MAS212 Scientific Computing and Simulation

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Today's lecture

- Scientific computing modules:
  - `numpy`
  - `matplotlib`
  - `scipy`
- Basic plotting
- Example #0: Lissajous curves
- Example #1: Monte Carlo integration
- Example #2: The logistic map
- Example #3: Quadratic maps and fractals

matplotlib

- `matplotlib` is a 2D plotting library for Python
- Home page: `http://matplotlib.org/`
- `matplotlib.pyplot` is a collection of command-style functions that make matplotlib work like MATLAB
- Tutorial: `http://matplotlib.org/users/pyplot_tutorial.html`

Plotting

Convention:

Import `pyplot` as follows:

```
>>> import matplotlib.pyplot as plt
```

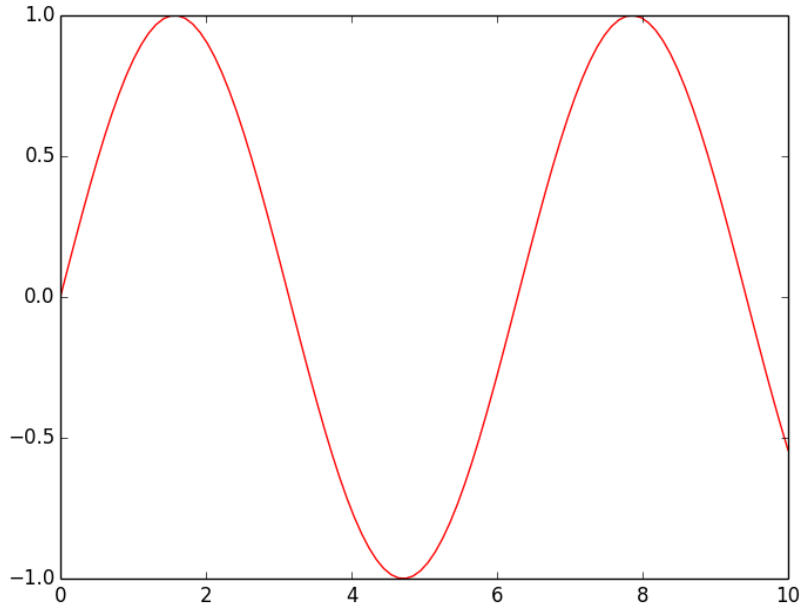
Jupyter Notebook

To include plots in your Jupyter Notebook, use:

```
%matplotlib inline
```

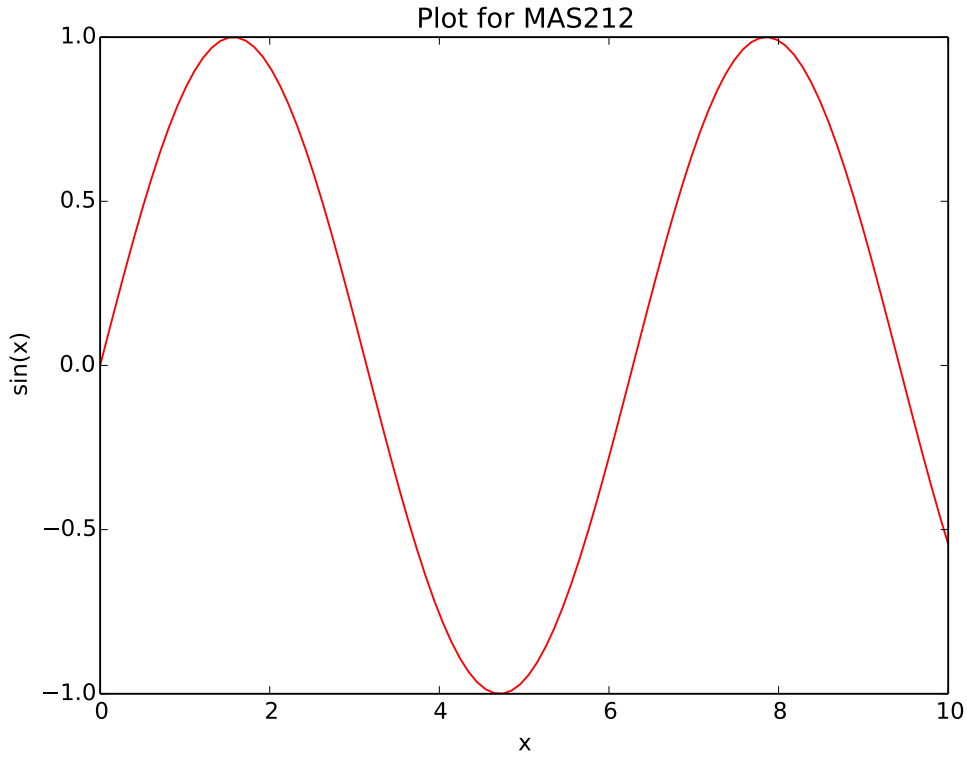
Plotting: Simple Example

```
>>> import numpy as np
>>> import matplotlib.pyplot as plt
>>> xs = np.linspace(0.0, 10.0, 100)  # 100 points
>>> ys = np.sin(xs)
>>> plt.plot(xs, ys, 'r-')  # red line
>>> plt.savefig('sin.png')  # save to file
>>> plt.show()
```



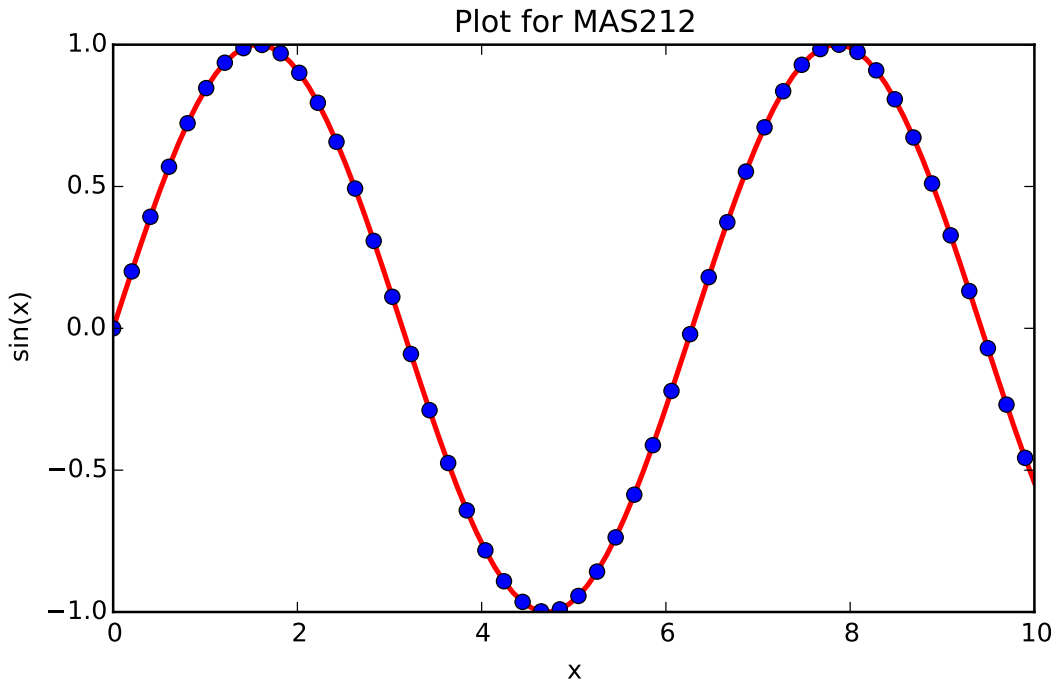
Plotting: Axis Labels

```
>>> plt.xlabel("x")
>>> plt.ylabel("sin(x)")
>>> plt.title("Plot for MAS212")
```



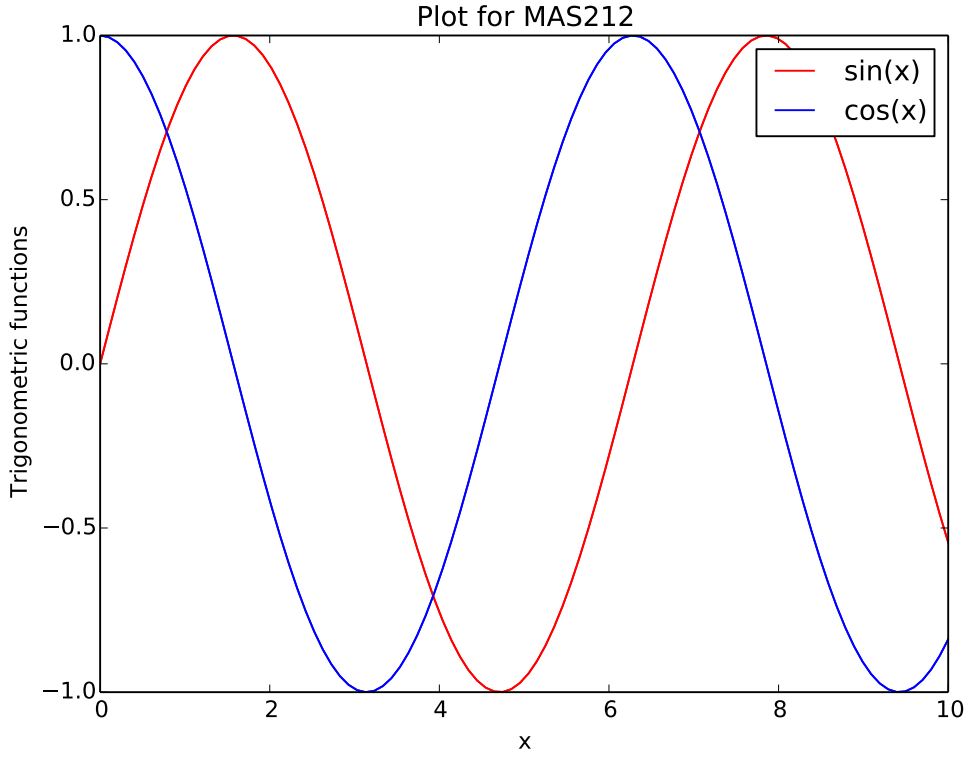
Plotting: Thicker lines. Points.

```
>>> plt.plot(xs, ys, 'r-', linewidth=2.0)  #  thicker red line
>>> plt.plot(xs[::2], ys[::2], 'bo')
# plot every other point as a blue filled circle
```

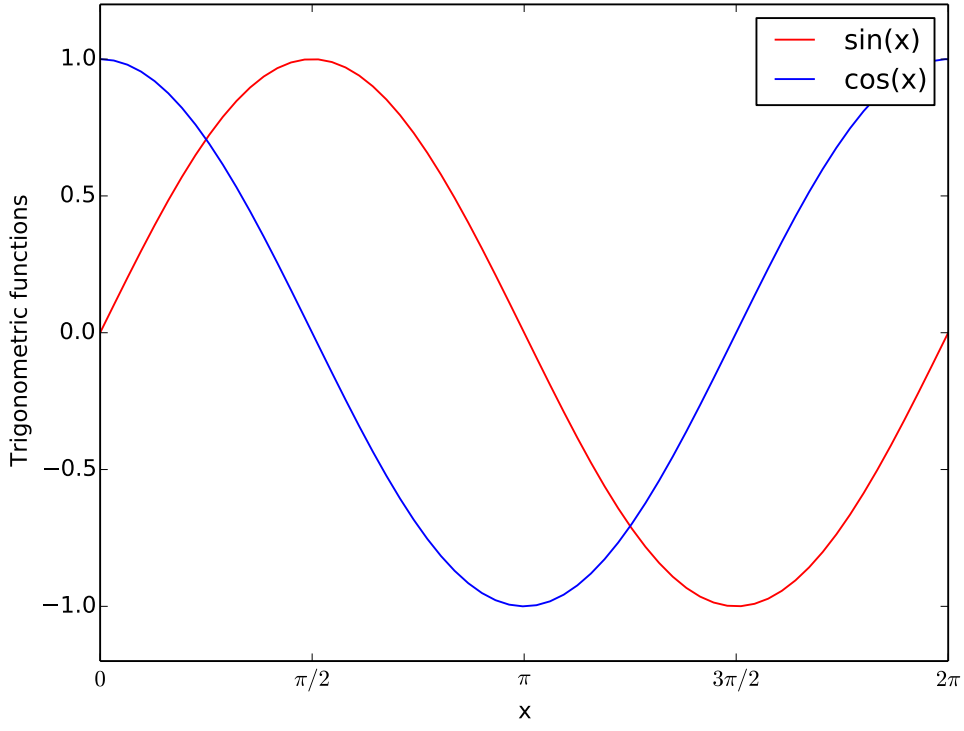


Plotting: Add a legend

```
>>> plt.plot(xs, np.sin(xs), 'r-', label="sin(x)")  # red line
>>> plt.plot(xs, np.cos(xs), 'b-', label="cos(x)")  # blue line
>>> plt.ylabel("Trigonometric functions")
>>> plt.legend()  # add a legend to the plot
```



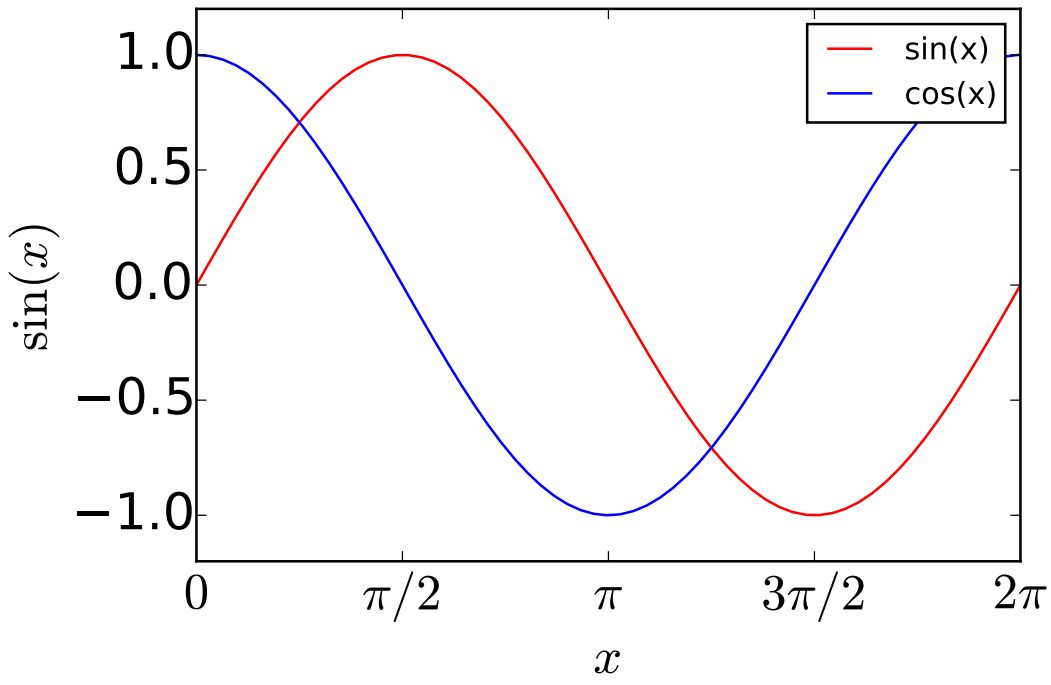
```
>>> plt.axis([0, 2.0*np.pi, -1.2, 1.2])
>>> # now set the ticks and labels on the x-axis.
>>> xtics = [0, np.pi/2.0, np.pi, 3*np.pi/2.0, 2*np.pi]
>>> xlabels = ['$0$', '$\pi/2$', '$\pi$', '$3\pi/2$', '$2\pi$']
>>> plt.xticks(xtics, xlabels)
```



How to improve readability?

1. Enlarge text elements using `fontsize` optional argument:

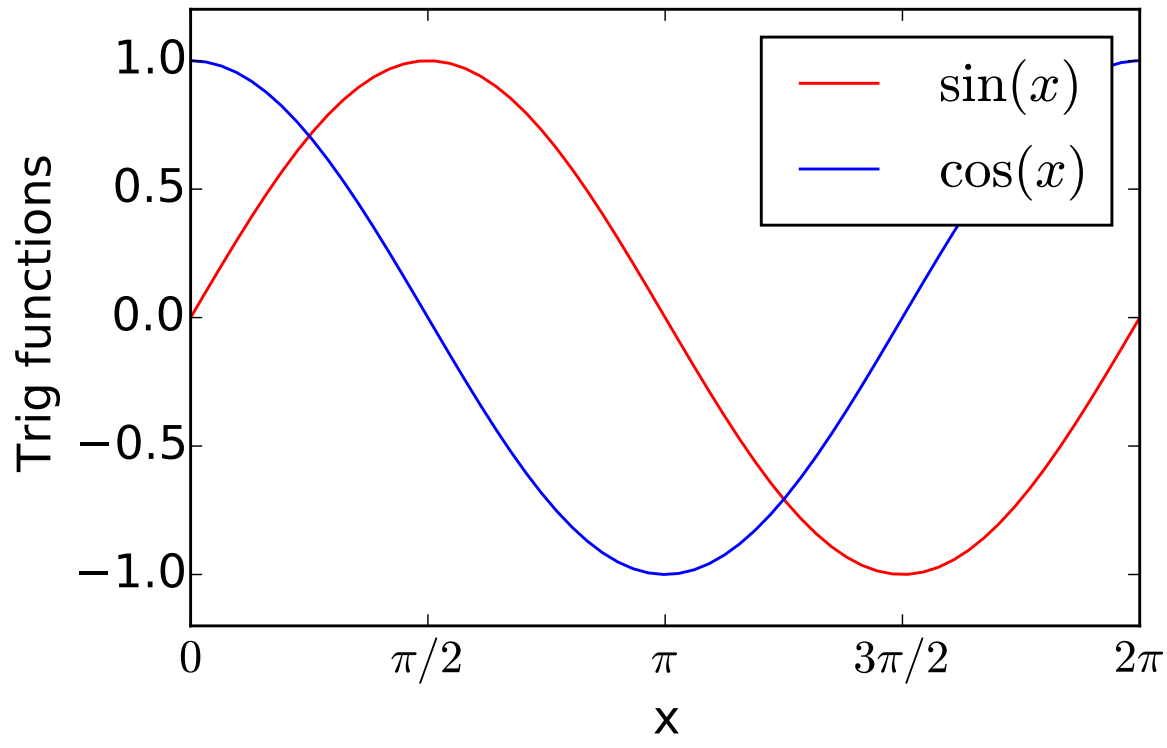
```
>>> plt.xticks(fontsize=20)
>>> plt.yticks(fontsize=20)
>>> plt.xlabel("$x$", fontsize=20)
>>> plt.ylabel("$\sin(x)$", fontsize=20)
```



How to improve readability?

2. Or: change default font size:

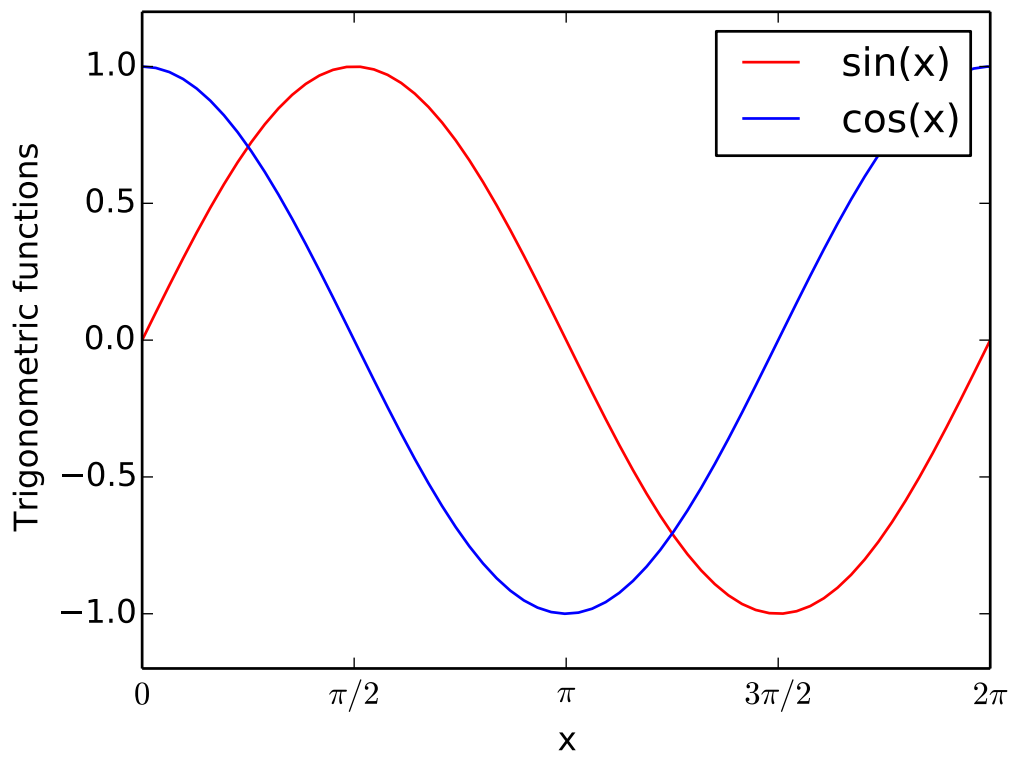
```
>>> plt.rcParams.update({'font.size': 16})
```



How to improve readability?

3. Or: Make all labels and lines bigger by making the plot smaller!

```
>>> F = plt.gcf()   # get current figure
>>> size = F.get_size_inches()
>>> fac = 0.7
>>> F.set_size_inches(size[0]*fac, size[1]*fac)
```



Example #0: Lissajous curves

- A Lissajous curve is the graph of a system of parametric equations:

$$x = A\sin(at + \delta), \quad y = B\sin(bt)$$

  where a, b, A, B, δ are constants and t is the parametric variable

- The appearance depends chiefly on the ratio a/b
  - $a/b = 1 \quad \Rightarrow$ ellipses, circles, lines
  - $a/b = 2, \delta = \pi/4 \quad \Rightarrow$ parabola
  - $a/b \in \mathbb{Q} \quad \Rightarrow$ closed curve

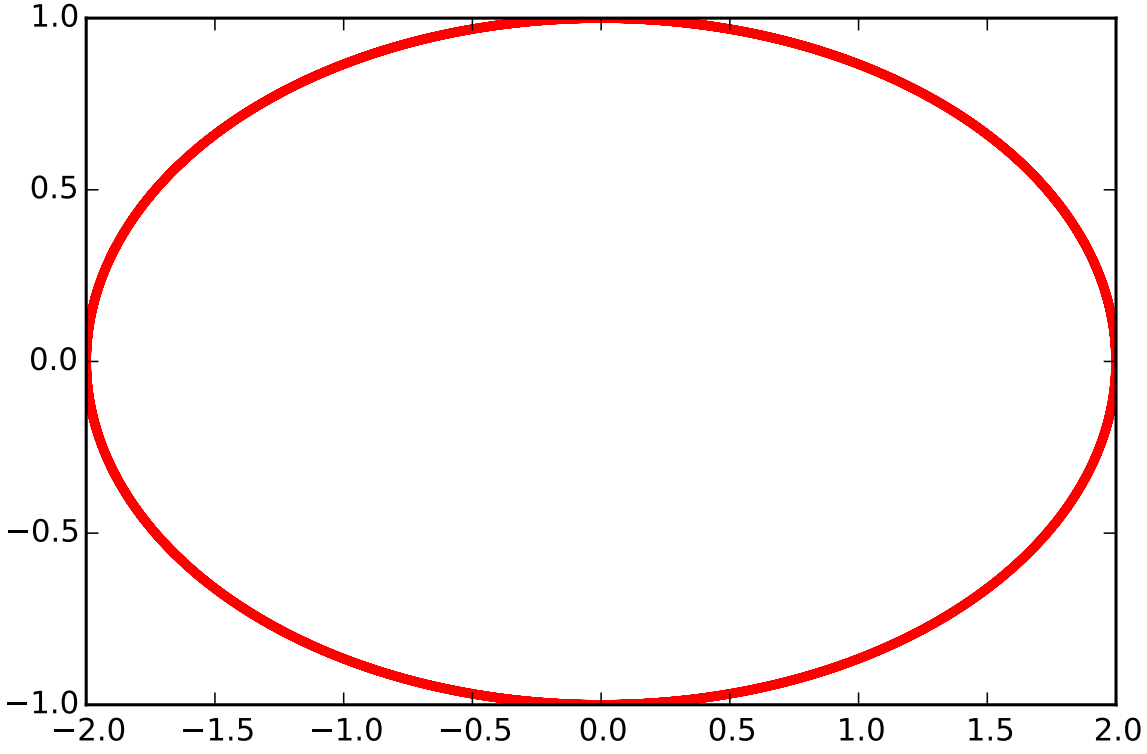
- If a/b is irrational, the curve does not close.

Example #0: Lissajous curves

```
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline

def plot_lissajous(b=1, a=1, A=2, B=1, d=np.pi/2):
    ts = np.linspace(0,30,600)
    plt.plot(A*np.sin(a*ts+d), B*np.sin(b*ts), 'r-', linewidth=3)
```

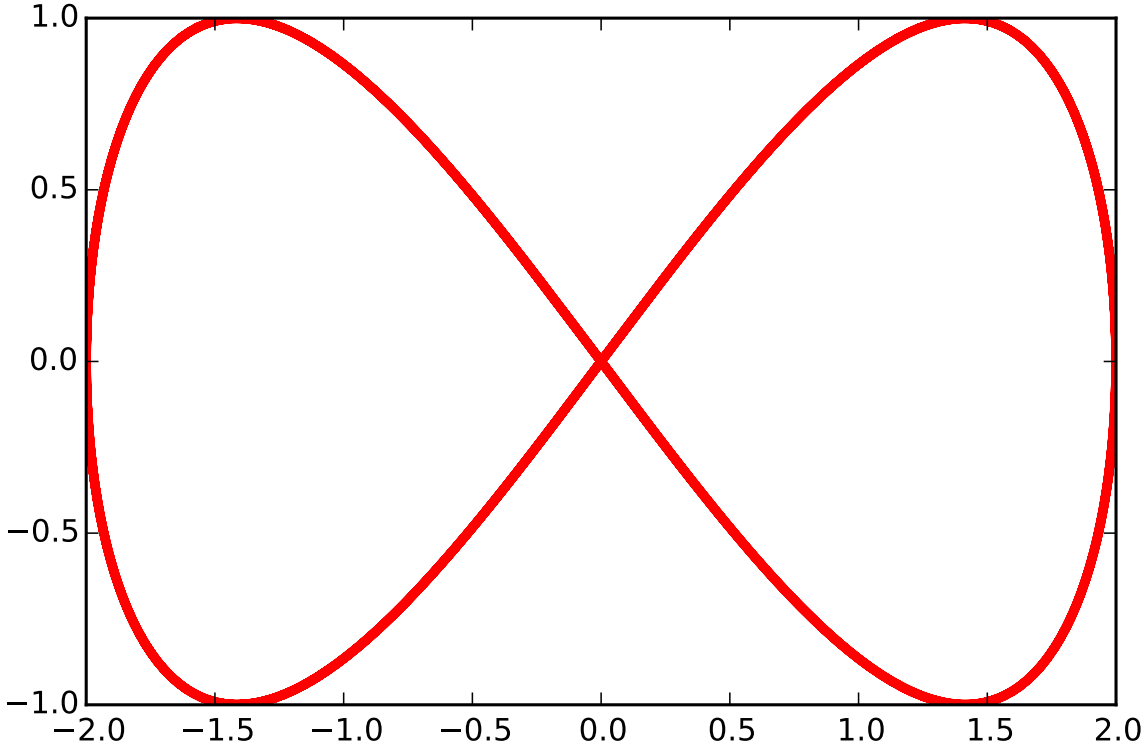
Example #0: Lissajous curves

```
plot_lissajous(b=1)
```



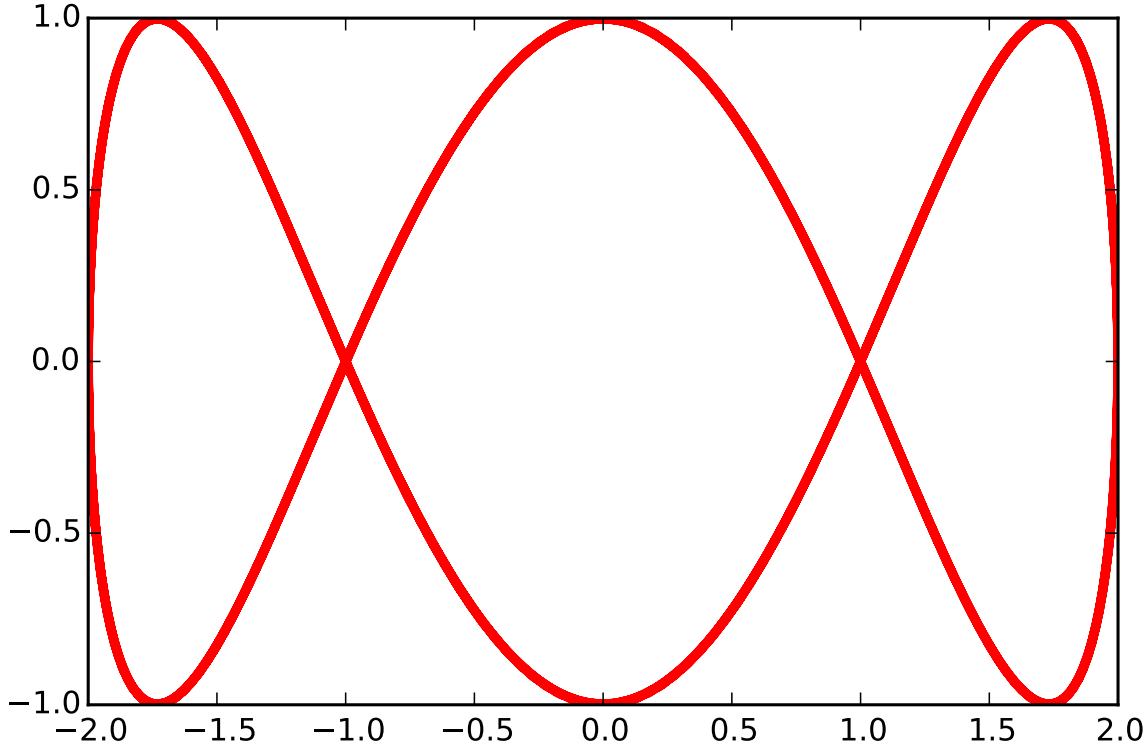
Example #0: Lissajous curves

```
plot_lissajous(b=2)
```



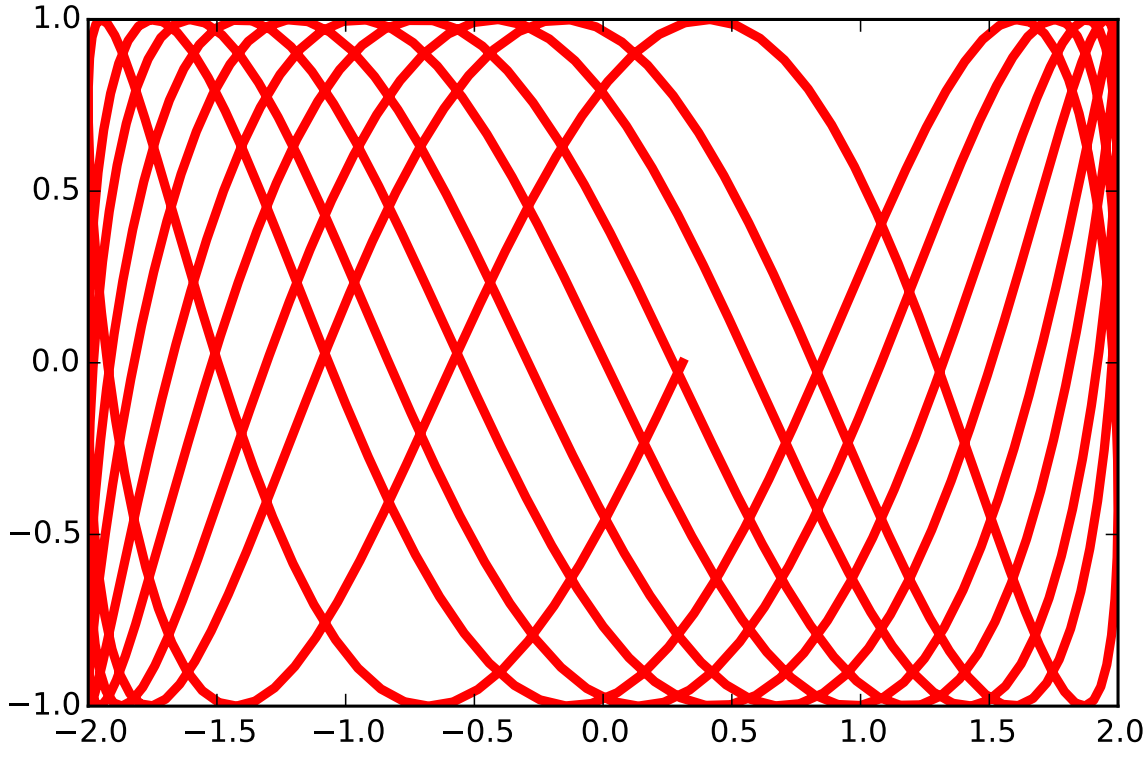
Example #0: Lissajous curves

```
plot_lissajous(b=3)
```



Example #0: Lissajous curves

```
plot_lissajous(b=np.pi)
```



- $b = \pi$ is **irrational** $\Rightarrow$ curve does not close.

Figures and subplots

- Plots are contained within a `Figure` object.
- Create a new figure with

```
fig = plt.figure()
```

- To add a new subplot to a figure:

```
ax1 = fig.add_subplot(2,2,1)
```

(This will add the first subplot to a 2×2 array of subplots).

- `ax1` is an `AxesSubplot` object
- `plot` function belongs to `AxesSubplot` object rather than `Figure`

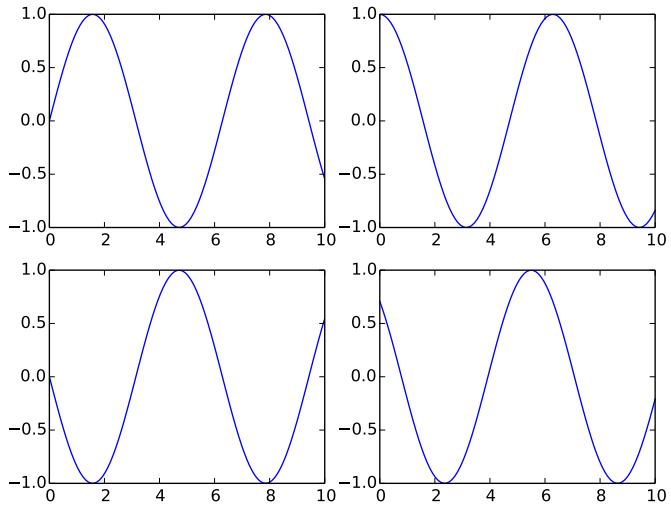
Figures and subplots

- Useful functions:

`plt.gcf()`	Get current figure
`plt.gca()`	Get current axes
`plt.clf()`	Clear figure
`plt.cla()`	Clear axes
`plt.close()`	Close plotting window

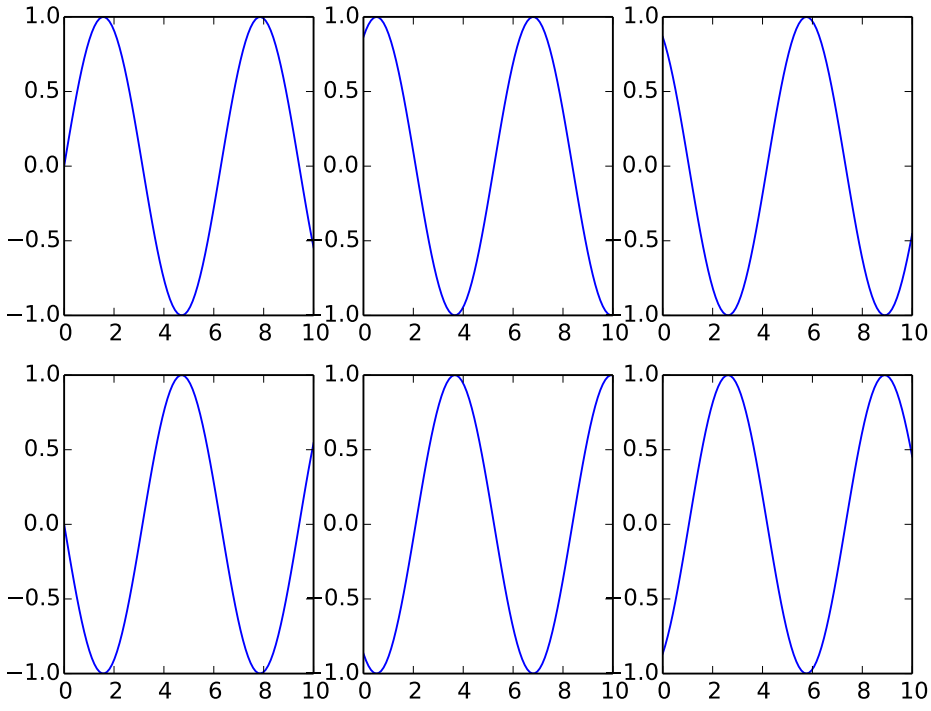
Multiple plots: method #1

```
>>> xs = np.linspace(0,10,100)
>>> f = plt.figure()
>>> ax = f.add_subplot(2,2,1)
>>> ax.plot(xs, np.sin(xs))
>>> ax = f.add_subplot(2,2,2)
>>> ax.plot(xs, np.sin(xs+np.pi/2.0))
>>> ax = f.add_subplot(2,2,3)
>>> ax.plot(xs, np.sin(xs+np.pi))
>>> ax = f.add_subplot(2,2,4)
>>> ax.plot(xs, np.sin(xs+3.0*np.pi/4.0))
```



Multiple plots: method #2

```
>>> fig, axes = plt.subplots(2,3)  # create 2 x 3 array of subplots
>>> axs = axes.flatten() # turn into 1D array.
>>> for i in range(len(axes)):
...     axs[i].plot(xs, np.sin(xs + 2.0*np.pi*i/len(axes)))
...
```



Multiple plots: method #2

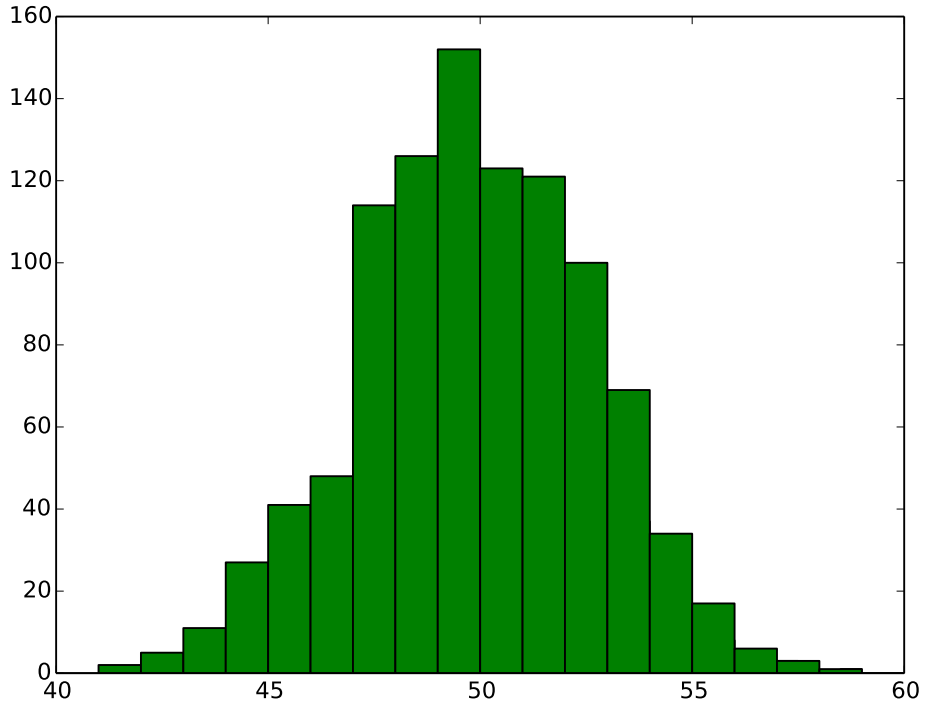
- I prefer method #2

```
>>> fig, axes = plt.subplots(2,3)
```

- This line returns a reference to the `Figure`, and to a 2×3 array of `AxesSubplot` objects
- Now refer to subplots by position in array, e.g. `axes[0,1]`.
- In the example above I looped over the array to quickly generate the subplots

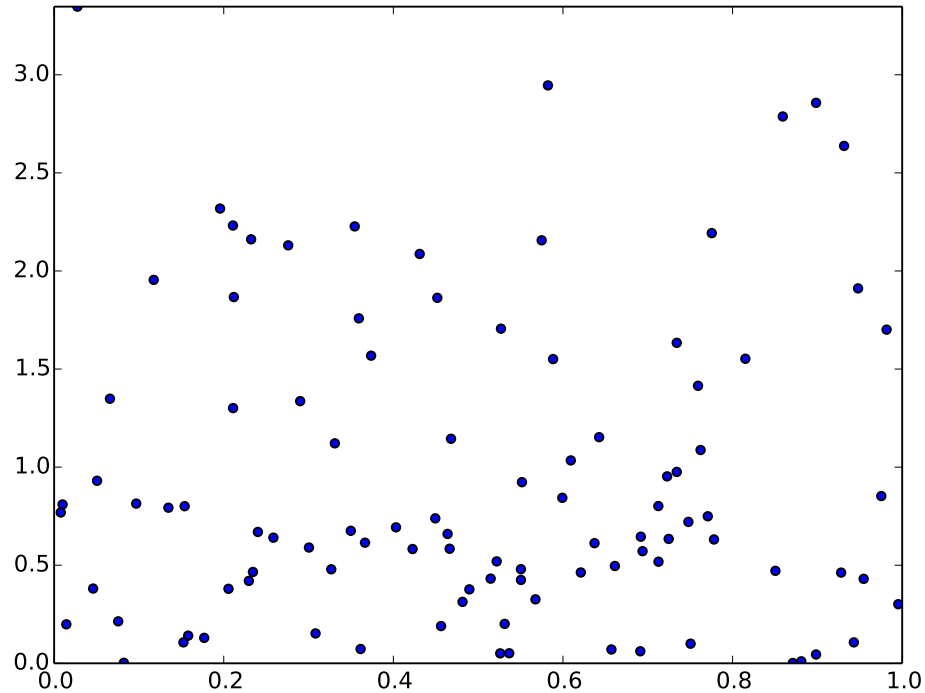
Histograms

```
>>> samplesize = 100
>>> Npts = 1000
>>> data = [sum(np.random.rand(samplesize)) for k in range(Npts)]
>>> plt.hist(np.array(data), bins=20, range=(40,60))
```



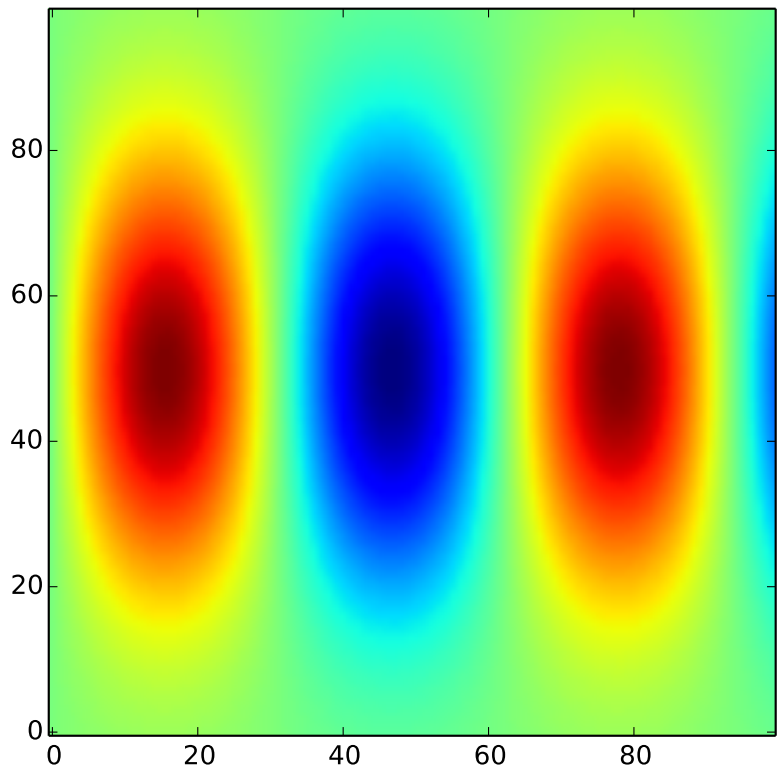
Scatter plots

```
>>> N = 100     # number of points
>>> xs = np.random.rand(N)     # uniform distribution [0,1]
>>> ys = -np.log(np.random.rand(N))  # Exponential distribution
>>> plt.axis([0,1,0,max(ys)])
[0, 1, 0, 3.347347821170366 4]
>>> plt.scatter(xs, ys)
```



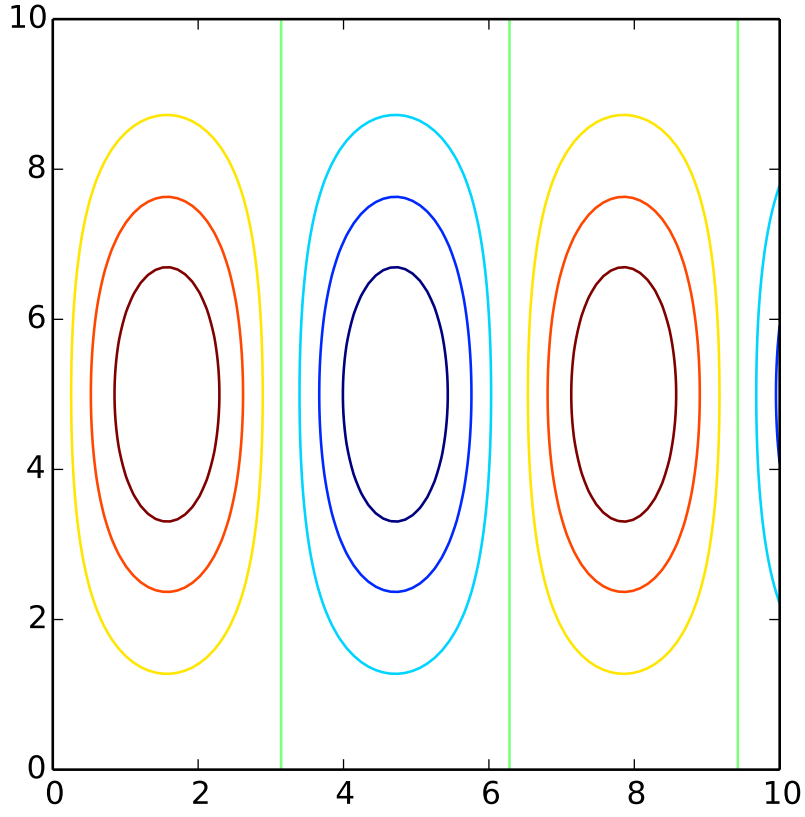
Colour map plots

```
>>> xs = np.linspace(0, 10, 100)
>>> y1 = np.sin(xs)
>>> y2 = np.exp(-(xs - 5.0)**2 / 10.0)
>>> zs = y1.reshape(len(y1), 1) * y2.reshape(1, len(y2))
>>> plt.gcf().set_size_inches(6,6)  # square
>>> plt.imshow(zs.T, origin='lower')
```



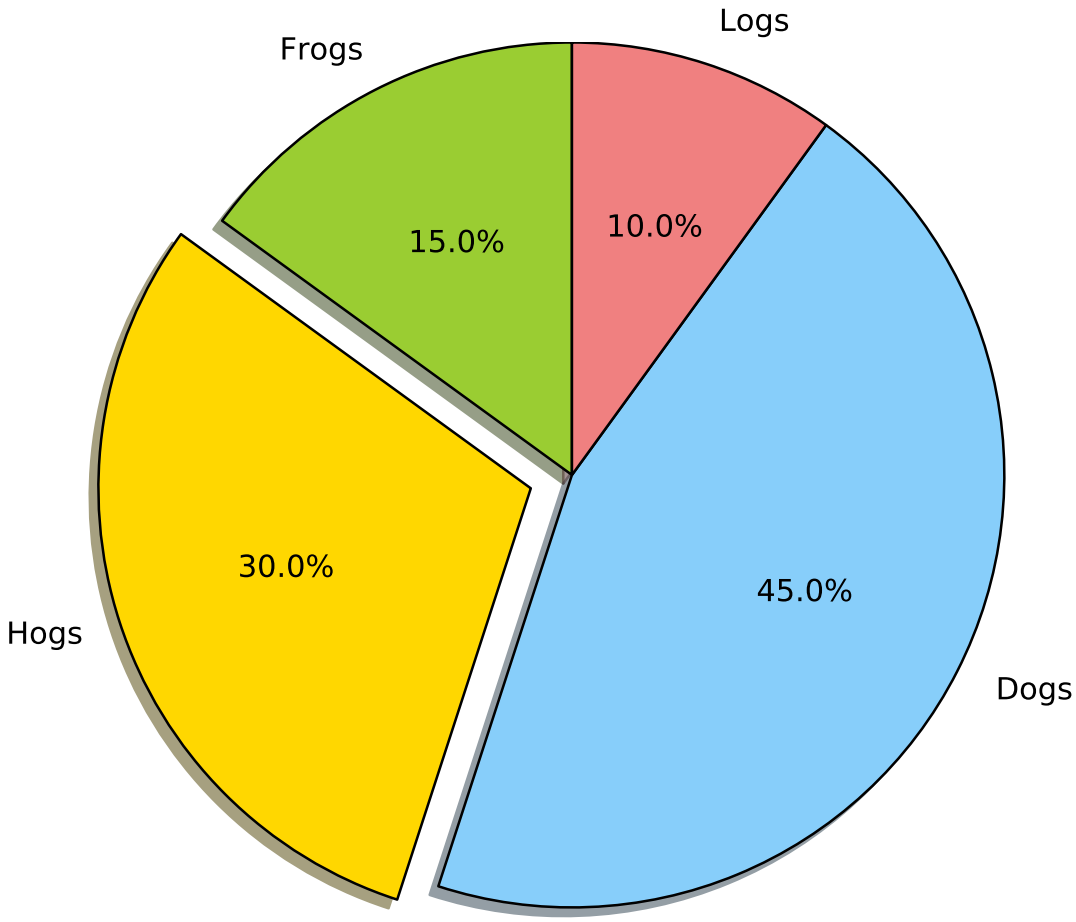
Contour plots

```
>>> plt.contour(xs, xs, z.T, origin='lower')
```

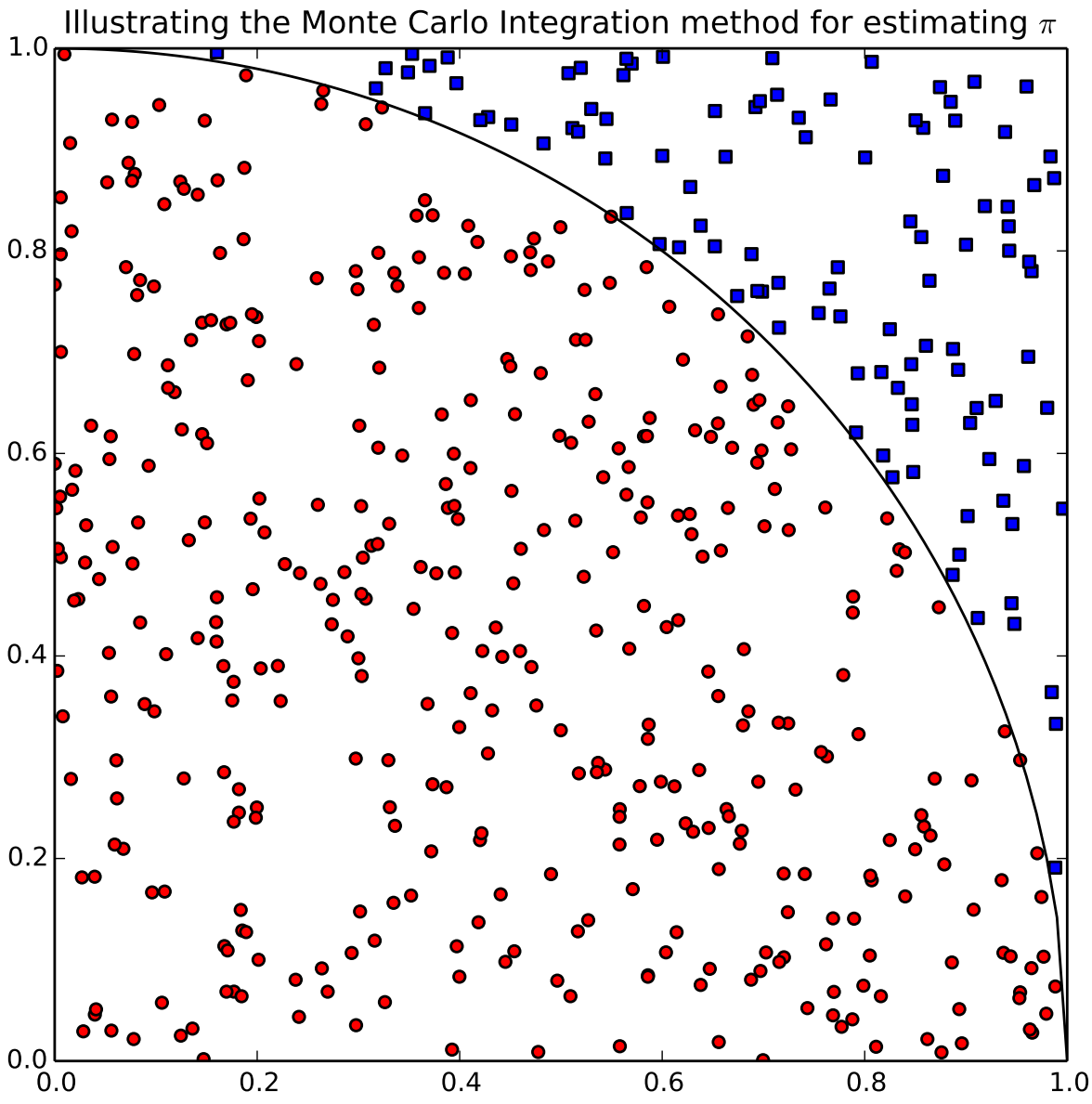


Pie charts

More example code at `http://matplotlib.org/examples/`



Example #1: Monte Carlo integration



Example #1: Monte Carlo integration

Algorithm:

- Generate a point in the unit square by drawing x, y from uniform distribution $[0, 1]$
- If $x^2 + y^2 \leq 1$, the point is inside the circle; else, outside.
- Let $n =$ num of points inside; $N =$ total number of points;
- Area of unit circle,

$$A = \pi \approx \frac{4n}{N}$$

- Hence we may use random numbers to estimate π.

```
import numpy as np
def estimate_pi(N):
    a = np.random.rand(2*N)
    b = a.reshape(2,N)
    c = b[0]**2 + b[1]**2
    return 4.0*c[c < 1.0].size / float(N)
```

```
>>> estimate_pi(10000)
3.1584
>>> estimate_pi(100000)
3.14348
>>> estimate_pi(1000000)
3.144024
>>> estimate_pi(10000000)
3.1419672
```

Example #1: Monte Carlo integration

- Suppose we use N points to get an estimate P for π. The error in the estimate is $\epsilon = P - \pi$.
- The error is probabilistic; ϵ is drawn from a probability distribution, which approaches a normal distribution as $N \to \infty$ (**central limit theorem**).
- The standard deviation σ in the error of the estimate scales as

$$\sigma \propto \frac{1}{\sqrt{N}}$$

- MC integration is an **inefficient** method for low-dimensional integrals
- It can be useful for d-dimensional integration when $d \gg 1$:

$$\sigma \propto N^{-1/2} \qquad \text{vs.} \qquad \sigma \propto N^{-k/d}$$

where k is the order of the standard integration method.

Example #2: The Logistic Map

A simple **non-linear** recurrence relation:

$$x \to rx(1 - x)$$

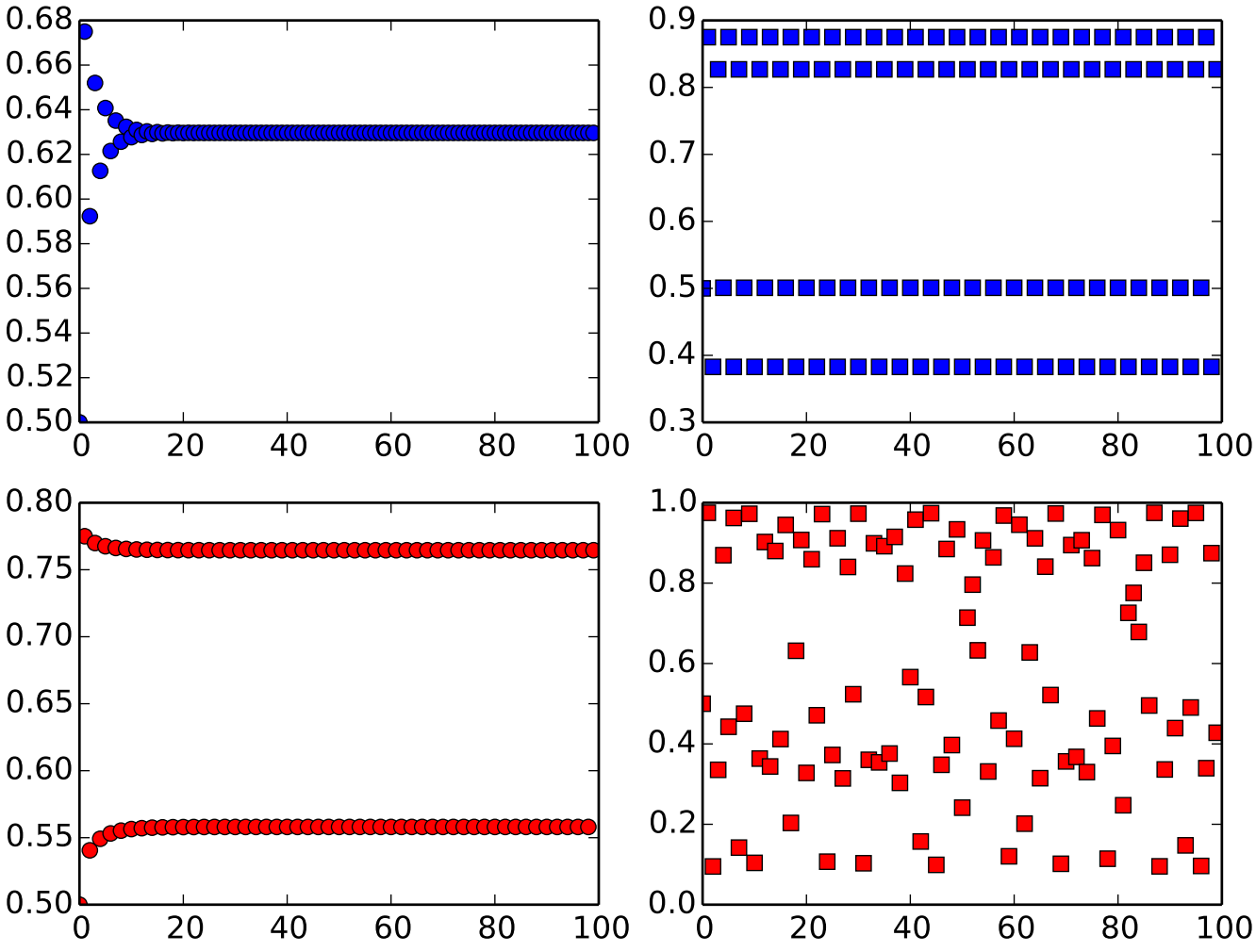
where μ is a parameter.

Originally used to model population dynamics.

Example #2: The Logistic Map

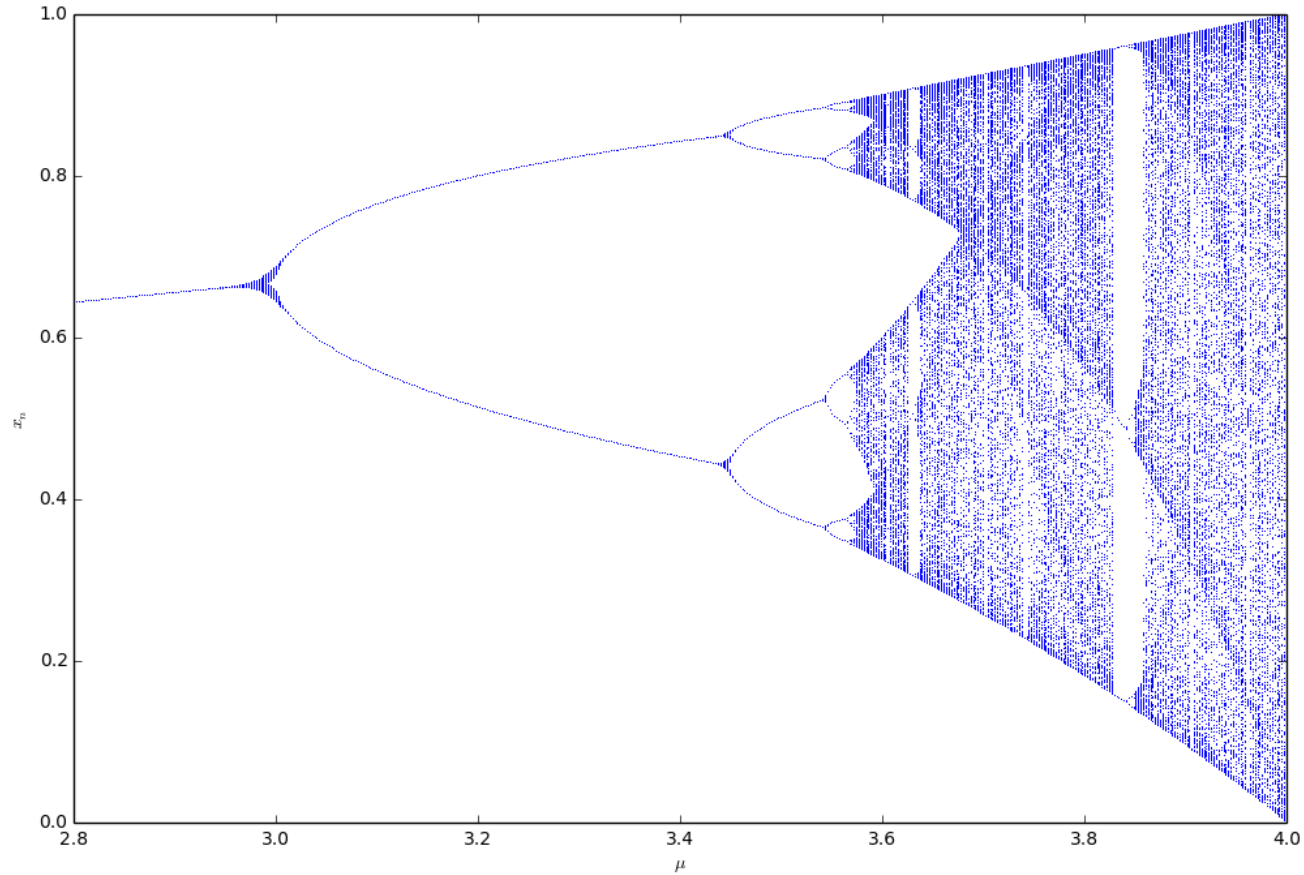
```
import numpy as np
import matplotlib.pyplot as plt

def logisticmap(r=2.0, N=100):
    xs = 0.5*np.ones(N)
    for i in np.arange(N-1):
        xs[i+1] = r*xs[i]*(1.0-xs[i])
    return xs

fig, ax = plt.subplots(2,2)
ax[0,0].plot(logisticmap(2.7), 'bo')
ax[1,0].plot(logisticmap(3.1), 'ro')
ax[0,1].plot(logisticmap(3.5), 'bs')
ax[1,1].plot(logisticmap(3.9), 'rs')
plt.show()
```

Example #2: The Logistic Map



- To plot pixels:

```
plt.plot(data, ',')  # comma
```



This is the bifurcation diagram for the logistic map ($\mu = r$ here).

Example #3: Quadratic maps $z \to z^2 + c$

- Consider an iterative map $z_{k+1} = f(z_k)$ generating a sequence $z_0, z_1, z_2, \ldots$ where

$$f(z_k) = z_k^2 + c, \qquad z_k, c \in \mathbb{C},$$

- The behaviour of the sequence depends on the starting value z_0 and the complex constant c
- Some possibilities: the sequence may
  - converge on an attractive **fixed point**, $f(z) = z$
  - repeat a sequence of period p, such that $f^p(z) = z$
  - **diverge** towards infinity, or
  - neither converge nor diverge but wander around

Definition: Julia set

The **Julia set** is the closure of the set of repelling periodic points.

Example #3: Quadratic maps $z \to z^2 + c$

Consider the special case $c = 0$:

- Three possibilities:
  1. $|z_0| < 1$: the sequence converges towards the **fixed point** at the origin
  2. $|z_0| > 1$: the sequence diverges, $|z_k| \to \infty$
  3. $|z_0| = 1$: the sequence remains on the unit circle.
- For $|z_0| = 1$, if $\arg(z_0) \in \mathbb{Q}$ the sequence is periodic, otherwise it is aperiodic.
- The Julia set is the unit circle.
- What happens when $c \neq 0$?

Example #3: Quadratic maps $z \to z^2 + c$

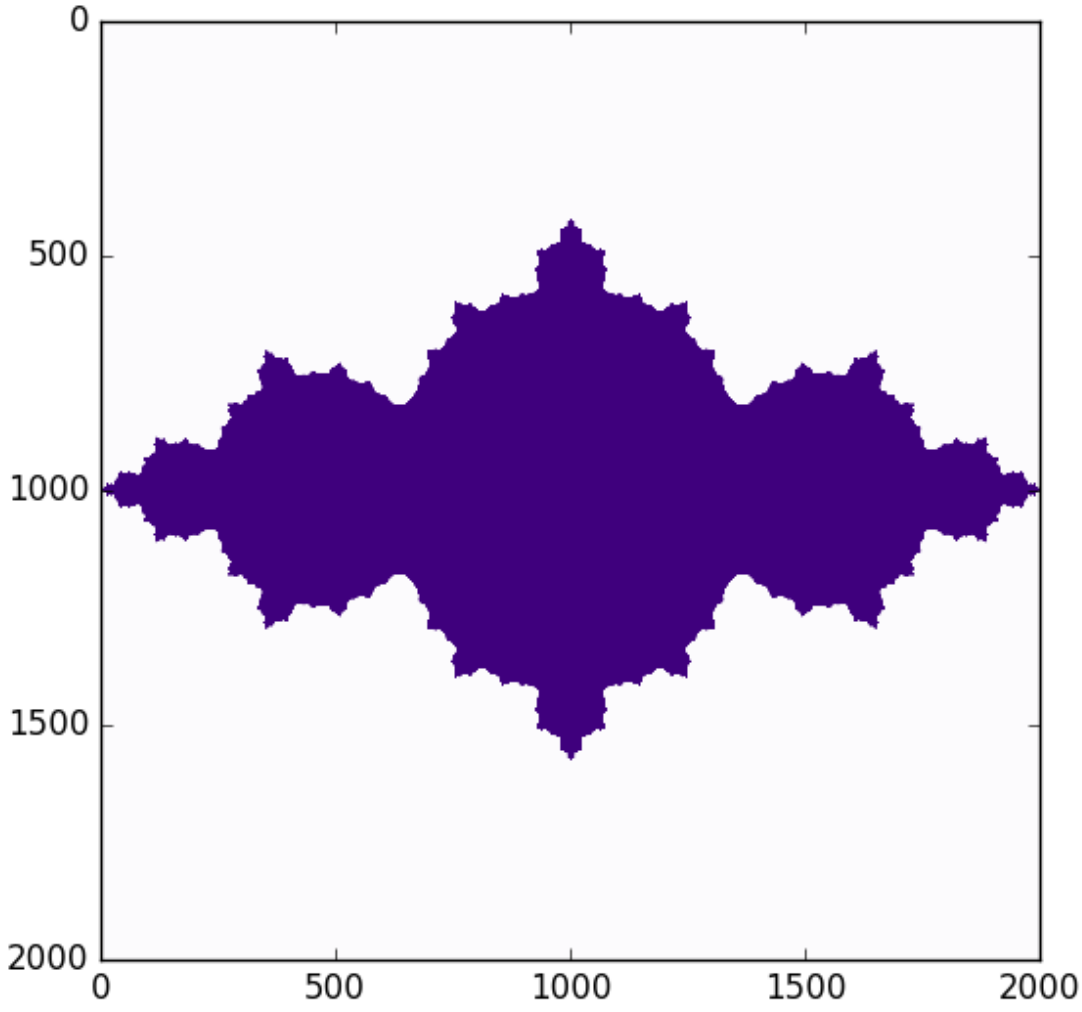
Exercise

- Make an $N \times N$ array of z_0 values, linearly-spaced across the complex domain $-d \leq \mathrm{Re}(z_0) \leq d$, $-d \leq \mathrm{Im}(z_0) \leq d$ for $d = 1.5$ (say)
- Apply the quadratic map N times to every value in the array.
- Construct the set of points S satisfying the condition $|z_N| < \alpha$, for $\alpha = 2$ (say).
- Colour the region S on the Argand diagram, using `plt.imshow()`

Example #3: Quadratic maps $z \to z^2 + c$

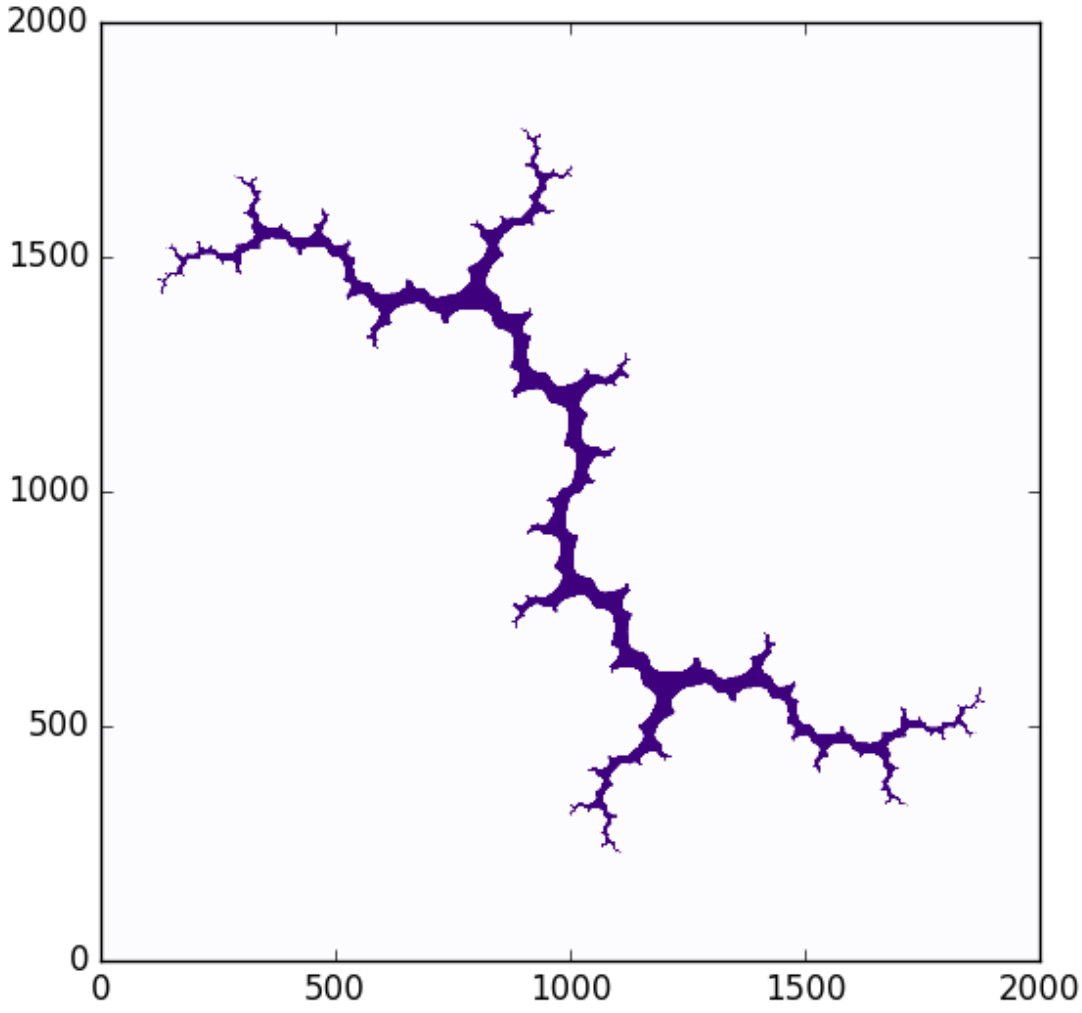
```
N = 2000
d = 1.5
xs = np.linspace(-d, d, N)
ys = np.linspace(-d, d, N)*1j
# use broadcasting to make an NxN array from rows/columns
zs = xs.reshape((1, N)) + ys.reshape((N, 1))
c = -0.75
for k in range(10):  # iterate
    zs = zs**2 + c   # ufunc acting on whole array
arr = (abs(zs) < 2.0)*1  # make an array of 1s (in S) and 0s
plt.imshow(arr, cmap='Purples', origin='lower')
plt.savefig("quadraticmap.png") # save to file
```

Example #3: Quadratic maps $z \to z^2 + c$



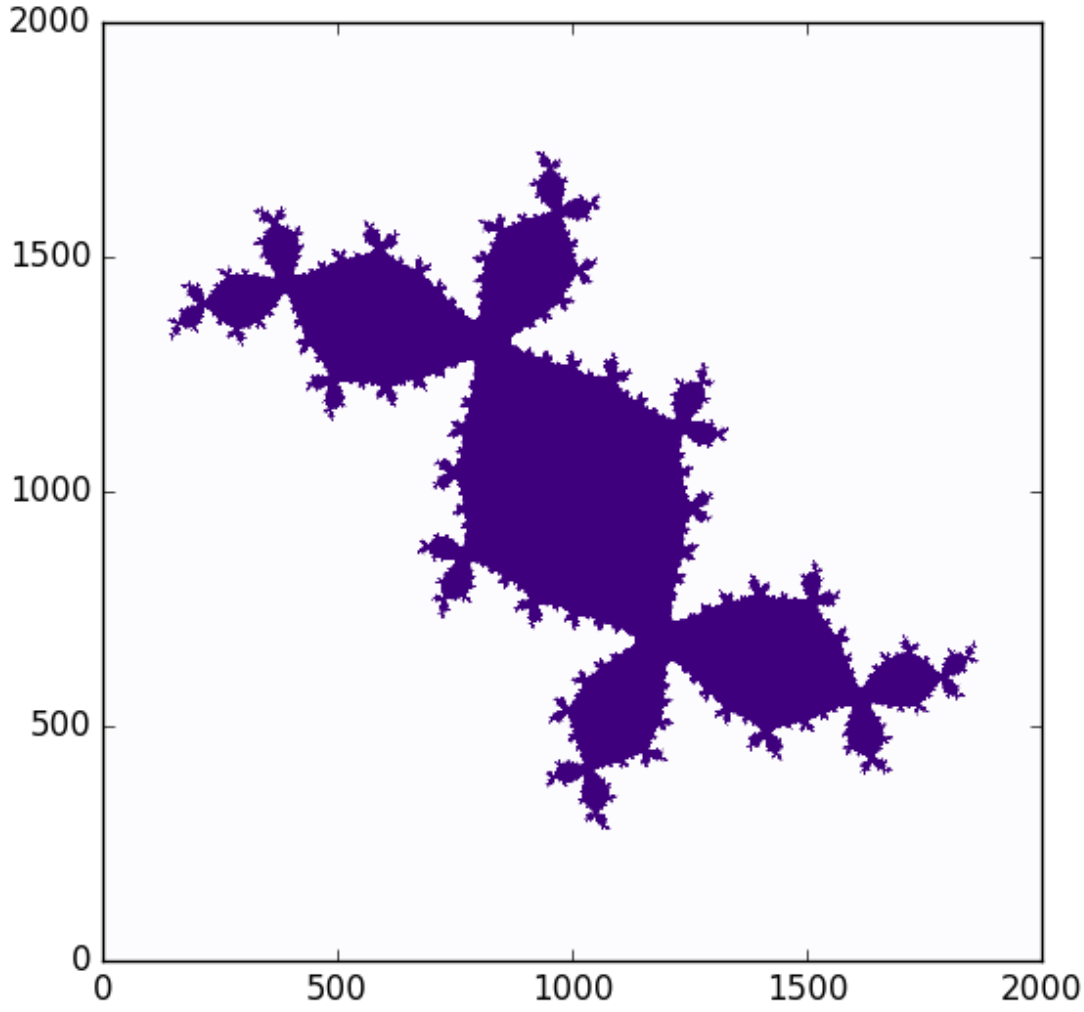
$c = -0.75$

Example #3: Quadratic maps $z \to z^2 + c$



$c = i$

Example #3: Quadratic maps $z \to z^2 + c$



$$c = -0.123 + 0.745i$$