SciPy

Intro to SciPy

- SciPy is a collection of numerical algorithms that is used with NumPy
- We'll give a brief overview of the algorithms and then look at the functions.

Subpackage	Description
cluster	Clustering algorithms
constants	Physical and mathematical constants
fftpack	Fast Fourier Transform routines
integrate	Integration and ordinary differential equation solvers
interpolate	Interpolation and smoothing splines
io	Input and Output
linalg	Linear algebra
ndimage	N-dimensional image processing
odr	Orthogonal distance regression
optimize	Optimization and root-finding routines
signal	Signal processing
sparse	Sparse matrices and associated routines
spatial	Spatial data structures and algorithms
special	Special functions
stats	Statistical distributions and functions
weave	C/C++ integration

(docs.scipy.org)

Conventions

- The SciPy docs recommend loading the various modules as:

```
import numpy as np
import scipy as sp
import matplotlib as mpl
import matplotlib.pyplot as plt
```

- Each subpackage must be imported separately:

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

  - Note that some popular functions are available in the main `scipy` namespace

Getting Help

- 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

Caveats

- 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.

Integration

Numerical Integration

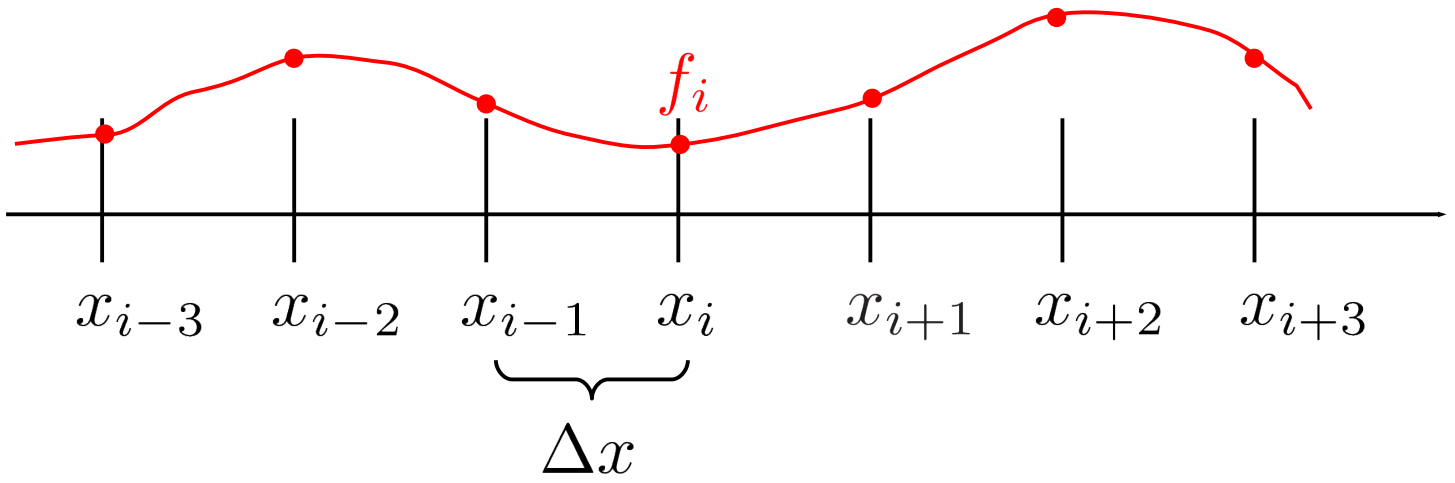
- We want to compute:

$$I = \int_a^b f(x)dx$$

- We can imagine 2 situations
  - 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
  - We have an analytic expression for f(x)
    - We have the freedom to pick our integration points, and this can allow us to optimize 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

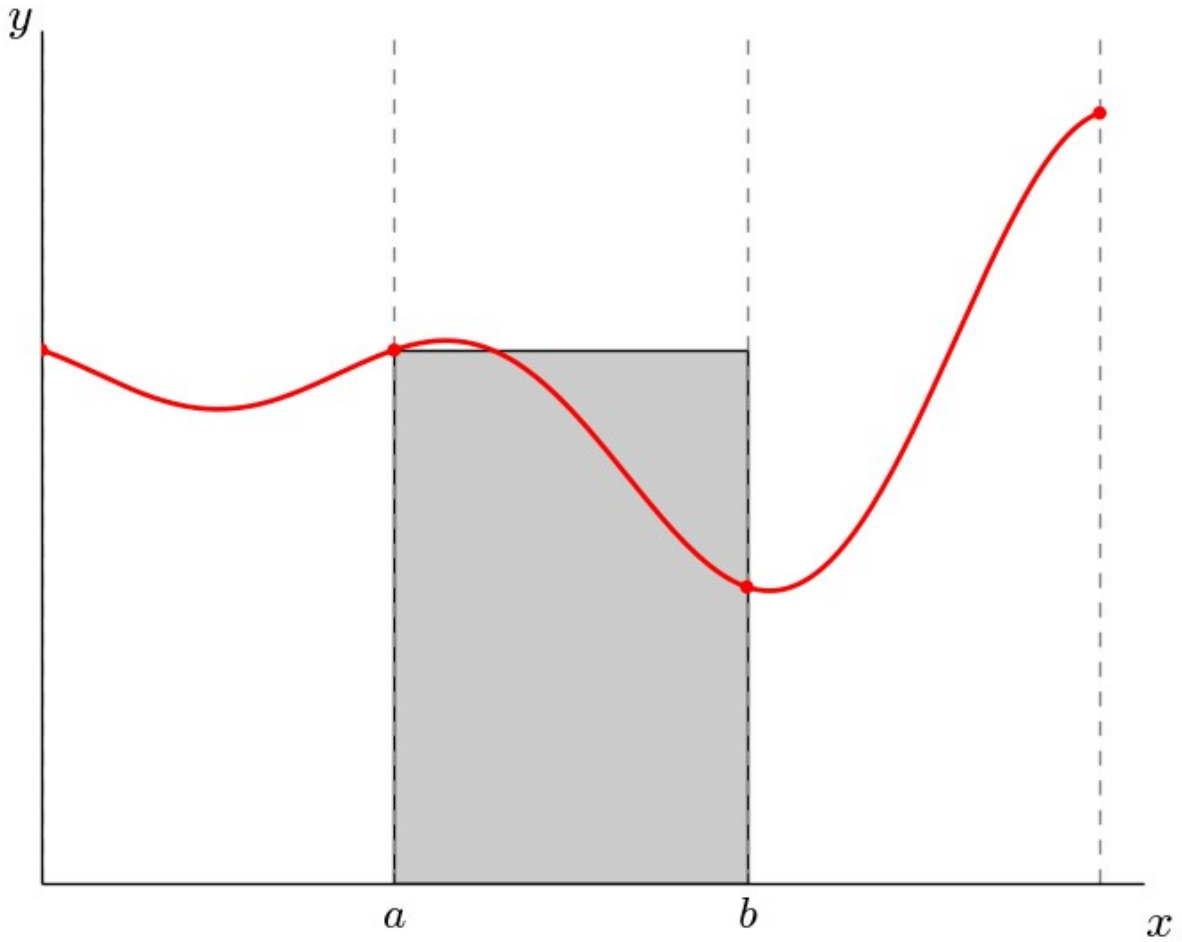
- Discretized data is represented at a finite number of locations
  - Integer subscripts are used to denote the position (index) on the grid
  - Structured/regular: spacing is constant



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

Numerical Integration

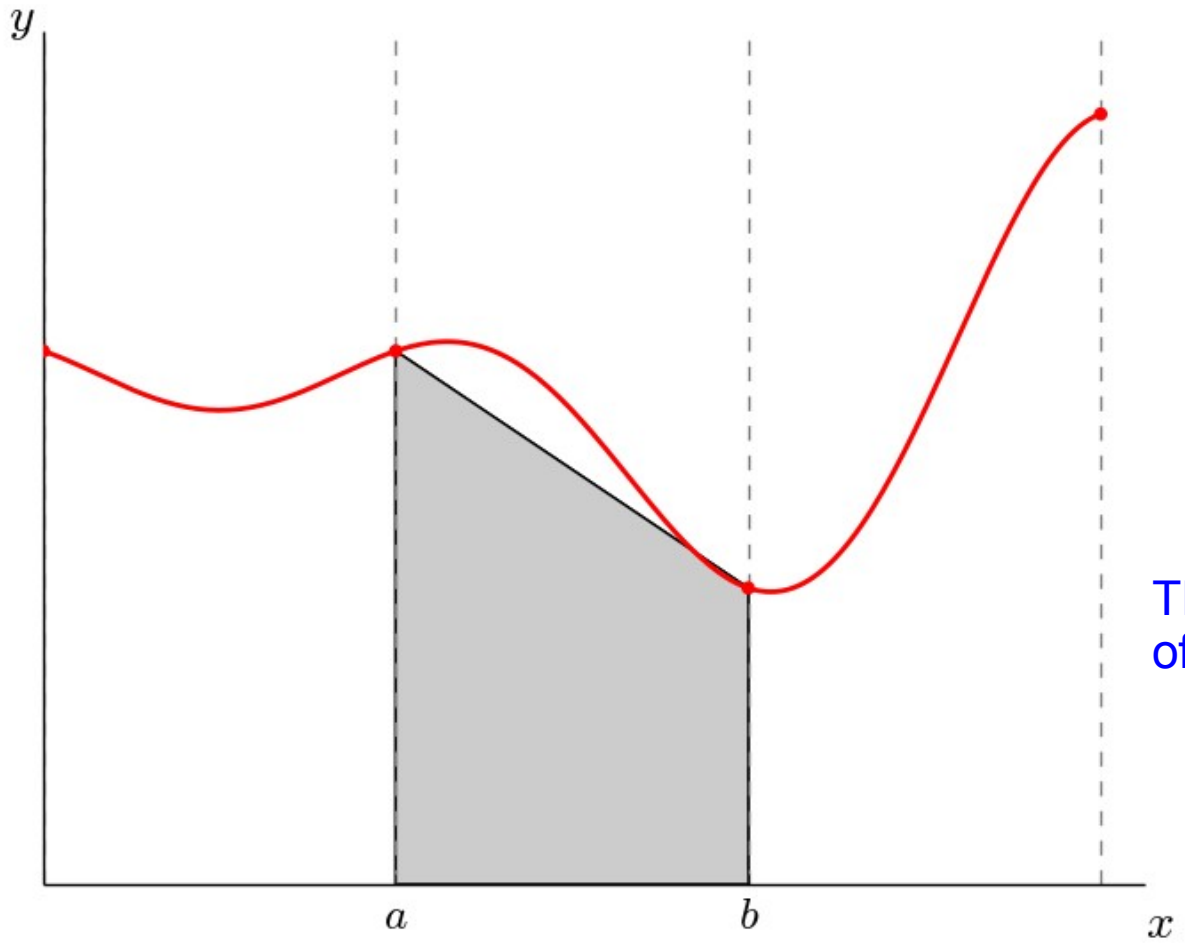
- Simplest case: piecewise constant interpolant (rectangle rule)



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

Numerical Integration

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



This is just the area of a trapezoid

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

Numerical Integration

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

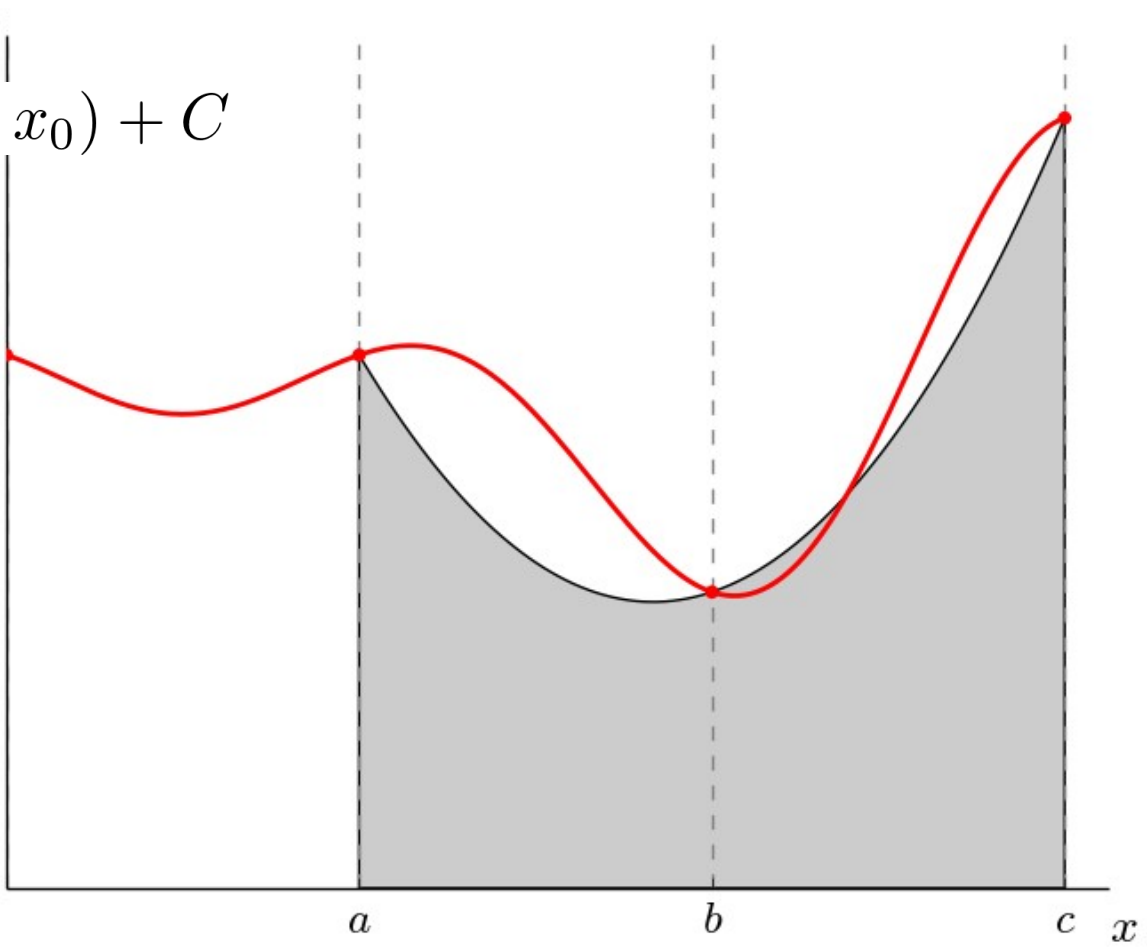
$$f(x) = A(x - x_0)^2 + B(x - x_0) + C$$

  - Solving:

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

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

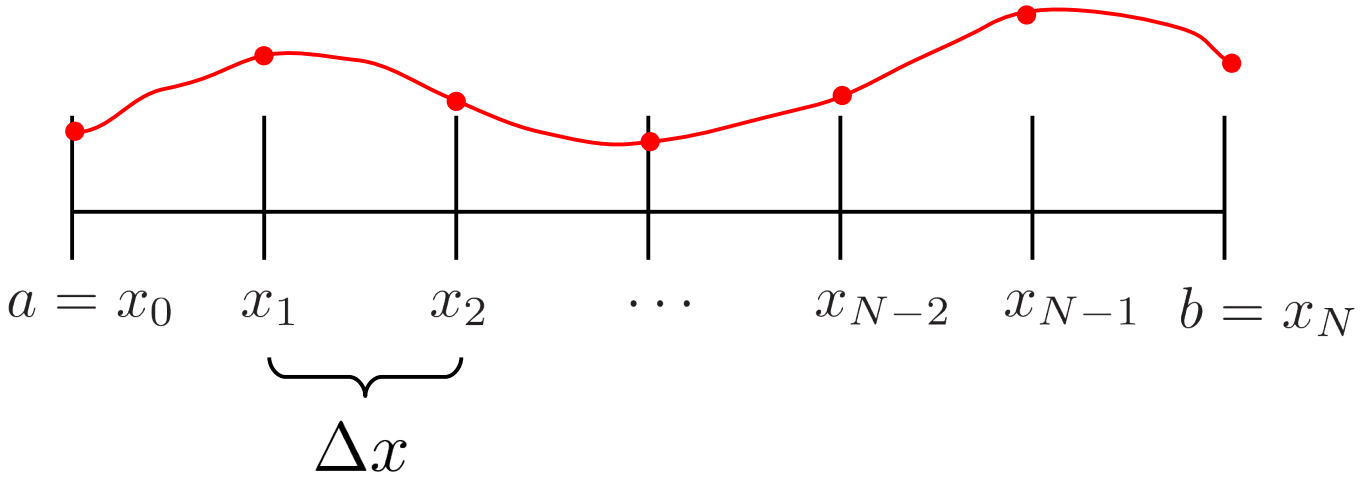
$$C = f_a$$



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

Compound Integration

- Break interval into chunks



$$I \equiv \int_a^b f(x)dx = \sum_{i=0}^{N-1} \underbrace{\int_{x_i}^{x_{i+1}} f(x)dx}$$

Integral over a single slab

Compound Integration

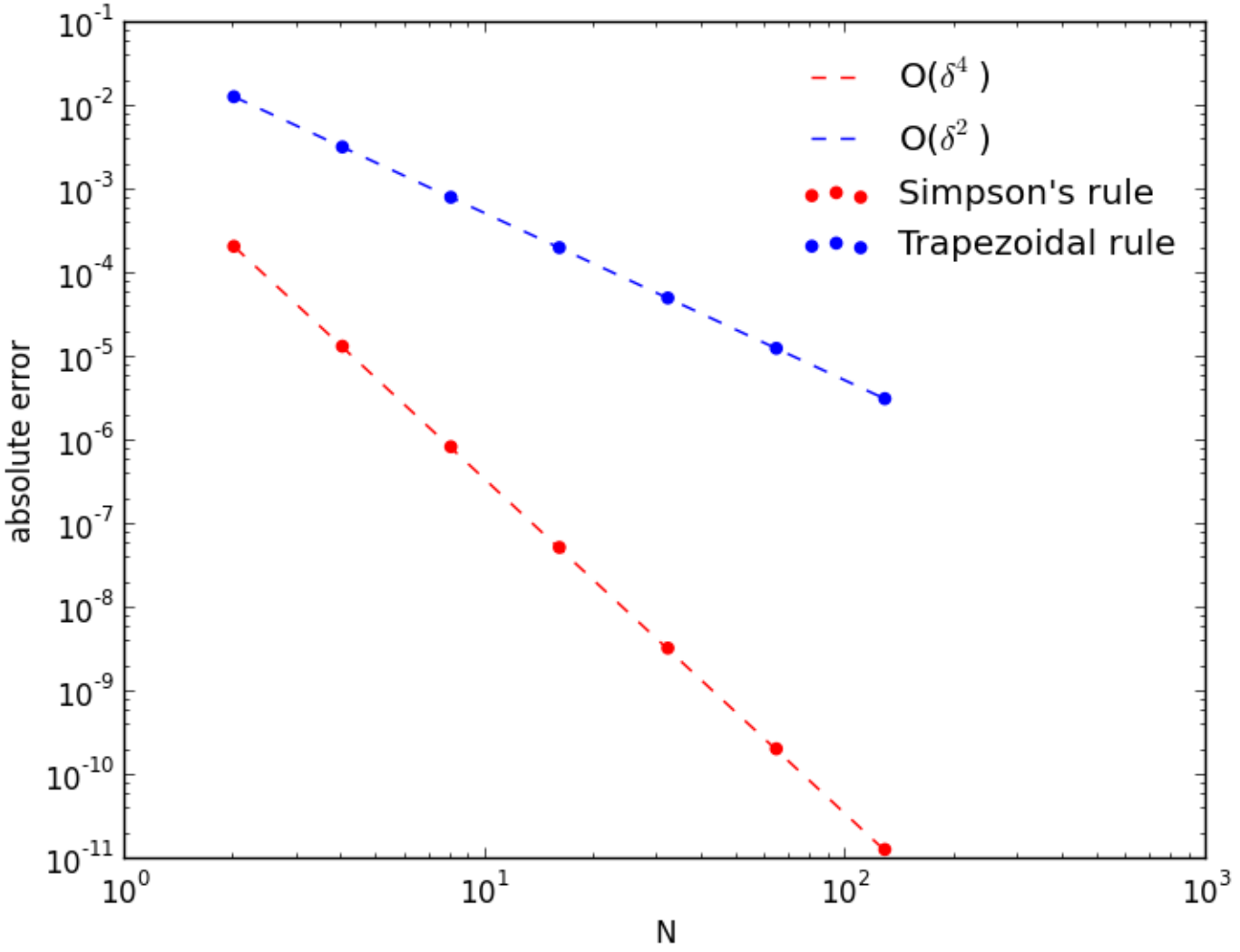
- Compound Trapezoidal

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

- 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

(Garcia, Ch. 10)

- 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

(Garcia, Ch. 10)

- 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.

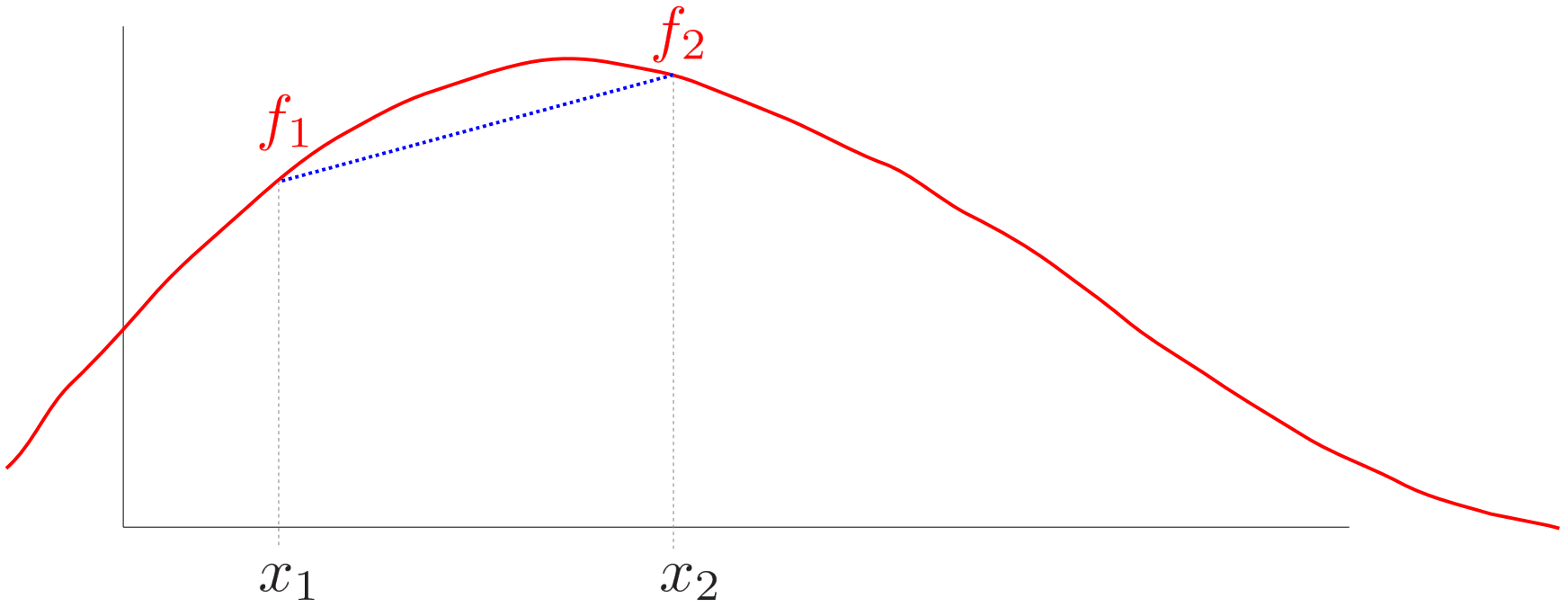
Interpolation

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:

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

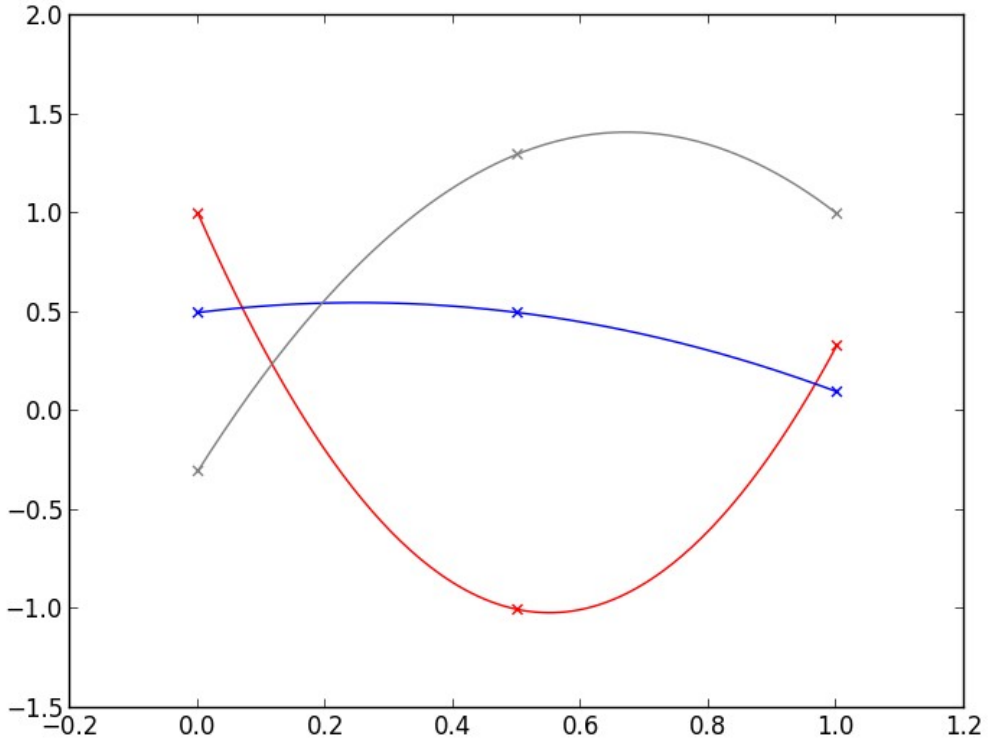
    - Basis function l_i is 0 at all x_j except for x_i (where it is 1)
  - Function value at x is:

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

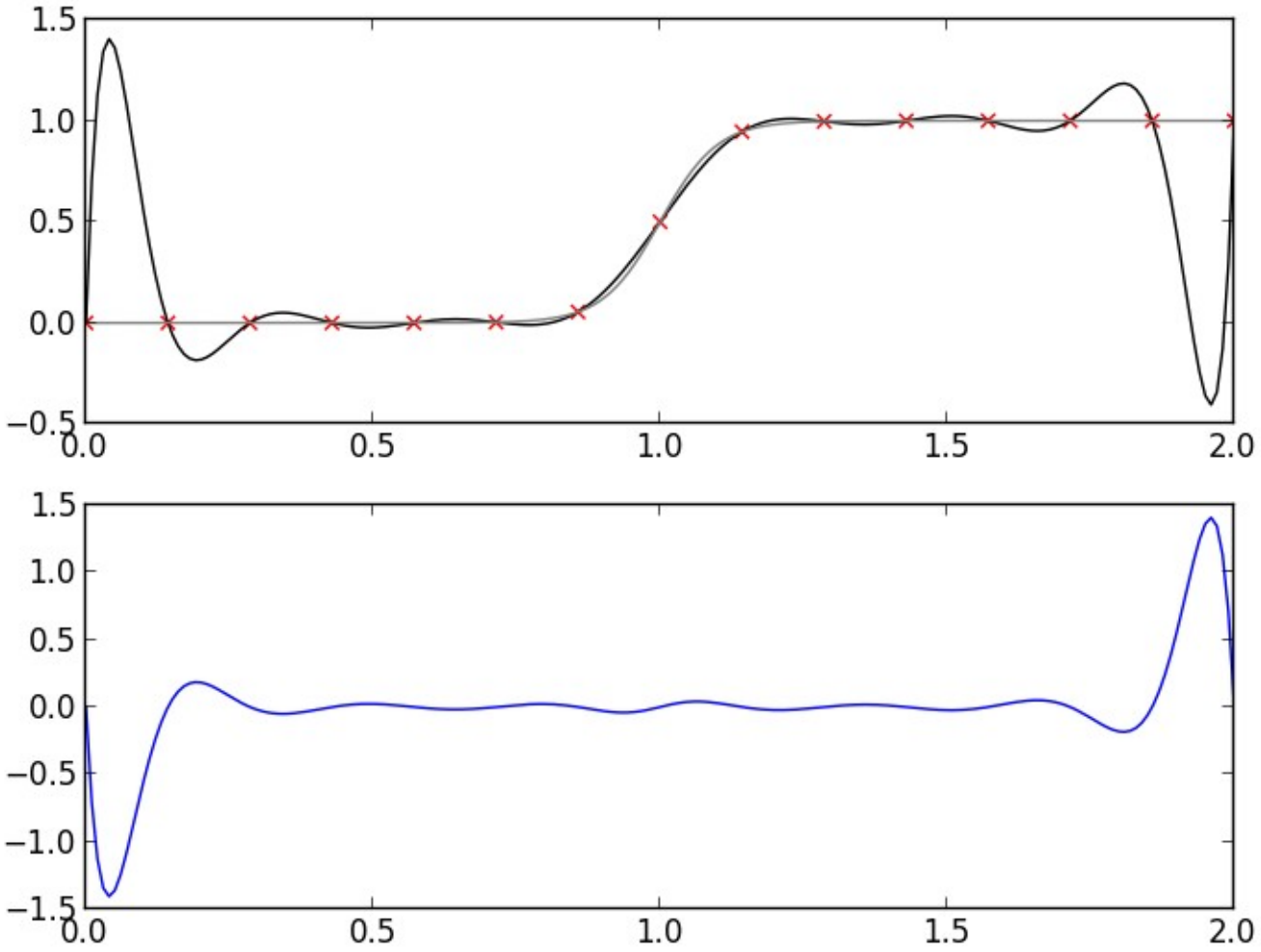
Lagrange Interpolation

- 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

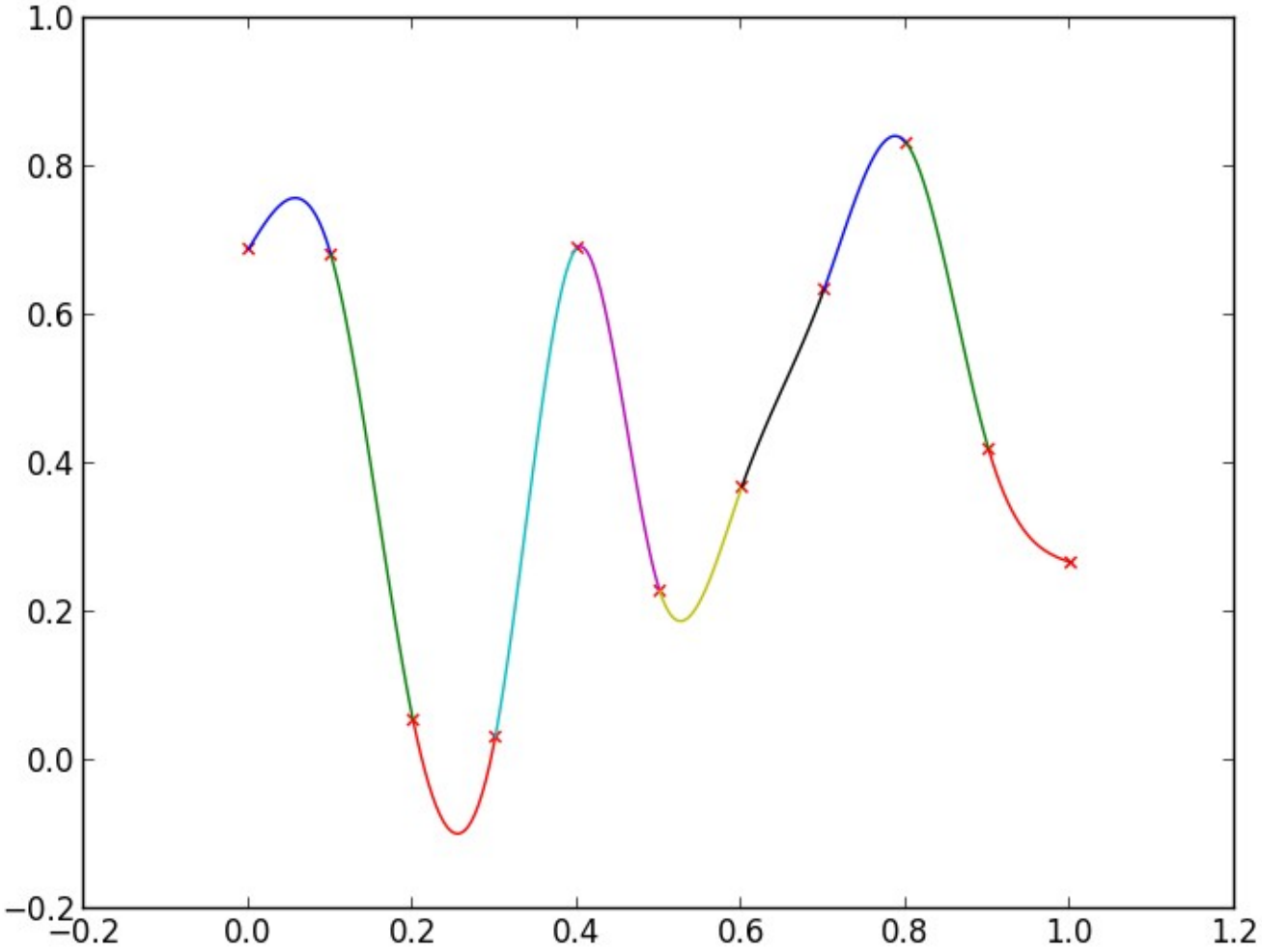


High-order is not always better: Interpolation through 15 points sampled uniformly from tanh(). The error is shown below.

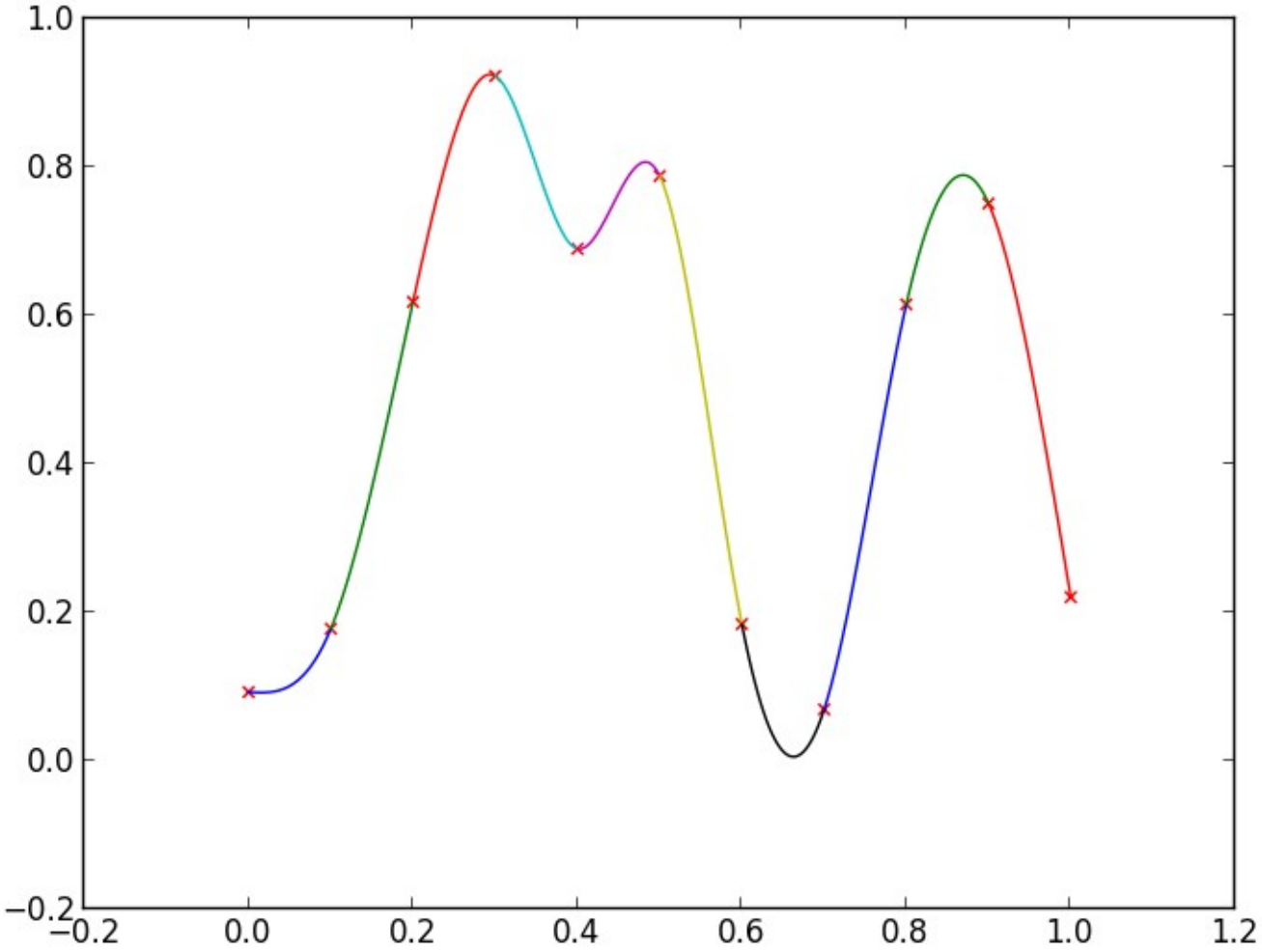
Splines

- 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

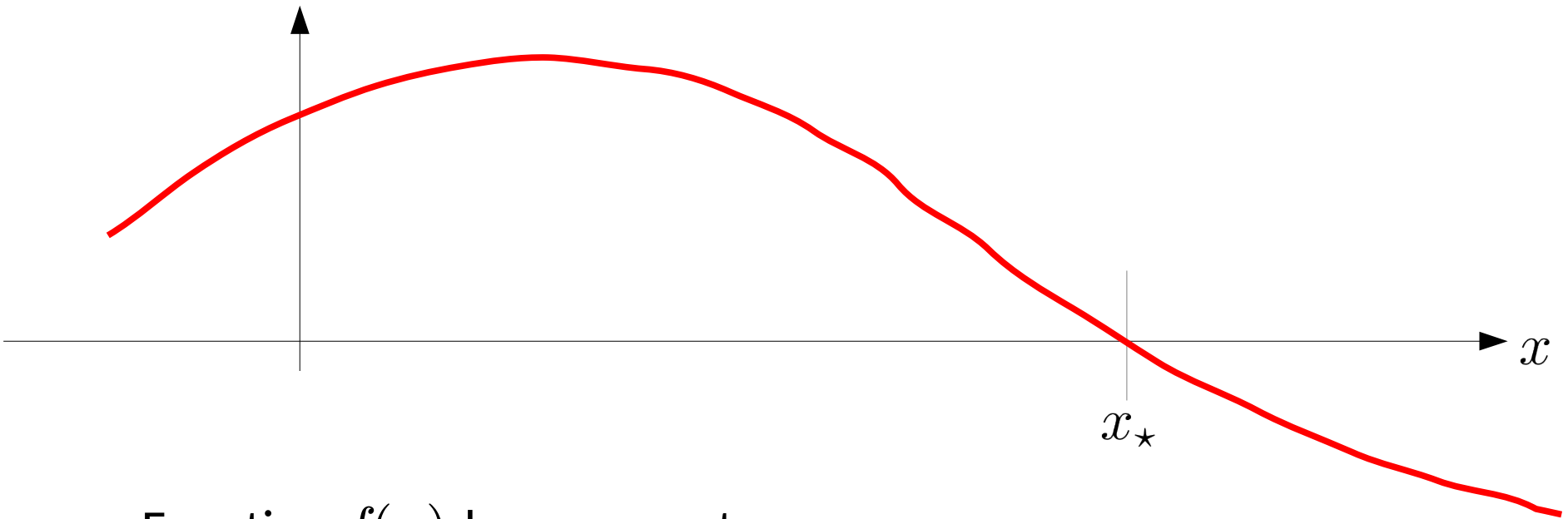
Cubic Splines

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

Root Finding

Root Finding

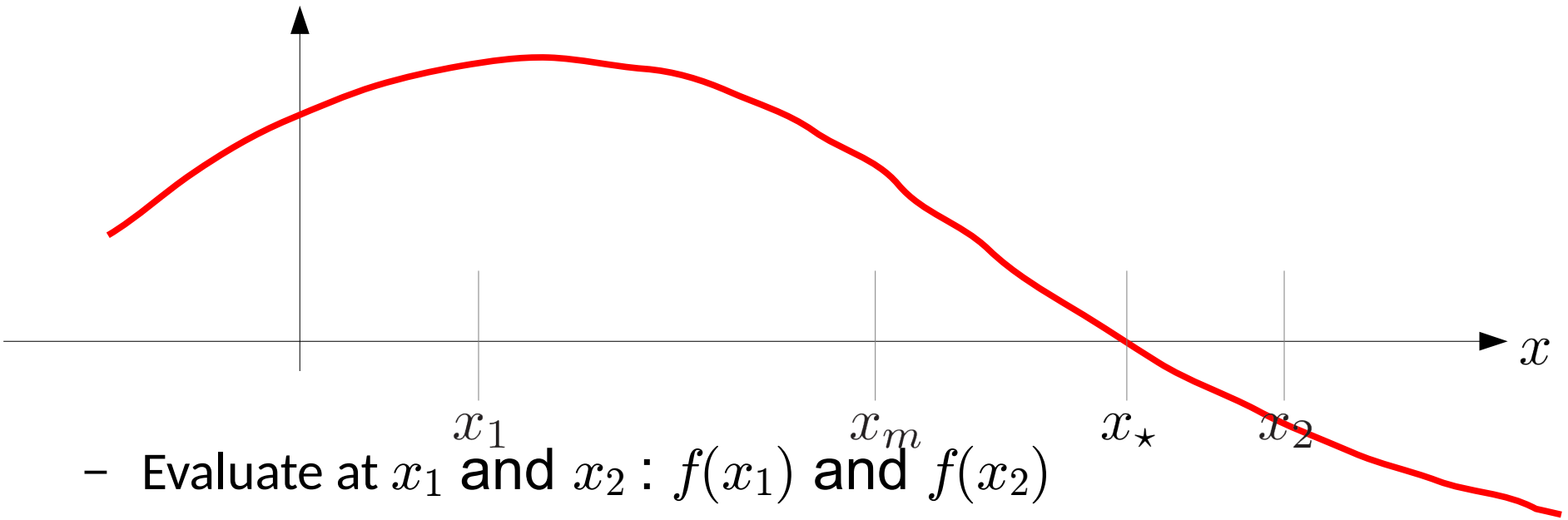
- Basic methods can be understood by looking at the function graphically



  - 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

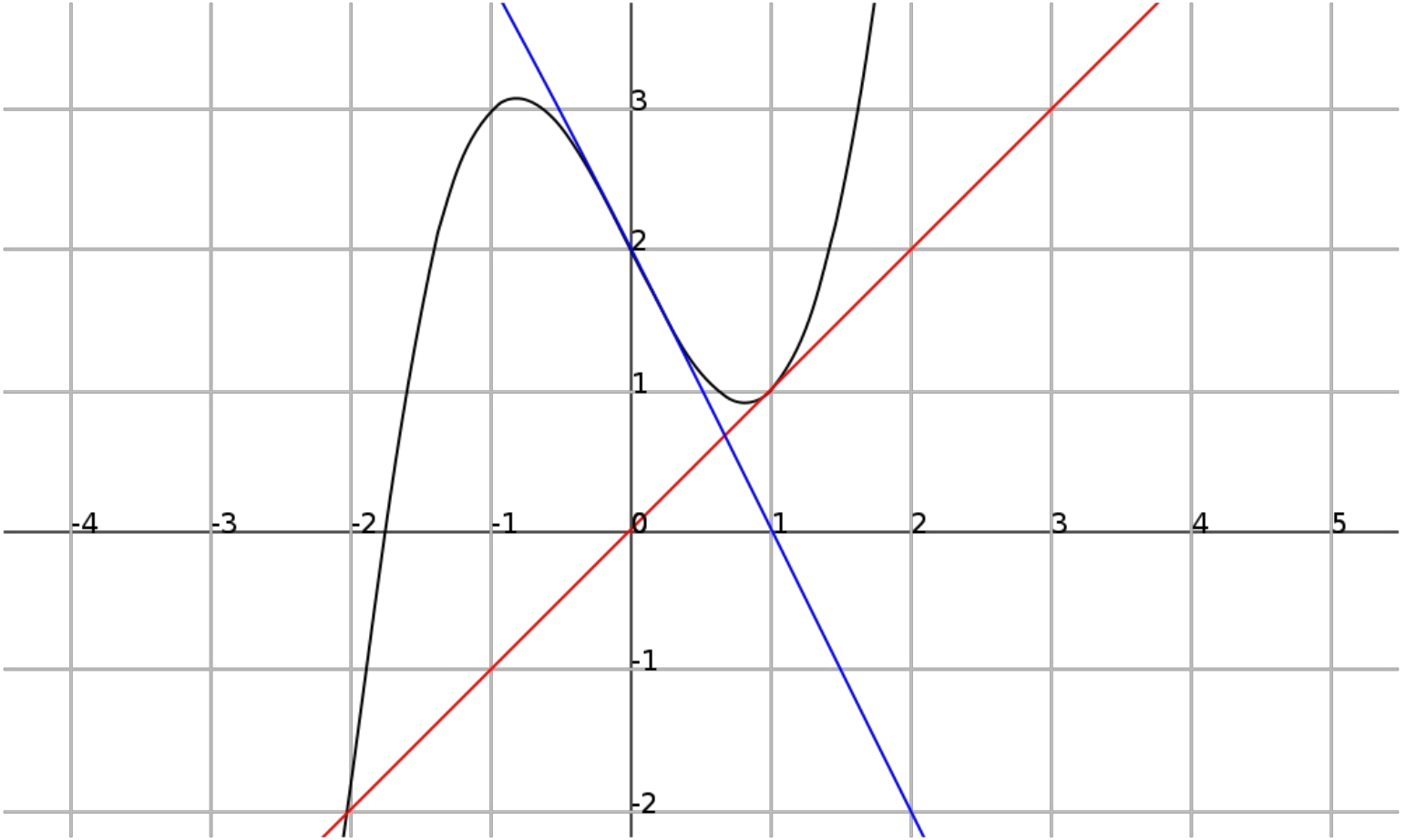
- Requirements for good convergence:
  - Derivative must exists and be non-zero in the interval near the root
  - Second derivative must be finite
  - x_0 must be close to the root
- Can be used with systems (we'll see this later)
- Multiple roots?
  - Generally: try to start with a good estimate*

*not a guarantee

Newton-Raphson

(Wikipedia)

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



(wikipedia)

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:

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

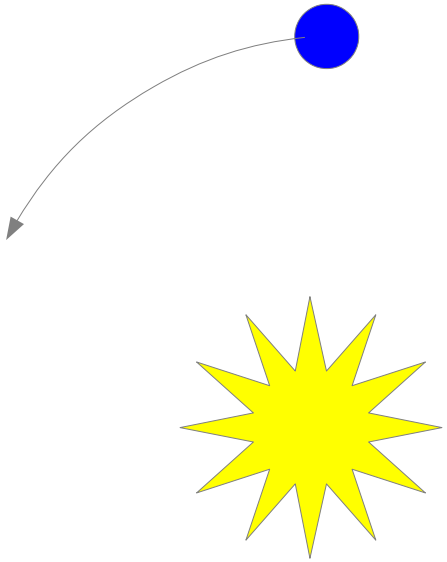
N equations + N unknowns

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: $\mathbf{J}\delta\mathbf{x}^{(k)} = -\mathbf{f}(\mathbf{x}^{(k)})\ , \quad \mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \delta\mathbf{x}^{(k)}$

ODEs

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):

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

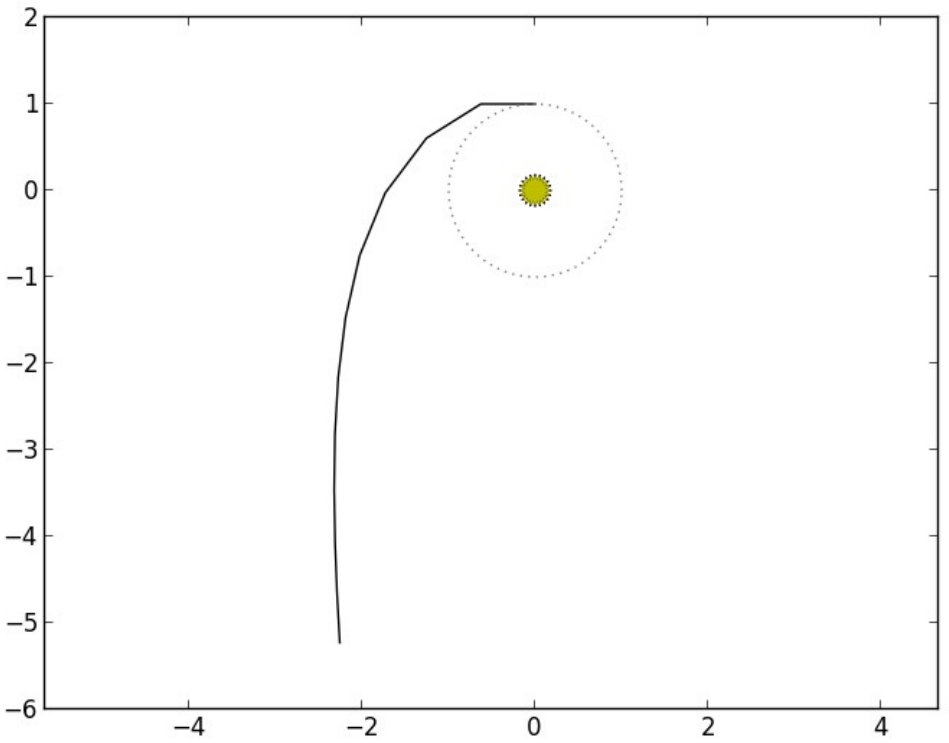
  - Work in units of AU, solar masses, and years
    - $GM = 4\ \pi^2$

Orbits: Euler's Method

- Simplest case: Euler's method

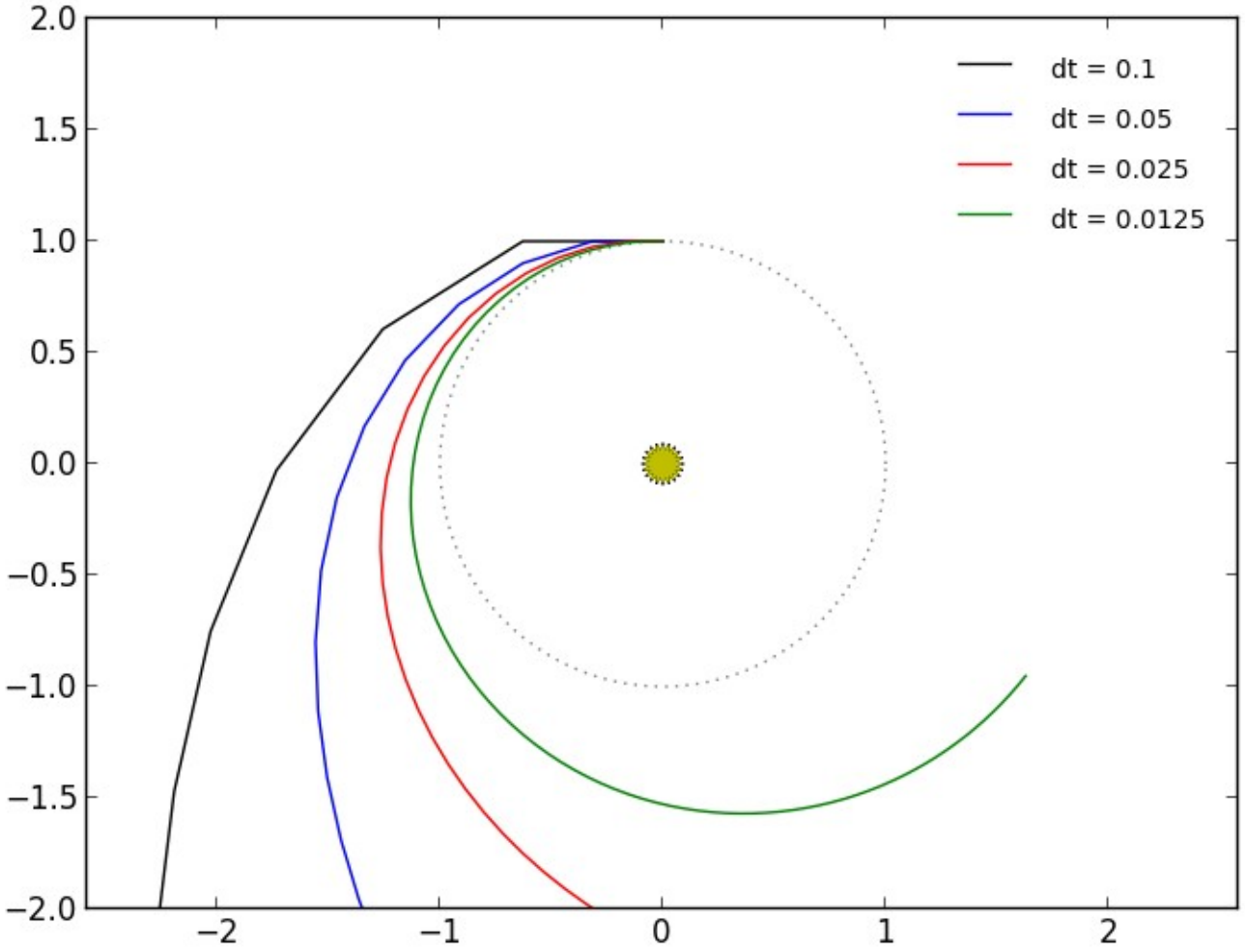
$$\mathbf{x}^{n+1} = \mathbf{x}^n + \tau \mathbf{v}^n \qquad \mathbf{v}^{n+1} = \mathbf{v}^n + \tau \mathbf{a}^n$$

- 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's 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:

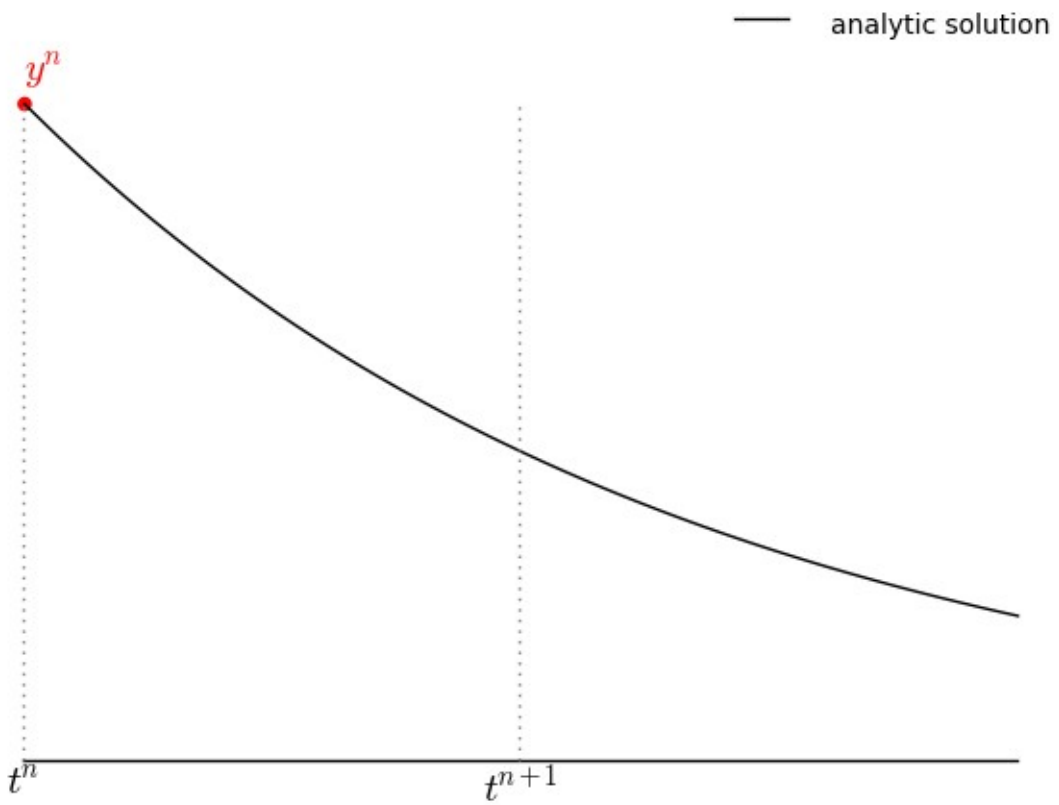
$$\mathbf{r}^{\star}=\mathbf{r}^{n}+(\tau/2)\mathbf{v}^{n}$$

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

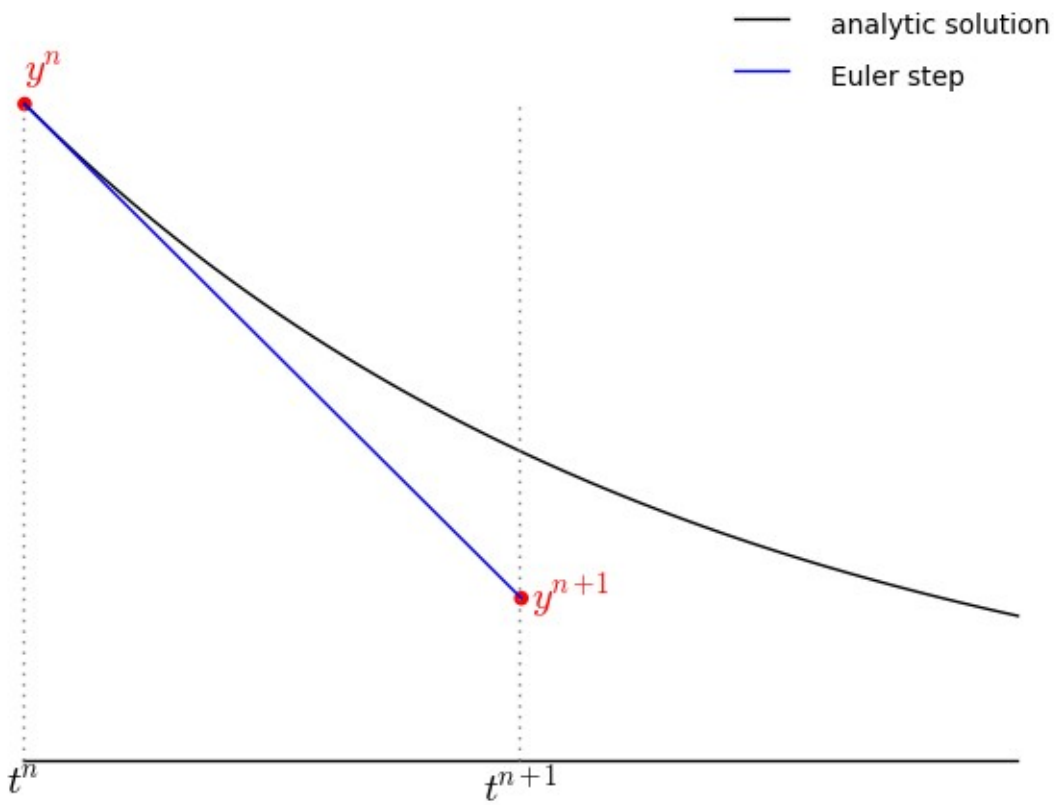
$$\mathbf{r}^{n+1}=\mathbf{r}^{n}+\tau\mathbf{v}^{\star}$$

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

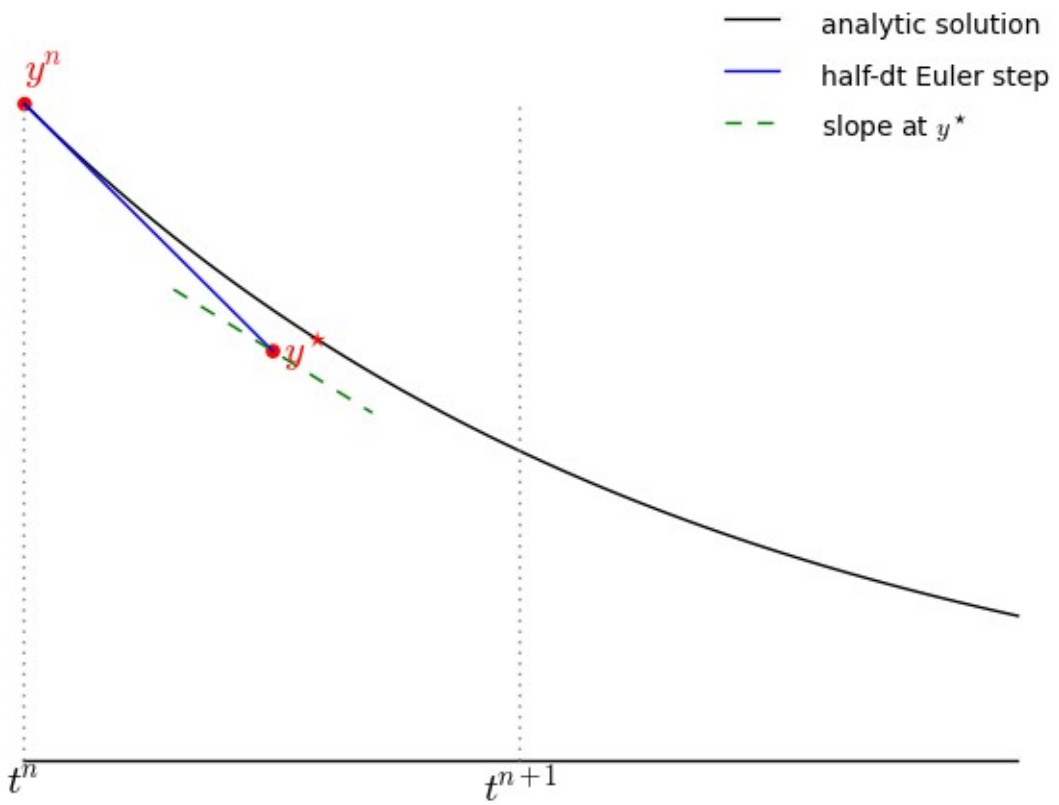
2nd-order Runge-Kutta



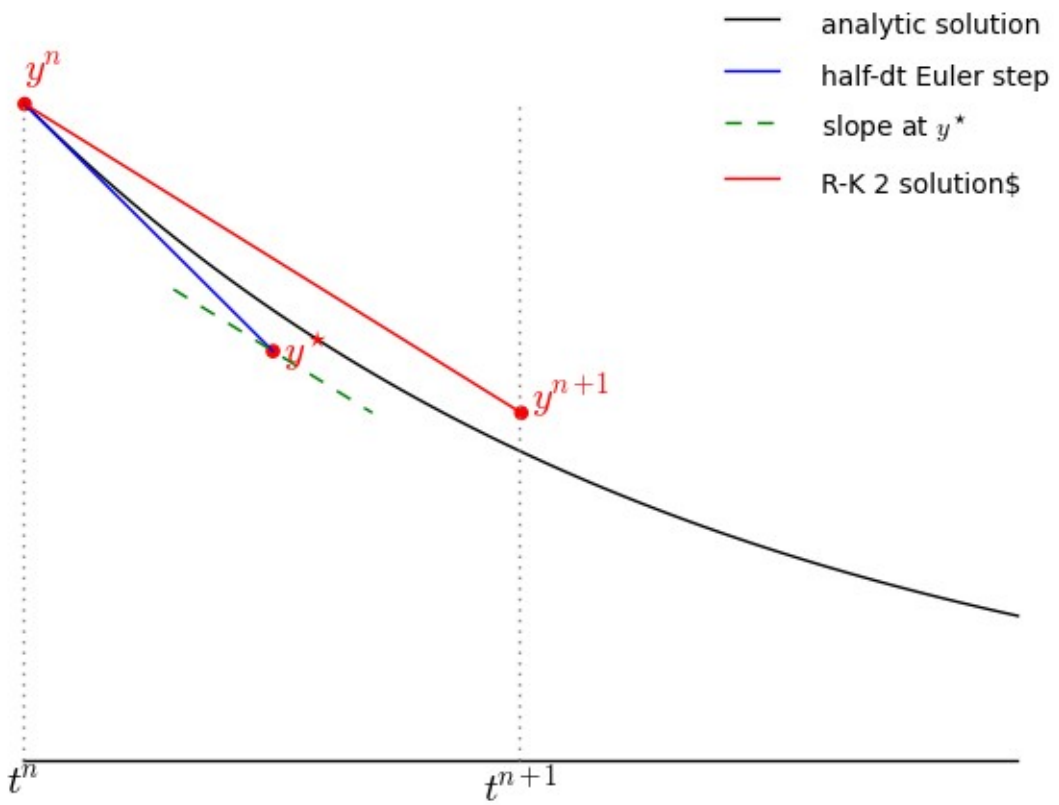
2nd-order Runge-Kutta



2nd-order Runge-Kutta



2nd-order Runge-Kutta



4th-order Runge-Kutta

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

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

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

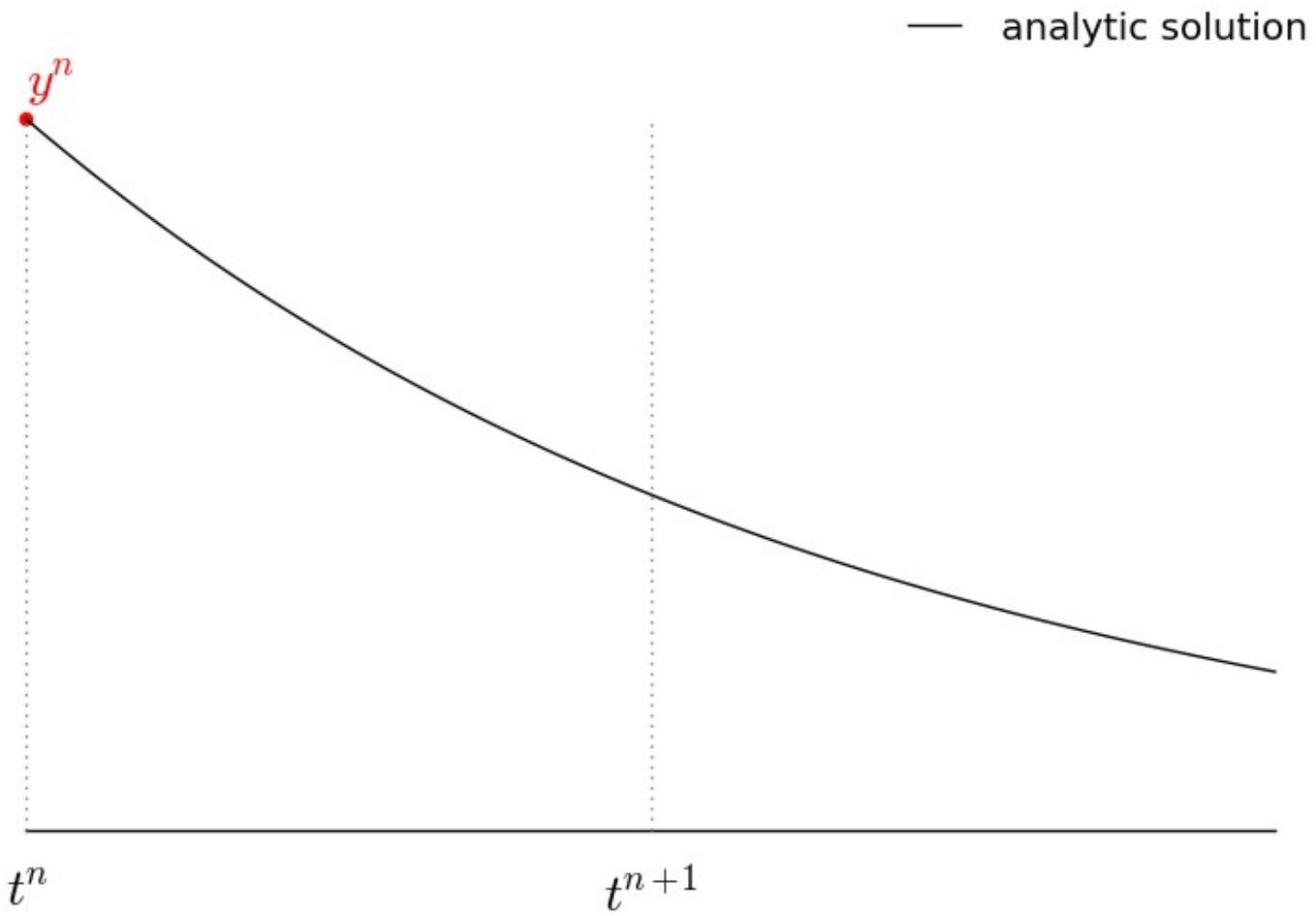
$$\mathbf{k}_2 = \mathbf{g}(t + \tfrac{\tau}{2}, \mathbf{y} + \tfrac{\tau}{2}\mathbf{k}_1)$$

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

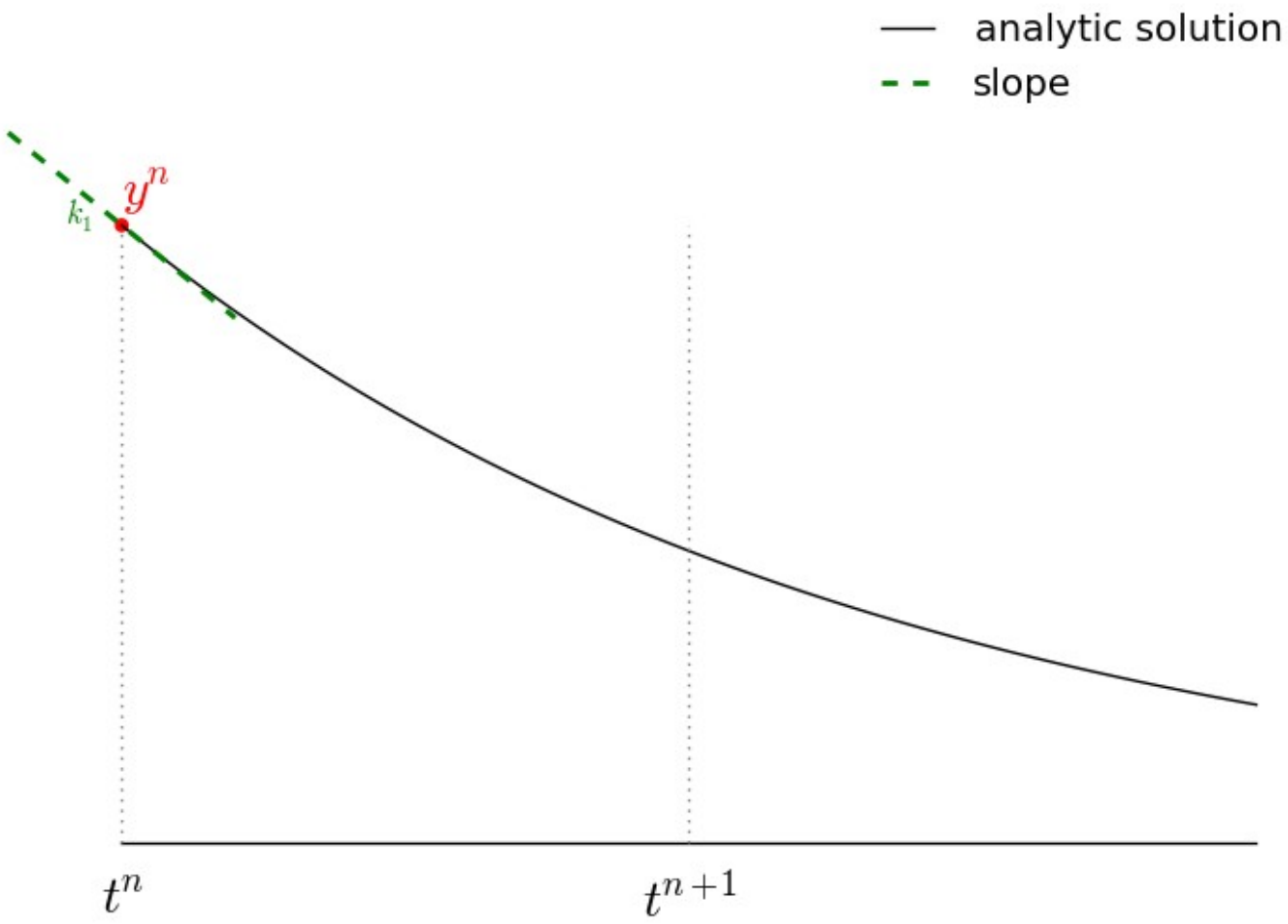
$$\mathbf{k}_4 = \mathbf{g}(t + \tau, \mathbf{y} + \tau\mathbf{k}_3)$$

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

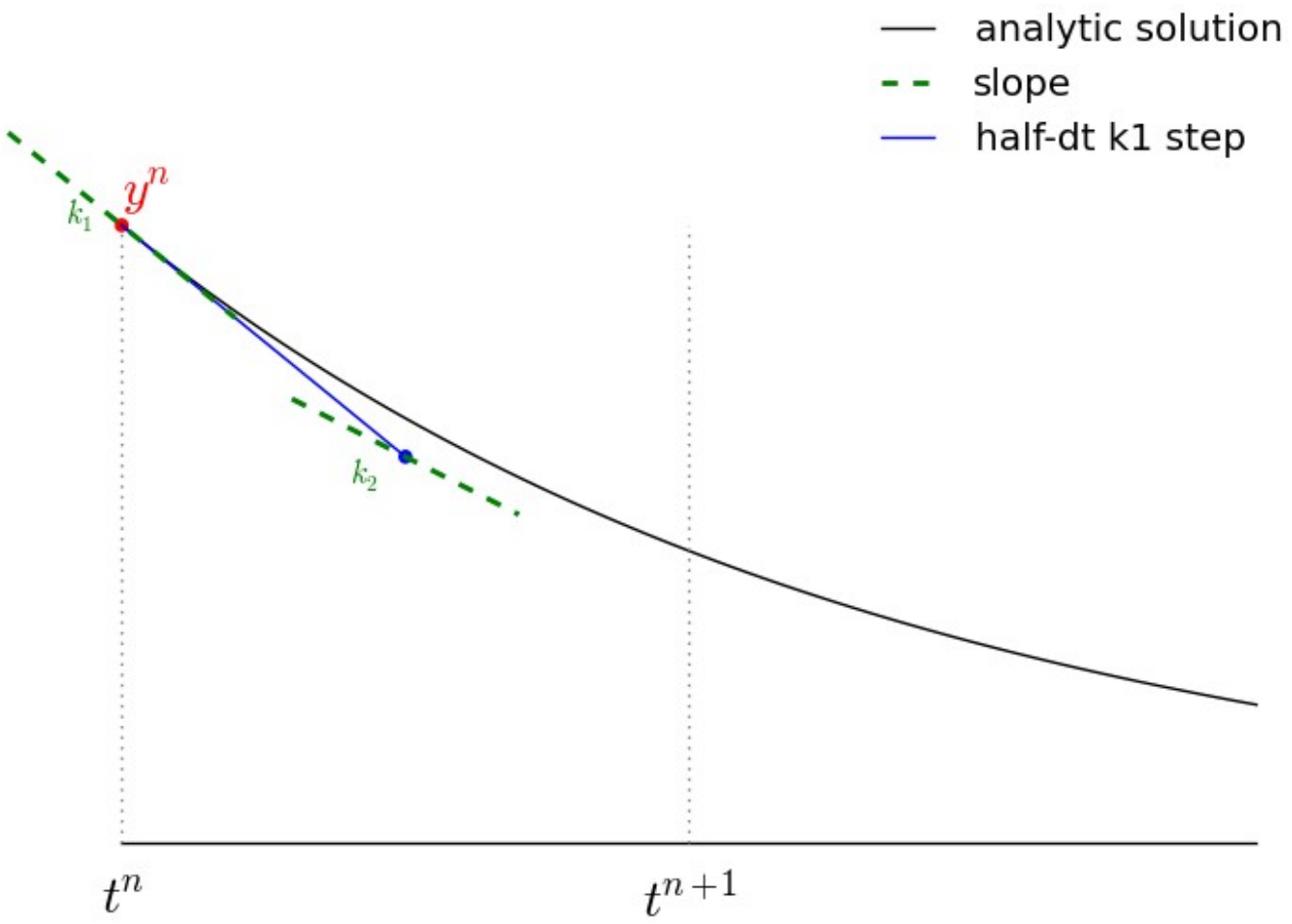
4th-order Runge-Kutta



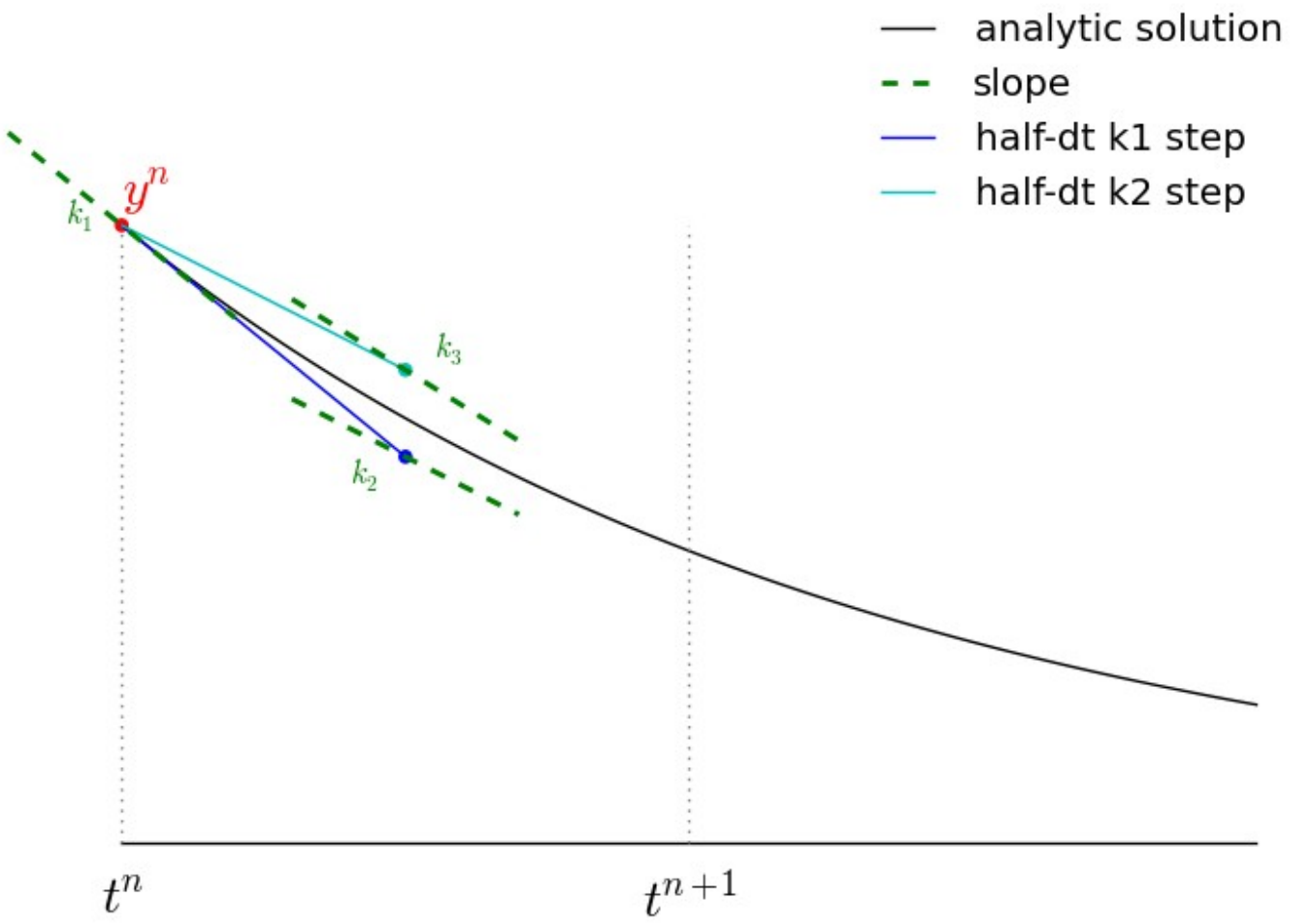
4^{th}-order Runge-Kutta



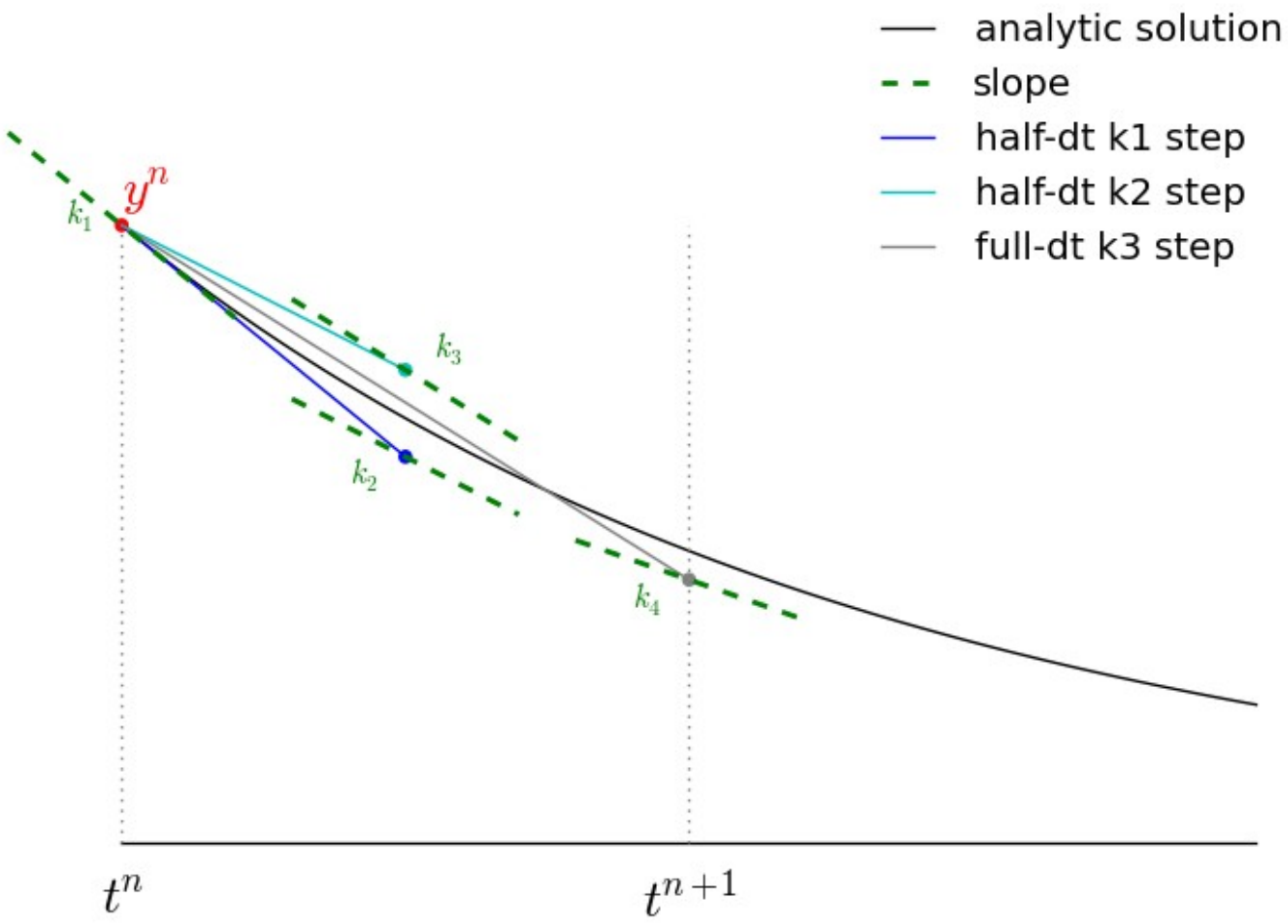
4th-order Runge-Kutta



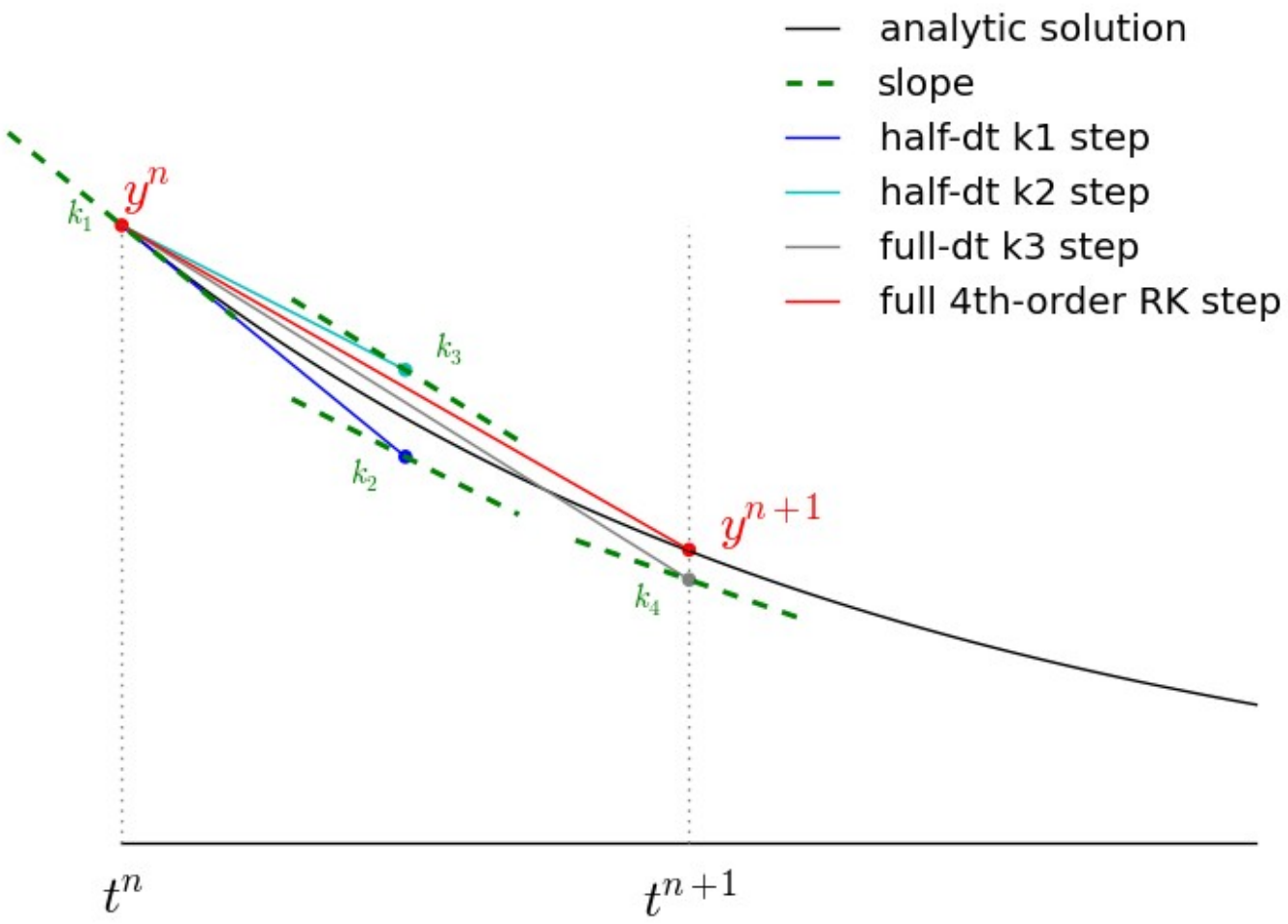
4^{th}-order Runge-Kutta



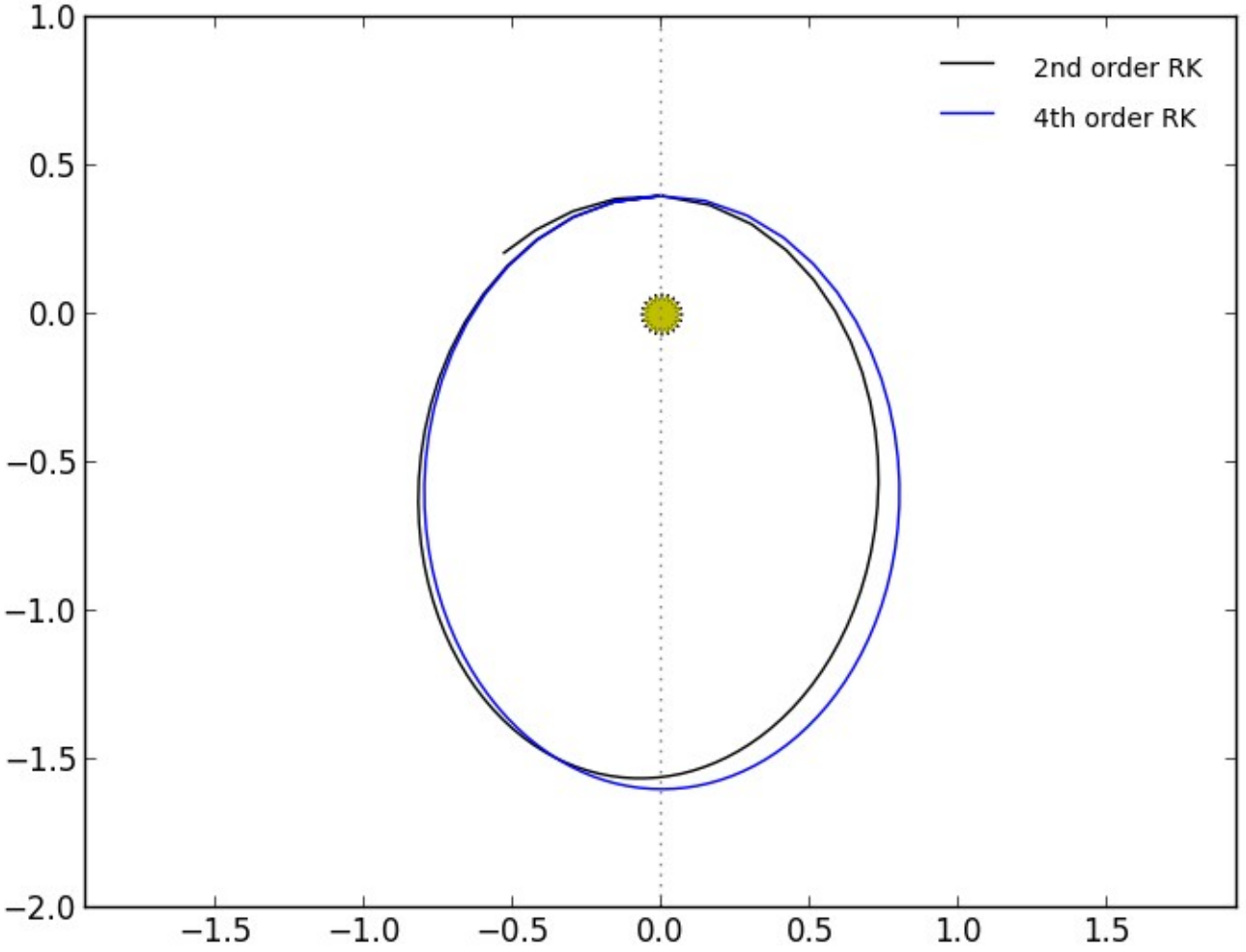
4th-order Runge-Kutta



4th-order Runge-Kutta

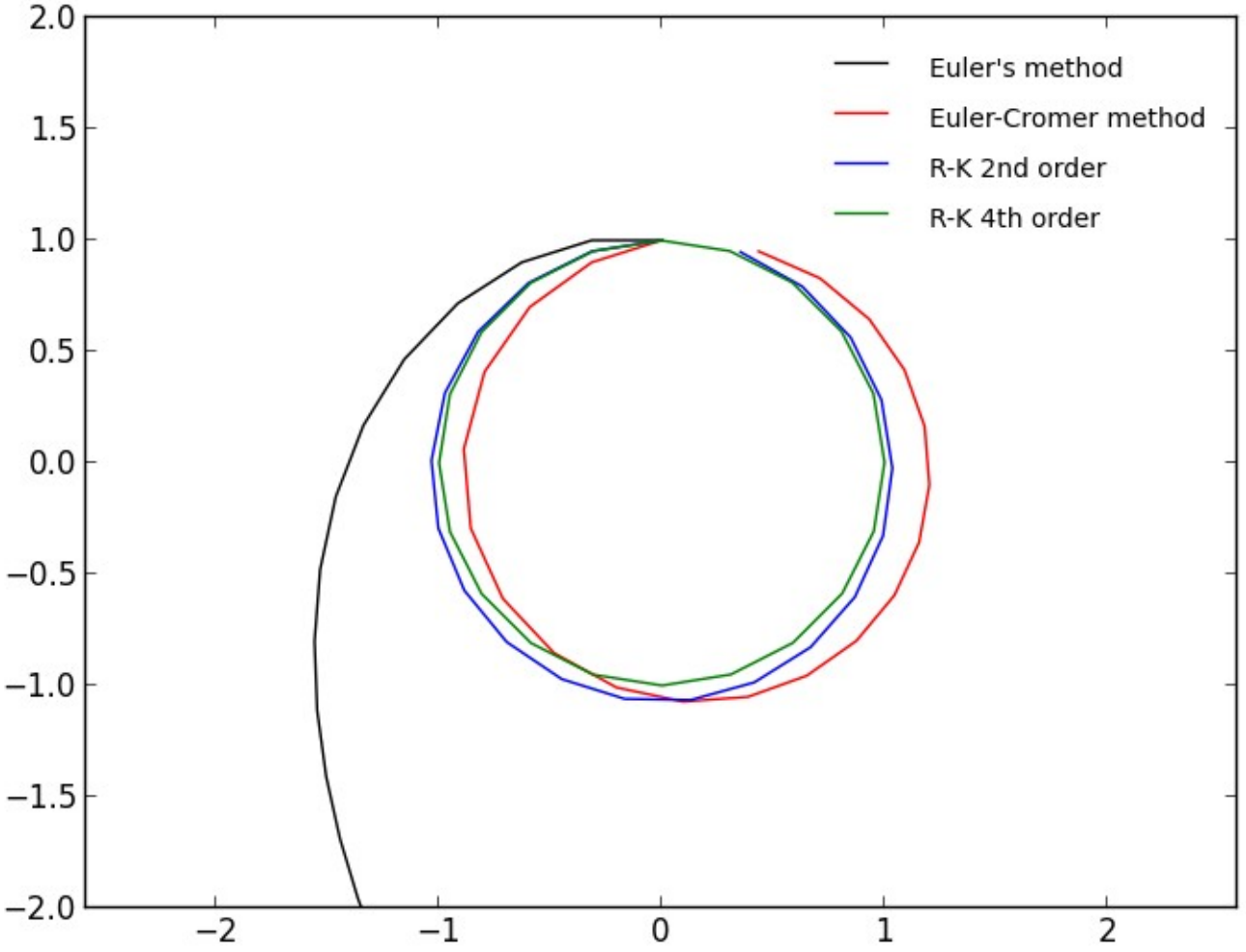


4th-order Runge-Kutta



This looks great! Let's look at the code...

4^{th}-order Runge-Kutta



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

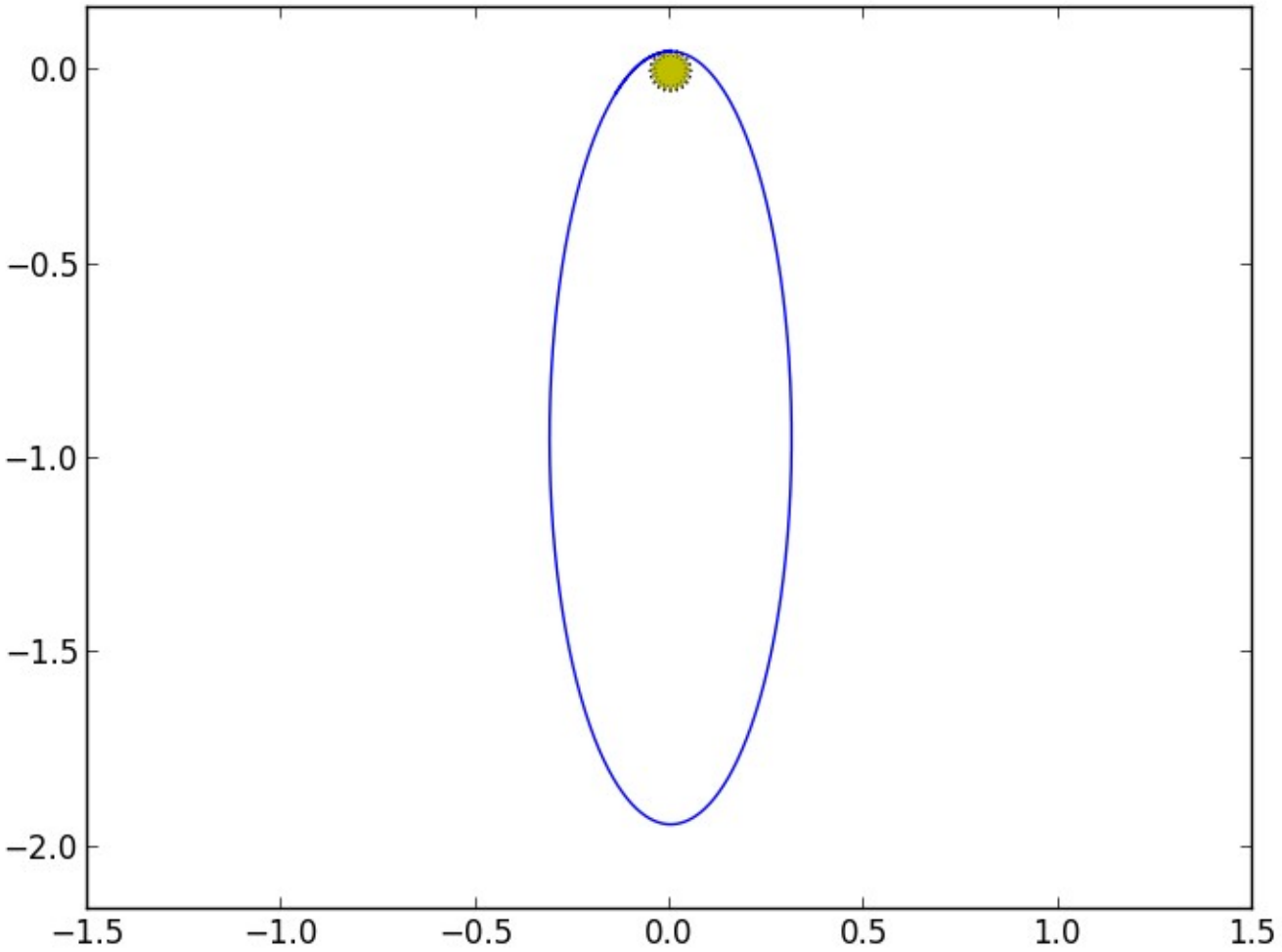
- Example from Garcia...

Ex: Highly Elliptical Orbit

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

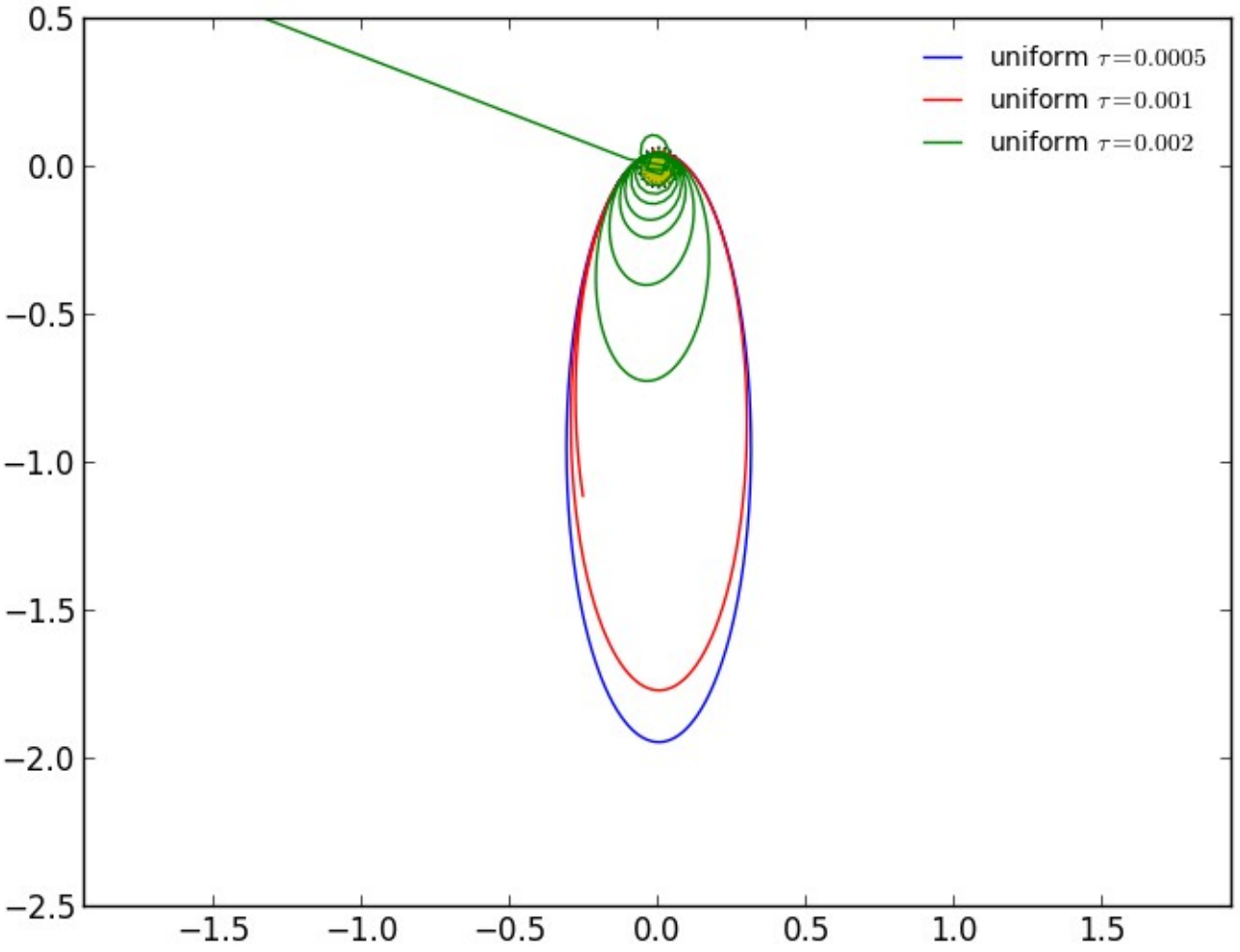
Just to get a reasonable-looking solution, we needed to use $\tau = 0.0005$

This takes 2001 steps



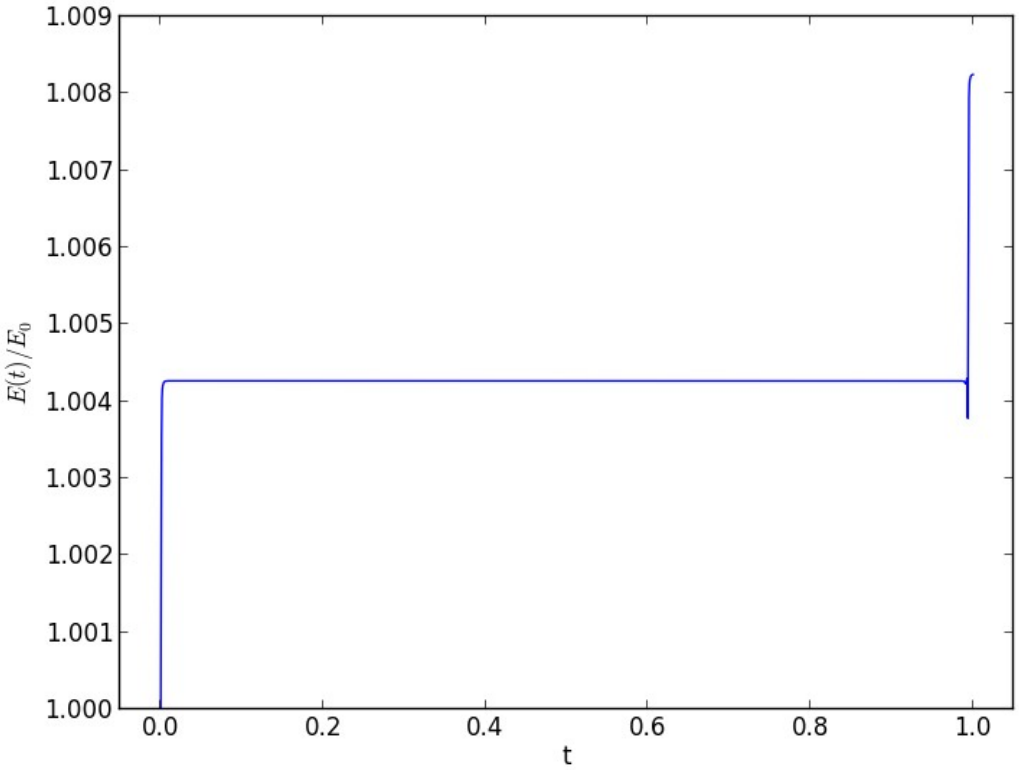
Ex: Highly-Elliptical Orbit

- Solutions with various uniform timesteps



Ex: Highly-Elliptical Orbit

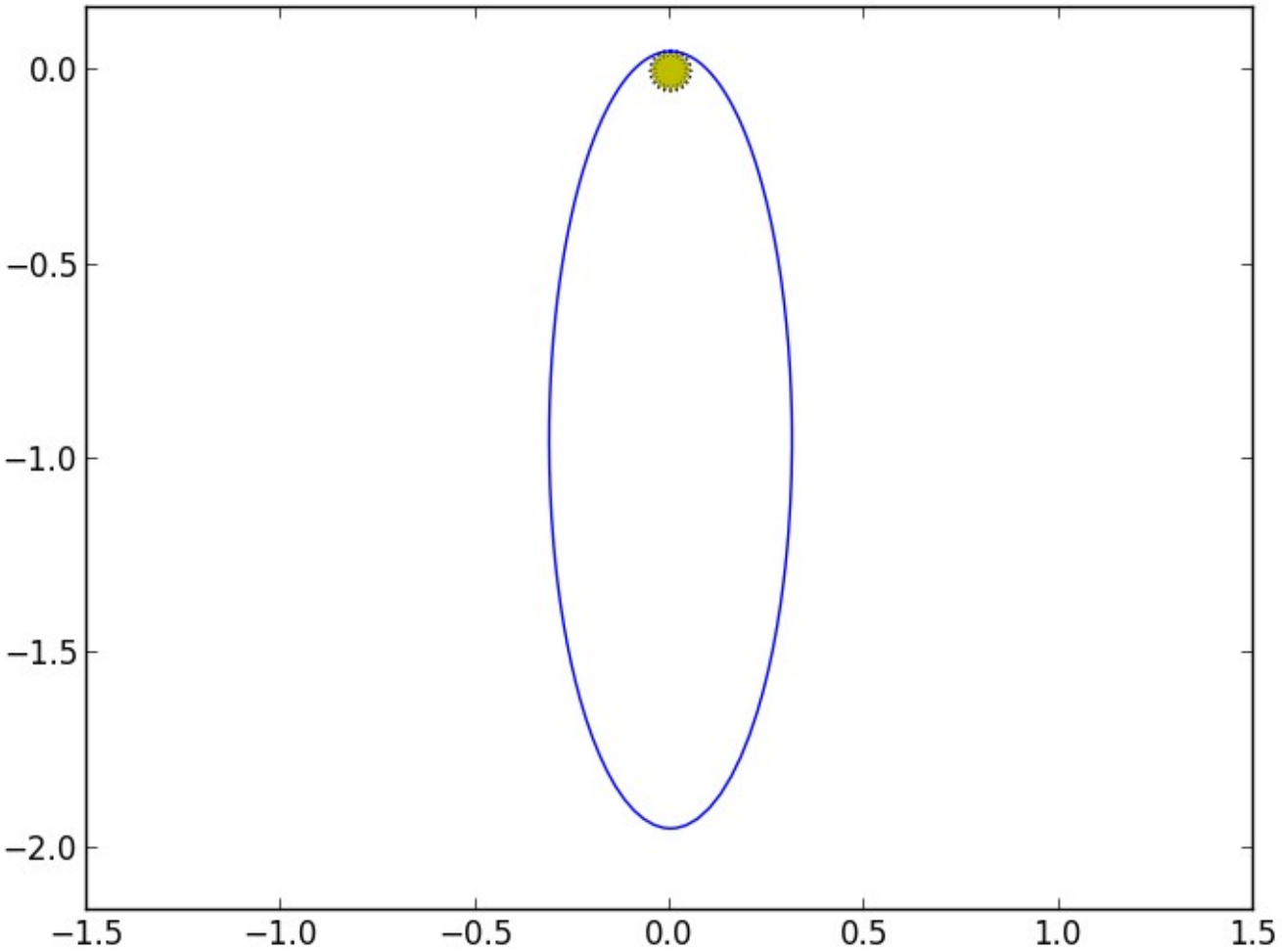
- Look at the total energy
  - At perihelion, conservation is the worse
  - Perihelion is where the velocity is greatest, and therefore the solution changes the fastest
- We can take a larger timestep at aphelion than perihelion



Adaptive Stepping

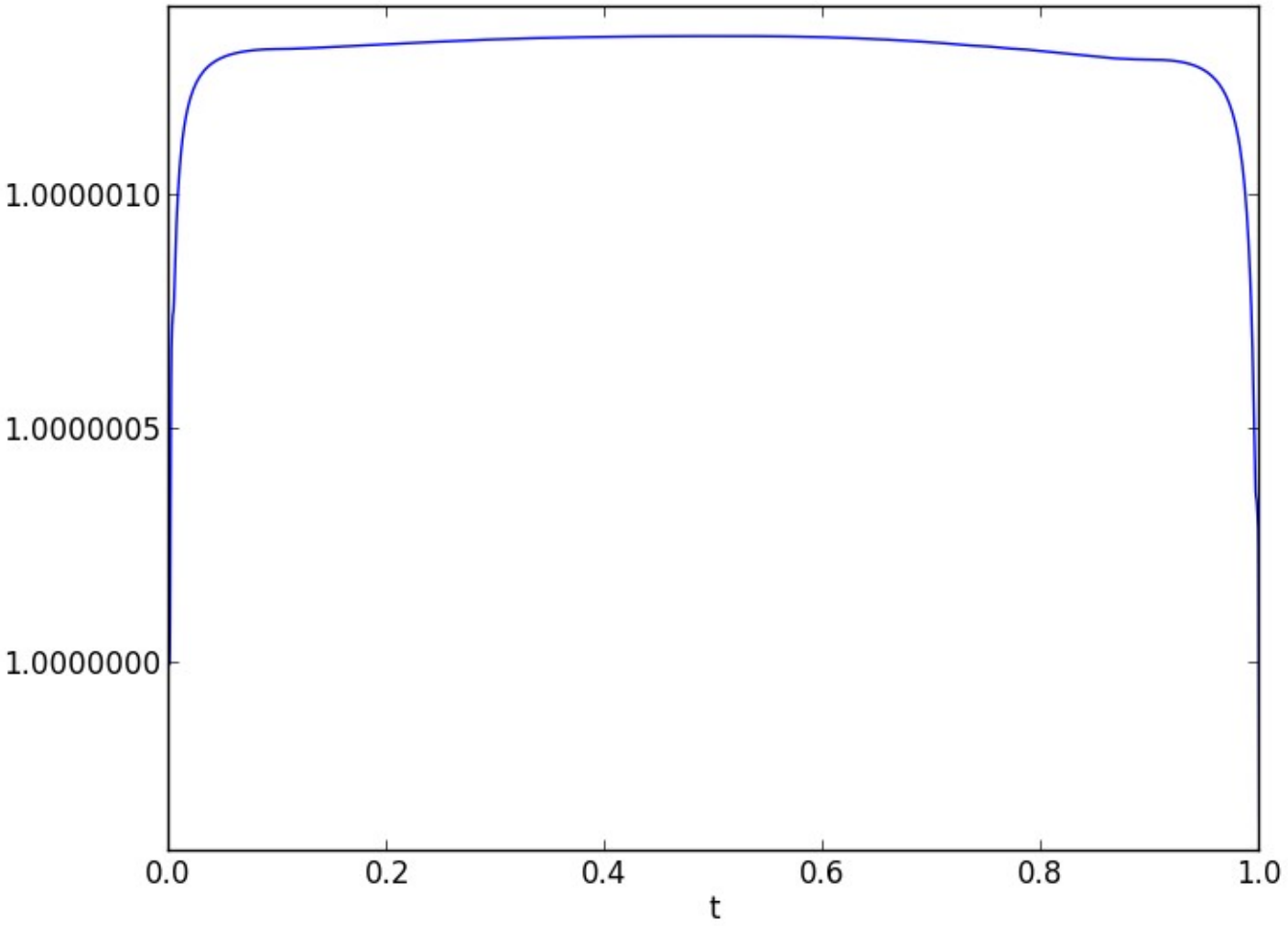
- Adaptive stepping, asking for $\epsilon = 10^{-7}$, with initial timestep the same as the non-adaptive case ($\tau = 0.005$)

This takes only 215 steps



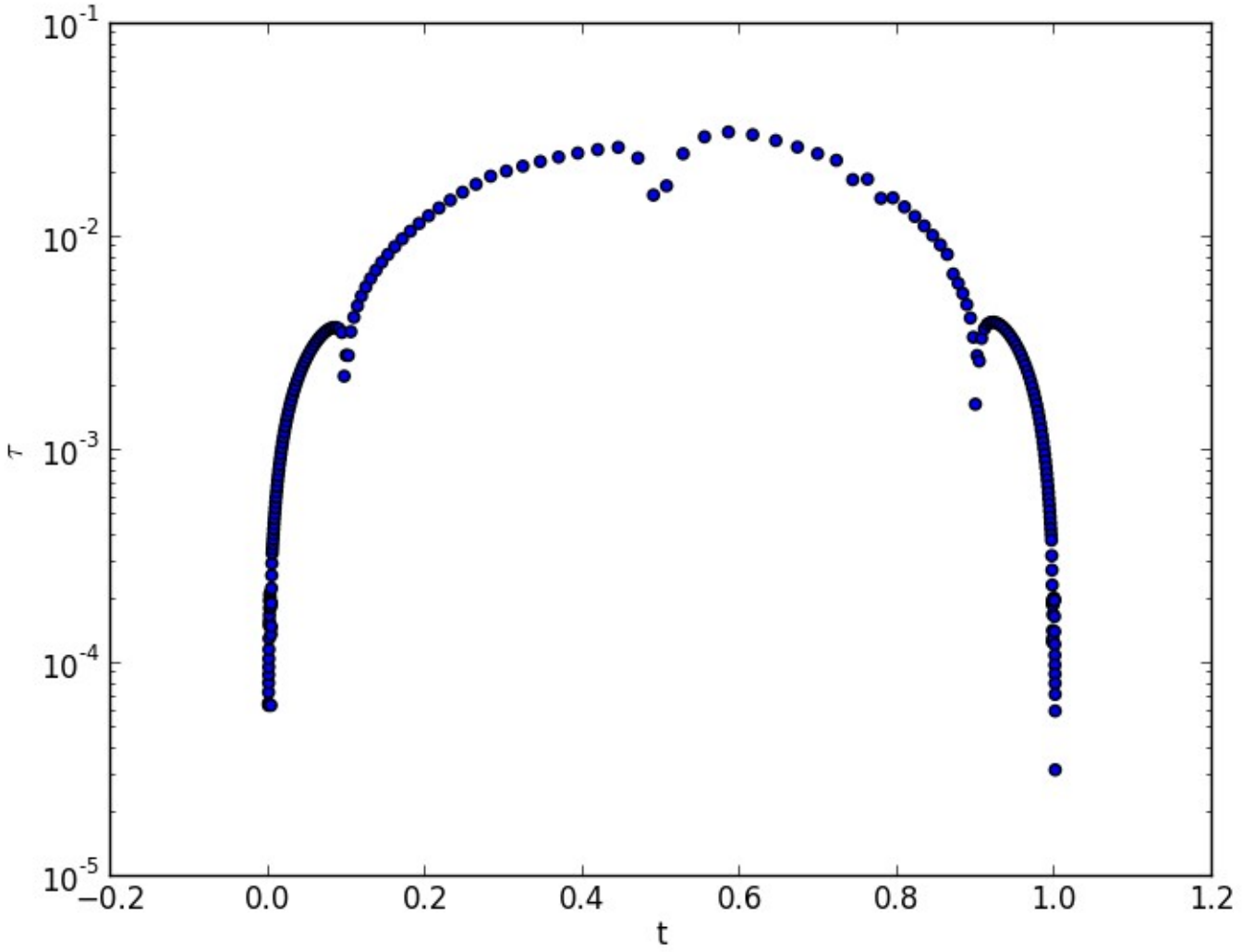
Adaptive Stepping

- 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

VODE

- For stiff systems, robust integration packages exist.
- VODE is a popular one (F77, but also in SciPy)
  - Uses a 5th-order implicit method, with error estimation (alternately, a 15th order explicit method)
  - Can either use a user-supplied Jacobian or compute one numerically
  - Two types of tolerances: absolute and relative—these have a big influence on your solution
  - Will do adaptive timesteps to reach your specified stop time

Fitting

Fitting Data

(discussion following Garcia)

- 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

Ex: Linear Regression

- 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

Errors 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

(Yakowitz and Szidarovszky)

- 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

FFTs

Fourier Transform

- Fourier transform converts a physical-space (or time series) representation of a function into frequency-space
  - Equivalent representation of the function, new view into its behavior
  - Inverse operation exists

$$F(k) = \int_{-\infty}^{\infty} f(x) e^{-2\pi i x k} dx \qquad f(x) = \int_{-\infty}^{\infty} F(k) e^{2\pi i x k} dk$$

- You can think of $F(k)$ as being the amount of the function f represented by a frequency k
- For discrete data, the discrete analog of the Fourier transform gives:
  - Amplitude and phase at discrete frequencies (wavenumbers)
  - Allows for an investigation into the periodicity of the discrete data
  - Allows for filtering in frequency-space

Discrete Fourier Transform

- The discrete Fourier transform (DFT) operates on discrete data
  - Usually we have evenly-spaced, real data
    - E.g. a time-series from an experiment
    - Simulation data for a velocity field
- DFT transforms the N spatial/temporal points into N frequency points
  - Transform: $$F_k = \sum_{n=0}^{N-1} f_n e^{-2\pi i n k/N}$$
  - Inverse: $$f_n = \frac{1}{N} \sum_{k=0}^{N-1} F_k e^{2\pi i n k/N}$$
  - This is the form used in NumPy, Garcia's text, and others

Discrete Fourier Transform

- What are the significance of the Re and Im parts?
  - Recall that we are integrating with $e^{-2\pi\, i\, k\, x}$
  - Euler's formula: $e^{i\, x} = \cos(x) + i\, \sin(x)$
  - Real part represents the cosine terms, symmetric functions
  - Imaginary part represents the sine terms, antisymmetric functions
  - Can also think in terms of an amplitude and a phase
  - If f_n is Real, then:

$$\mathrm{Re}(F_k) = \sum_{n=0}^{N-1} f_n \cos\left(\frac{2\pi n k}{N}\right) \qquad \mathrm{Im}(F_k) = \sum_{n=0}^{N-1} f_n \sin\left(\frac{2\pi n k}{N}\right)$$

- An FFT is simply an efficient way to implement the sums in the DFT

Python/NumPy's FFT

- `numpy.fft`: http://docs.scipy.org/doc/numpy/reference/routines.fft.html
- `fft`/`ifft`: 1-d data
  - By design, the k=0, … N/2 data is first, followed by the negative frequencies. These later are not relevant for a real-valued f(x)
  - k's can be obtained from `fftfreq(n)`
  - `fftshift(x)` shifts the k=0 to the center of the spectrum
- `rfft`/`irfft`: for 1-d real-valued functions. Basically the same as `fft`/`ifft`, but doesn't return the negative frequencies
- 2-d and n-d routines analogously defined

Real Space vs. Frequency Space

- Imagine transforming a real-valued function, f , with N data points
  - The FFT of f will have $N/2$ complex data points
  - Same amount of information in each case, but each complex point corresponds to 2 real numbers.
    - This is a consequence of the analytic Fourier transform satisfying $F(-k) = F^{\star}(k)$ if $f(x)$ is real
  - Most FFT routines will return N complex points—half of them are duplicate, i.e. they don't add to the information content
    - Often, there are specific implementations optimized for the case where the function is real (e.g. rfft)
  - This affects normalization (note k=0 different)
- This is also referred to as aliasing.
- The maximum frequency, $1/\ (2\ \Delta x)$ is called the Nyquist frequency

Normalization

- When plotting, we want to put the physical scale back in, as well as make the correspondence to the continuous representation
  - Wavenumber to frequency:
    - In index space, the smallest wavelength is from one cell to the next, and the smallest frequency is 1/N
    - Adding points to our data means we open up higher and higher frequencies
    - Lowest frequency: 1/L; highest frequency: 1/Δx
  - Amplitudes: rewrite inverse expression:

This is what we plot

$$f_n = \frac{1}{N}\sum_{n=0}^{N-1} F_k e^{2\pi i n k/N} = \underbrace{\sum_{n=0}^{N-1}\left(\frac{F_k}{N}\right) e^{2\pi i n k/N}}$$

This looks like the continuous form

  - Another interpretation: $F_k \,/\, N \Leftrightarrow F_k\, dk$

FFT Tips

- Different FFT codes make different assumptions about the normalization, etc.
- Make sure the FFT does what you expect it should be working on a single-frequency sine first.

Linear Algebra

Numerical Linear Algebra

- The basic problem we wish to solve is: $A\,x = b$
  - It is generally simpler to solve this system directly than to first find the inverse and then multiply A^{-1} b
- Gaussian elimination works with a general matrix
  - Faster methods exist for banded, sparse, symmetric, … matrices
  - Explicit code for doing Gaussian elimination posted on our course page. See any numerical text for a discussion of the algorithm.

Gaussian Elimination

- The main, general technique for solving a linear system $Ax=b$ is Gaussian-Elimination
  - Doesn't require computing an inverse
  - For special matrices, faster techniques may apply
- Forward-elimination + Back-substitution steps
- Round-off can cause issues and lead to systems that are unsolvable
  - Example from Garcia

$$\begin{aligned} \epsilon x_1 + x_2 + x_3 &= 5 \\ x_1 + x_2 &= 3 \\ x_1 + x_3 &= 4 \end{aligned}$$

in limit $\epsilon \to 0$

Gaussian Elimination

- Worked ex (from Garcia):

$$\begin{aligned} x_1 + x_2 + x_3 &= 6 \\ -x_1 + 2x_2 &= 3 \\ 2x_1 + x_3 &= 5 \end{aligned}$$

- Eliminate x_1 from the second and third eqs

$$\begin{aligned} x_1 + x_2 + x_3 &= 6 \\ 3x_2 + x_3 &= 9 \\ -2x_2 - x_3 &= -7 \end{aligned}$$

- Eliminate x_2 from the last eq.

$$\begin{aligned} x_1 + x_2 + x_3 &= 6 \\ 3x_2 + x_3 &= 9 \\ -\tfrac{1}{3}x_3 &= -1 \end{aligned}$$

Forward elimination

Gaussian Elimination

```
/                                \   /         \
|  4.000   3.000   4.000  10.000 |   |  2.000  |
|  2.000  -7.000   3.000   0.000 |   |  6.000  |
| -2.000  11.000   1.000   3.000 |   |  3.000  |
|  3.000  -4.000   0.000   2.000 |   |  1.000  |
\                                /   \         /

/                                \   /         \
|  3.000  -4.000   0.000   2.000 |   |  1.000  |
|  0.000  -4.333   3.000  -1.333 |   |  5.333  |
|  0.000   8.333   1.000   4.333 |   |  3.667  |
|  0.000   8.333   4.000   7.333 |   |  0.667  |
\                                /   \         /

/                                \   /         \
|  3.000  -4.000   0.000   2.000 |   |  1.000  |
|  0.000   8.333   4.000   7.333 |   |  0.667  |
|  0.000   0.000  -3.000  -3.000 |   |  3.000  |
|  0.000   0.000   5.080   2.480 |   |  5.680  |
\                                /   \         /

/                                \   /         \
|  3.000  -4.000   0.000   2.000 |   |  1.000  |
|  0.000   8.333   4.000   7.333 |   |  0.667  |
|  0.000   0.000   5.080   2.480 |   |  5.680  |
|  0.000   0.000   0.000  -1.535 |   |  6.354  |
\                                /   \         /

/                                \   /         \
|  3.000  -4.000   0.000   2.000 |   |  1.000  |
|  0.000   8.333   4.000   7.333 |   |  0.667  |
|  0.000   0.000   5.080   2.480 |   |  5.680  |
|  0.000   0.000   0.000  -1.535 |   |  6.354  |
\                                /   \         /
```

Sometimes we do partial pivoting: swap rows to put the one with the largest (scaled) element on top.

solved x: [6.04615385 2.21538462 3.13846154 -4.13846154]
A.x: [2. 6. 3. 1.]

Caveats

- Singular matrix
  - If the matrix has no determinant, then we cannot solve the system
  - Common way for this to enter: one equation in our system is a linear combination of some others
  - Not always easy to detect from the start

Gaussian Elimination

- Condition number
  - Measure of how close to singular we are
  - Think of it as a measure of how much x would change due to a small change in b (large condition number means G-E inaccurate)
  - Formal definition: $\mathrm{cond}(A) = \|A\|\|A^{-1}\|$
    - Further elucidation requires defining the norm
  - Rule of thumb (Yakowitz & Szidarovszky, Eq. 2.31):
    - If $x^\star$ is the exact solution and x is the computed solution, then

$$\frac{\|x^\star - x\|}{\|x^\star\|} \approx \mathrm{cond}(A) \cdot \epsilon_{\mathrm{machine}}$$

- Simple ill-conditioned example: see G. J. Tee, ACM SIGNUM Newsletter, v. 7, issue 3, Oct. 1972, p. 19 (posted)

Tridiagonal Solve

- Tridiagonal systems come up very often in physical systems
- Efficient, O(N), algorithm derived from looking at the Gaussian elimination sequence (see e.g. Wikipedia):
  - Standard data layout.

$$\begin{pmatrix} b_0 & c_0 & & & & & \\ a_1 & b_1 & c_1 & & & & \\ & a_2 & b_2 & c_2 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & a_{N-2} & b_{N-2} & c_{N-2} \\ & & & & & a_{N-1} & b_{N-1} \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ \vdots \\ x_{N-2} \\ x_{N-1} \end{pmatrix} = \begin{pmatrix} d_0 \\ d_1 \\ d_2 \\ \vdots \\ \vdots \\ d_{N-2} \\ d_{N-1} \end{pmatrix}$$

Note that $a_0 = c_{N-1} = 0$

LU Decomposition

- LU Decomposition is an alternate to Gaussian elimination
  - See Pang/Wikipedia for details
- Basic idea:
  - Find upper and lower triangular matrices such that $A = LU$
  - Express $Ax = b$ as $Ly = b$ and $Ux = y$
  - Most of the work in the solve is in doing the decomposition, so if you need to solve for many different b's, this is more efficient
- This is often used in stiff integration packages

BLAS/LINPACK/LAPACK

- BLAS (basic linear algebra subroutines)
  - These are the standard building blocks (API) of linear algebra on a computer (Fortran and C)
  - Most linear algebra packages formulate their operations in terms of BLAS operations
  - Three levels of functionality:
    - Level 1: vector operations ($\alpha\ x + y$)
    - Level 2: matrix-vector operations ($\alpha\ A\ x + \beta\ y$)
    - Level 3: matrix-matrix operations ($\alpha\ A\ B + \beta\ C$)
  - Available on pretty much every platform
    - Some compilers provide specially optimized BLAS libraries (-lblas) that take great advantage of the underlying processor instructions
    - ATLAS: automatically tuned linear algebra software

BLAS/LINPACK/LAPACK

- LINPACK
  - Older standard linear algebra package from 1970s designed for architectures available then
  - Superseded by LAPACK

See Top 500 list

- LAPACK
  - The standard for linear algebra
  - Built upon BLAS
  - Routines named in the form `xyyzzz`
    - `x` refers to the data type (s/d are single/double precision floating, c/z are single/double complex)
    - `yy` refers to the matrix type
    - `zzz` refers to the algorithm (e.g. `sgebrd` = single precision bi-diagonal reduction of a general matrix)
  - Ex: single precision routines: http://www.netlib.org/lapack/single/

Table 2.1: Matrix types in the LAPACK naming scheme

BD	bidiagonal
DI	diagonal
GB	general band
GE	general (i.e., unsymmetric, in some cases rectangular)
GG	general matrices, generalized problem (i.e., a pair of general matrices)
GT	general tridiagonal
HB	(complex) Hermitian band
HE	(complex) Hermitian
HG	upper Hessenberg matrix, generalized problem (i.e a Hessenberg and a triangular matrix)
HP	(complex) Hermitian, packed storage
HS	upper Hessenberg
OP	(real) orthogonal, packed storage
OR	(real) orthogonal
PB	symmetric or Hermitian positive definite band
PO	symmetric or Hermitian positive definite
PP	symmetric or Hermitian positive definite, packed storage
PT	symmetric or Hermitian positive definite tridiagonal
SB	(real) symmetric band
SP	symmetric, packed storage
ST	(real) symmetric tridiagonal
SY	symmetric
TB	triangular band
TG	triangular matrices, generalized problem (i.e., a pair of triangular matrices)
TP	triangular, packed storage
TR	triangular (or in some cases quasi-triangular)
TZ	trapezoidal
UN	(complex) unitary
UP	(complex) unitary, packed storage

http://www.netlib.org/lapack/lug/node24.html

Python Support for Linear Algebra

- Basic methods in numpy.linalg
  - http://docs.scipy.org/doc/numpy/reference/routines.linalg.html
- More general stuff in SciPy (scipy.linalg)
  - http://docs.scipy.org/doc/scipy/reference/linalg.html
- SciPy calls the LAPACK routines under the hood (in the SciPy docs, you can click on the “source” link to see the explicit calls).

Python Support for Linear Algebra

- Numpy has a matrix type built from the array class
  - `*` operator works element by element for arrays but does matrix product for matrices
  - Vectors are automatically converted into 1×N or N×1 matrices
  - Matrix objects cannot be > rank 2
  - Matrix has `.H`, `.I`, and `.A` attributes (transpose, inverse, as array)
  - See http://www.scipy.org/NumPy_for_Matlab_Users for more details
- Some examples…
  - http://www.scipy.org/Tentative_NumPy_Tutorial