

Computational Environments and Toolchains

Topic 02 — Scientific Computing using Python

Lecture 03 — scipy

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Outline

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

Outline

1. SciPy

1.1	Introduction	3
1.2	Integration	7
1.3	Interpolation	20
1.4	Root Finding	30
1.5	ODEs	38
1.6	Curve Fitting	65

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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.

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Numerical Integration

We want to compute:

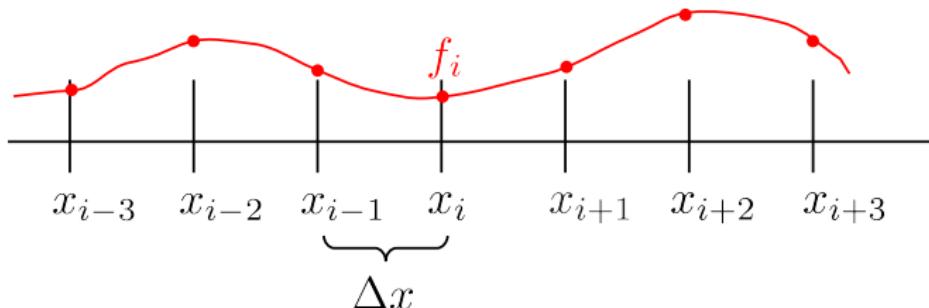
$$I = \int_a^b f(x) \, dx \quad (1)$$

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

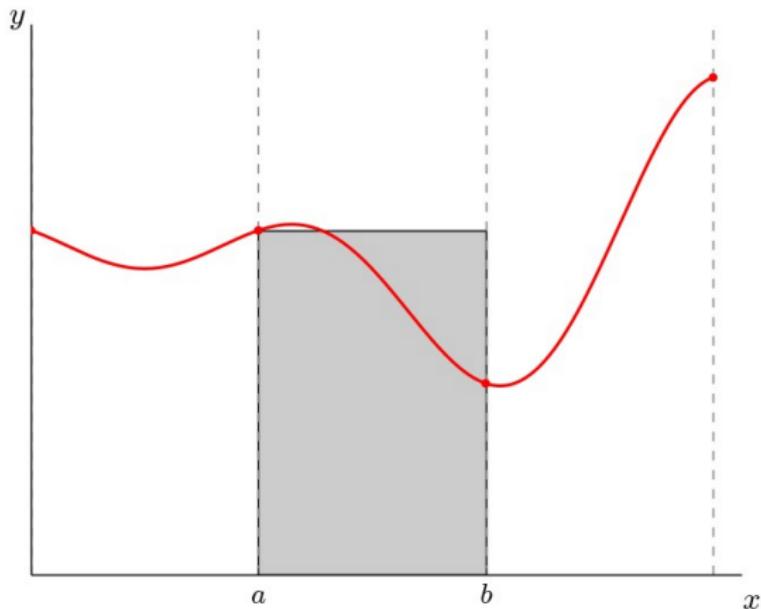
- Discretized data is represented at a finite number of locations
 - Integer subscripts are used to denote the position (index) on the grid
 - Structured/regular: spacing is constant



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

Rectangular Rule

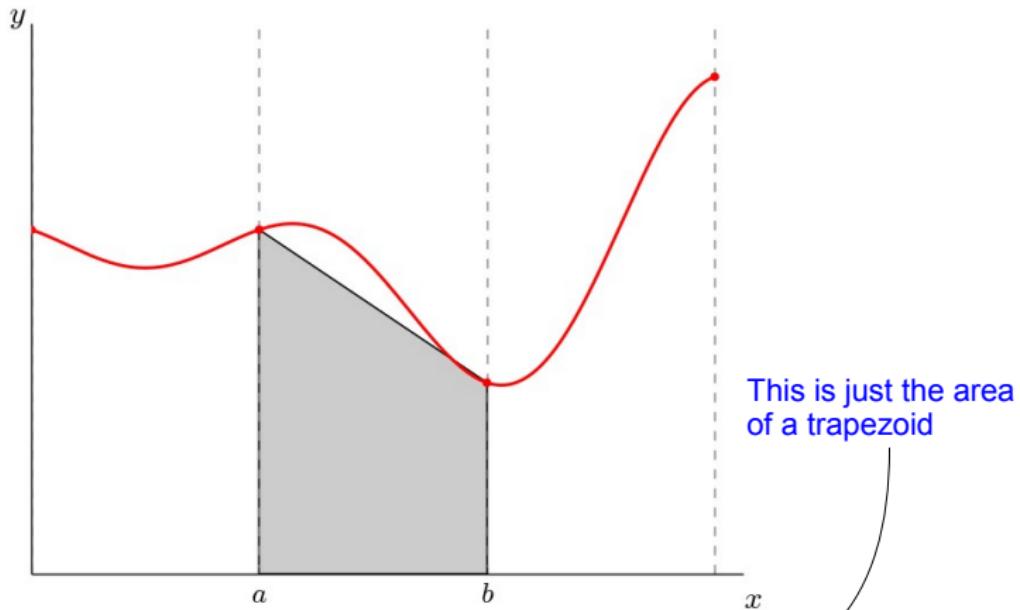
- Simplest case: piecewise constant interpolant ([rectangle rule](#))



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

Trapezoidal Rule

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



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

Simpson's Rule

- Piecewise quadratic interpolant (**Simpson's rule**)

- 3 unknowns and 3 points

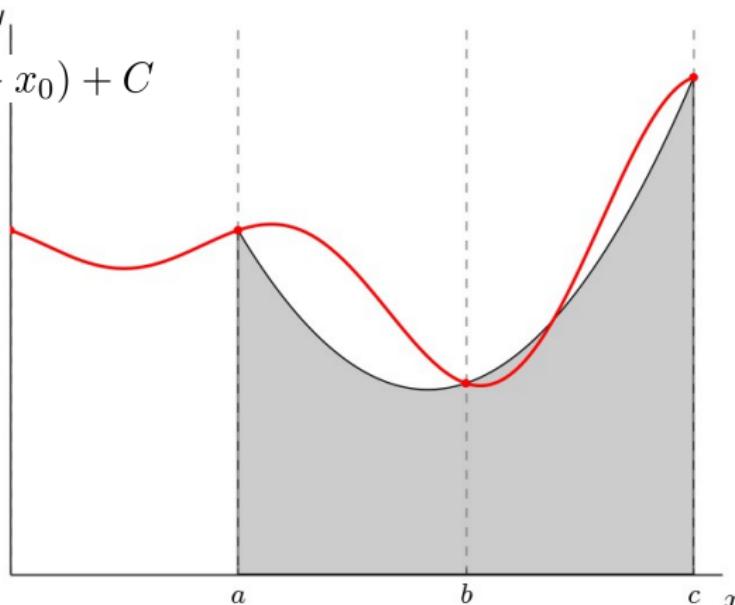
$$f(x) = A(x - x_0)^2 + B(x - x_0) + C$$

- **Solving:**

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

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

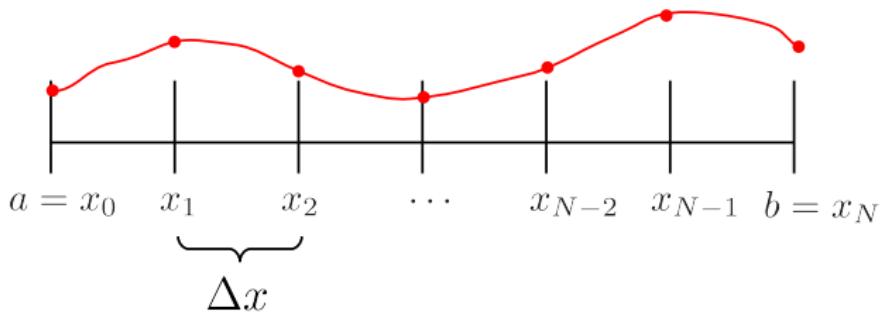
$$C = f_a$$



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

Compound Integration

- Break interval into chunks



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

Integral over a
single slab

Compound Integration

- Compound Trapezoidal

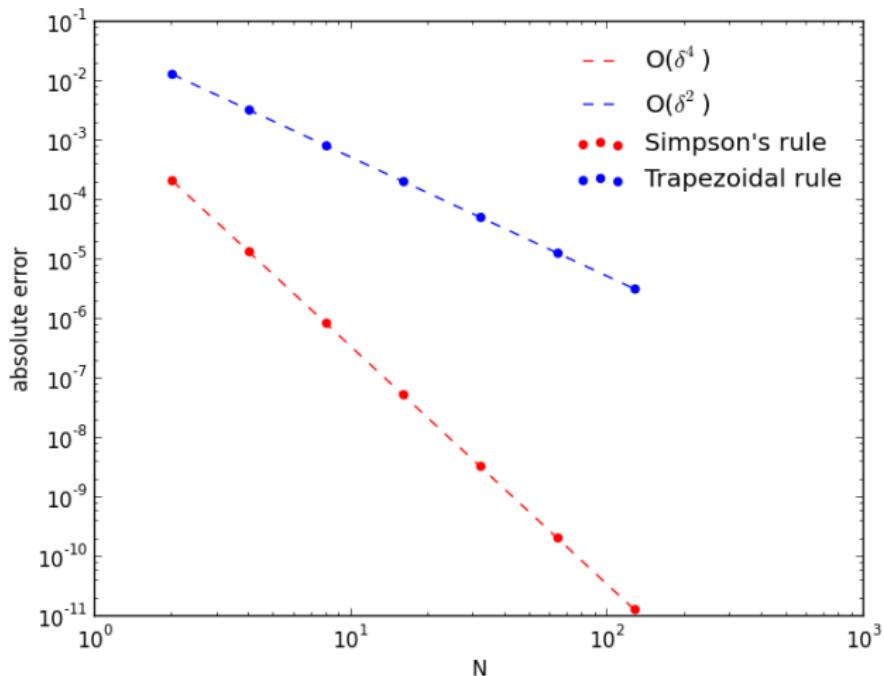
$$\int_a^b f(x)dx = \frac{\Delta x}{2} \sum_{i=0}^{N-1} (f_i + f_{i+1}) + \mathcal{O}(\Delta x^2)$$

- 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

$$\int_a^b f(x)dx \approx w_1f(x_1) + \dots w_Nf(x_N)$$

- 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

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

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

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

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
$(-1, 1)$	$(1 - x)^\alpha(1 + x)^\beta$, $\alpha, \beta > -1$	Jacobi polynomials	25.4.33 ($\beta = 0$)	Gauss–Jacobi quadrature
$(-1, 1)$	$\frac{1}{\sqrt{1 - x^2}}$	Chebyshev polynomials (first kind)	25.4.38	Chebyshev–Gauss quadrature
$[-1, 1]$	$\sqrt{1 - x^2}$	Chebyshev polynomials (second kind)	25.4.40	Chebyshev–Gauss quadrature
$[0, \infty)$	e^{-x}	Laguerre polynomials	25.4.45	Gauss–Laguerre quadrature
$[0, \infty)$	$x^\alpha e^{-x}$	Generalized Laguerre polynomials		Gauss–Laguerre quadrature
$(-\infty, \infty)$	e^{-x^2}	Hermite polynomials	25.4.46	Gauss–Hermite quadrature

(Wikipedia)

- 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:

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

```
erf(1) (exact):          0.84270079295
3-point trapezoidal:    0.825262955597 -0.017437837353
3-point Simpson's:      0.843102830043 0.000402037093266
3-point Gauss-Legendre: 0.842690018485 -1.0774465204e-05
```

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

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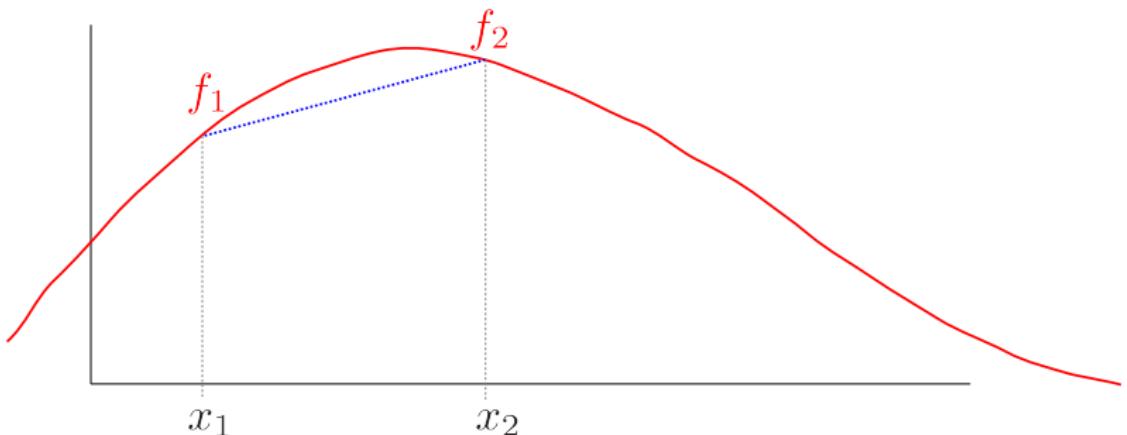
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Interpolation

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

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

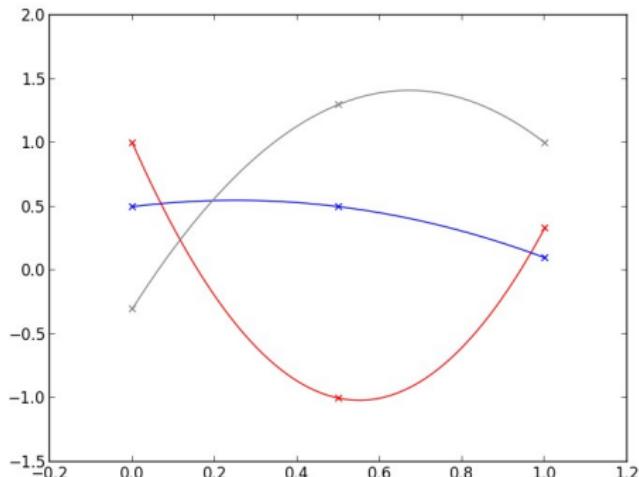
- Basis function l_i is 0 at all x_j except for x_i (where it is 1)
- Function value at x is:

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

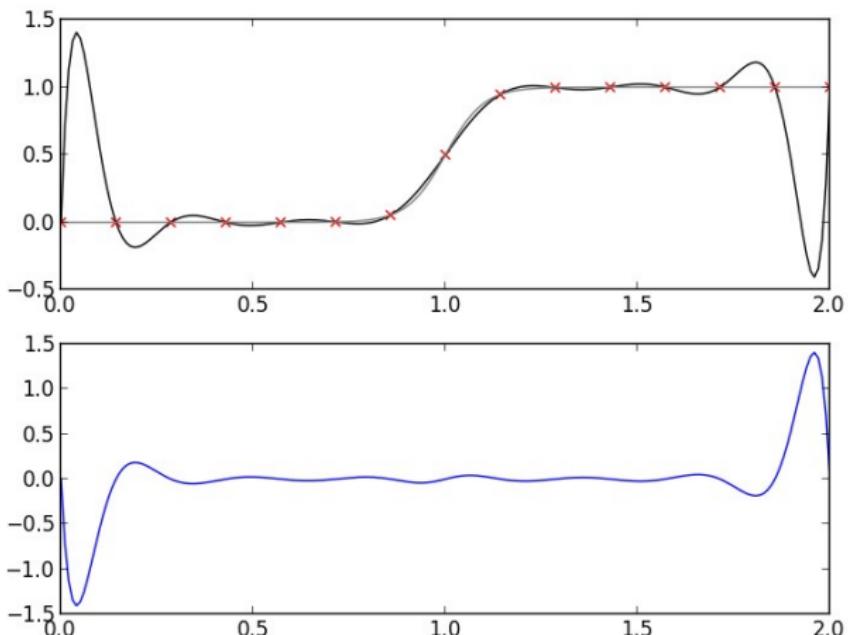
Lagrange Interpolation

- 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

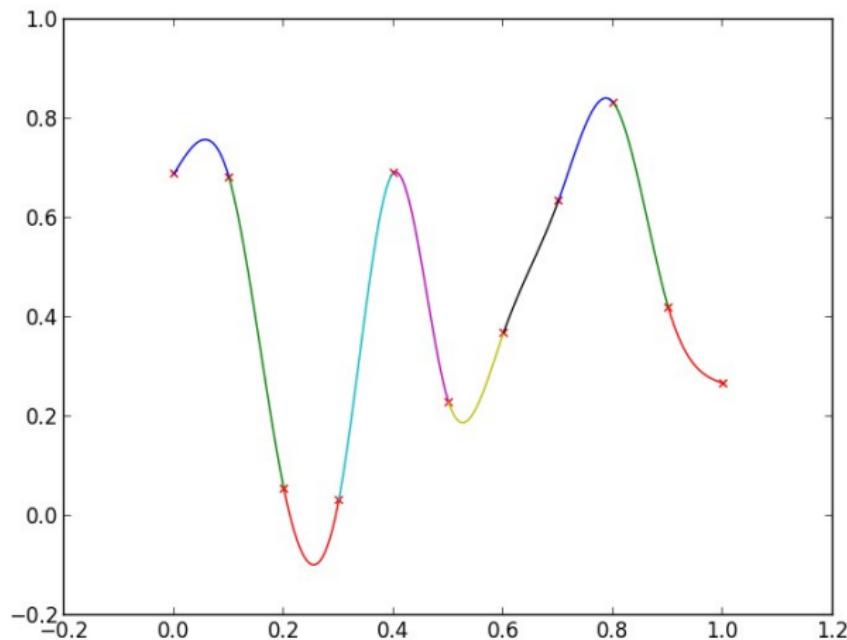


High-order is not always better: Interpolation through 15 points sampled uniformly from $\tanh()$. The error is shown below.

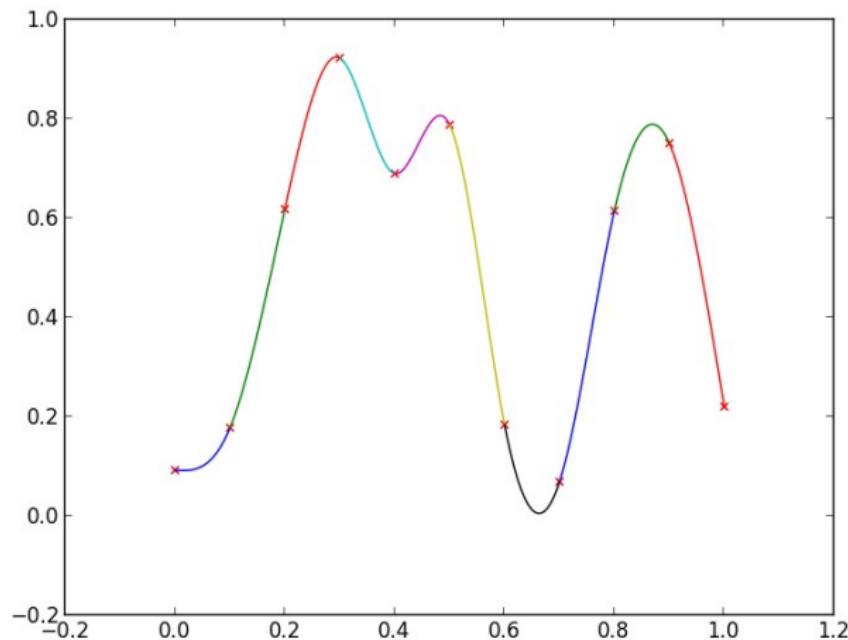
Splines

- 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

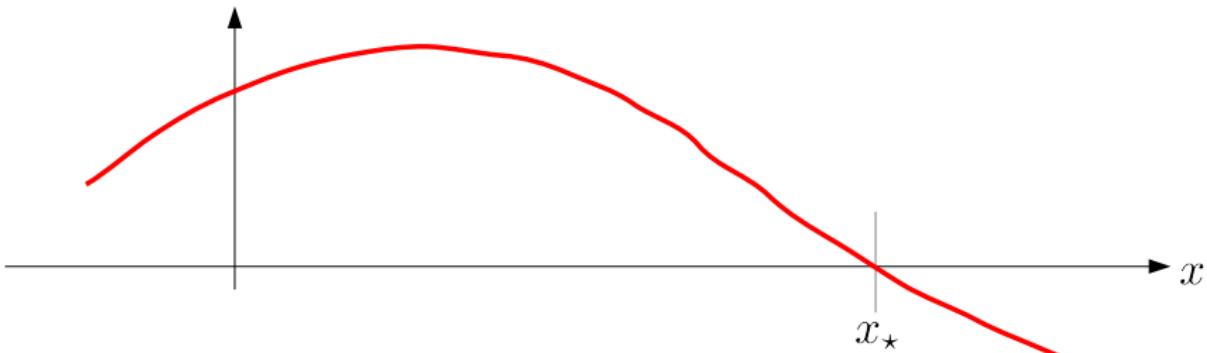
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Root Finding

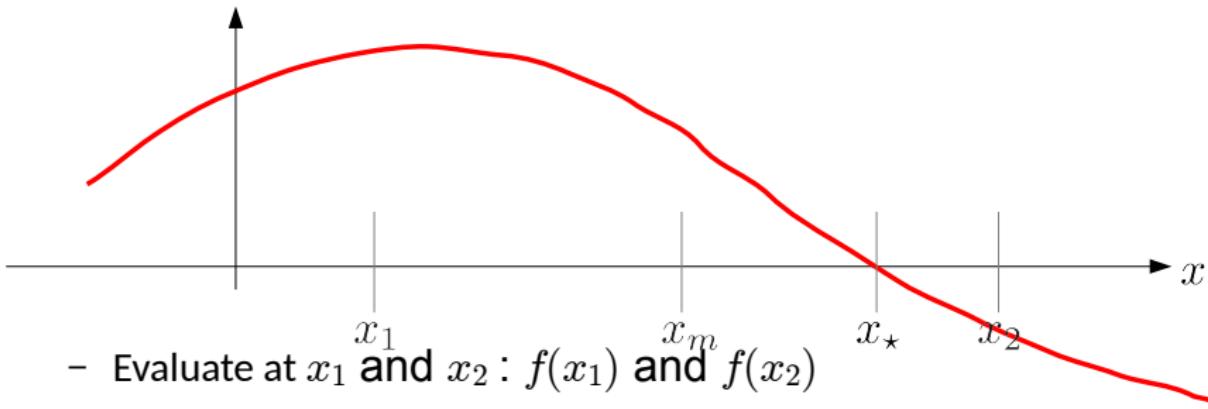
- Basic methods can be understood by looking at the function graphically



- Function $f(x)$ has a zero at x_*
- 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:

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

- 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 $< \epsilon$
- Converges fast: usually only a few iterations are needed

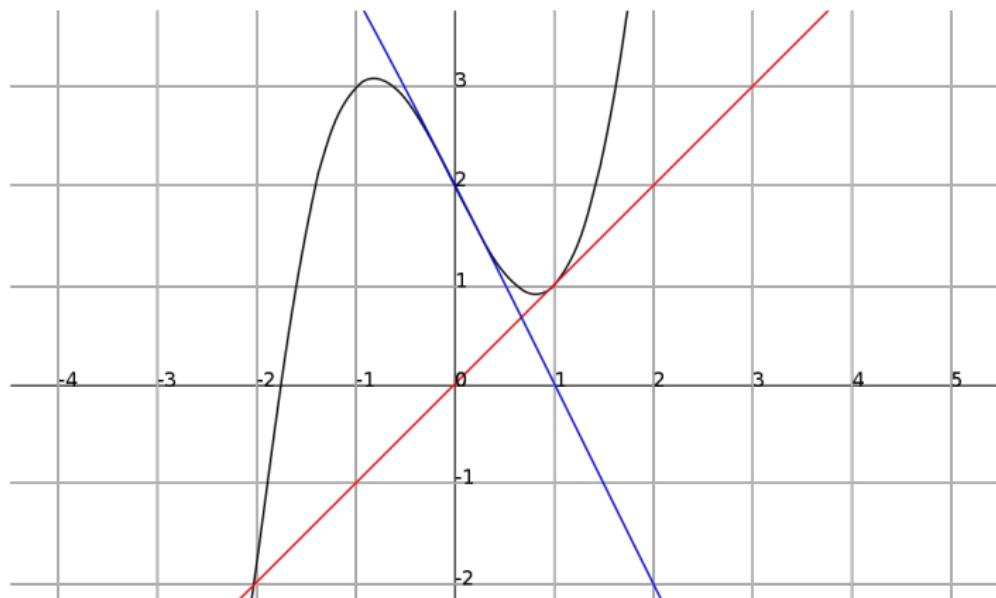
Newton-Raphson

- 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 $0 \rightarrow 1 \rightarrow 0 \rightarrow 1 \rightarrow 0 \dots$
 - 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: $\mathbf{f}(\mathbf{x})$
 - $\mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x}) \ f_2(\mathbf{x}) \ f_3(\mathbf{x}) \dots \ f_N(\mathbf{x}))^T$
 - Column vector of unknowns: $\mathbf{x} = (x_1 \ x_2 \ x_3 \dots \ x_N)^T$
- We want to find the zeros:
 - Initial guess: $\mathbf{x}^{(0)}$
 - Taylor expansion:

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



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

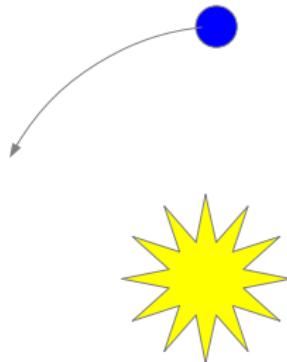
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ODEs

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



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

- 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

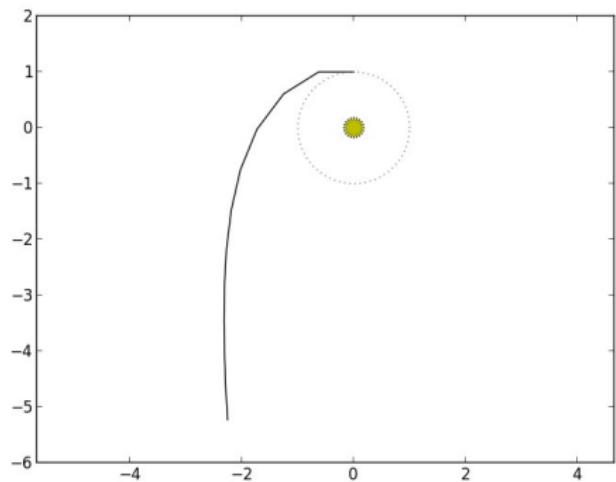
$$\mathbf{x}^{n+1} = \mathbf{x}^n + \tau \mathbf{v}^n \quad \mathbf{v}^{n+1} = \mathbf{v}^n + \tau \mathbf{a}^n$$

- Need to specify a semi-major axis and eccentricity
- Initial conditions:

– $x = 0, y = a(1 - e)$

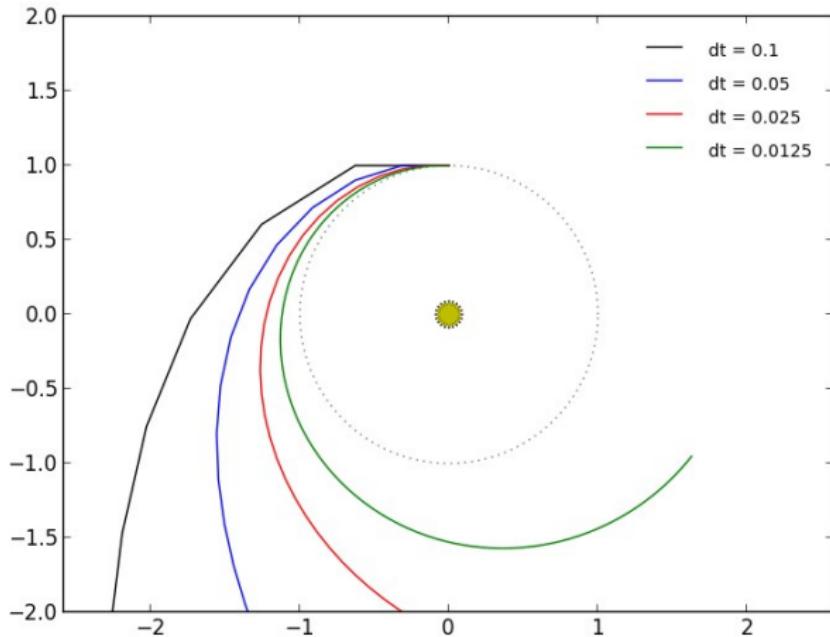
– $u = -\sqrt{\frac{GM}{a}} \frac{1+e}{1-e}, v = 0$

– 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:

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

- 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:

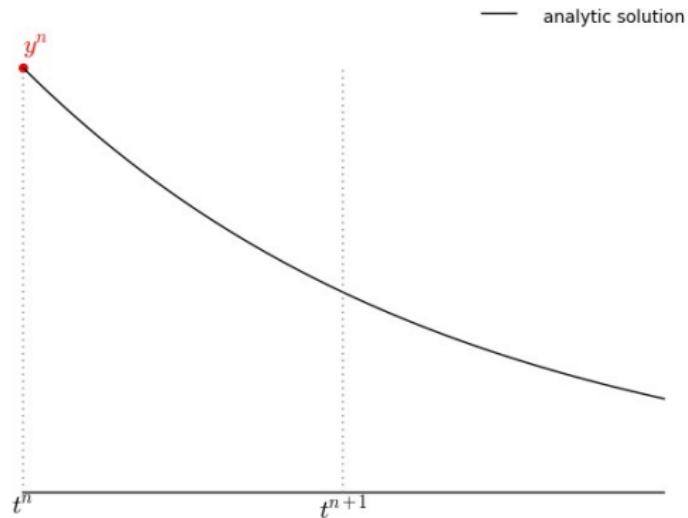
$$\mathbf{r}^* = \mathbf{r}^n + (\tau/2) \mathbf{v}^n$$

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

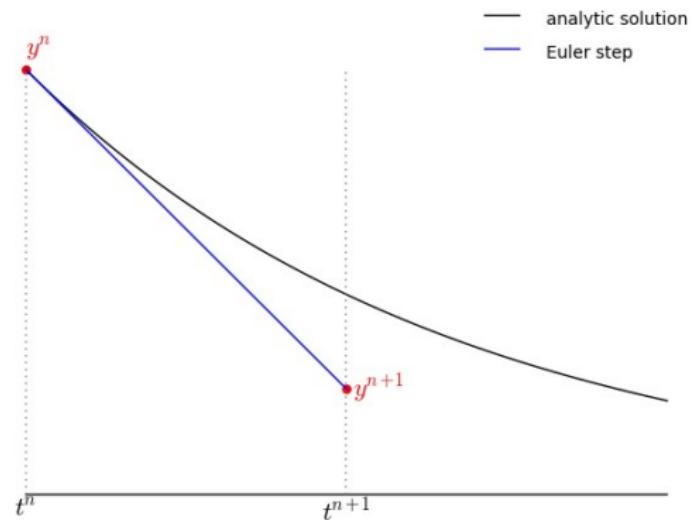
$$\mathbf{r}^{n+1} = \mathbf{r}^n + \tau \mathbf{v}^*$$

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

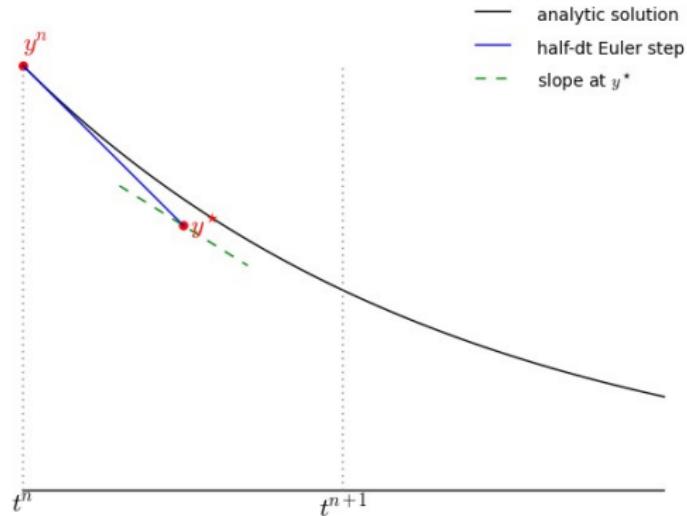
2nd Runge-Kutta Methods



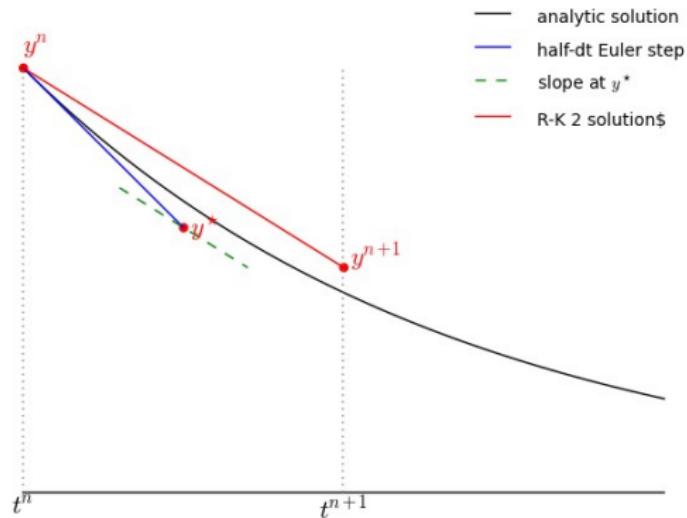
2nd Runge-Kutta Methods



2nd Runge-Kutta Methods



2nd Runge-Kutta Methods



4th Runge-Kutta Methods

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

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

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

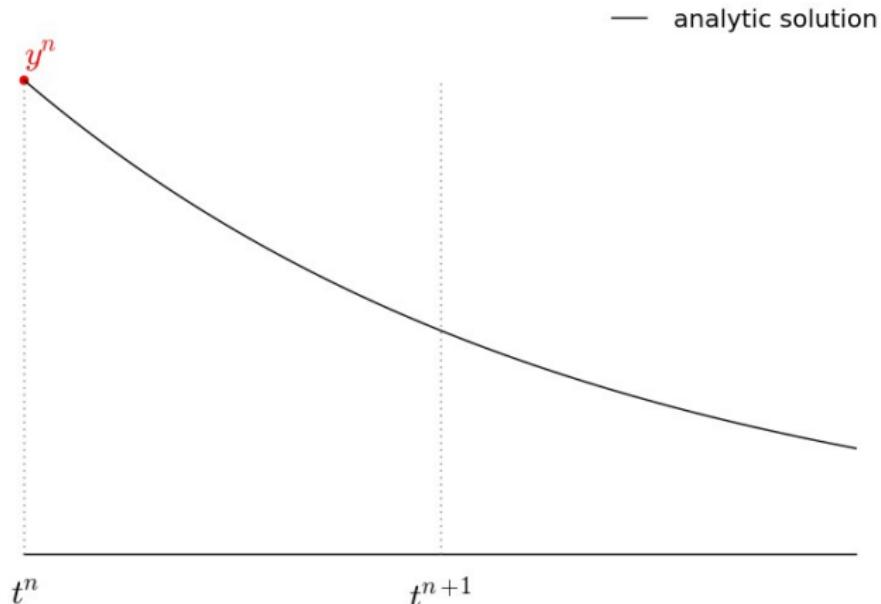
$$\mathbf{k}_2 = \mathbf{g}\left(t + \frac{\tau}{2}, \mathbf{y} + \frac{\tau}{2}\mathbf{k}_1\right)$$

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

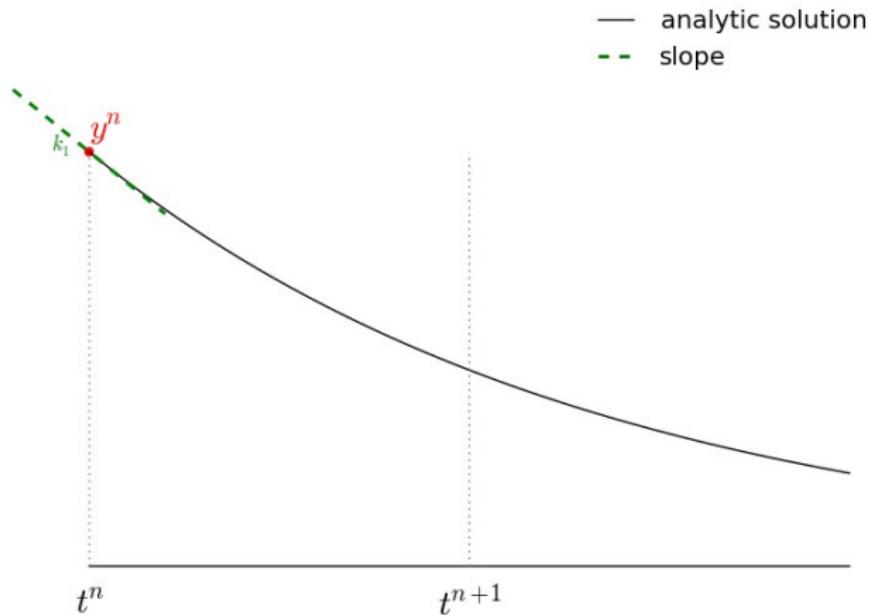
$$\mathbf{k}_4 = \mathbf{g}(t + \tau, \mathbf{y} + \tau\mathbf{k}_3)$$

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

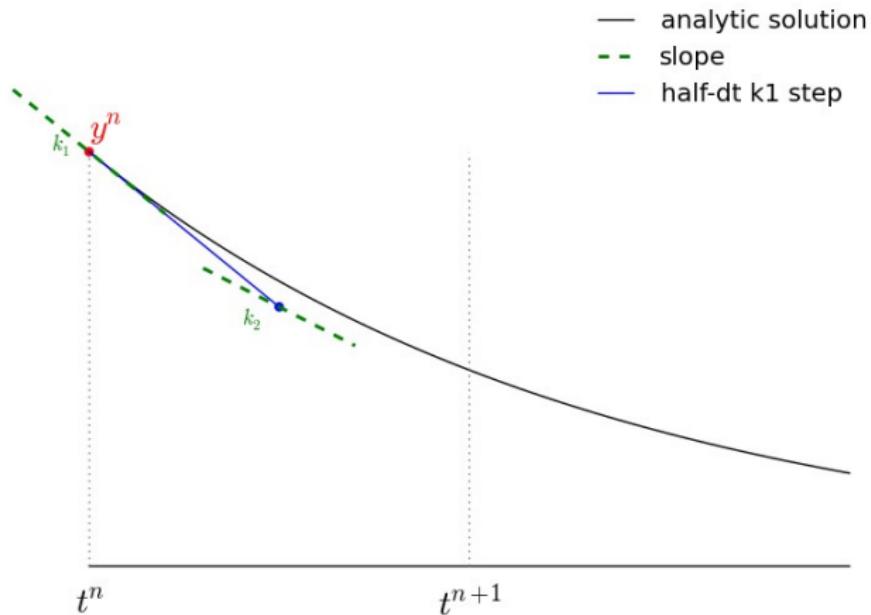
4th Runge-Kutta Methods



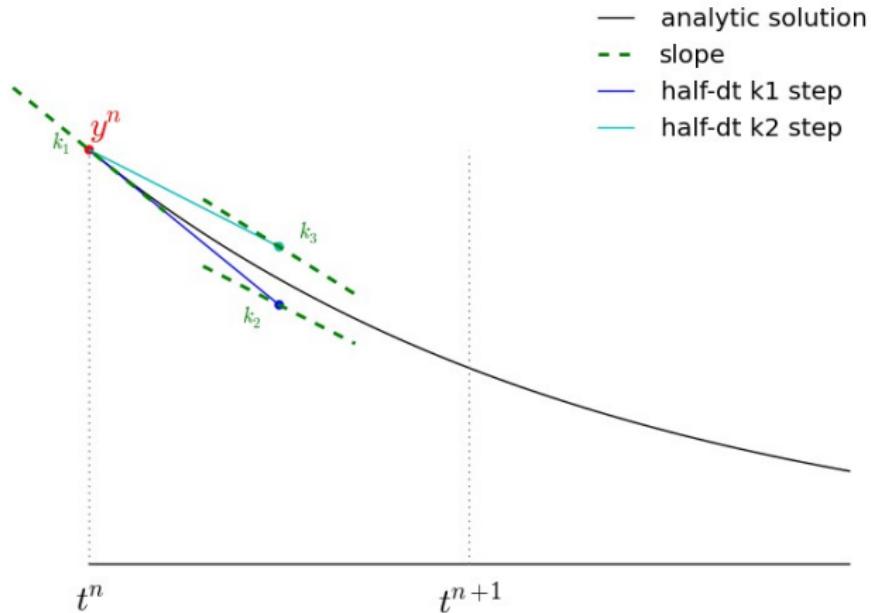
4th Runge-Kutta Methods



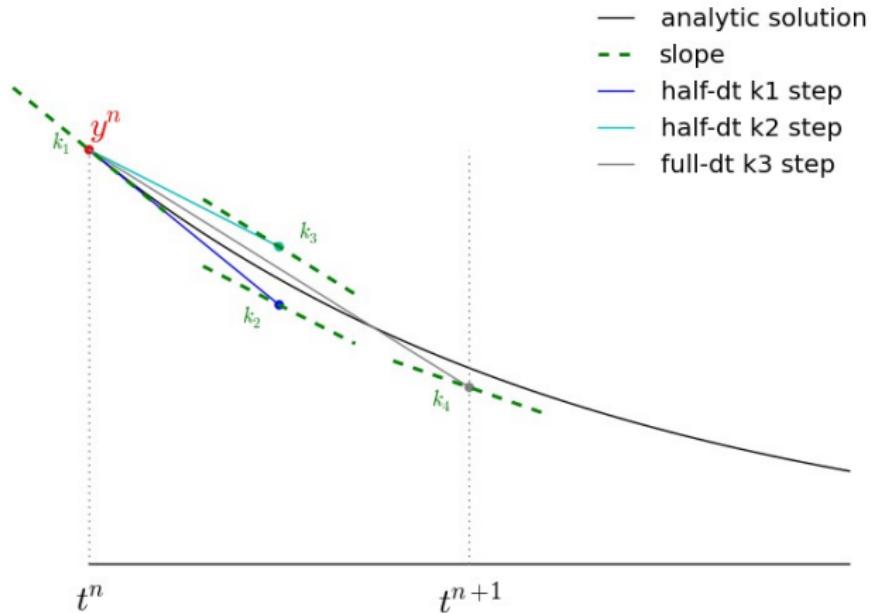
4th Runge-Kutta Methods



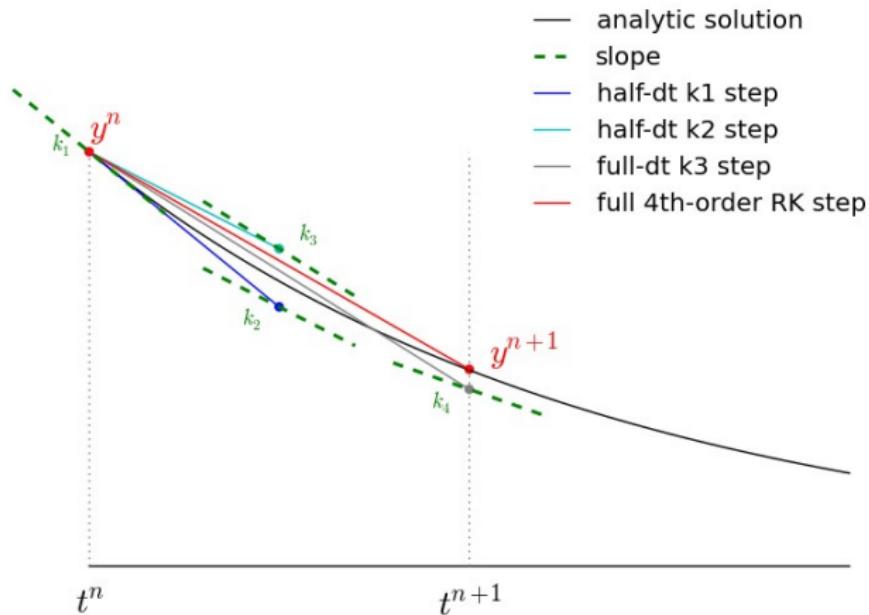
4th Runge-Kutta Methods



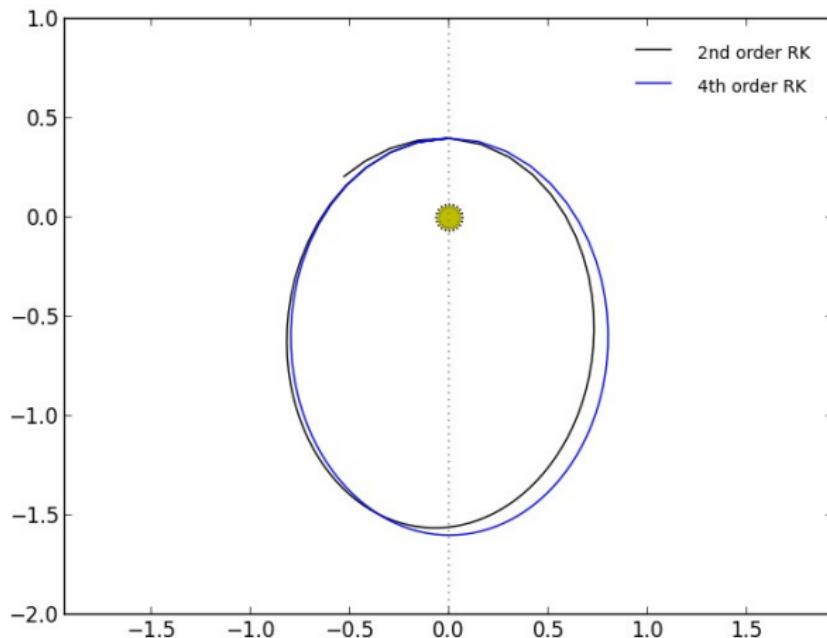
4th Runge-Kutta Methods



4th Runge-Kutta Methods

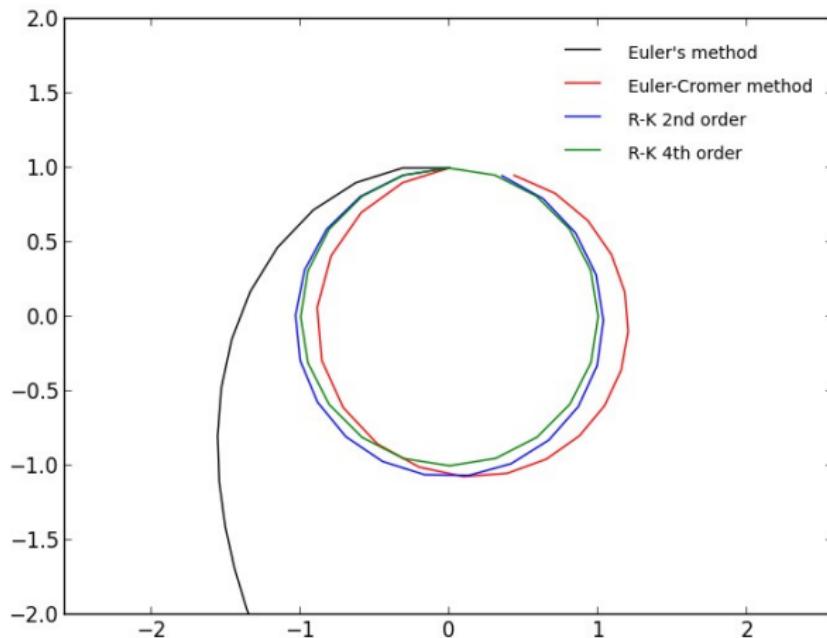


4th Runge-Kutta Methods



This looks great!

4th Runge-Kutta Methods



Even with a coarse timestep, RK4 does very well.

Adaptive Stepping

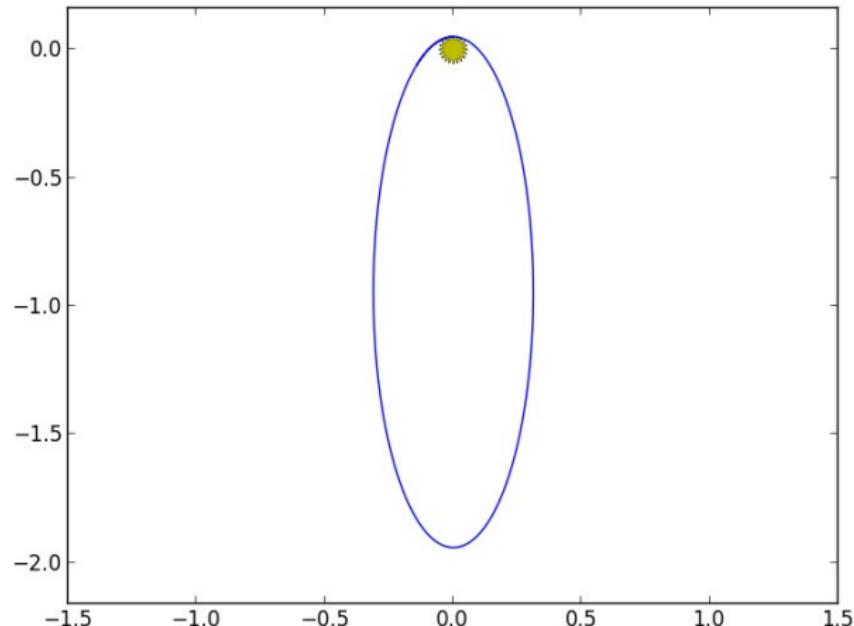
- We need a smaller timestep where the solution changes most rapidly
 - We can get away with large timesteps in regions of slow evolution
- Monitoring the error can allow us to estimate the optimal timestep to reach some desired accuracy
- Lot's of different techniques for this in the literature
 - Take 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

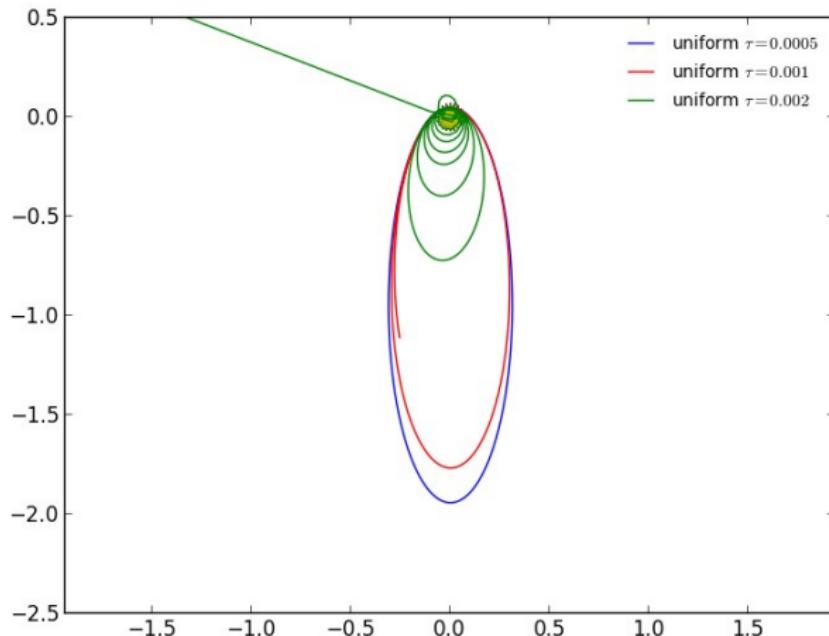
Just to get a reasonable-looking solution, we needed to use $\tau = 0.0005$

This takes 2001 steps



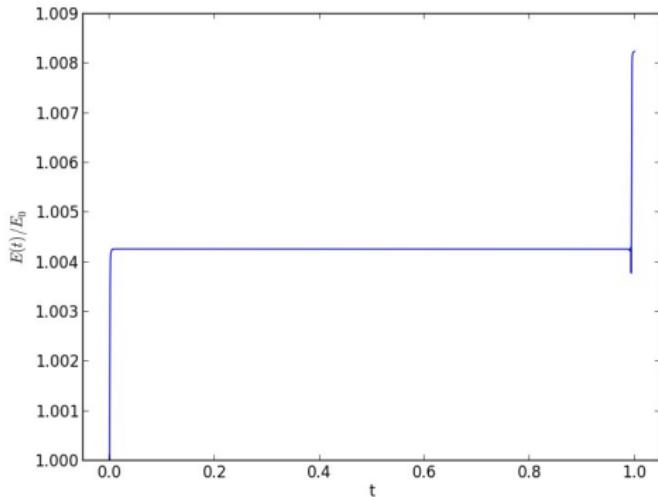
Example: Highly Elliptical Orbit

- Solutions with various uniform timesteps



Example: Highly Elliptical Orbit

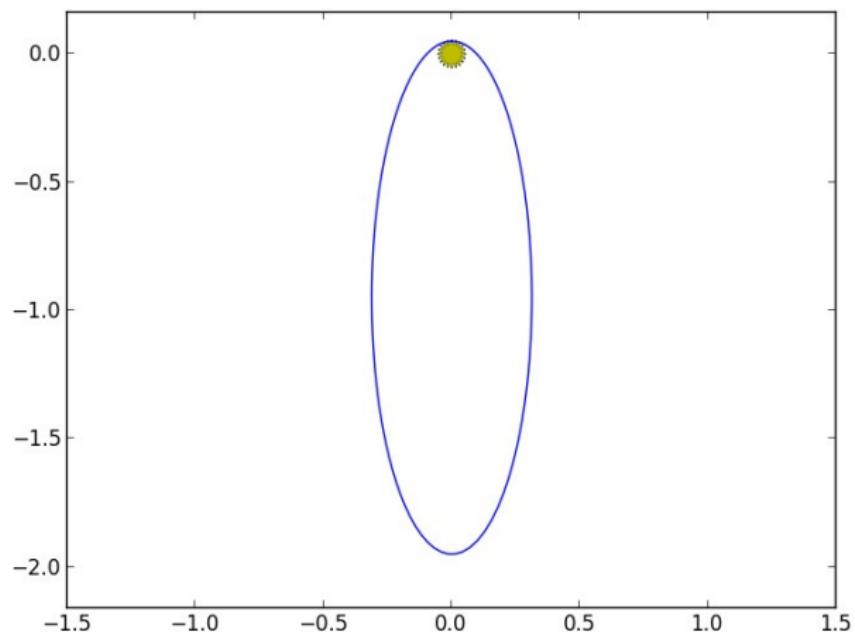
- Look at the total energy
 - At perihelion, conservation is the worse
 - Perihelion is where the velocity is greatest, and therefore the solution changes the fastest
- We can take a larger timestep at aphelion than perihelion



Example: Highly Elliptical Orbit

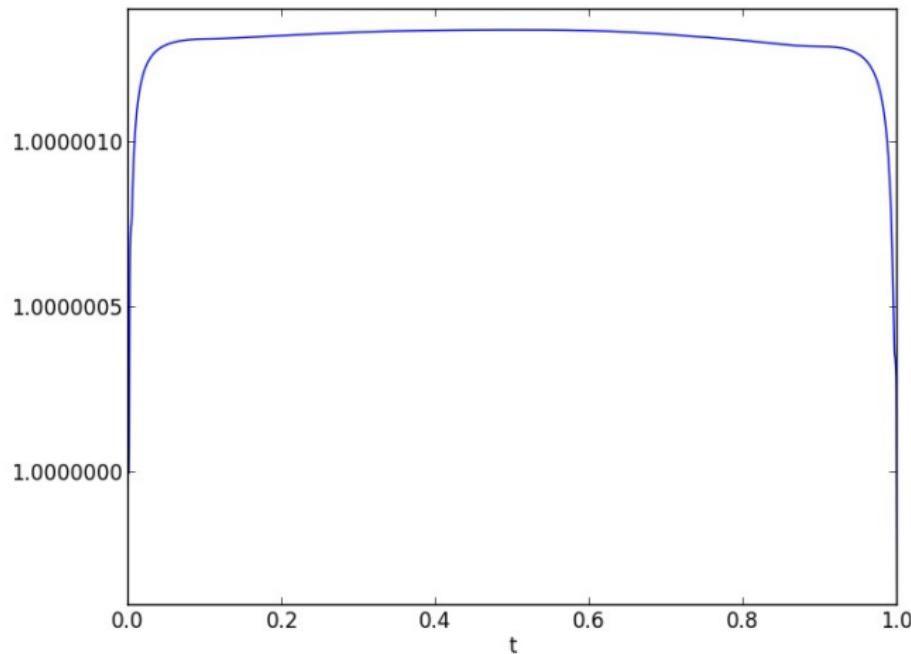
- Adaptive stepping, asking for $\epsilon = 10^{-7}$, with initial timestep the same as the non-adaptive case ($\tau = 0.005$)

This takes only 215 steps



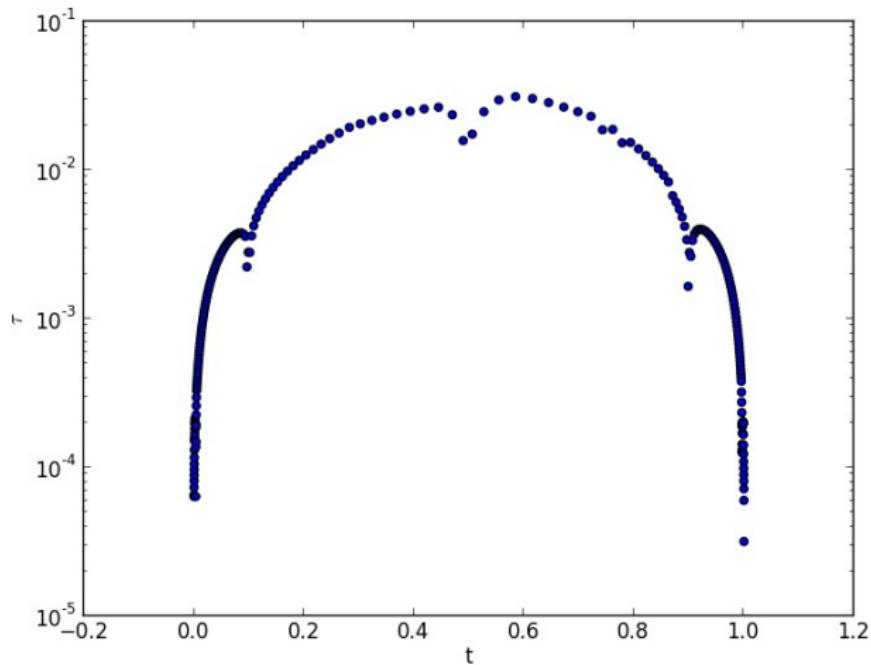
Adaptive Stepping

- 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

1. SciPy

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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:

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

- Define:

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

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

- 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 Y s may be nonlinear but we are still linear in the a s
- 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:

$$\text{Var}(a_1 + a_2 x_i - y_i) = \text{Var}(a_2 x_i - y_i)$$

$$= a_2^2 \text{Var}(x_i) + \text{Var}(y_i) = a_2^2 \sigma_{x,i}^2 + \sigma_{y,i}^2$$

(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:

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

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

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