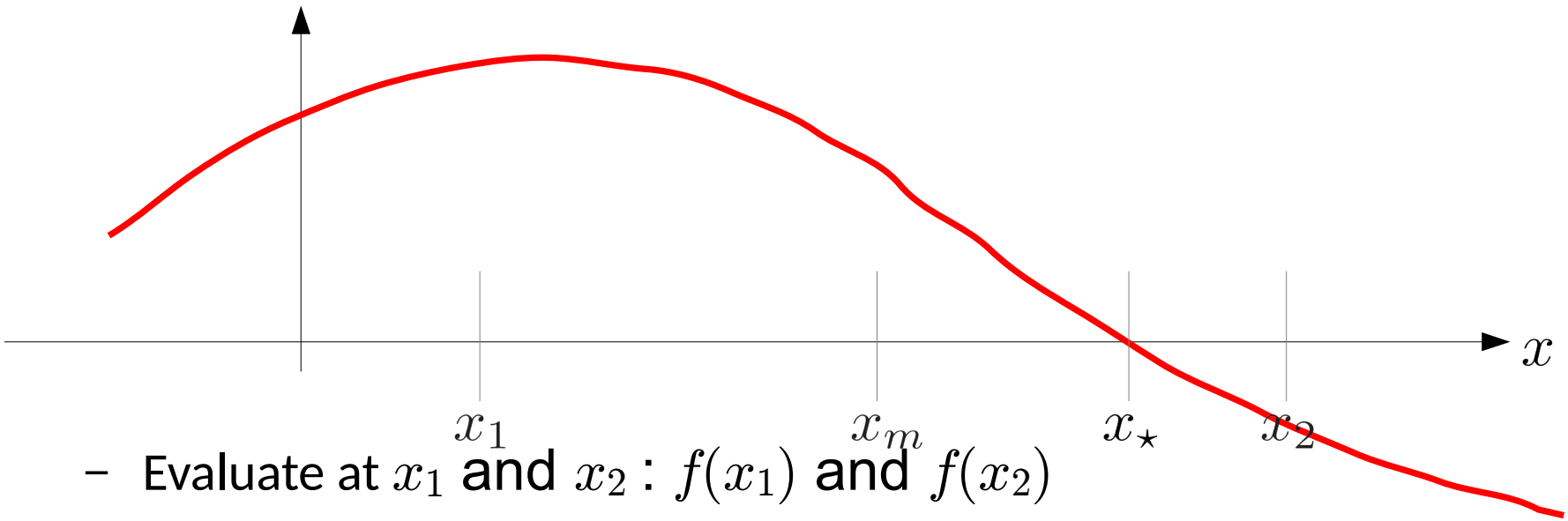
- Basic methods can be understood by looking at the function graphically



  - Function $f(x)$ has a zero at $x_\star$
  - Note the sign of $f(x)$ changes at the root

Bisection

- Simplest method: bisection



  - Evaluate at x_1 and x_2 : $f(x_1)$ and $f(x_2)$
  - If these are different signs, then the root lies between them
  - Evaluate at the midpoint: $x_m = (x_1 + x_2)/2$ getting $f(x_m)$
  - The root lies in one of the two intervals—repeat the process

Newton-Raphson

- If we know df/dx we can do better
  - Start with an initial guess, x_0, that is "close" to the root
  - Taylor expansion:

$$f(x_0 + \delta) \approx f(x_0) + f'(x_0)\delta + ...$$

  - If we are close, then

$$f(x_0 + \delta) \approx 0 \longrightarrow \delta = -\frac{f(x_0)}{f'(x_0)}$$

  - Update

$$x_1 = x_0 + \delta$$

  - We can continue, iterating again and again, until the change in the root < ε
- Converges fast: usually only a few iterations are needed

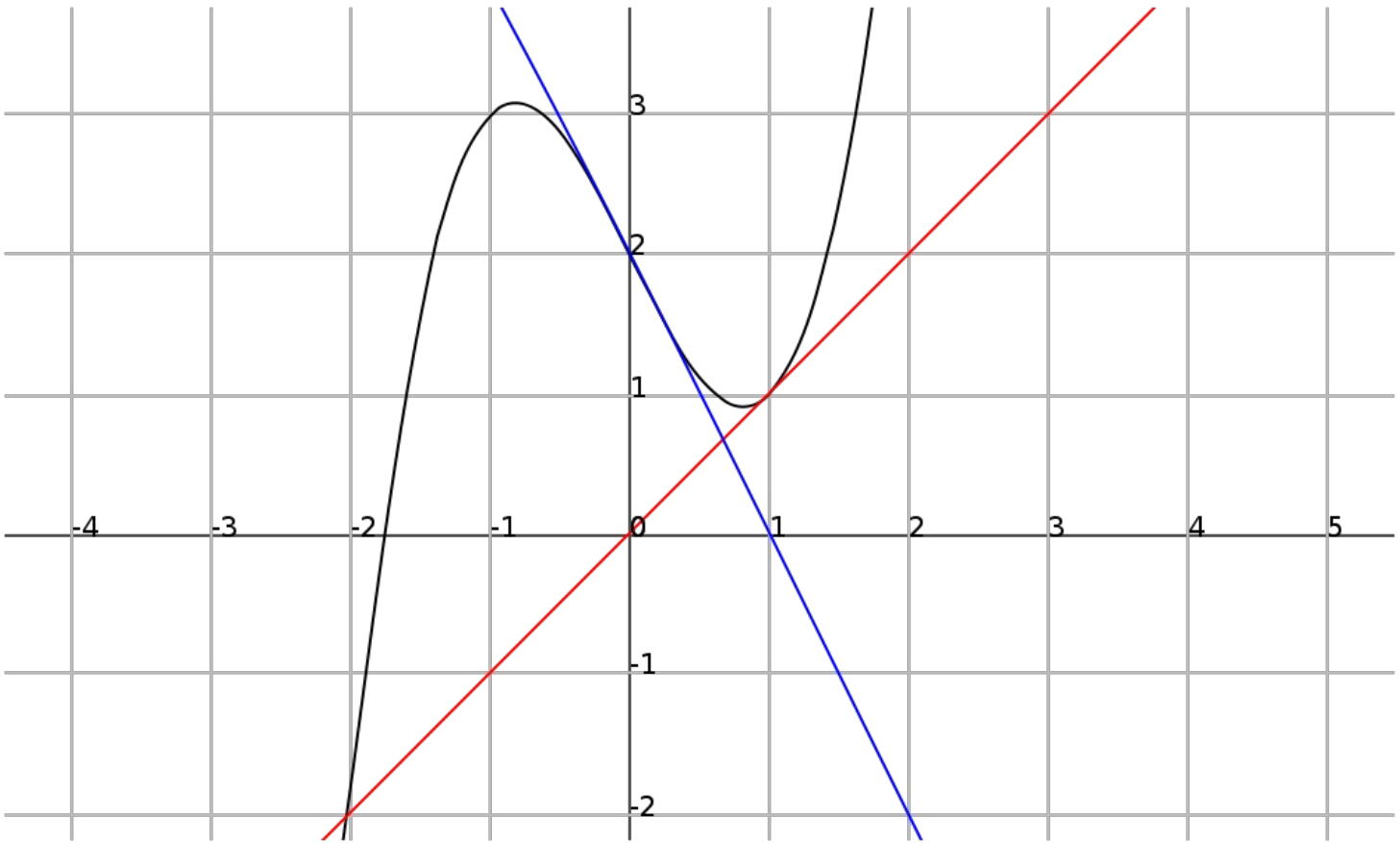
Newton-Raphson

- Requirements for good convergence:
  - Derivative must exists and be non-zero in the interval near the root
  - Second derivative must be finite
  - x_0 must be close to the root
- Can be used with systems (we'll see this later)
- Multiple roots?
  - Generally: try to start with a good estimate*

*not a guarantee

Newton-Raphson

- Consider $f(x) = x^3 - 2x + 2$
  - Start with $0 \rightarrow 1 \rightarrow 0 \rightarrow 1 \rightarrow 0$ ...
  - Cycle



Secant Method

- If we don't know df/dx, we can still use the same ideas
  - We need to initial guesses: x_{-1} and x_0
  - Use approximate derivative

$$x_1 = x_0 - \frac{f(x_0)}{[f(x_0) - f(x_{-1})]/(x_0 - x_{-1})}$$

    - Used when an analytic derivative is unavailable, or too expensive to compute (e.g. EOS)
- Brent's method combines bisection, secant, and other methods to provide a very reliable method

Multivariate Newton's Method

- Imagine a vector function: $\mathbf{f}(\mathbf{x})$
  - $\mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x})\ f_2(\mathbf{x})\ f_3(\mathbf{x})\ \ldots\ f_N(\mathbf{x}))^T$
  - Column vector of unknowns: $\mathbf{x} = (x_1\ x_2\ x_3\ \ldots\ x_N)^T$
- We want to find the zeros:
  - Initial guess: $\mathbf{x}^{(0)}$
  - Taylor expansion:

$$f_i(\mathbf{x}^{(0)} + \delta\mathbf{x}) \approx 0 = f_i(\mathbf{x}^{(0)}) + \sum_{j=1}^{N} \frac{\partial f_i}{\partial x_j}\delta x_j + \ldots$$

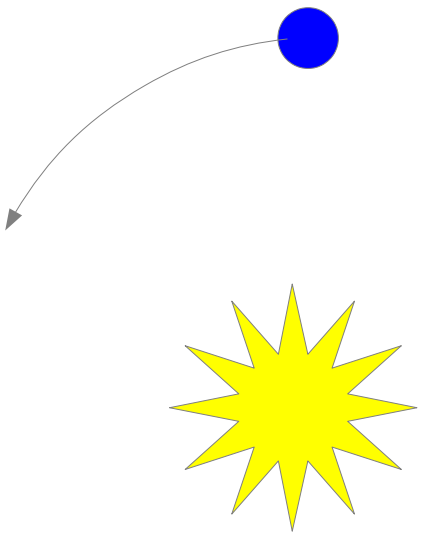
N equations + N unknowns

This is the Jacobian

  - Update to initial guess is: $\delta\mathbf{x} = -\mathbf{J}^{-1}\mathbf{f}(\mathbf{x}^{(0)})$
    - Cheaper to solve the linear system than to invert the Jacobian
  - Iterate: $\mathbf{J}\delta\mathbf{x}^{(k)} = -\mathbf{f}(\mathbf{x}^{(k)})\ , \quad \mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \delta\mathbf{x}^{(k)}$

Outline

ODEs



- Consider orbits around the Sun
  - Another simple system that allows us to explore the properties of ODE integrators

$$\dot{\mathbf{x}} = \mathbf{v} \qquad \dot{\mathbf{v}} = -\frac{GM\mathbf{r}}{r^3}$$

  - Kepler's law (neglecting orbiting object mass):

$$4\pi^2 a^3 = GM_\star P^2$$

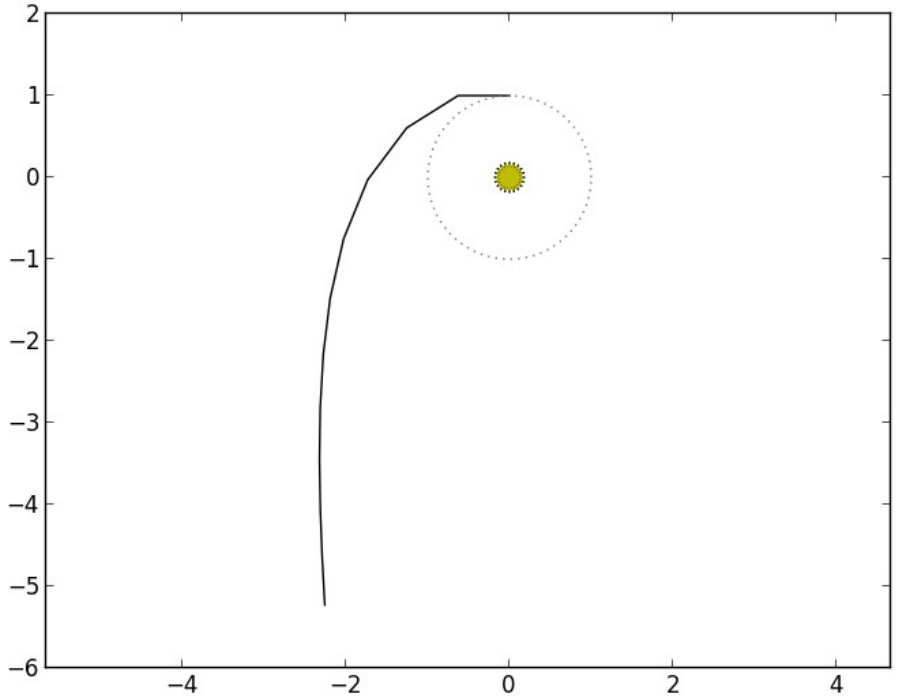
  - Work in units of AU, solar masses, and years
    - $GM = 4\ \pi^2$

Orbits: Euler Method

- Simplest case: Euler's method

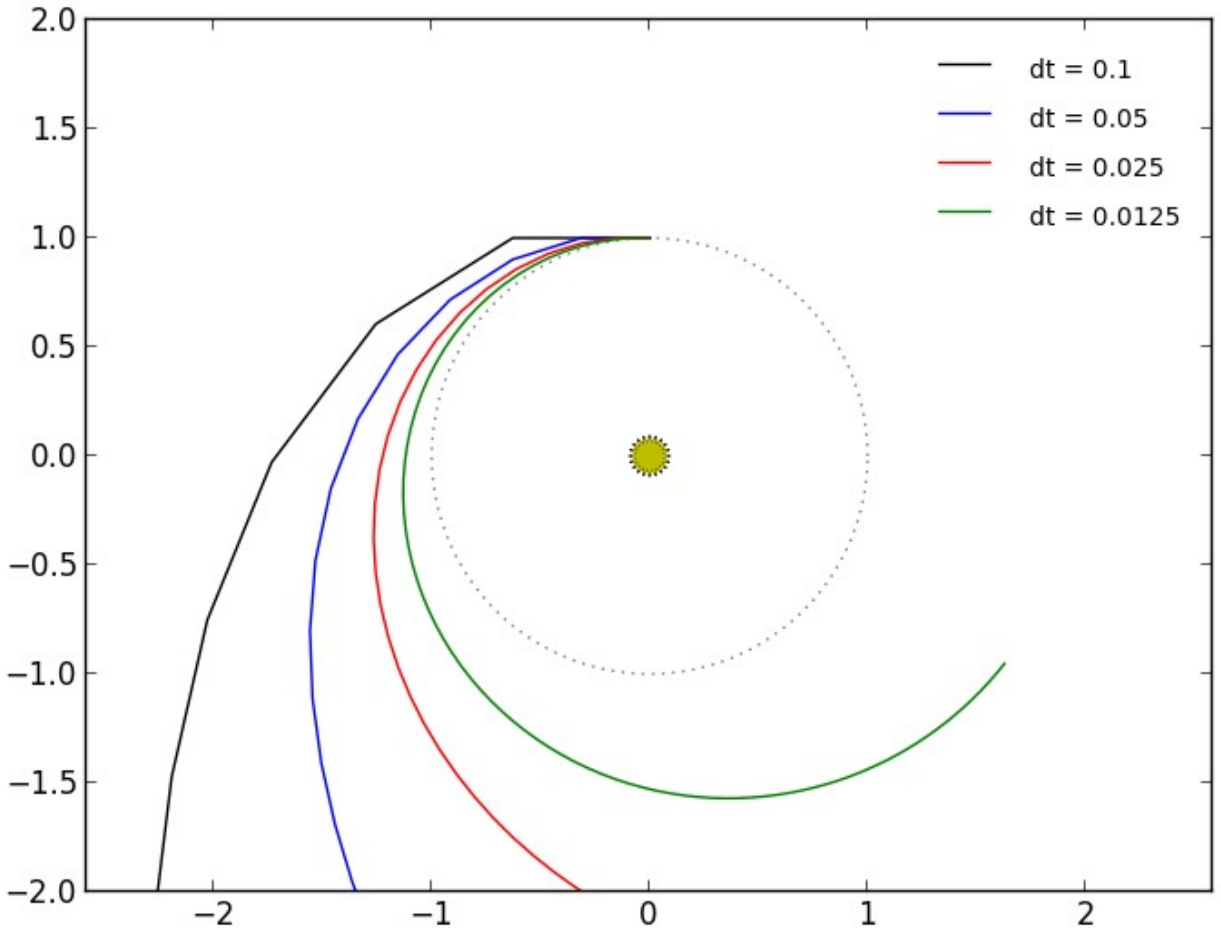
$$\mathbf{x}^{n+1} = \mathbf{x}^n + \tau \mathbf{v}^n \qquad \mathbf{v}^{n+1} = \mathbf{v}^n + \tau \mathbf{a}^n$$

- Need to specify a semi-major axis and eccentricity
- Initial conditions:
  - $x = 0,\ y = a(1-e)$
  - $u = -\sqrt{\frac{GM}{a}\frac{1+e}{1-e}},\ v = 0$
  - This is counter-clockwise orbiting



Our planet escapes—clearly energy is not conserved here!

Orbits: Euler Method



Things get better with a smaller timestep, but this is still first-order

Let's look at the code and see how small we need to get a closed circle

Higher Order Methods

- Midpoint or 2nd order Runge-Kutta:

$$\frac{\mathbf{r}^{n+1} - \mathbf{r}^n}{\tau} = \mathbf{v}^{n+1/2} + \mathcal{O}(\tau^2) \qquad \frac{\mathbf{v}^{n+1} - \mathbf{v}^n}{\tau} = \mathbf{a}^{n+1/2} + \mathcal{O}(\tau^2)$$

- The updates are then:

$$\mathbf{r}^{n+1} = \mathbf{r}^n + \tau \mathbf{v}^{n+1/2} + \mathcal{O}(\tau^3)$$

$$\mathbf{v}^{n+1} = \mathbf{v}^n + \tau \mathbf{a}^{n+1/2} + \mathcal{O}(\tau^3)$$

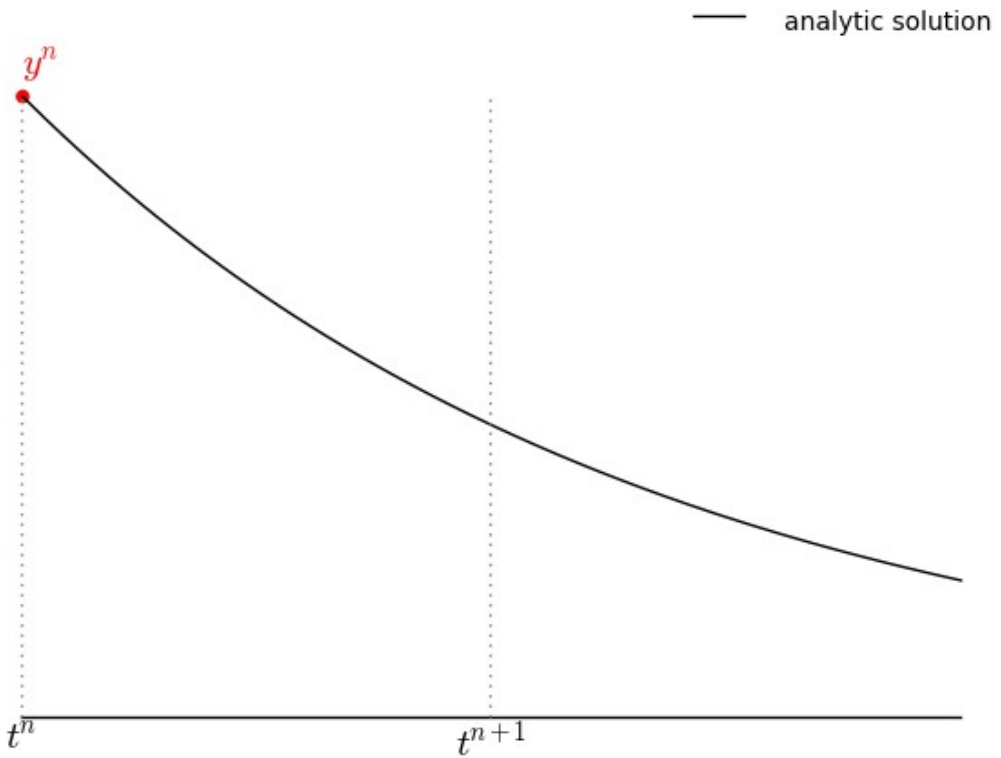
- This is third-order accurate (locally), to start things off, we do:

$$\mathbf{r}^\star = \mathbf{r}^n + (\tau/2)\mathbf{v}^n$$
$$\mathbf{v}^\star = \mathbf{v}^n + (\tau/2)\mathbf{a}^n$$

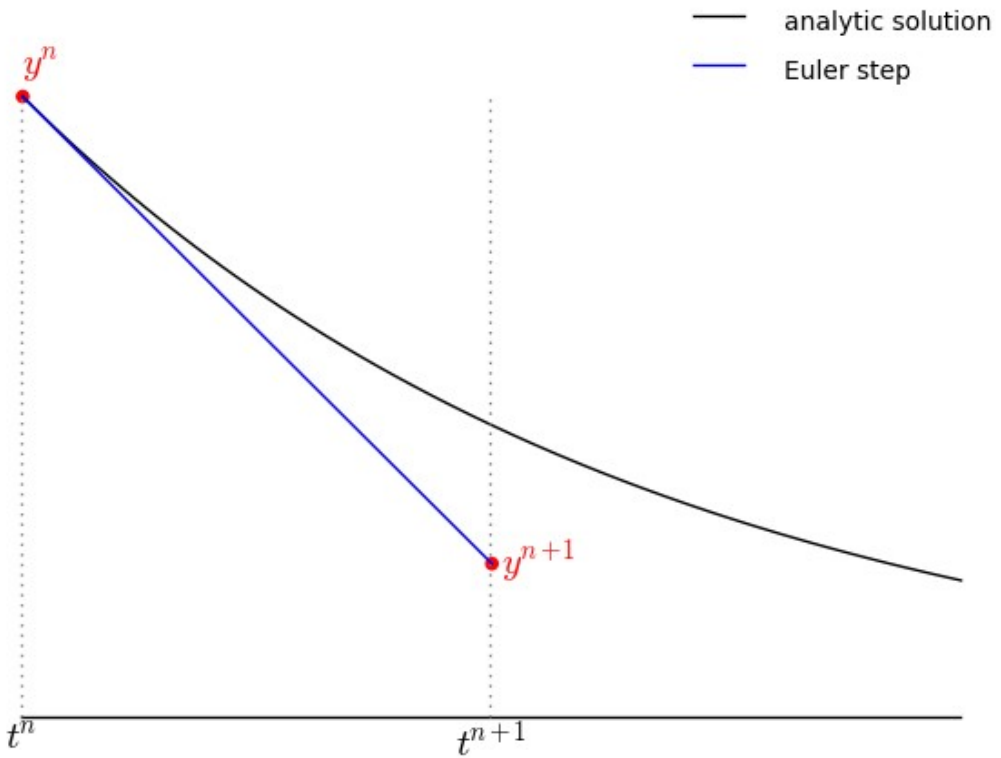
$$\mathbf{r}^{n+1} = \mathbf{r}^n + \tau \mathbf{v}^\star$$

$$\mathbf{v}^{n+1} = \mathbf{v}^n + \tau \mathbf{a}(\mathbf{r}^\star)$$

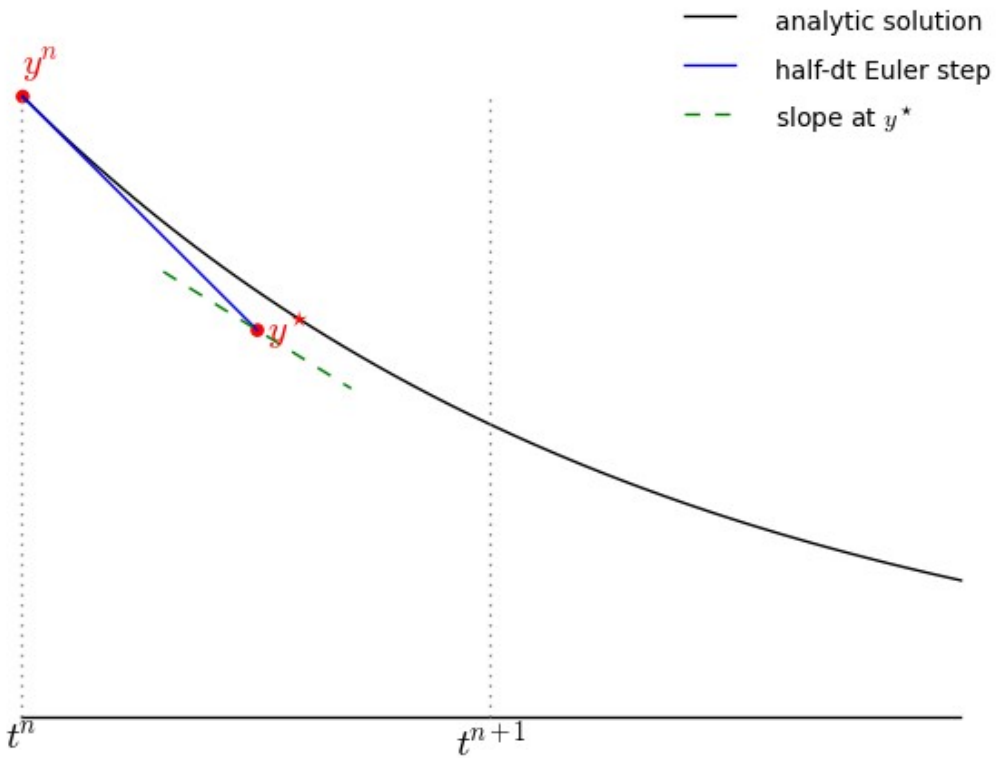
2nd Runge-Kutta Methods



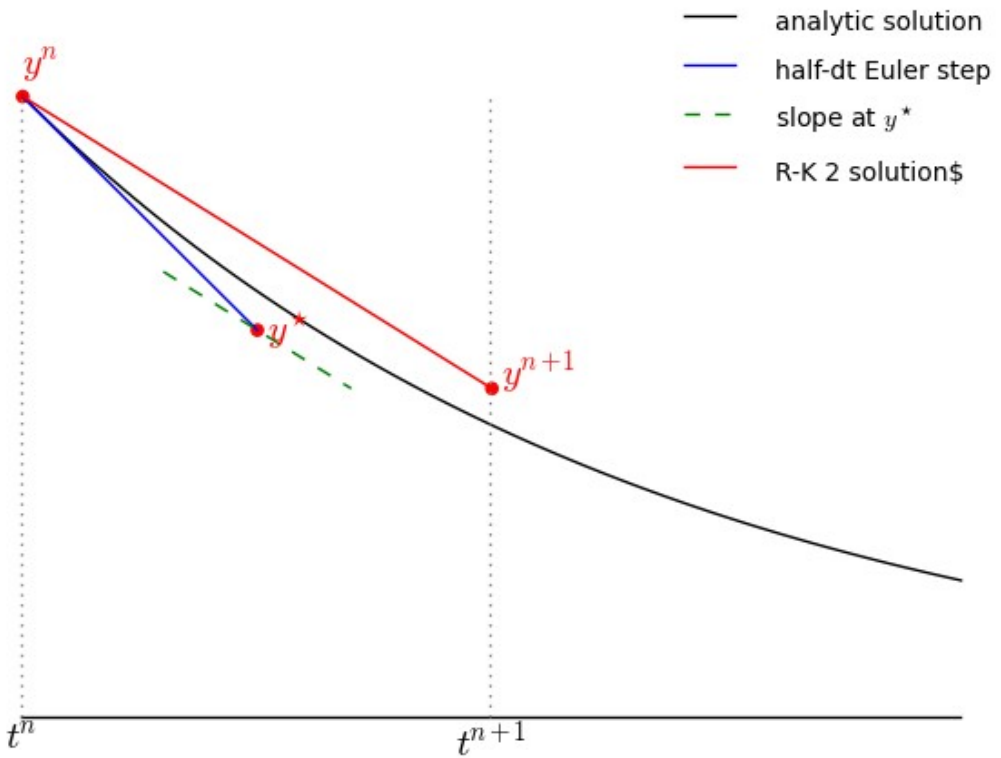
2nd Runge-Kutta Methods



2nd Runge-Kutta Methods



2nd Runge-Kutta Methods



4^{th} Runge-Kutta Methods

- One of the most popular methods is 4^{th}-order Runge-Kutta
  - Consider system: $\dot{\mathbf{y}} = \mathbf{g}(t, \mathbf{y})$
  - Update through τ :

$$\mathbf{y}^{n+1} = \mathbf{y}^n + \frac{\tau}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4) + \mathcal{O}(\tau^5)$$

$$\mathbf{k}_1 = \mathbf{g}(t, \mathbf{y})$$

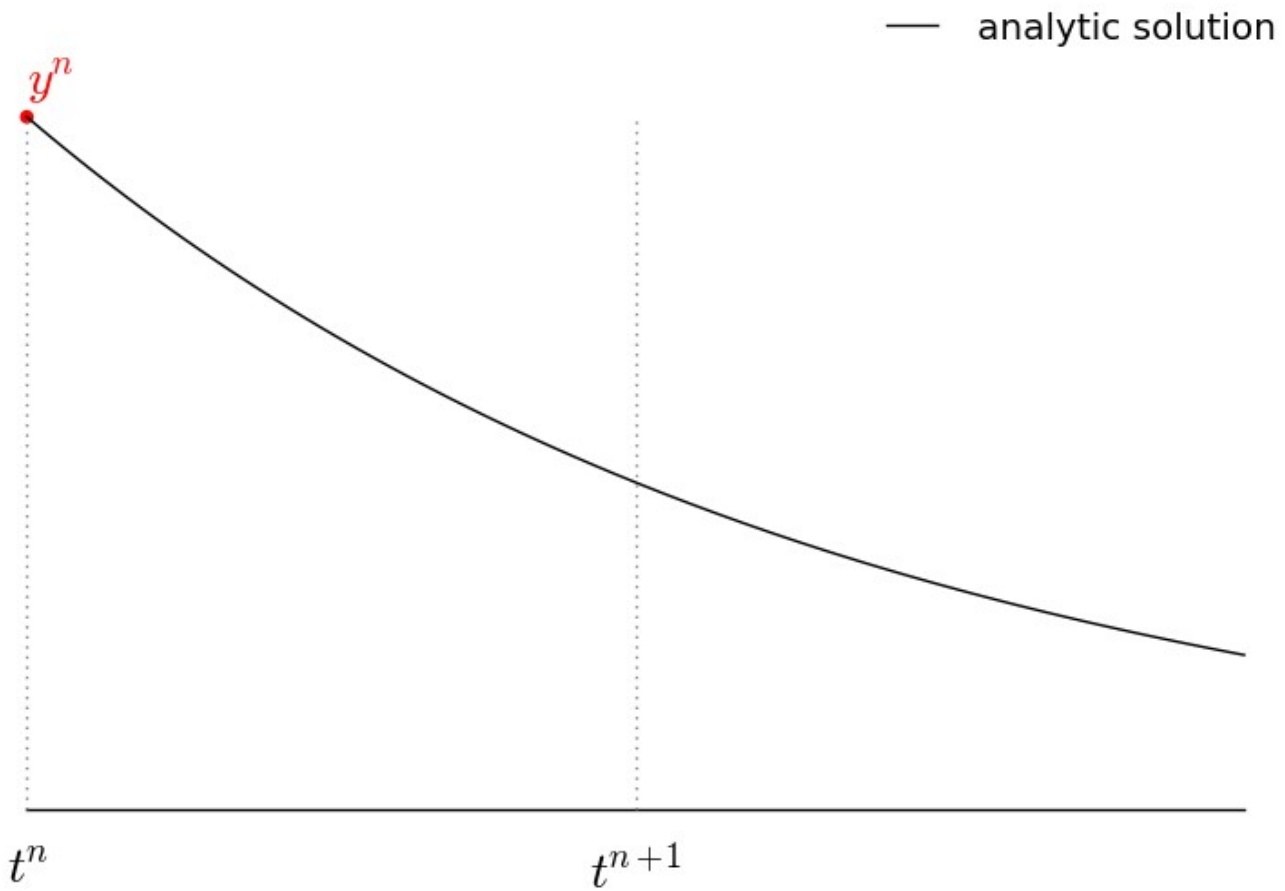
$$\mathbf{k}_2 = \mathbf{g}(t + \tfrac{\tau}{2}, \mathbf{y} + \tfrac{\tau}{2}\mathbf{k}_1)$$

$$\mathbf{k}_3 = \mathbf{g}(t + \tfrac{\tau}{2}, \mathbf{y} + \tfrac{\tau}{2}\mathbf{k}_2)$$

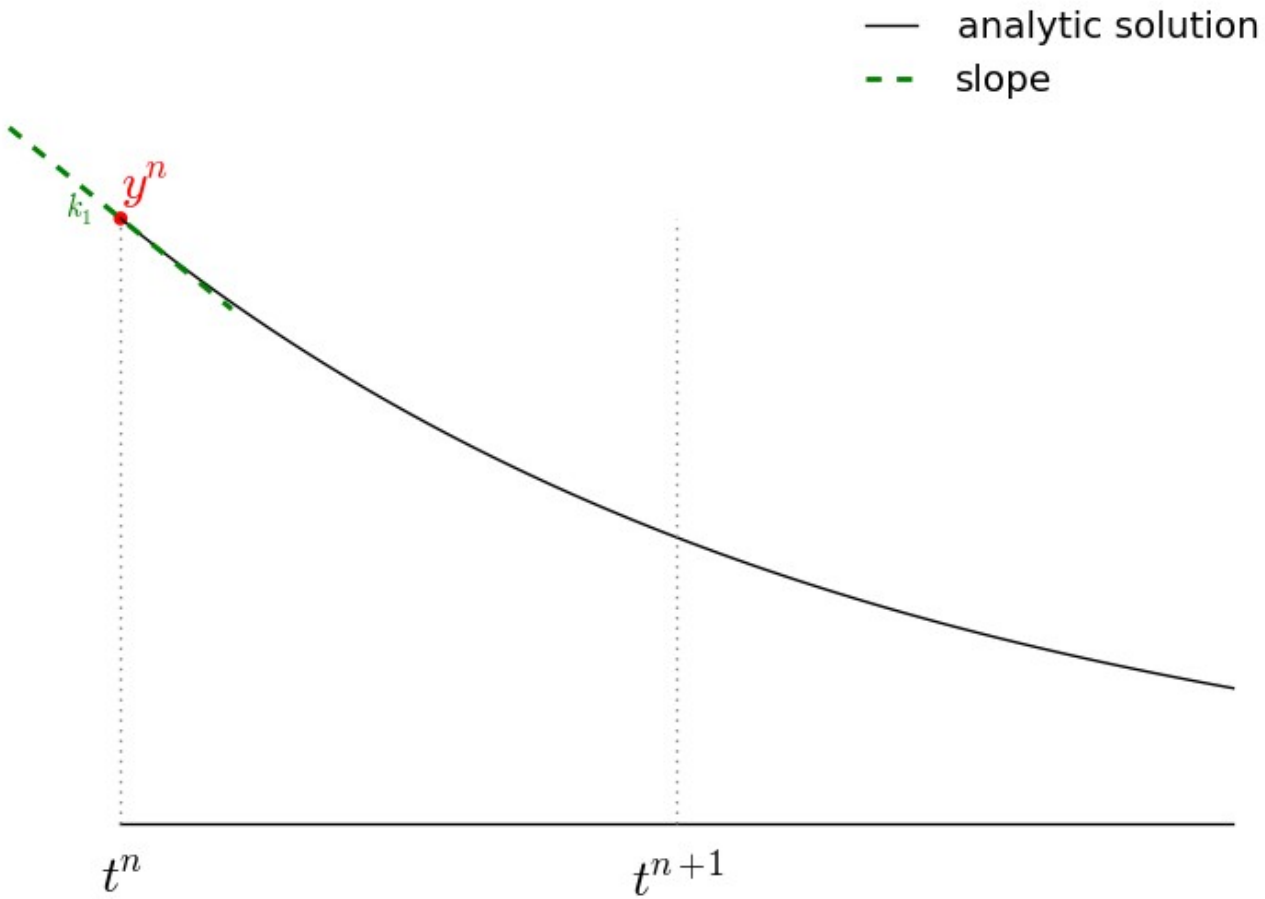
$$\mathbf{k}_4 = \mathbf{g}(t + \tau, \mathbf{y} + \tau\mathbf{k}_3)$$

- Notice the similarity to Simpson's integration
- Derivation found in many analysis texts

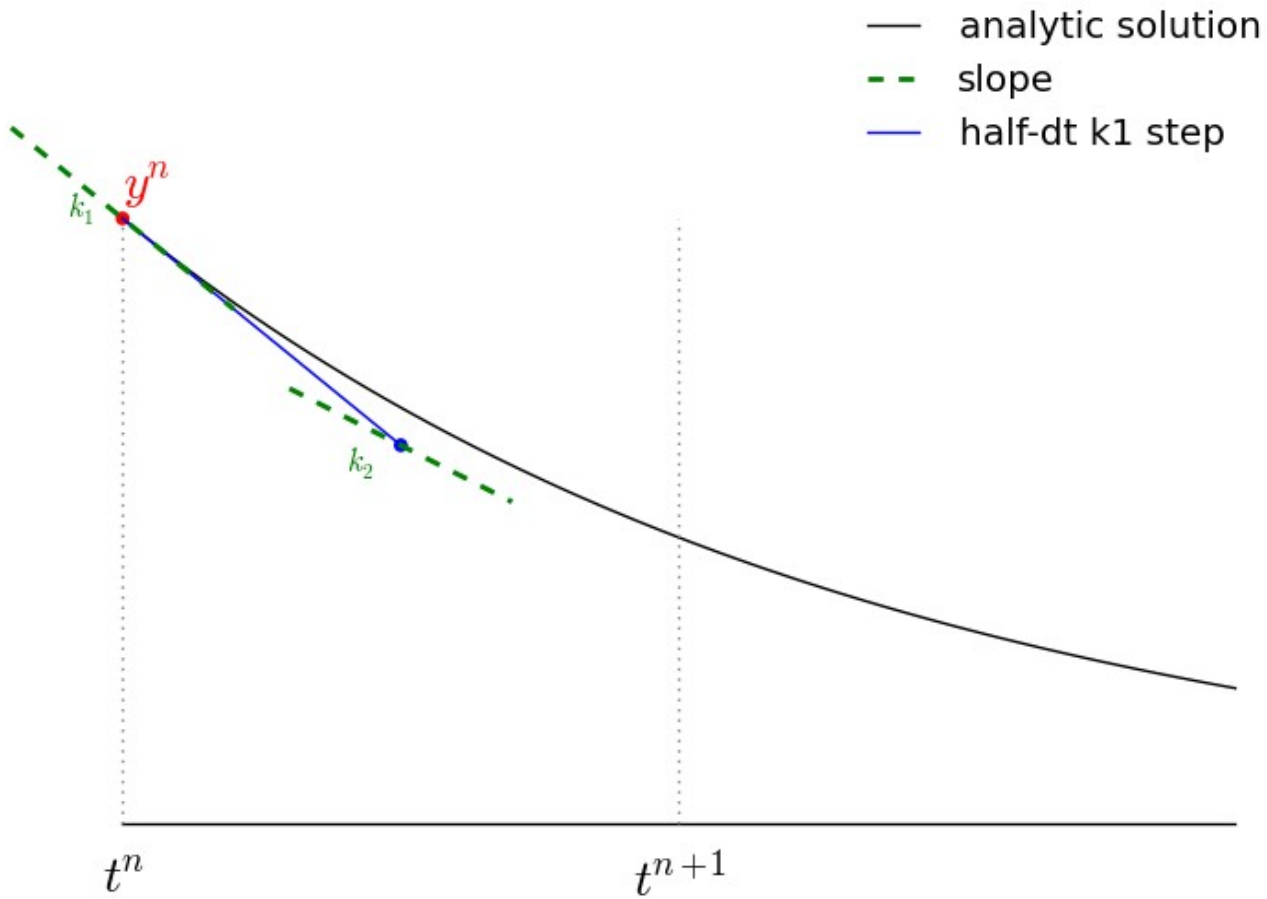
4^{th} Runge-Kutta Methods



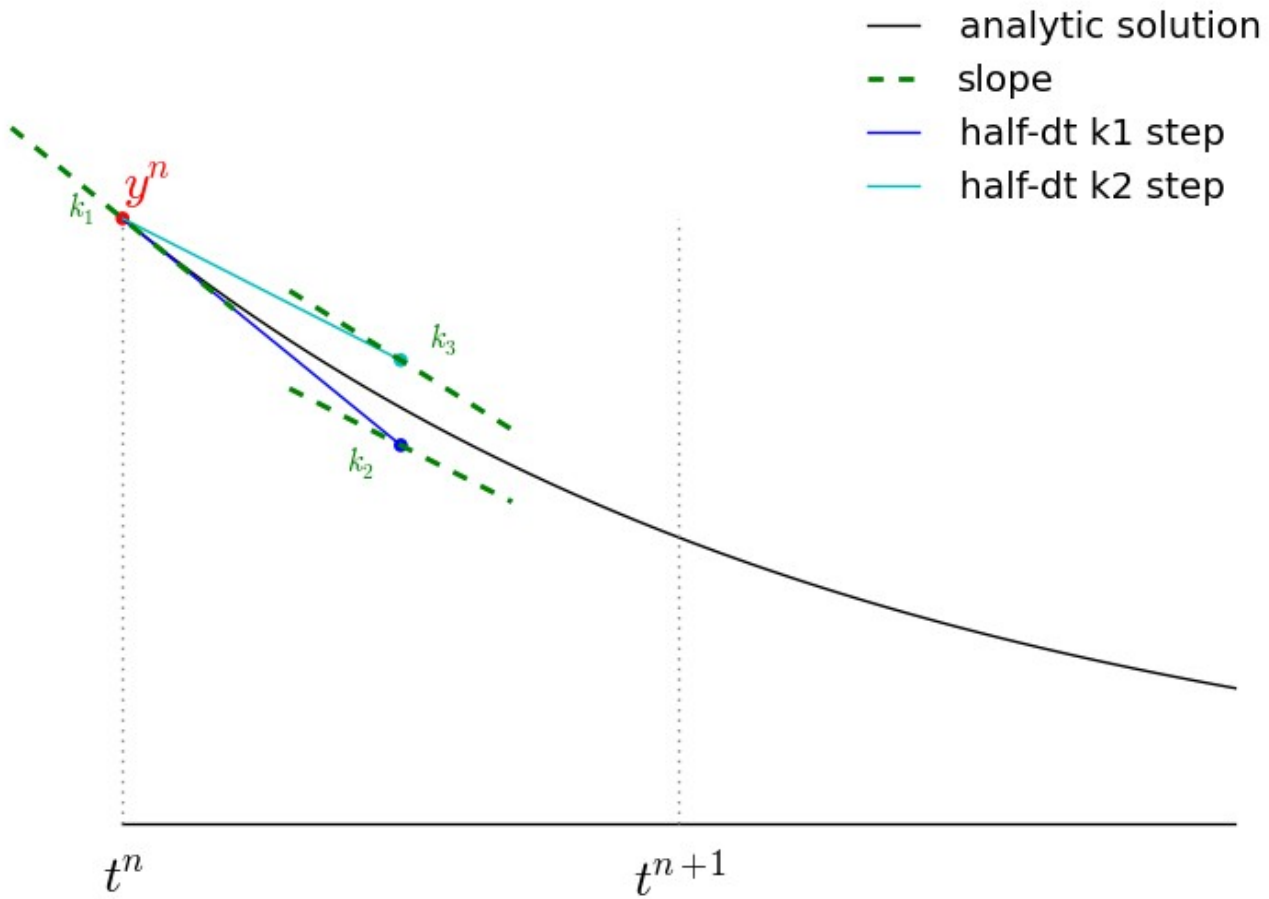
4^{th} Runge-Kutta Methods



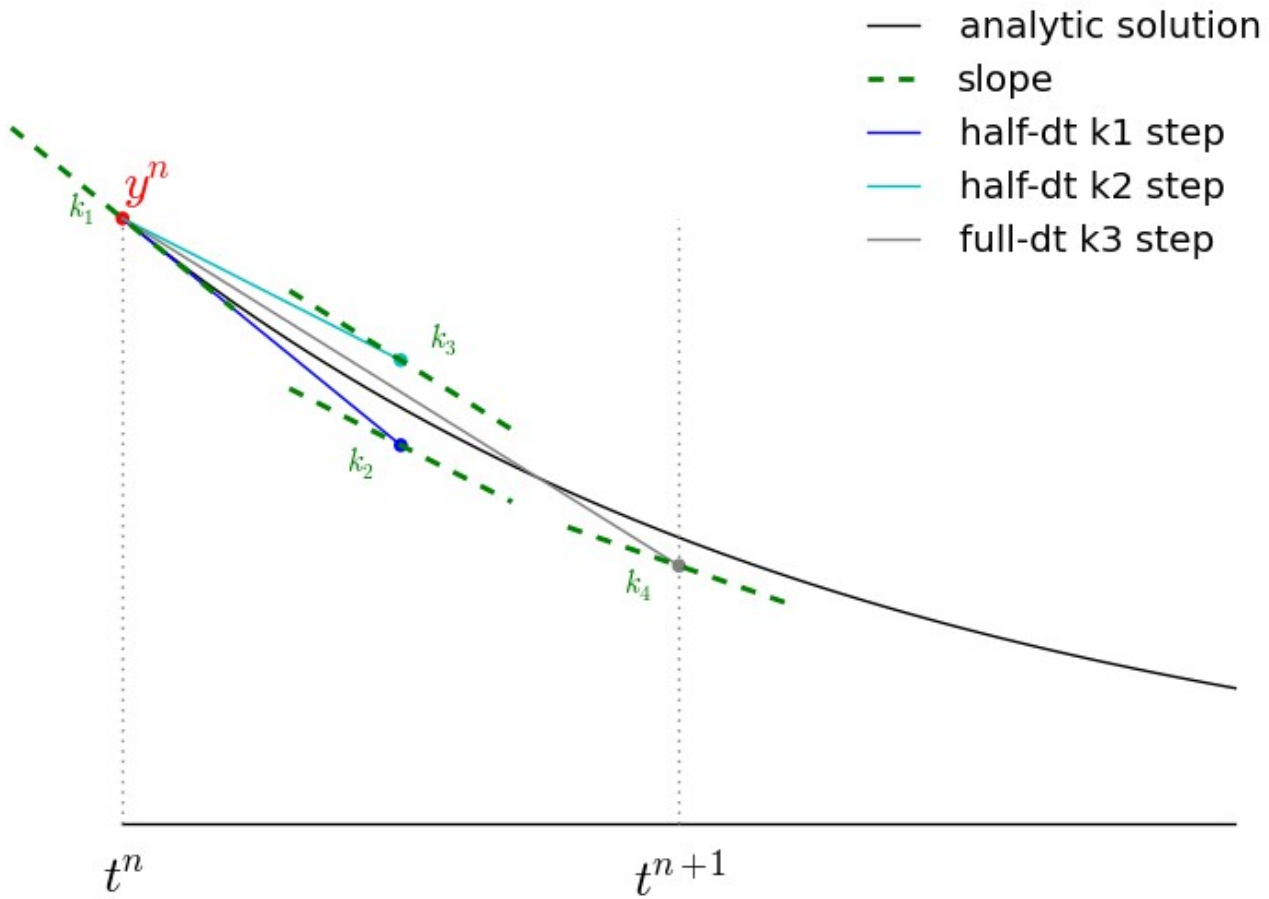
4^{th} Runge-Kutta Methods



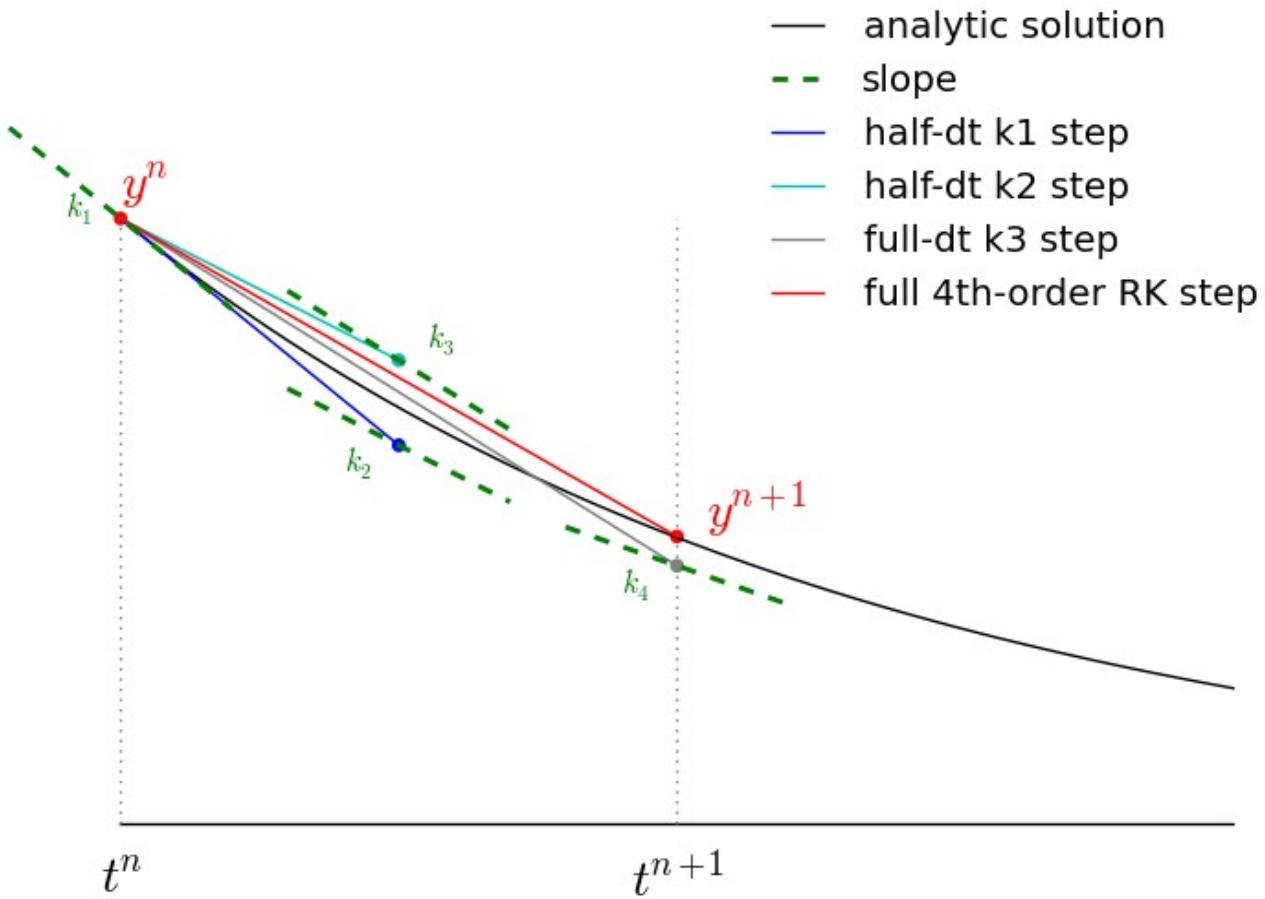
4^{th} Runge-Kutta Methods



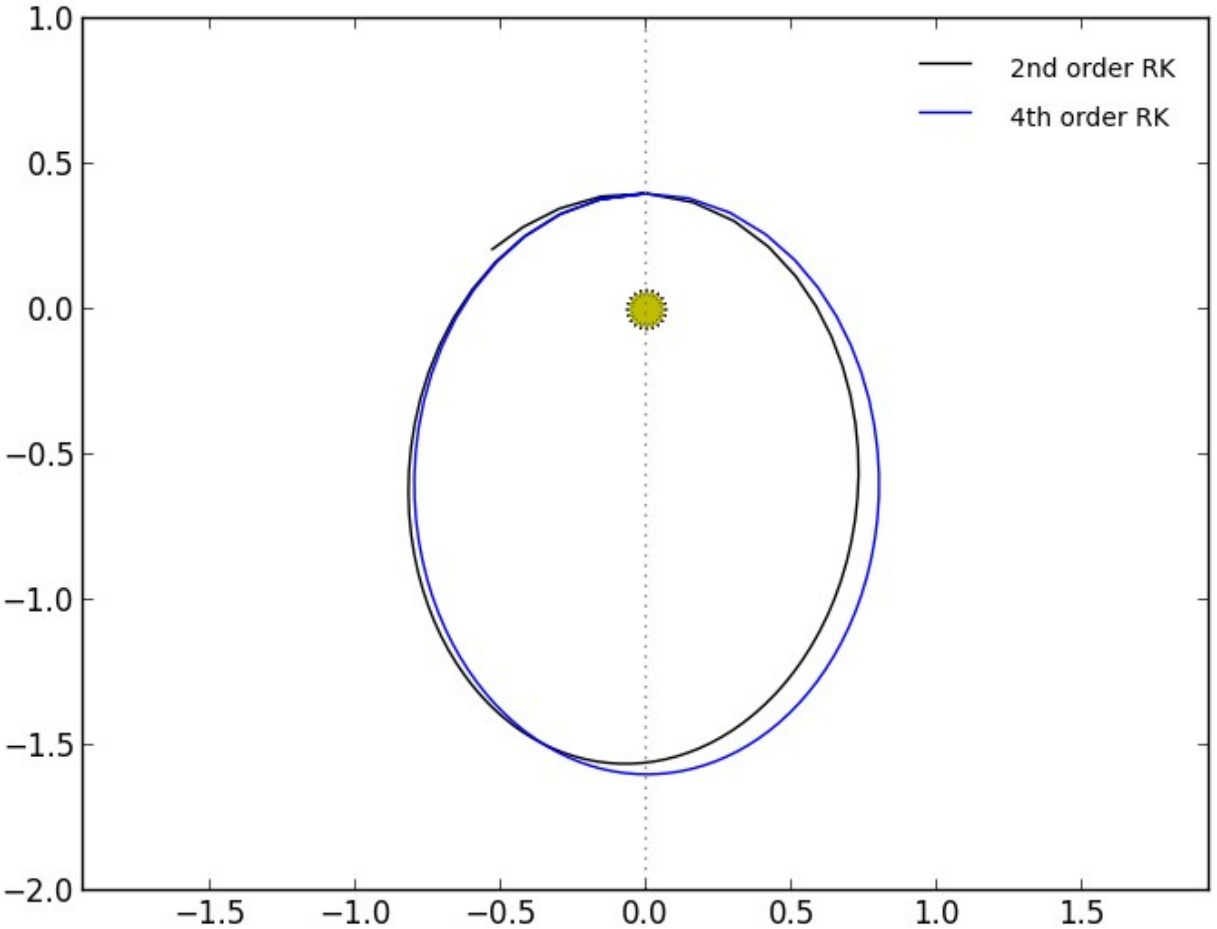
4^{th} Runge-Kutta Methods



4^{th} Runge-Kutta Methods

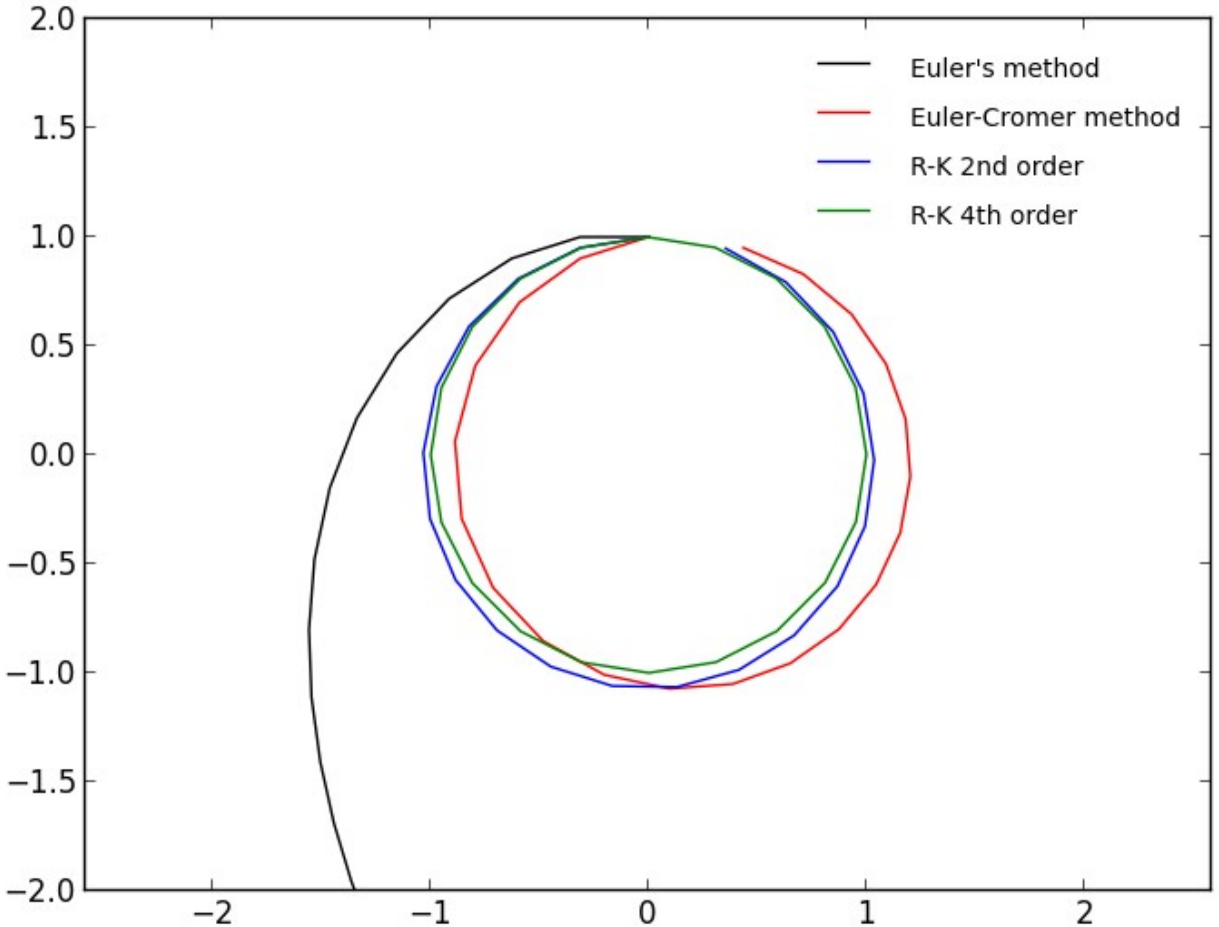


4^{th} Runge-Kutta Methods



This looks great!

4^{th} Runge-Kutta Methods



Even with a coarse timestep, RK4 does very well.

Adaptive Stepping

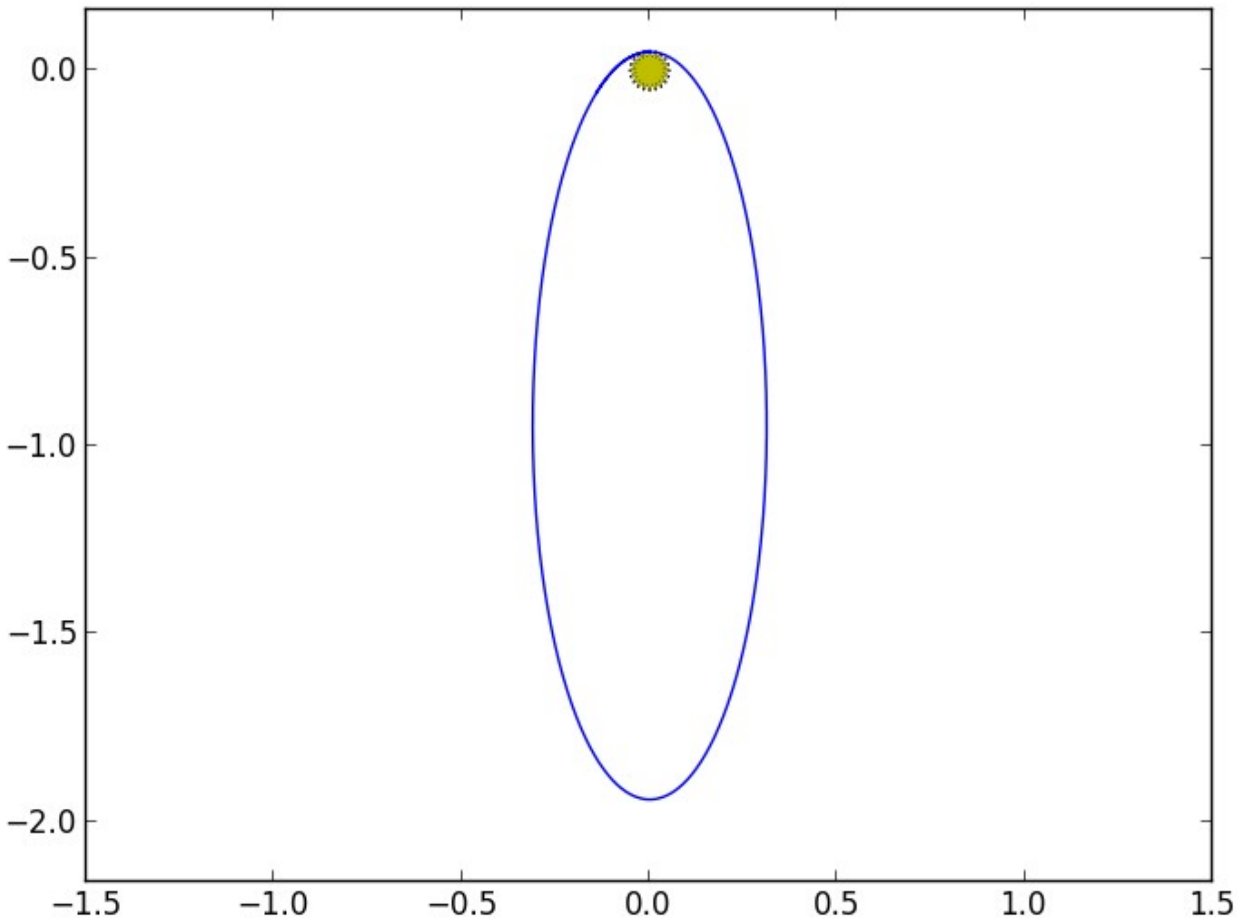
- We need a smaller timestep where the solution changes most rapidly
  - We can get away with large timesteps in regions of slow evolution
- Monitoring the error can allow us to estimate the optimal timestep to reach some desired accuracy
- Lot's of different techniques for this in the literature
  - Take two half steps and compare to one full state
  - Compare higher and lower order methods

Example: Highly Elliptical Orbit

- Consider a highly elliptical orbit: a = 1.0, e = 0.95
  - Sun-grazing comet

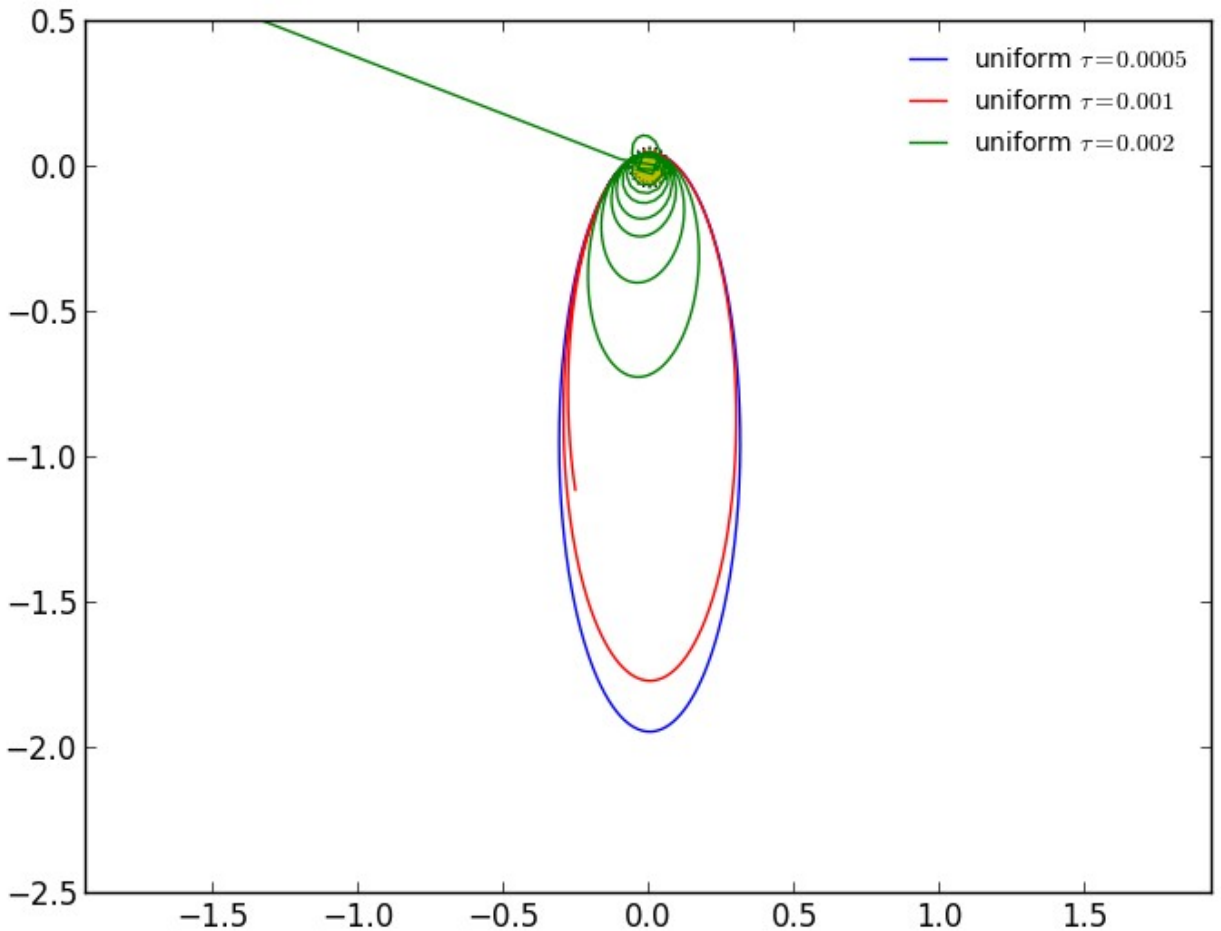
Just to get a reasonable-looking solution, we needed to use $\tau = 0.0005$

This takes 2001 steps



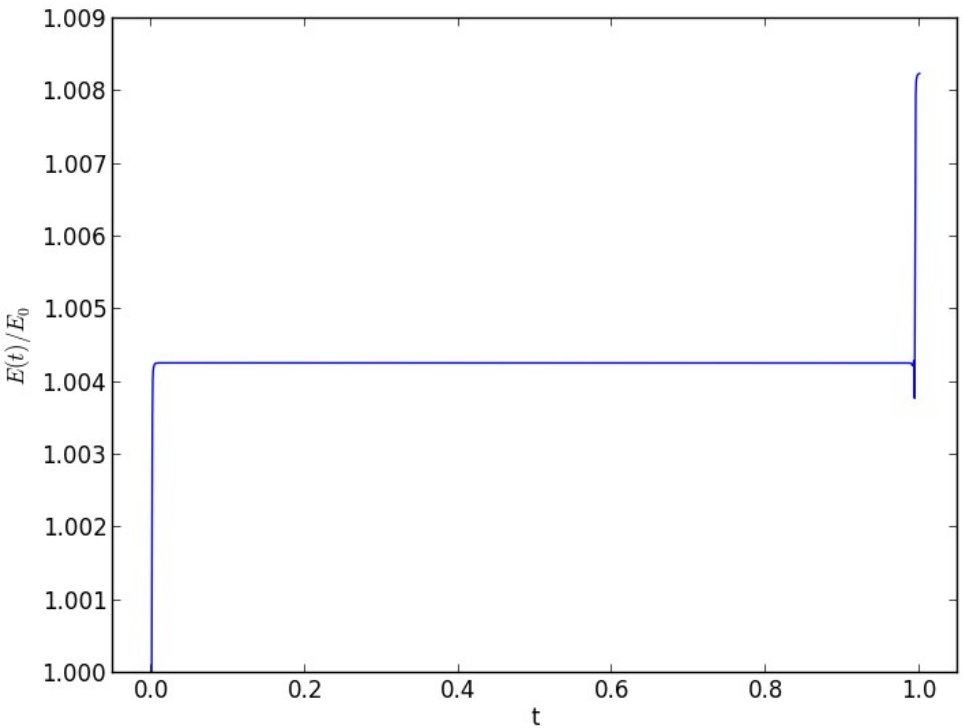
Example: Highly Elliptical Orbit

- Solutions with various uniform timesteps



Example: Highly Elliptical Orbit

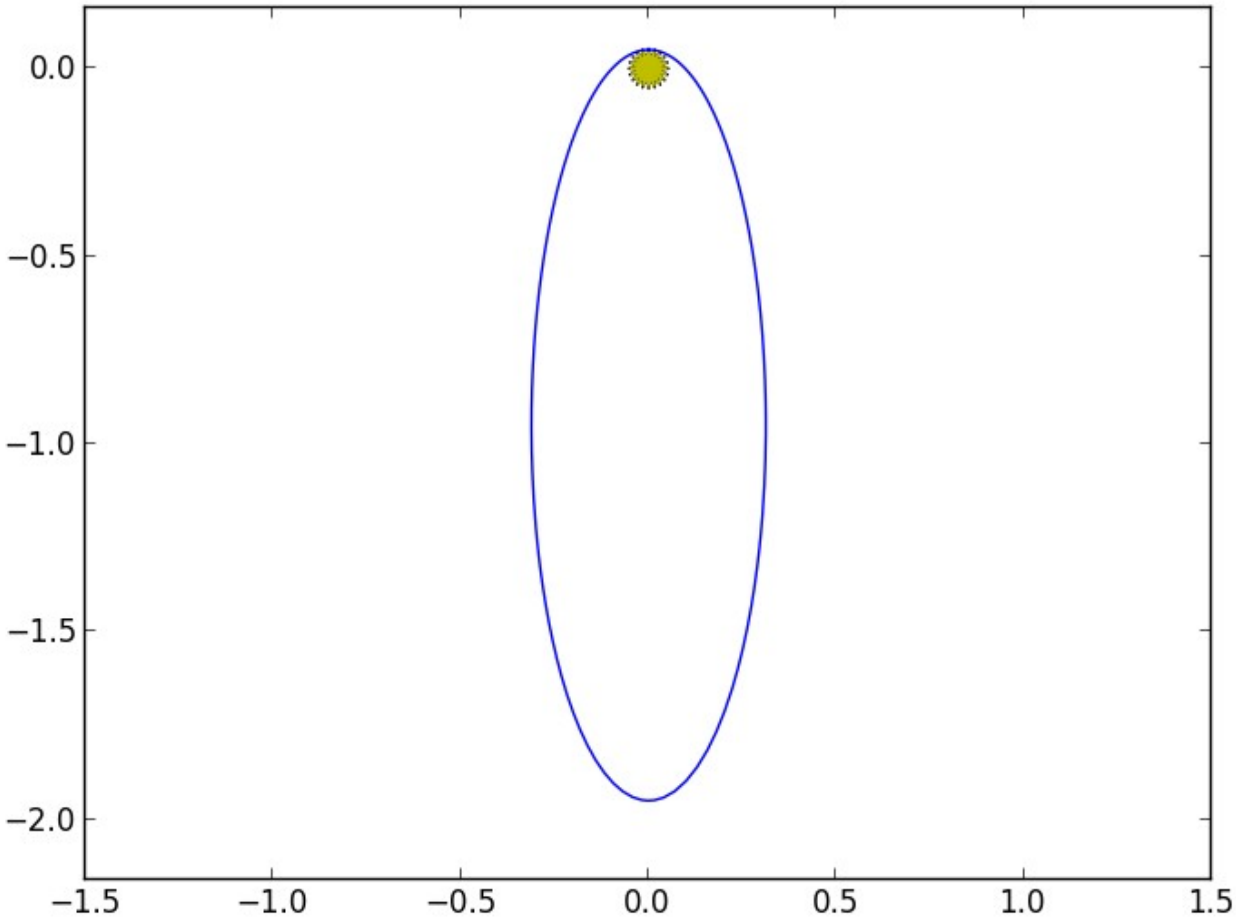
- Look at the total energy
  - At perihelion, conservation is the worse
  - Perihelion is where the velocity is greatest, and therefore the solution changes the fastest
- We can take a larger timestep at aphelion than perihelion



Example: Highly Elliptical Orbit

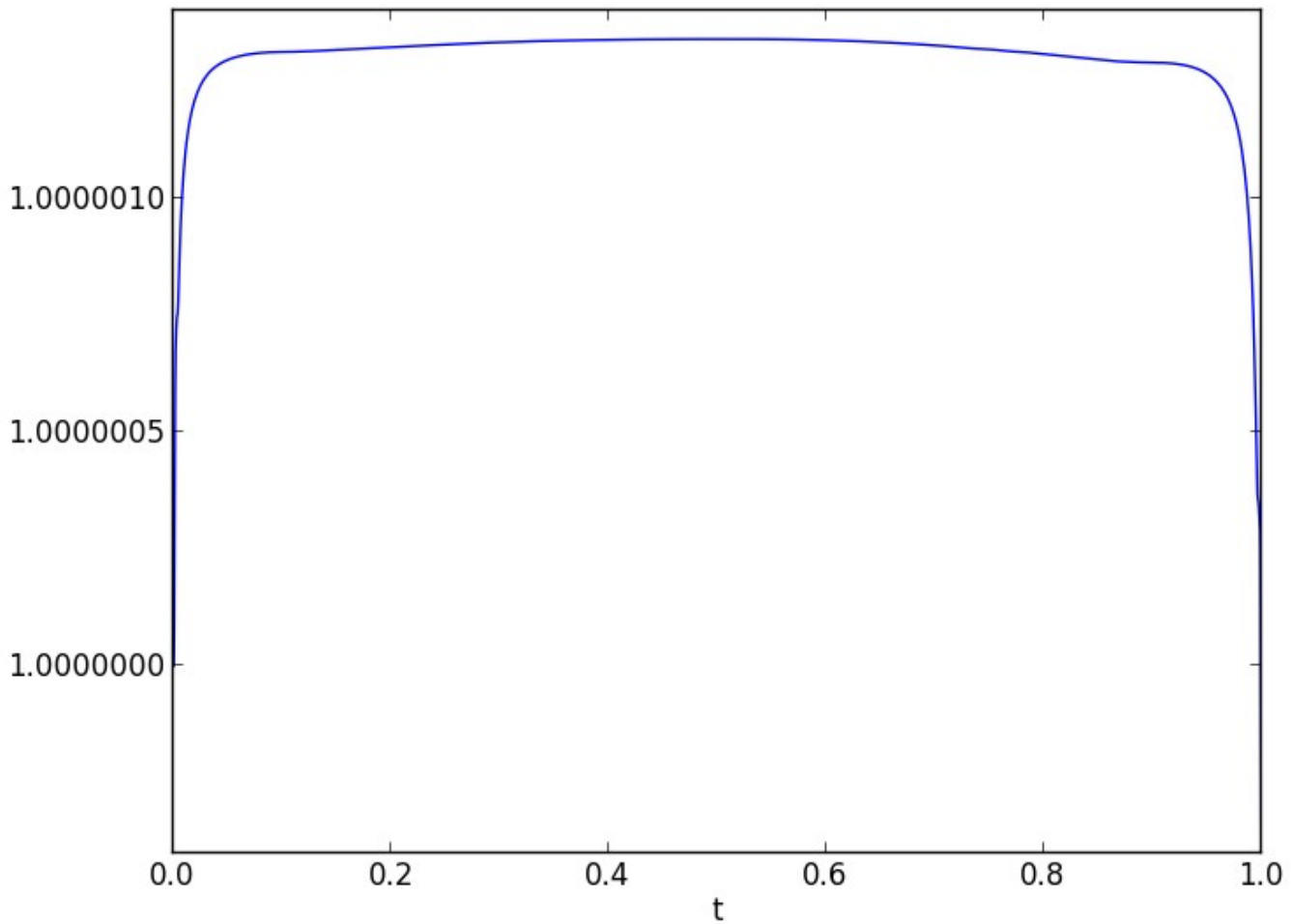
- Adaptive stepping, asking for $\epsilon = 10^{-7}$, with initial timestep the same as the non-adaptive case ($\tau = 0.005$)

This takes only 215 steps



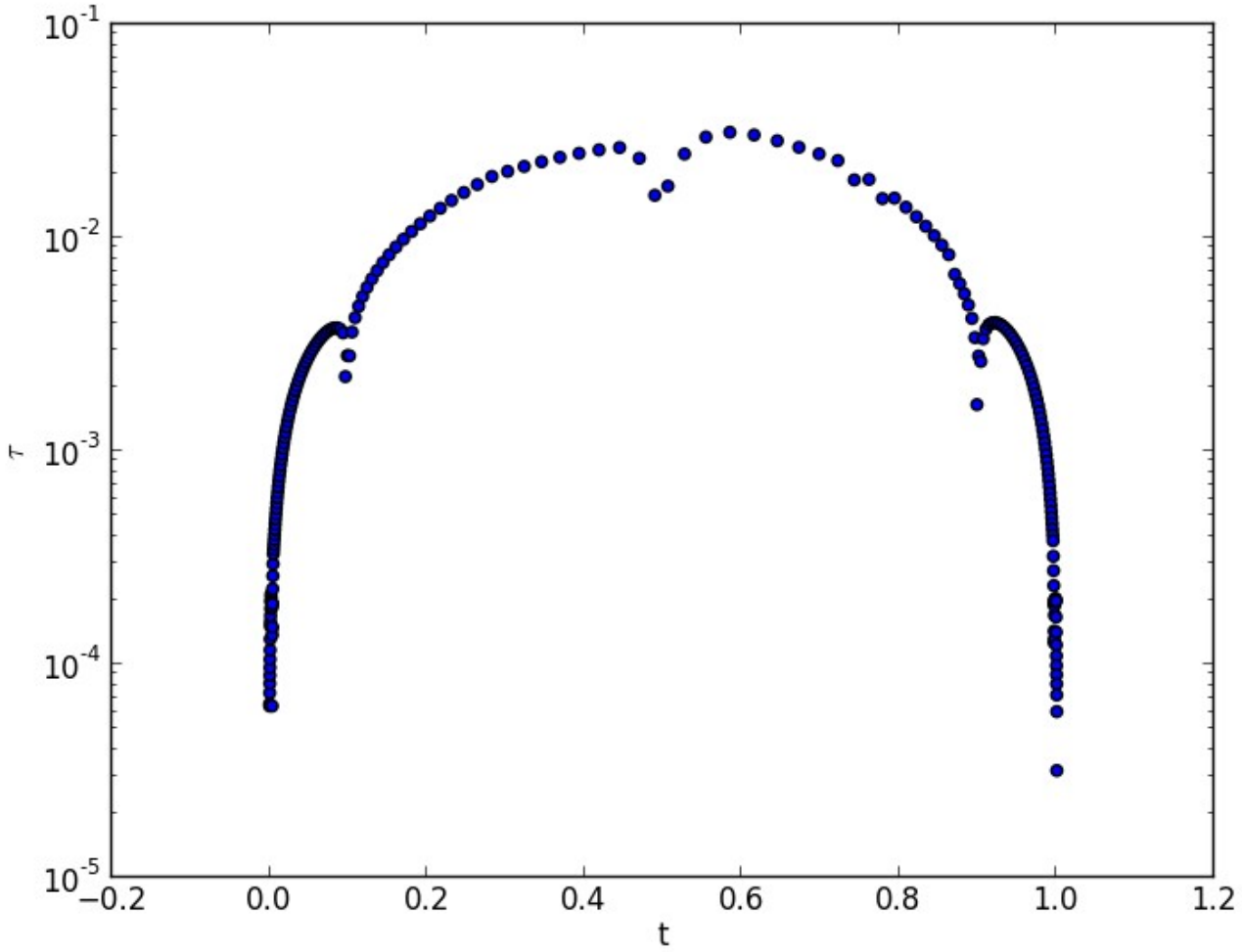
Adaptive Stepping

- Energy conservation is now far superior



Adaptive Stepping

- Timestep varies significantly over the evolution



Adaptive Stepping / Error Estimation

- You should always perform some sort of error estimation
- Specifying absolute and relative errors in the state variables ensures you know about the quality of the solution
- The SciPy ODE packages can control all of this for you

Stiff Equations / Implicit Methods

- Consider the ODE (example from Byrne & Hindmarsh 1986):

$$\dot{y} = -10^3(y - e^{-t}) - e^{-t}$$

$$y(0) = 0$$

- This has the exact solution:

$$y(t) = e^{-t} - e^{-10^3 t}$$

  - Looking at this, we see that there are two characteristic timescales for change, $\tau_1 = 1$ and $\tau_2 = 10^{-3}$
  - A problem with dramatically different timescales for change is called stiff

- Stiff ODEs can be hard for the methods we discussed so far
  - Stability requires that we evolve on the shortest timescale

Outline

Fitting Data

- We get experimental/observational data as a sequence of times (or positions) and associate values
  - N points: (x_i, y_i)
  - Often we have errors in our measurements at each of these values: σ_i for each y_i
- To understand the trends represented in our data, we want to find a simple functional form that best represents the data—this is the fitting problem
  - The `scipy.optimize` module offers routines to do fitting
- We'll look at least squares fitting
  - Two cases: general linear and nonlinear

Fitting Data

- We want to fit our data to a function: $Y(x, \{a_j\})$
  - Here, the a_j are a set of parameters that we can adjust
  - We want to find the optimal set of a_j that make Y best represent our data
- The distance between a point and the representative curve is

$$\Delta_i = Y(x_i, \{a_j\}) - y_i$$

  - Least squares fit minimizes the sum of the squares of all these errors
  - With error bars, we weight each distance error by the uncertainty in that measurement, giving:

$$\chi^2(\{a_j\}) = \sum_{i=1}^{N} \left(\frac{\Delta_i}{\sigma_i} \right)^2$$

This is what we minimize

Example: Linear Regression (Least Squares)

- Minimization: derivative of χ^2 with respect to all parameters is zero:

$$\frac{\partial \chi^2}{\partial a_1} = 2\sum_{i=1}^{N} \frac{a_1 + a_2 x_i - y_i}{\sigma_i^2} = 0 \qquad \frac{\partial \chi^2}{\partial a_2} = 2\sum_{i=1}^{N} \frac{a_1 + a_2 x_i - y_i}{\sigma_i^2} x_i = 0$$

  - Define:

$$S = \sum_{i=1}^{N} \frac{1}{\sigma_i^2} \qquad \xi_1 = \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2} \qquad \xi_2 = \sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2}$$

$$\eta = \sum_{i=1}^{N} \frac{y_i}{\sigma_i^2} \qquad \mu = \sum_{i=1}^{N} \frac{x_i y_i}{\sigma_i^2}$$

- Result: simple linear system to solve:

$$a_1 S + a_2 \xi_1 - \eta = 0$$

$$a_1 \xi_1 + a_2 \xi_2 - \mu = 0$$

Goodness of the Fit

- Typically, if M is the number of parameters (2 for linear), then $N \gg M$
  - Average pointwise error should be $|y_i - Y(x_i)| \sim \sigma_i$
  - Number of degrees of freedom is $N - M$
    - i.e. larger M makes it easier to fit all the points
    - See discussion in Numerical Recipes for more details and limitations
  - Putting these ideas into the χ^2 expression suggests that we consider

$$\frac{\chi^2}{N - M}$$

    - If this is < 1, then the fit is good
    - But watch out, $\ll 1$ may also mean our errors were too large to begin with, we used too many parameters, ...

General Linear Least Squares

- Garcia and Numerical Recipes provide a good discussion here
- We want to fit to

$$Y(x;\{a_j\}) = \sum_{j=1}^{M} a_j Y_j(x)$$

  - Note that the Ys may be nonlinear but we are still linear in the as
  - Here, Y_j are our basis set—they can be x^j in which case we fit to a general polynomial
- Minimize:

$$\frac{\partial \chi^2}{\partial a_j} = \frac{\partial}{\partial a_j} \sum_{i=1}^{N} \frac{1}{\sigma_i^2} \left\{ \sum_{k=1}^{M} a_k Y_k(x_i) - y_i \right\}^2 = 0 \longrightarrow$$

$$\sum_{i=1}^{N} \sum_{k=1}^{M} \frac{Y_j(x_i)}{\sigma_i} \frac{Y_k(x_i)}{\sigma_i} a_k = \sum_{i=1}^{N} \frac{Y_j(x_i)}{\sigma_i} \frac{y_i}{\sigma_i}$$

Linear system

Error bars in Both x and y

- Depending on the experiment, you may have errors in the dependent variable
  - For linear regression, our function to minimize becomes:

$$\chi^2(a_1, a_2) = \sum_{i=1}^{N} \frac{(a_1 + a_2 x_i - y_i)^2}{\sigma_{y,i}^2 + a_2^2 \sigma_{x,i}^2}$$

    - Denominator is the total variance of the linear combination we are minimizing:

$$\begin{aligned} \mathrm{Var}(a_1 + a_2 x_i - y_i) &= \mathrm{Var}(a_2 x_i - y_i) \\ &= a_2^2 \mathrm{Var}(x_i) + \mathrm{Var}(y_i) = a_2^2 \sigma_{x,i}^2 + \sigma_{y,i}^2 \end{aligned}$$

      (think about propagation of errors)
- We cannot solve analytically for the parameters, but we can use our root finding techniques on this.
  - See NR and references therein for more details

General Non-linear Fitting

- Consider fitting directly to a function where the parameters enter nonlinearly:

$$f(a_0, a_1) = a_0 e^{a_1 x}$$

  - We want to minimize

$$Q \equiv \sum_{i=1}^{N} (y_i - a_0 e^{a_1 x_i})^2$$

  - Set the derivatives to zero:

$$f_0 \equiv \frac{\partial Q}{\partial a_0} = \sum_{i=1}^{N} e^{a_1 x_i} \left(a_0 e^{a_1 x_i} - y_i\right) = 0$$

$$f_1 \equiv \frac{\partial Q}{\partial a_1} = \sum_{i=1}^{N} x_i e^{a_1 x_i} \left(a_0 e^{a_1 x_i} - y_i\right) = 0$$

- This is a nonlinear system—we use something like the multivariate root find