Visualization and optimization

- Jupyter
- Matplotlib
- scipy.optimize.minimize

The Jupyter Notebook

The Jupyter Notebook is an open-source web application that allows you to create and share documents that contain live code, equations, visualizations and narrative text. Uses include: data cleaning and transformation, numerical simulation, statistical modeling, data visualization, machine learning, and much more.

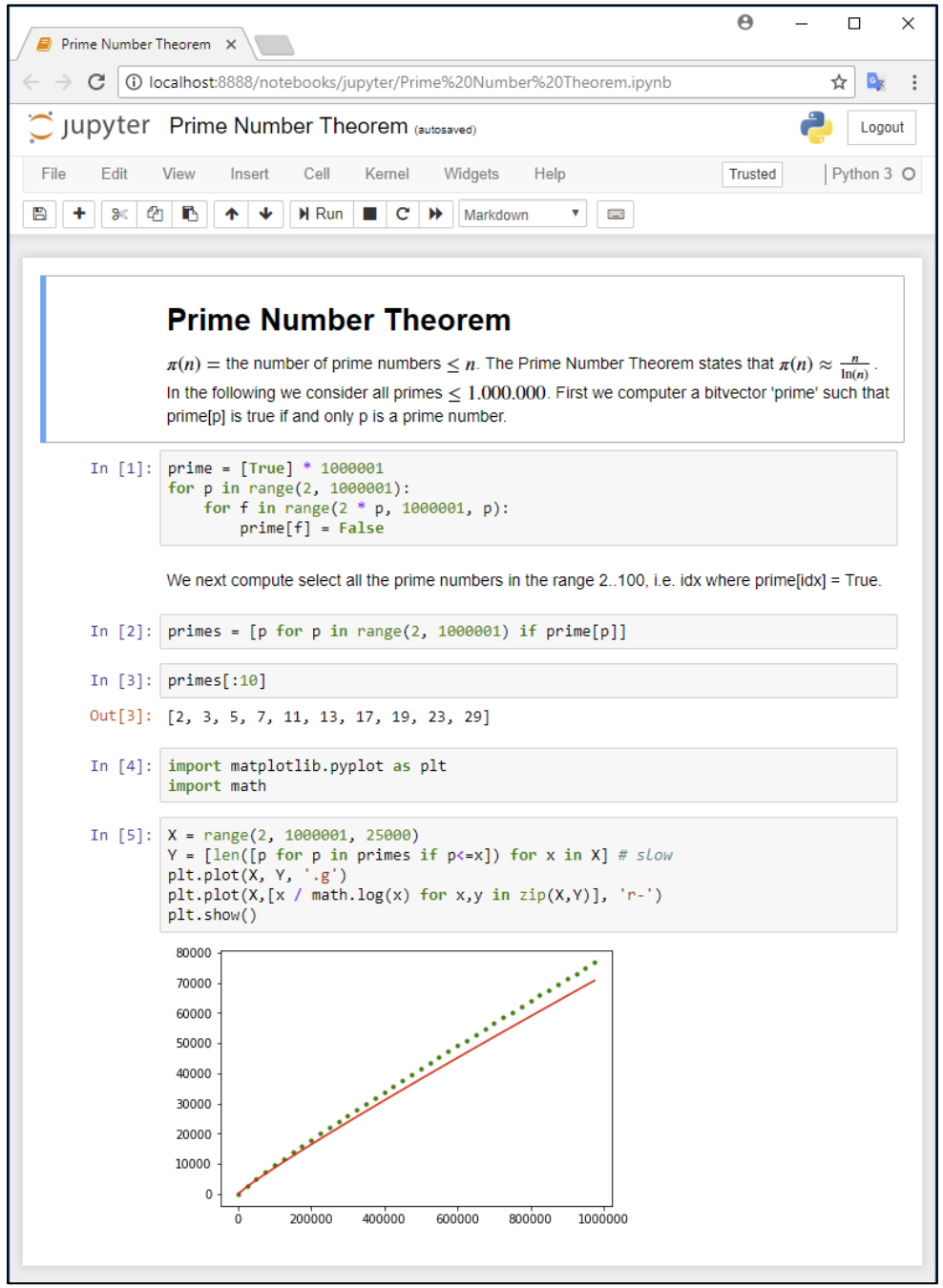
jupyter.org

python

IP[y]:
IPython

jupyter

Jupyter Server
(e.g. running on
local machine)



Web Browser

User

cells

python code

formatted text: Markdown / LaTeX / HTML / ...

python shell output

matplotlib / numpy / ... output

Prime Number Theorem

localhost:8888/notebooks/jupyter/Prime%20Number%20Theorem.ipynb

jupyter Prime Number Theorem (autosaved)

Logout

File Edit View Insert Cell Kernel Widgets Help Trusted Python 3

Run Markdown

Prime Number Theorem

$\pi(n) =$ the number of prime numbers $\leq n$. The Prime Number Theorem states that $\pi(n) \approx \frac{n}{\ln(n)}$.
In the following we consider all primes $\leq 1.000.000$. First we computer a bitvector 'prime' such that prime[p] is true if and only p is a prime number.

In [1]:
```
prime = [True] * 1000001
for p in range(2, 1000001):
    for f in range(2 * p, 1000001, p):
        prime[f] = False
```

We next compute select all the prime numbers in the range 2..100, i.e. idx where prime[idx] = True.

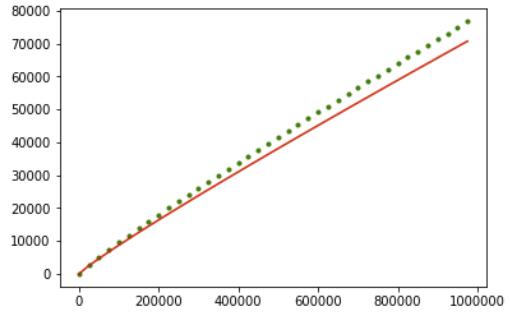
In [2]:
```
primes = [p for p in range(2, 1000001) if prime[p]]
```

In [3]:
```
primes[:10]
```

Out[3]:
```
[2, 3, 5, 7, 11, 13, 17, 19, 23, 29]
```

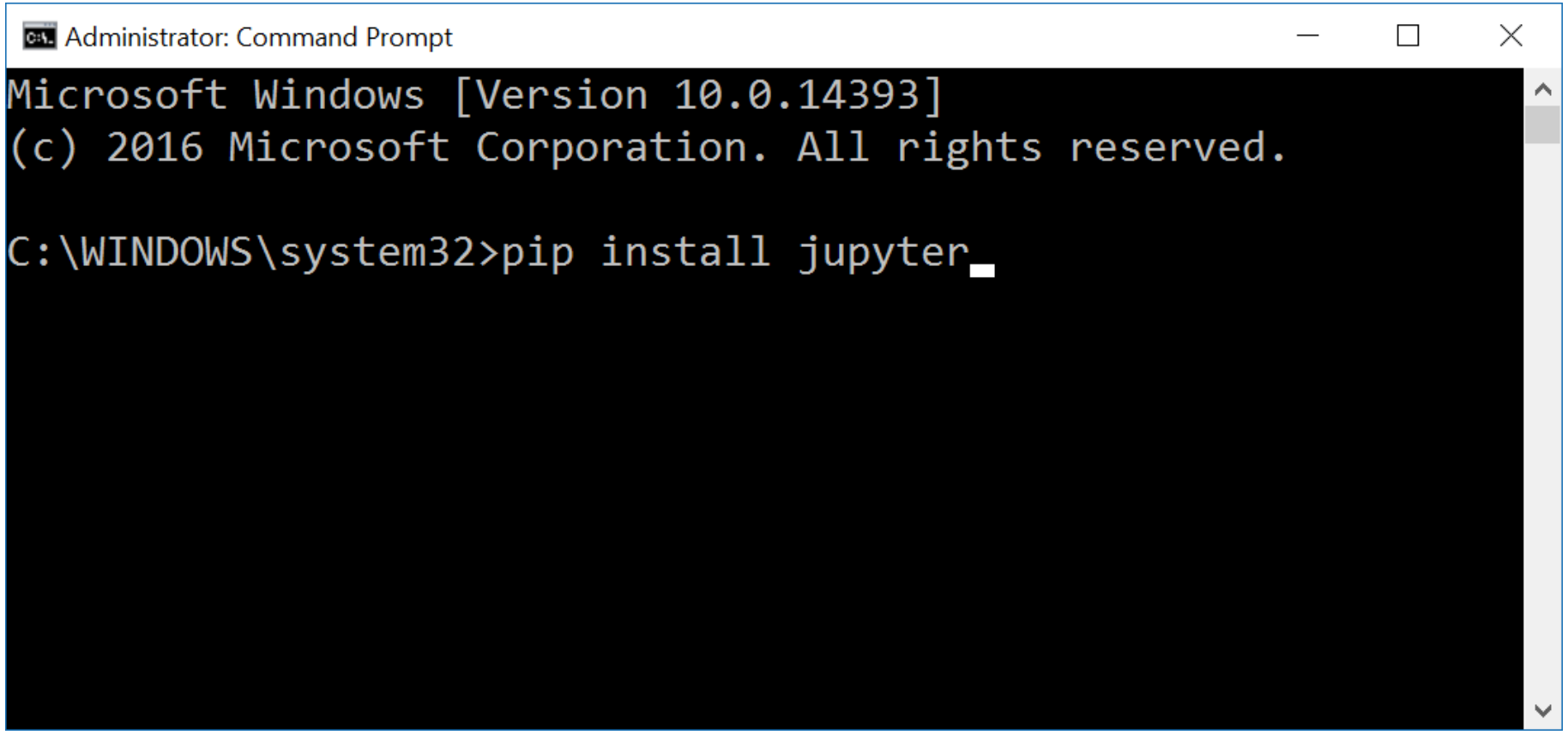
In [4]:
```
import matplotlib.pyplot as plt
import math
```

In [5]:
```
X = range(2, 1000001, 25000)
Y = [len([p for p in primes if p<=x]) for x in X] # slow
plt.plot(X, Y, '.g')
plt.plot(X,[x / math.log(x) for x,y in zip(X,Y)], 'r-')
plt.show()
```



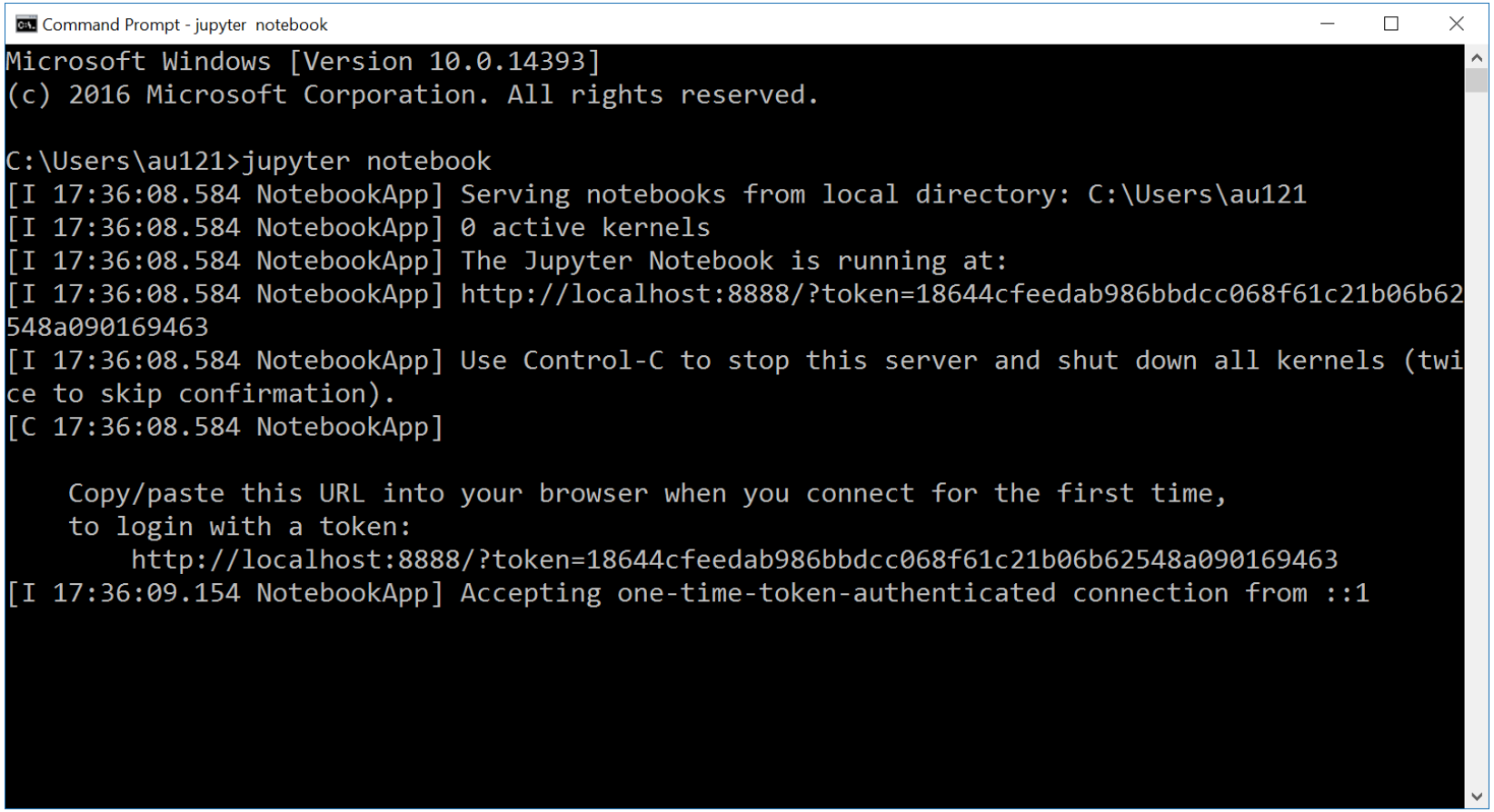
Jupyter - installing

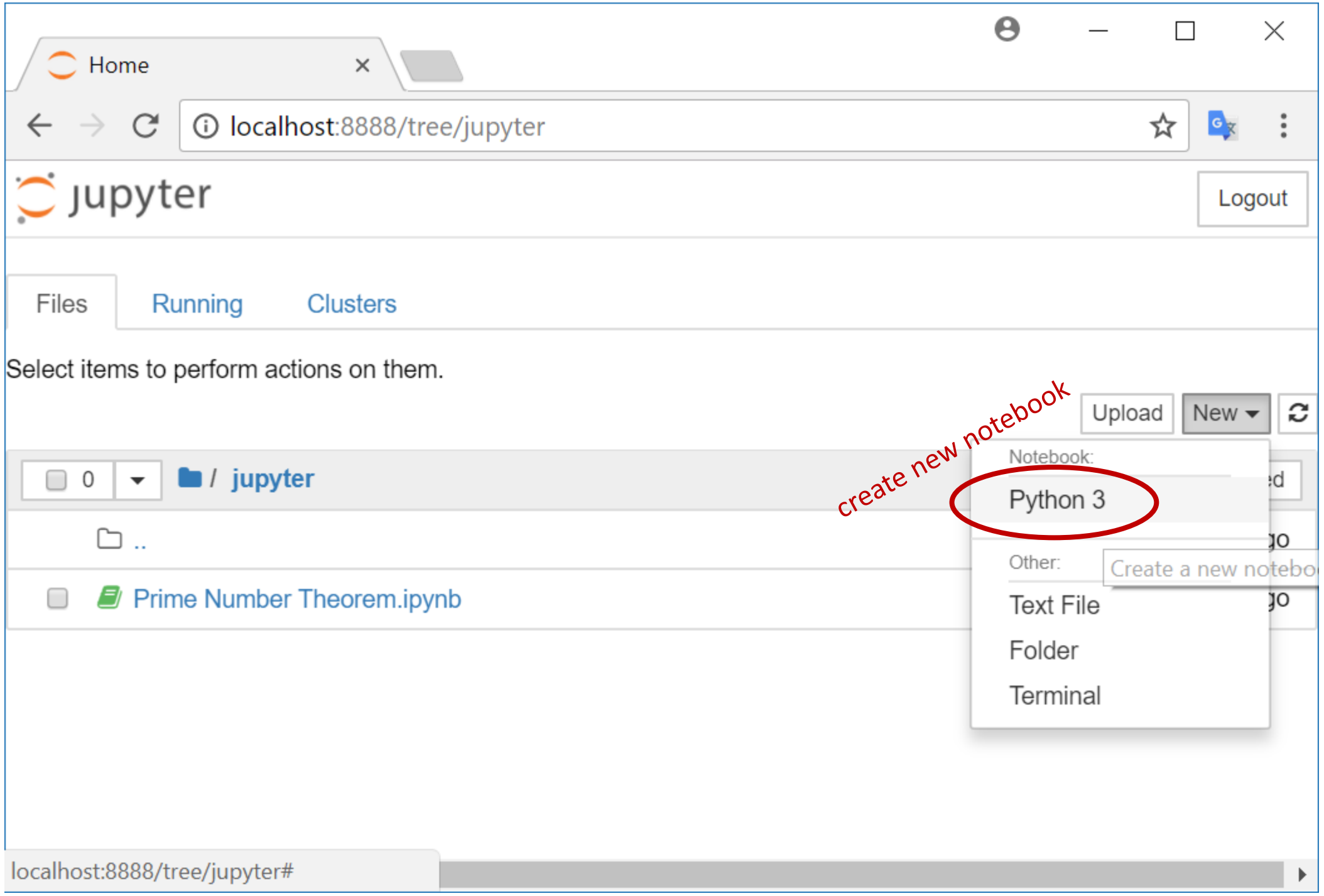
- Open a windows shell and run: `pip install jupyter`



Jupyter – launching the jupyter server

- Open a windows shell and run: `jupyter notebook`




Home
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Clusters
Select items to perform actions on them.
create new notebook
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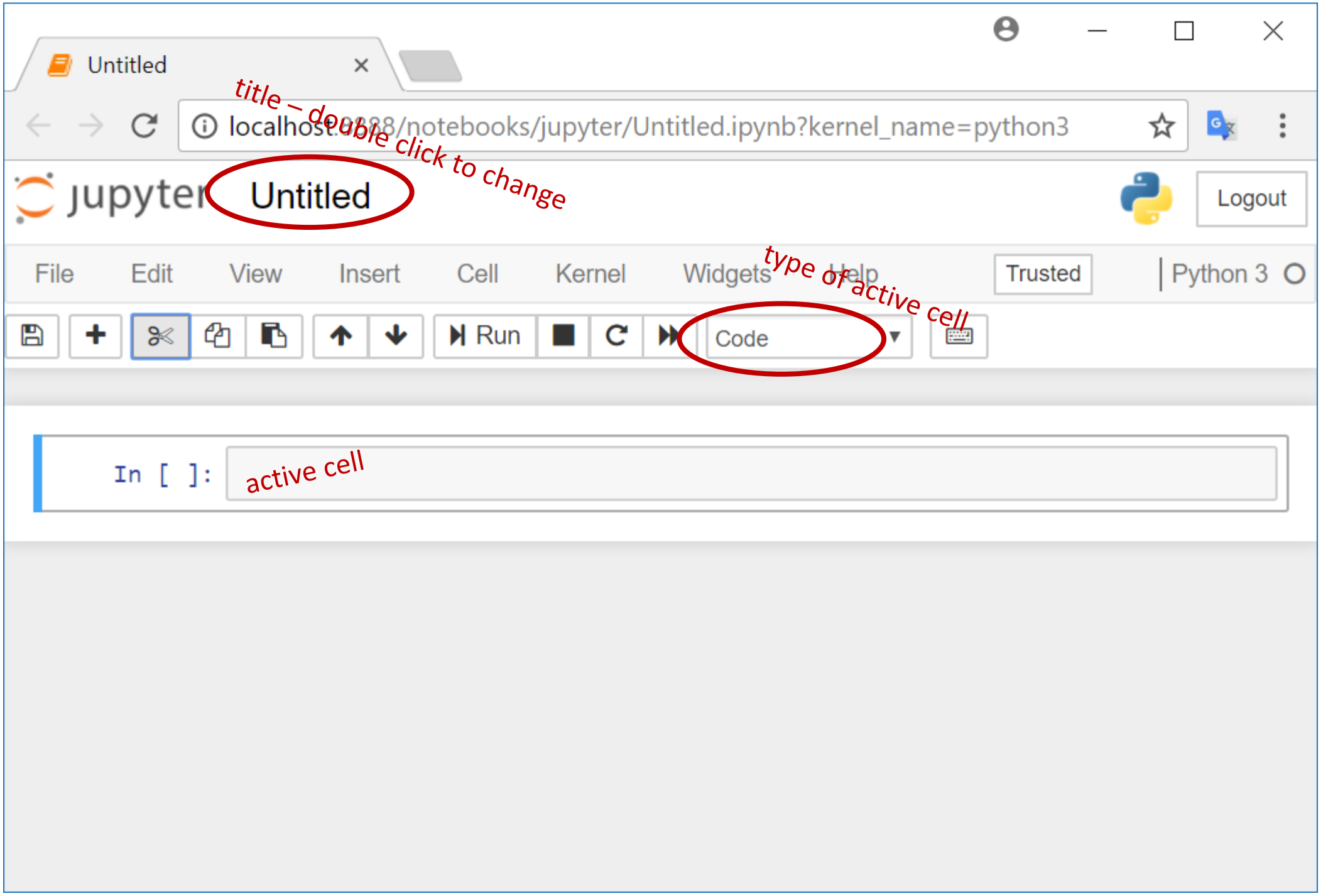
Prime Number Theorem.ipynb
Notebook:
Python 3
Other:
Create a new notebo
Text File
Folder
Terminal
localhost:8888/tree/jupyter#


Untitled
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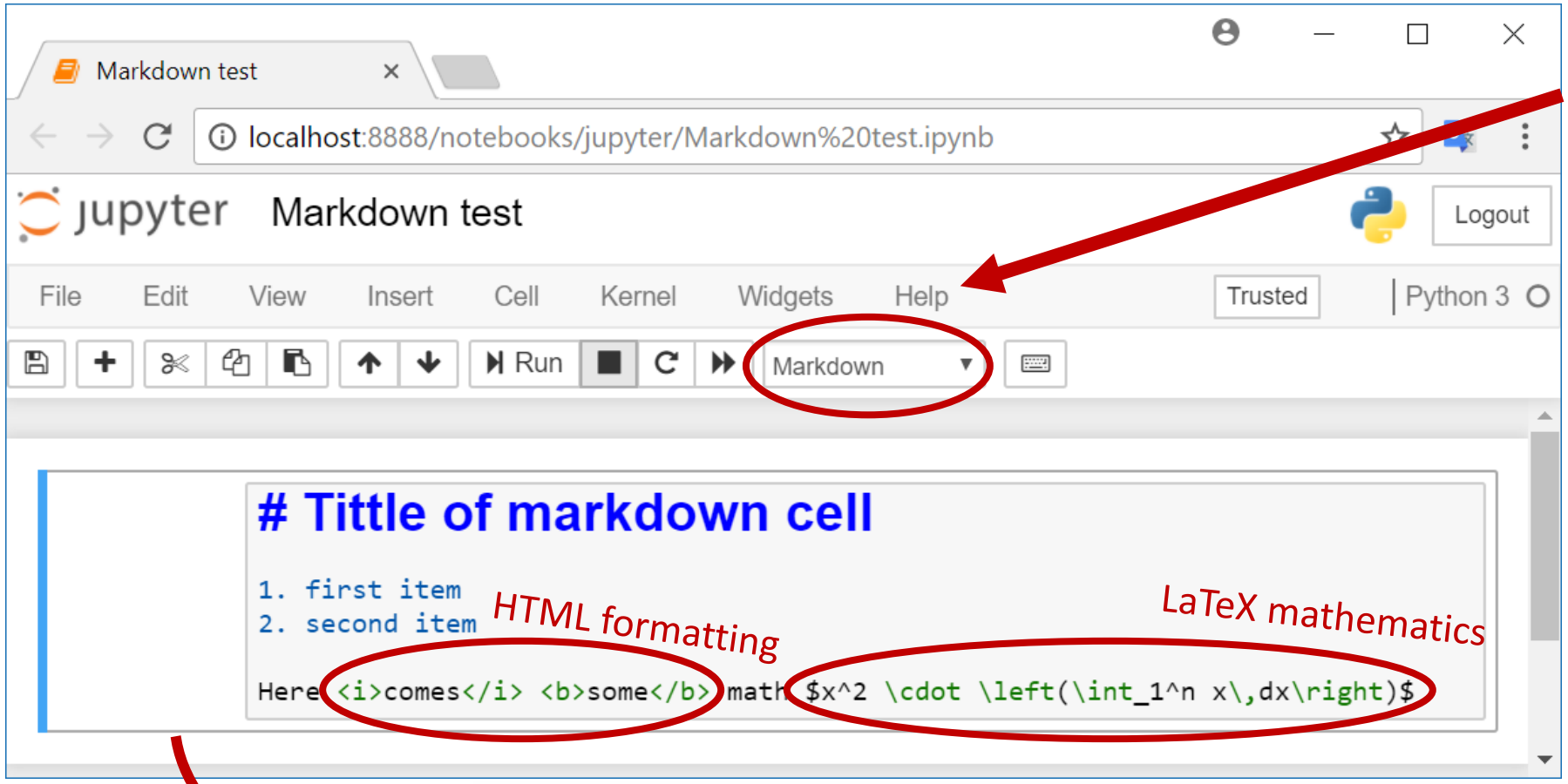


Try:
Help > User Interface Tour
Help > Markdown

after pressing
Ctrl + Enter (evaluates)
Alt + Enter (evaluates + new cell)

Tittle of markdown cell

1. first item
2. second item

Here *comes* **some** math $x^2 \cdot \left(\int_1^n x\,dx\right)$

github.com/adam-p/markdown-here/wiki/Markdown-Cheatsheet

Jupyter

- Widespread tool used for data science applications
- Documentation, code for data analysis, and resulting visualizations are stored in one common format
- Easy to update visualizations
- Works with about 100 different programming languages (not only Python 3), many special features, ...
- Easy to share data analysis

- *Many online tutorials and examples are available*

Matplotlib is a Python 2D plotting library which produces publication quality figures in a variety of hardcopy formats and interactive environments across platforms. Matplotlib can be used in Python scripts, the Python and IPython shells, the Jupyter notebook, web application servers, and four graphical user interface toolkits.

Matplotlib tries to make easy things easy and hard things possible. You can generate plots, histograms, power spectra, bar charts, errorcharts, scatterplots, etc., with just a few lines of code. For simple plotting the pyplot module provides a MATLAB-like interface, particularly when combined with IPython. For the power user, you have full control of line styles, font properties, axes properties, etc, via an object oriented interface or via a set of functions familiar to MATLAB users.

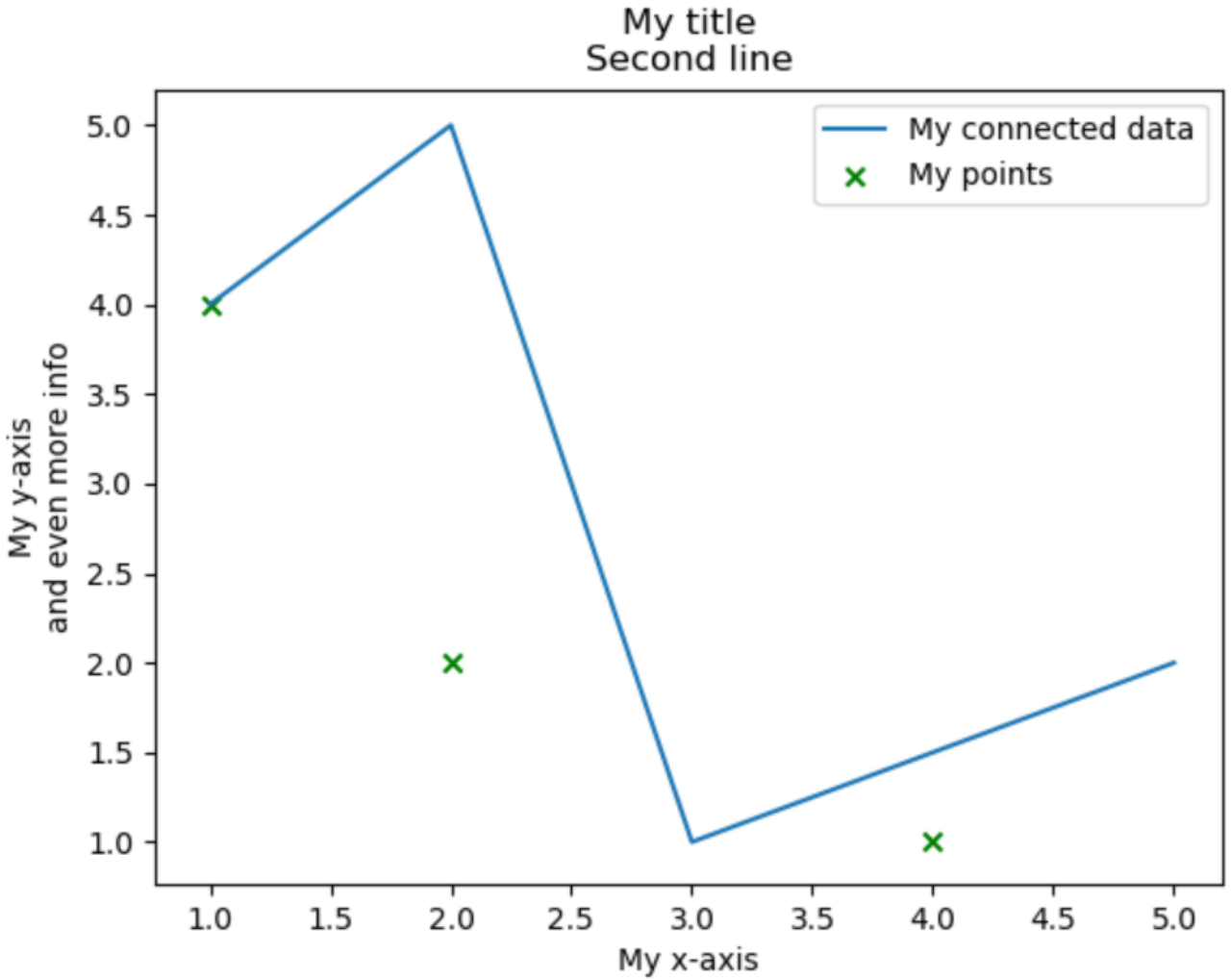
matplotlib.org

Some simple matplotlib examples

Plot and Scatter

matplotlib-plot.py

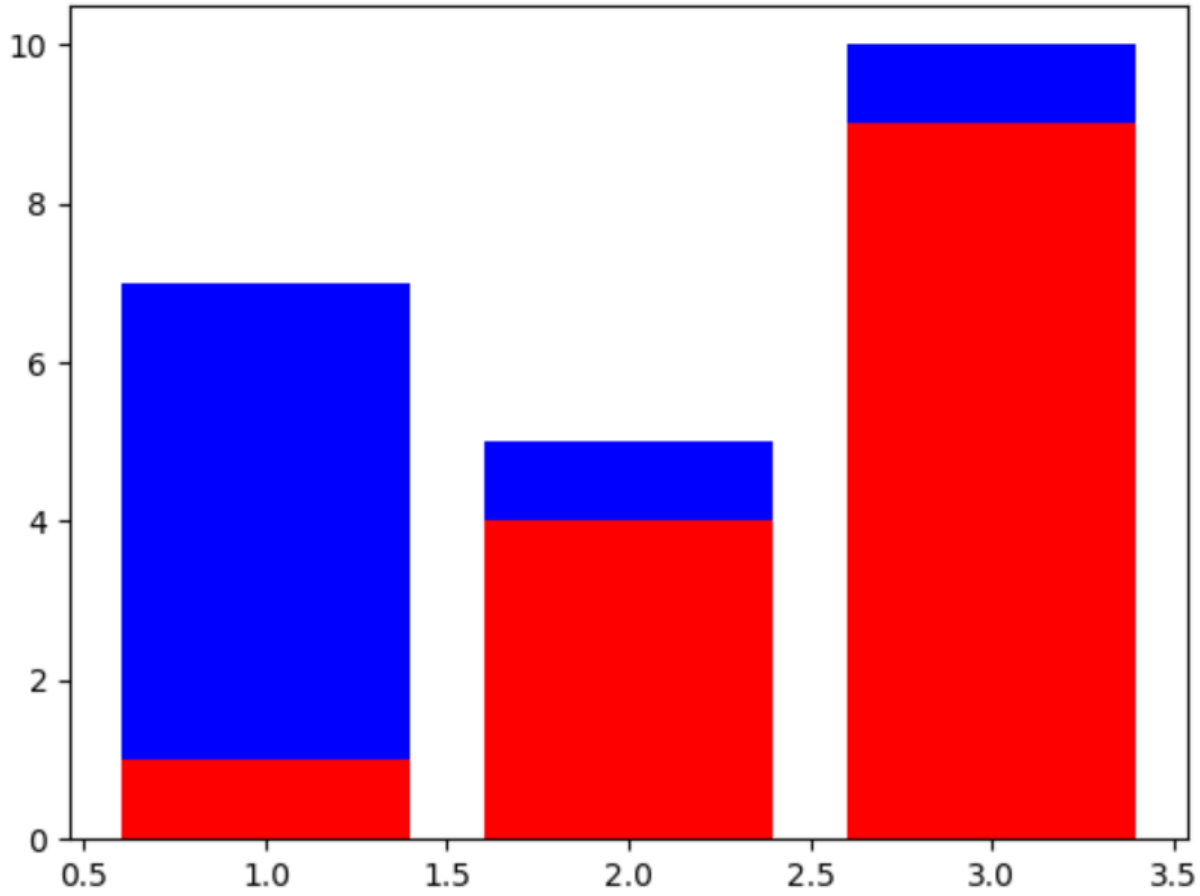
```
import matplotlib.pyplot as plt

x1 = [1, 2, 3, 5]
y1 = [4, 5, 1, 2]

x2 = [1, 2, 4]
y2 = [4, 2, 1]

plt.plot(x1, y1, label='My connected data')
plt.scatter(x2, y2, label='My points',
            marker='x', color='green')
plt.xlabel('My x-axis')
plt.ylabel('My y-axis\nand even more info')
plt.title('My title\nSecond line')
plt.legend()
plt.show()
```



Bars

matplotlib-bars.py

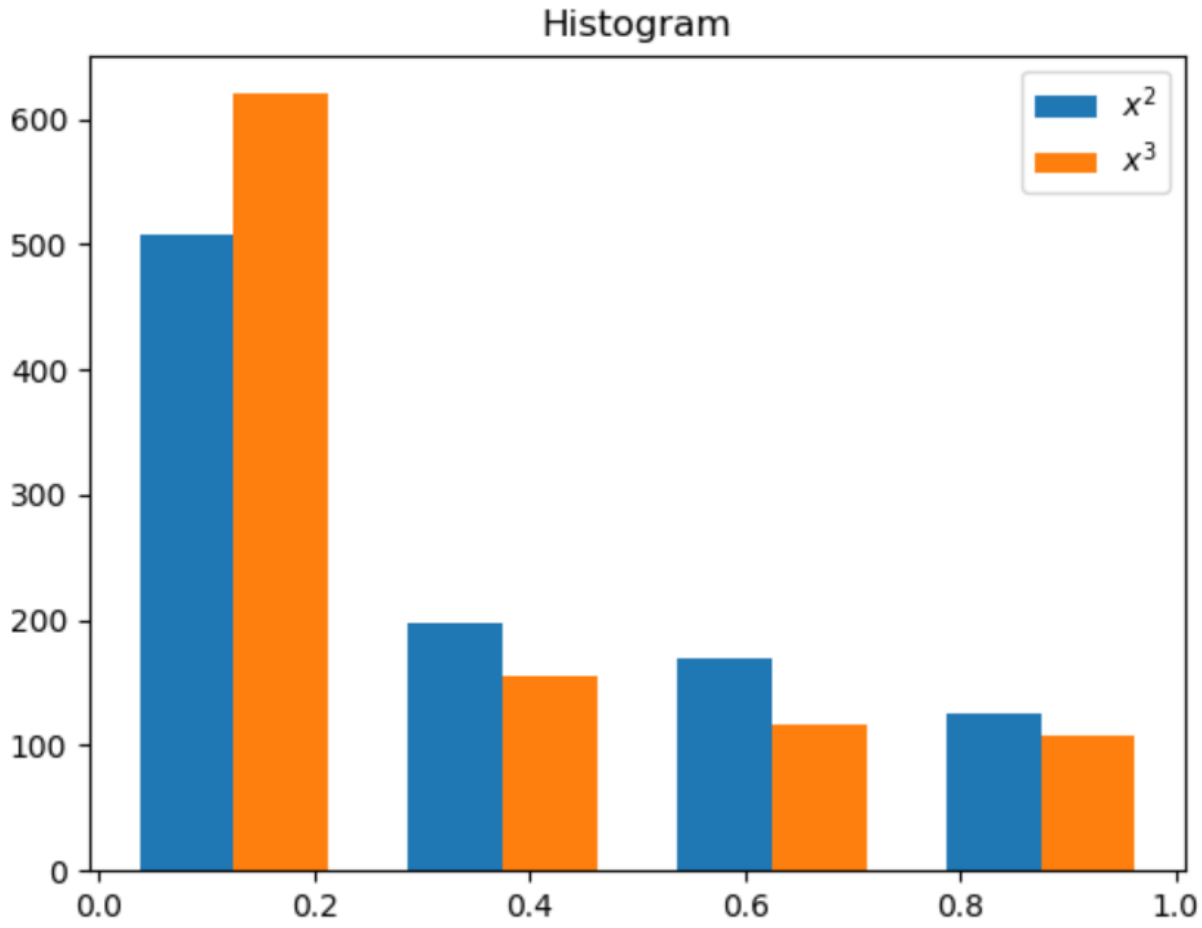
```
import matplotlib.pyplot as plt

x = [1, 2, 3]
y = [7, 5, 10]

plt.bar(x, y, color='blue')
plt.bar(x, [v**2 for v in x], color='red')
plt.show()
```



Histogram

matplotlib-histogram.py

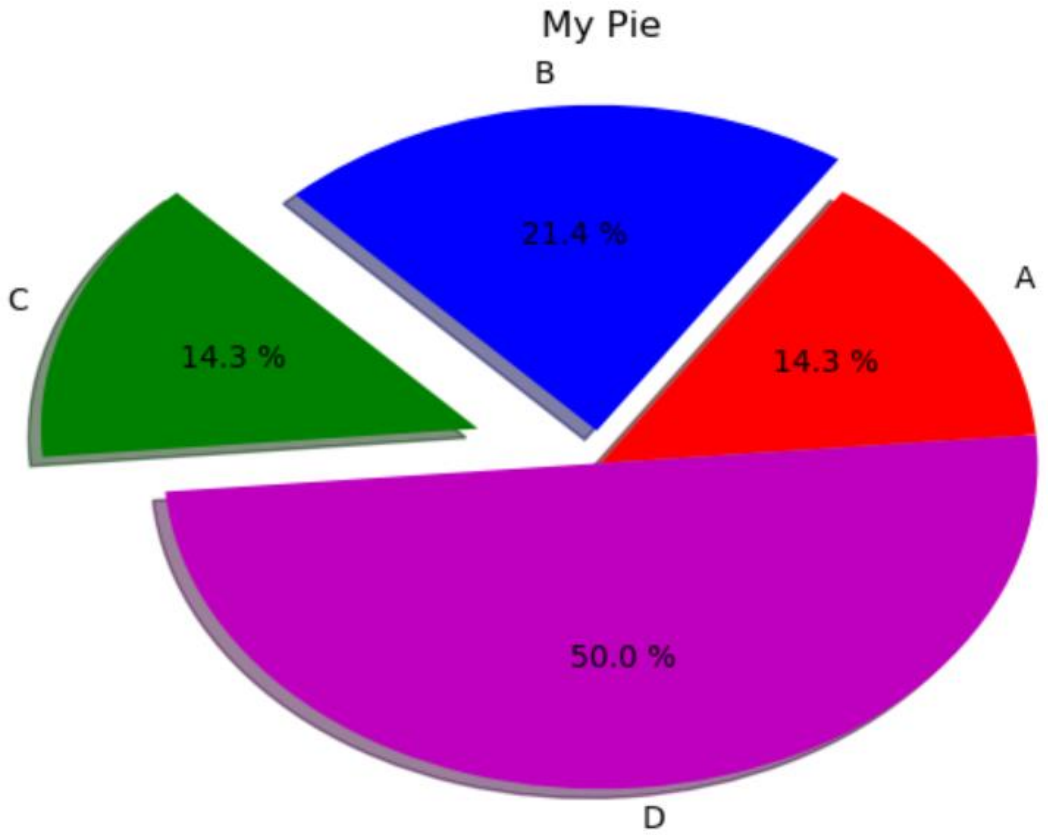
```
import matplotlib.pyplot as plt
from random import random

values1 = [random()**2 for _ in range(1000)]
values2 = [random()**3 for _ in range(1000)]

bins = [0.0, 0.25, 0.5, 0.75, 1.0]

plt.hist([values1, values2], bins, histtype='bar',
         rwidth=0.7, label=['$x^2$', '$x^3$'])
plt.title('Histogram')
plt.legend()
plt.show()
```



Pie

matplotlib-pie.py

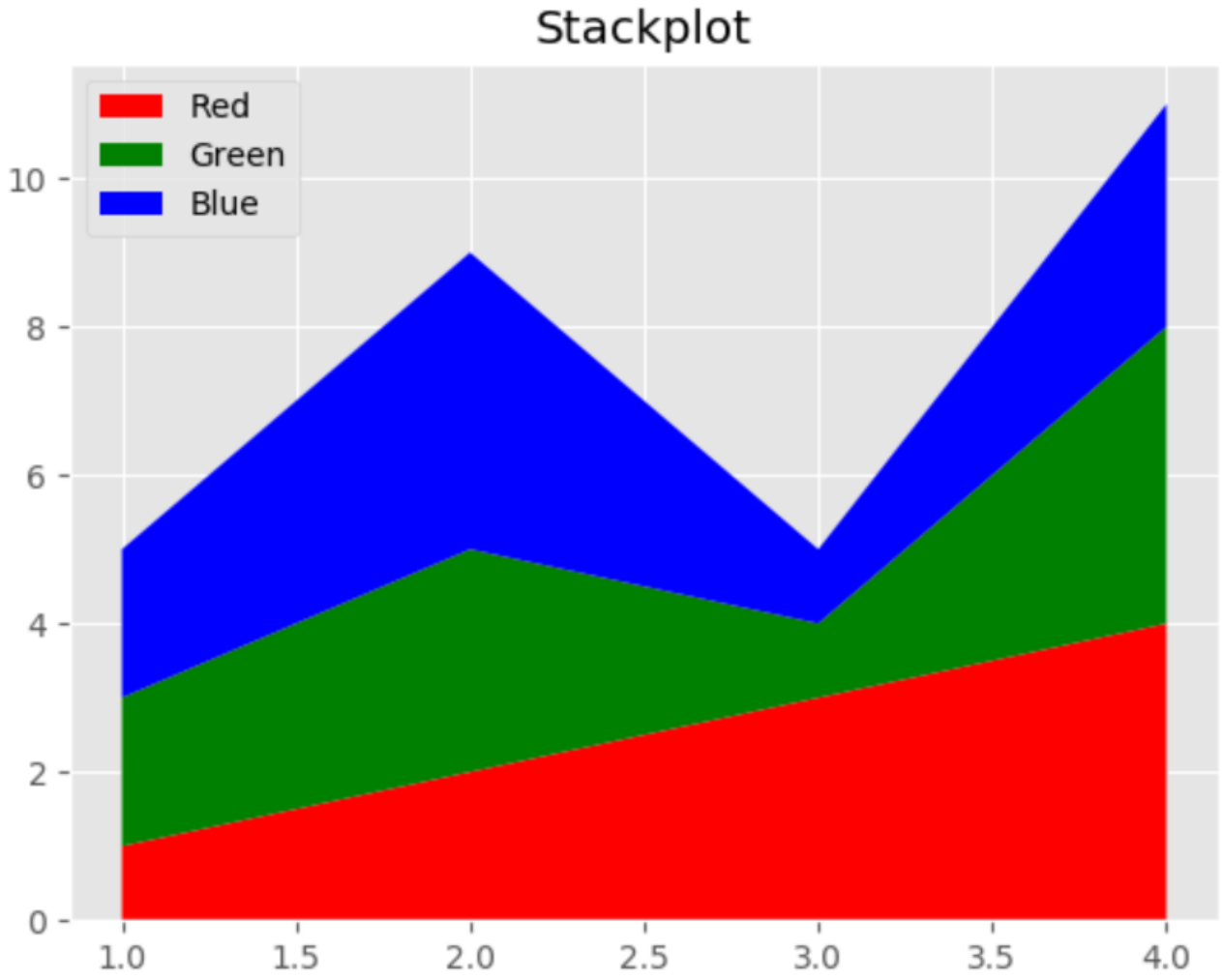
```
import matplotlib.pyplot as plt

plt.title('My Pie')
plt.pie([2, 3, 2, 7],
        labels=['A','B','C','D'],
        colors=['r', 'b', 'g', 'm'],
        startangle=5,
        shadow=True,
        explode=(0, 0.1, 0.3, 0),
        autopct='%1.1f %%'  # percent formatting
        )
plt.show()
```



Stackplot

matplotlib-stackplot.py

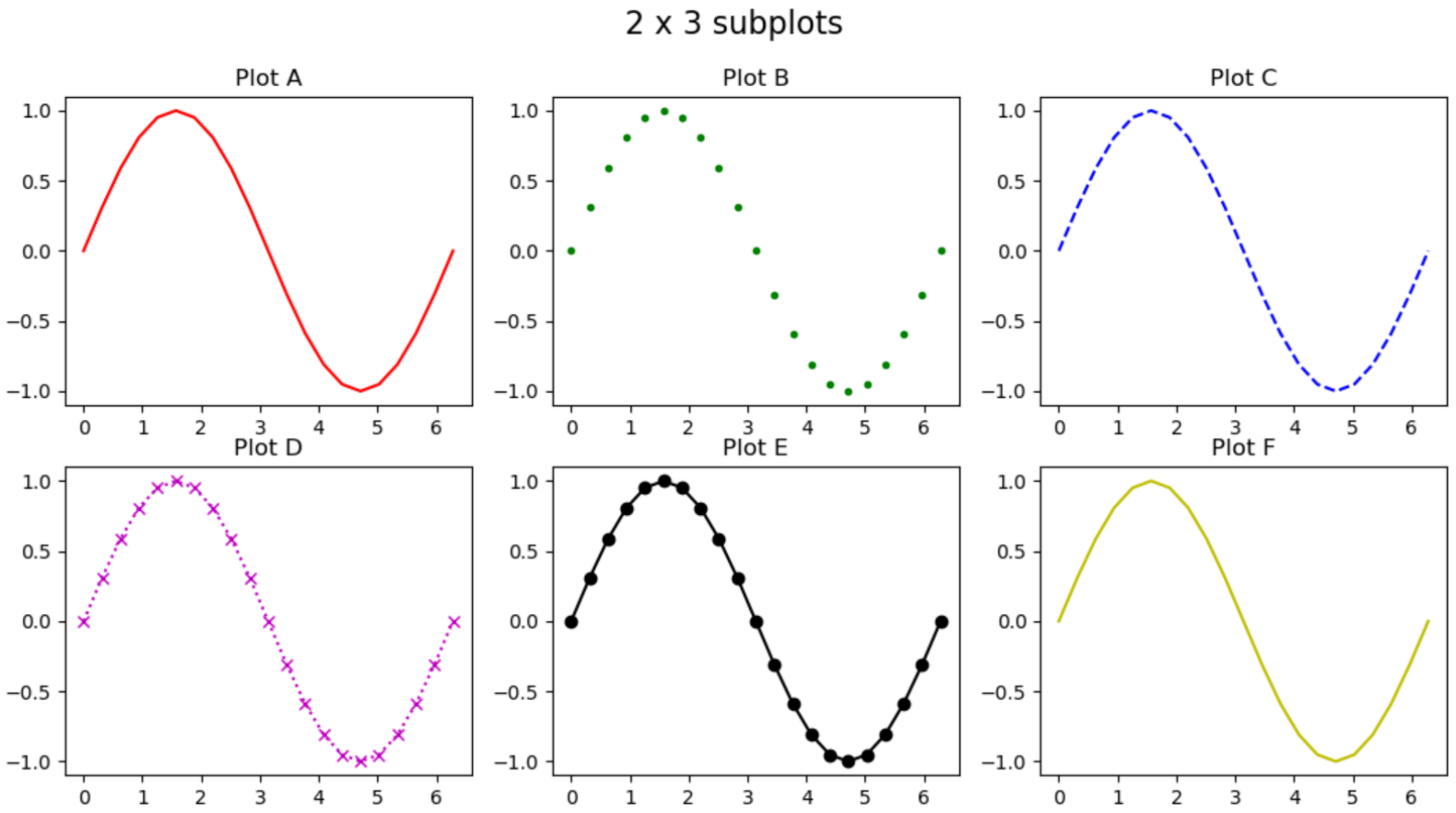
```
import matplotlib.pyplot as plt
from matplotlib import style

style.use('ggplot')

x = [1, 2, 3, 4]

y1 = [1, 2, 3, 4]
y2 = [2, 3, 1, 4]
y3 = [2, 4, 1, 3]

plt.title('Stackplot')

plt.stackplot(x, y1, y2, y3,
              colors=['r', 'g', 'b'],
              labels=["Red", "Green", "Blue"])
plt.grid(True)
plt.legend(loc=2)
plt.show()
```



Subplots (2 rows, 3 columns)

matplotlib-subplots.py

```
import matplotlib.pyplot as plt
import math

x_min, x_max, n = 0, 2 * math.pi, 20

x = [x_min + (x_max - x_min) * i / n
     for i in range(n + 1)]
y = [math.sin(v) for v in x]

plt.subplot(2, 3, 1)
plt.plot(x, y, 'r-')
plt.title('Plot A')

plt.subplot(2, 3, 2)
plt.plot(x, y, 'g.')
plt.title('Plot B')

plt.subplot(2, 3, 3)
plt.plot(x, y, 'b--')
plt.title('Plot C')

plt.subplot(2, 3, 4)
plt.plot(x, y, 'mx:')
plt.title('Plot D')

plt.subplot(2, 3, 5)
plt.plot(x, y, 'ko-')
plt.title('Plot E')

plt.subplot(2, 3, 6)
plt.plot(x, y, 'y')
plt.title('Plot F')

plt.suptitle('2 x 3 subplots', fontsize=16)

plt.show()
```

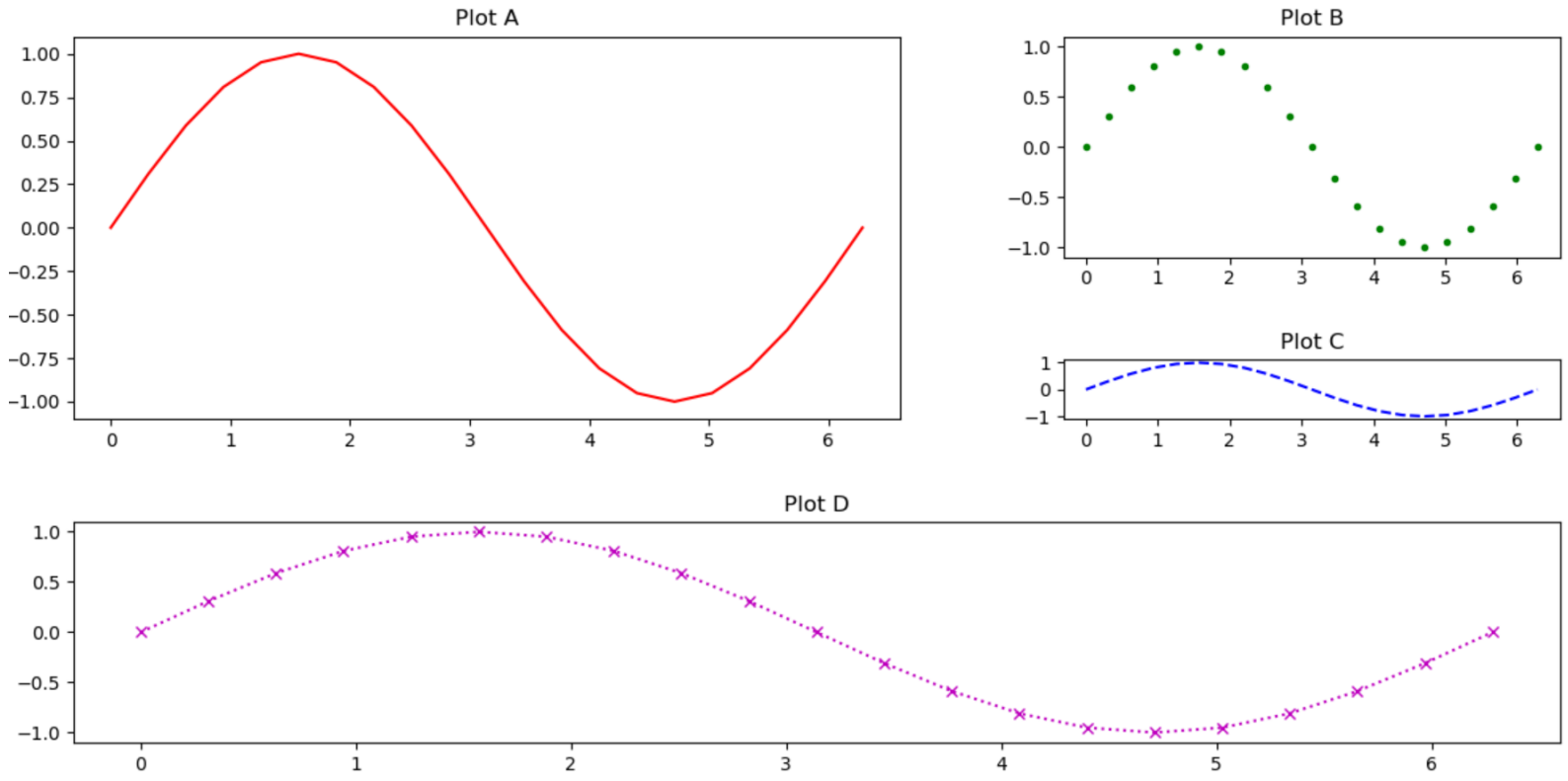


subplot2grid (5 x 5)

matplotlib-subplots.py

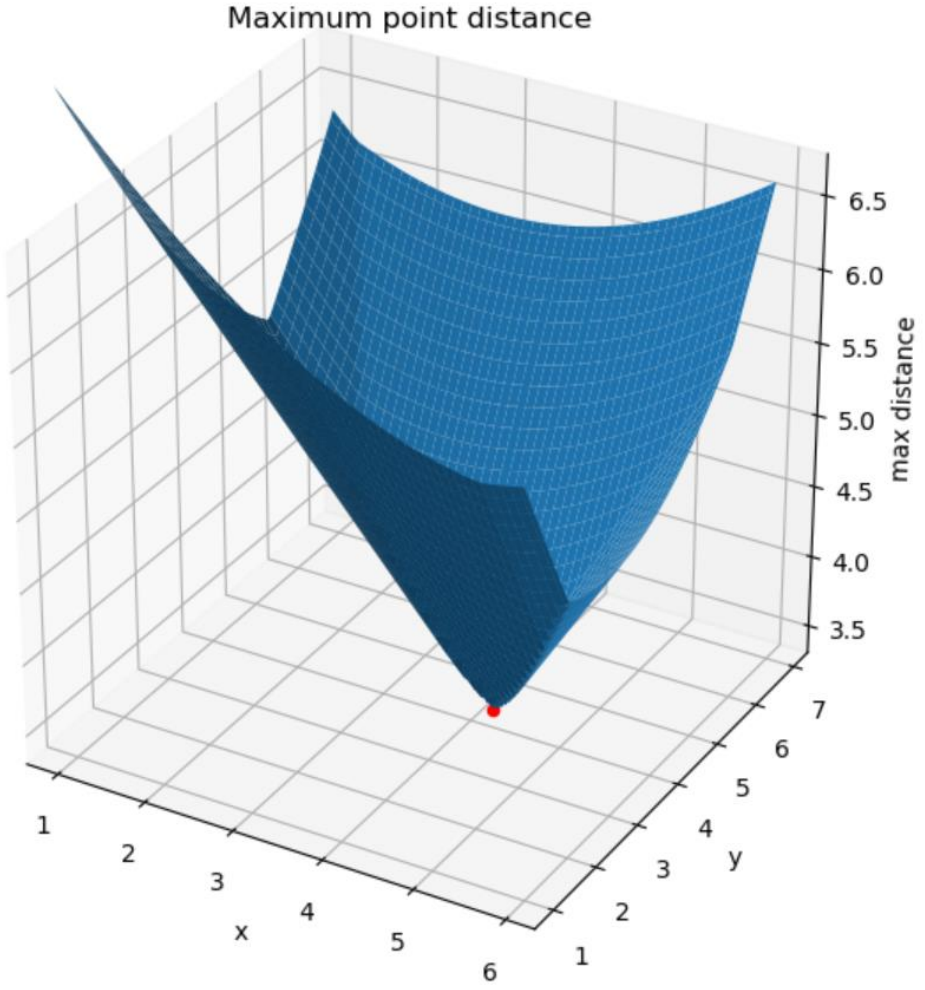
```
import matplotlib.pyplot as plt
import math

x_min, x_max, n = 0, 2 * math.pi, 20

x = [x_min + (x_max - x_min) * i / n
     for i in range(n + 1)]
y = [math.sin(v) for v in x]

plt.subplot2grid((5, 5), (0,0),
                 rowspan=3, colspan=3)
plt.plot(x, y, 'r-')
plt.title('Plot A')

plt.subplot2grid((5, 5), (0,3),
                 rowspan=2, colspan=2)
plt.plot(x, y, 'g.')
plt.title('Plot B')

plt.subplot2grid((5, 5), (2,3),
                 rowspan=1, colspan=2)
plt.plot(x, y, 'b--')
plt.title('Plot C')

plt.subplot2grid((5, 5), (3,0),
                 rowspan=2, colspan=5)
plt.plot(x, y, 'mx:')
plt.title('Plot D')

plt.tight_layout()
plt.show()
```

upper left corner



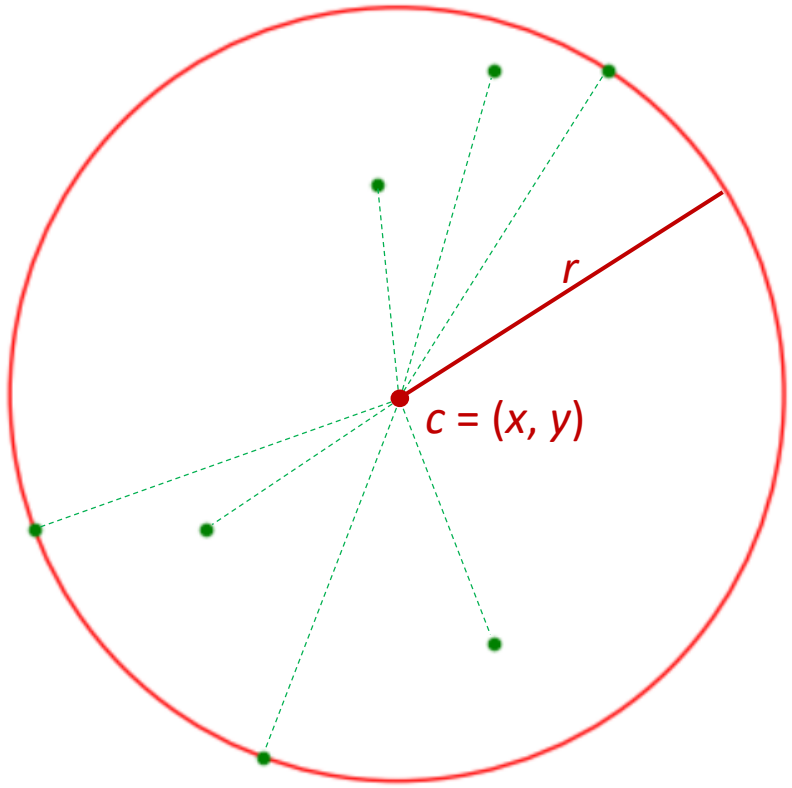
scipy.optimize.minimize

- Find point p minimizing function f
- Supports 13 algorithms – but no guarantee that result correct
- Knowledge about optimization will help you know what optimization algorithm to select and what parameters to provide for better results
- WARNING
  Many solvers return the wrong value



https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.minimize.html

Example: Minimum enclosing circle

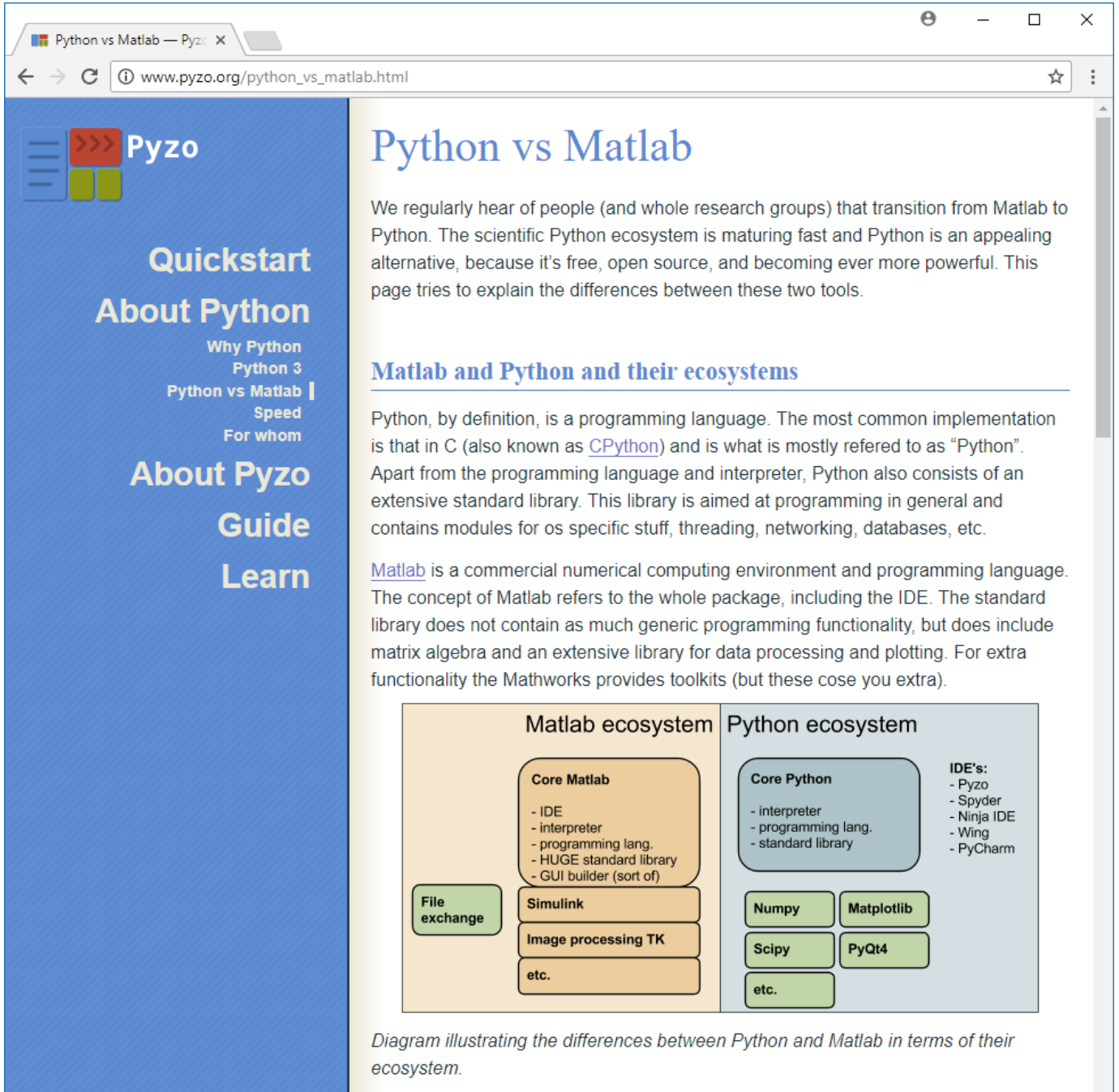


- Find c such that $r = \max_p |p - c|$ is minimized
- A solution is characterized by either 1) three points on circle, where the triangle contains the circle center 2) two opposite points on diagonal
- Try a standard numeric minimization solver
- ⚠ Computation involves max and $\sqrt{x}$, which can be hard for numeric optimization solvers

Python/scipy vs MATLAB

Some basic differences

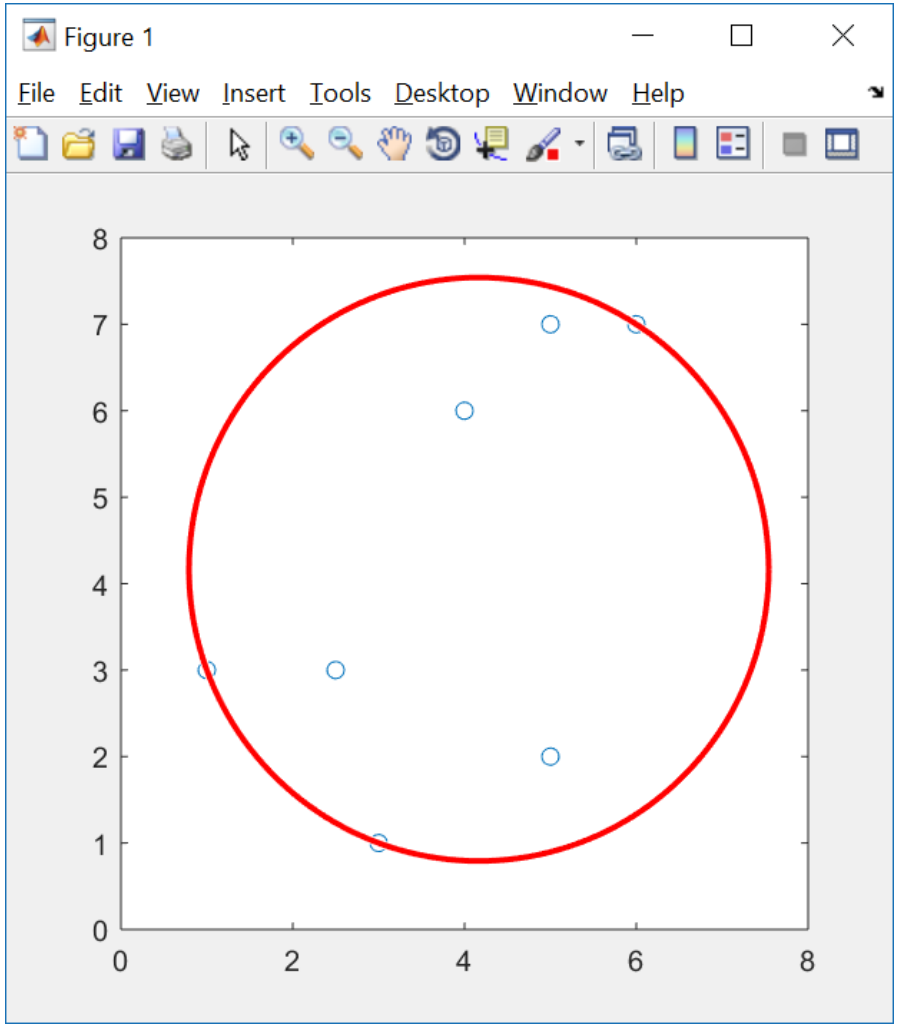
- "**end**" closes a MATLAB block
- "**;**" at end of command avoids command output
- a(1) instead a[i]
- 1st element of a list a(1)
- a(i:j) includes both a(i) and a(j)



Minimum enclosing circle in MATLAB

enclosing_circle.m

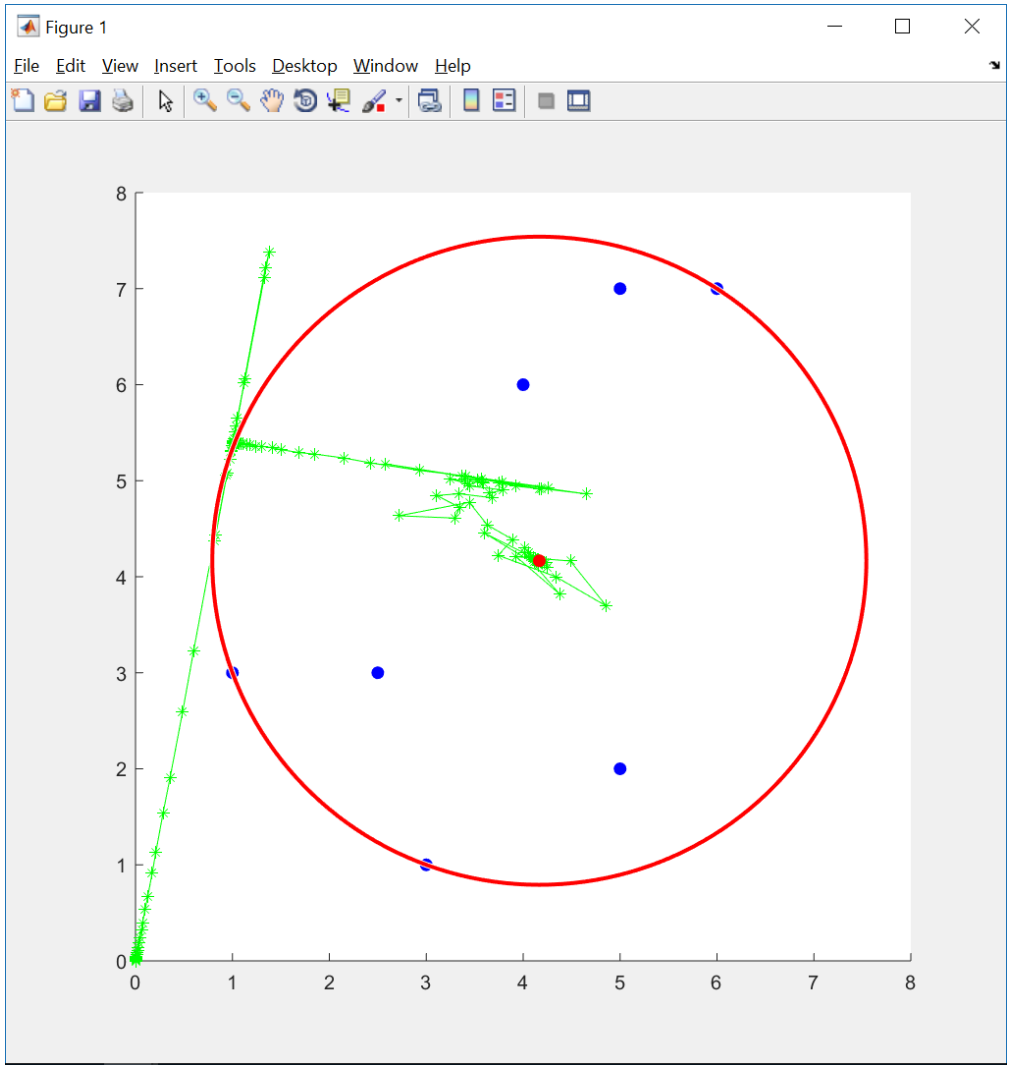
```
% Minimum enclosing circle of a point set
% fminsearch uses the Nelder-Mead algorithm

global x y
x = [1.0, 3.0, 2.5, 4.0, 5.0, 6.0, 5.0];
y = [3.0, 1.0, 3.0, 6.0, 7.0, 7.0, 2.0];
c = fminsearch(@(x) max_distance(x), [0,0]);
plot(x, y, "o");
viscircles(c, max_distance(c));

function dist = max_distance(p)
    global x y
    dist = 0.0;
    for i=1:length(x)
        dist = max(dist, pdist([p; x(i), y(i)],
                               'euclidean'));
    end
end
```



Minimum enclosing circle in MATLAB (trace)

enclosing_circle_trace.m

```
global x y trace_x trace_y

x = [1.0, 3.0, 2.5, 4.0, 5.0, 6.0, 5.0];
y = [3.0, 1.0, 3.0, 6.0, 7.0, 7.0, 2.0];
trace_x = [];
trace_y = [];

c = fminsearch(@(x) max_distance(x), [0,0]);

hold on
plot(x, y, "o", 'color', 'b', 'MarkerFaceColor', 'b');
plot(trace_x, trace_y, "*-", "color", "g");
plot(c(1), c(2), "o", 'color', 'r', 'MarkerFaceColor', 'r');
viscircles(c, max_distance(c),"color","red");

function dist = max_distance(p)
    global x y trace_x trace_y
    trace_x = [trace_x, p(1)];
    trace_y = [trace_y, p(2)];

    dist = 0.0;
    for i=1:length(x)
        dist = max(dist, pdist([p; x(i), y(i)], 'euclidean' ));
    end
end
```



Minimum enclosing circle in Python

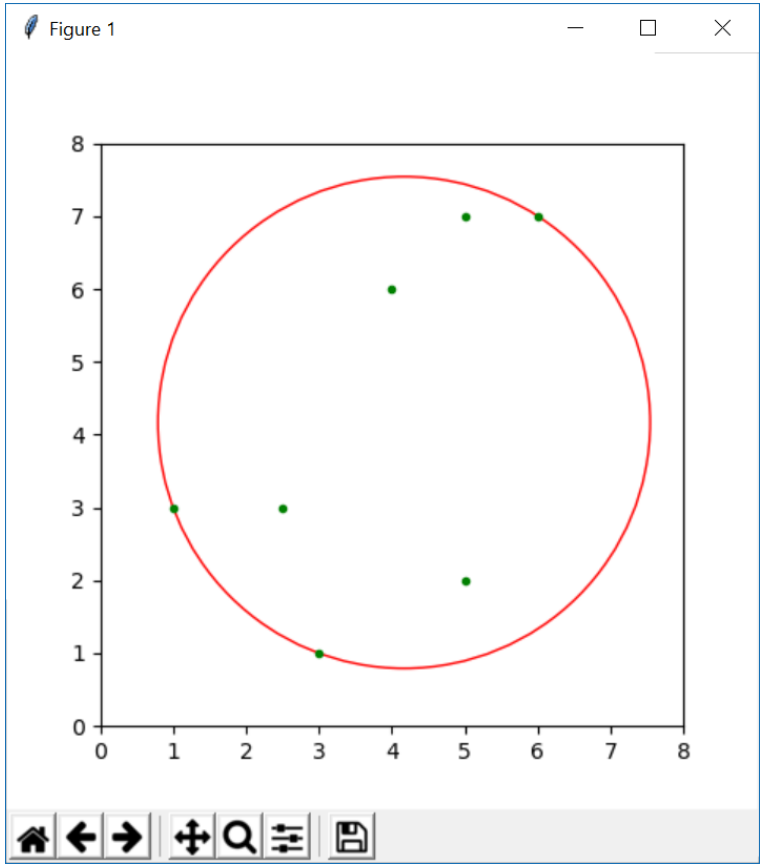
enclosing_circle.py

```
from math import sqrt
from scipy.optimize import minimize
import matplotlib.pyplot as plt

x = [1.0, 3.0, 2.5, 4.0, 5.0, 6.0, 5.0]
y = [3.0, 1.0, 3.0, 6.0, 7.0, 7.0, 2.0]

def dist(p, q):
    return sqrt((p[0]-q[0])**2 + (p[1]-q[1])**2)
def max_distance(c):
    return max([dist(p, c) for p in zip(x, y)])

c = minimize(max_distance, [0.0, 0.0], \
             method="nelder-mead").x
ax = plt.gca()
ax.set_xlim((0, 8))
ax.set_ylim((0, 8))
ax.set_aspect("equal")
plt.plot(x, y, "g.")
ax.add_artist(plt.Circle(c, max_distance(c), \
                         color="r", fill=False))
plt.show()
```

import modules

force optimization method

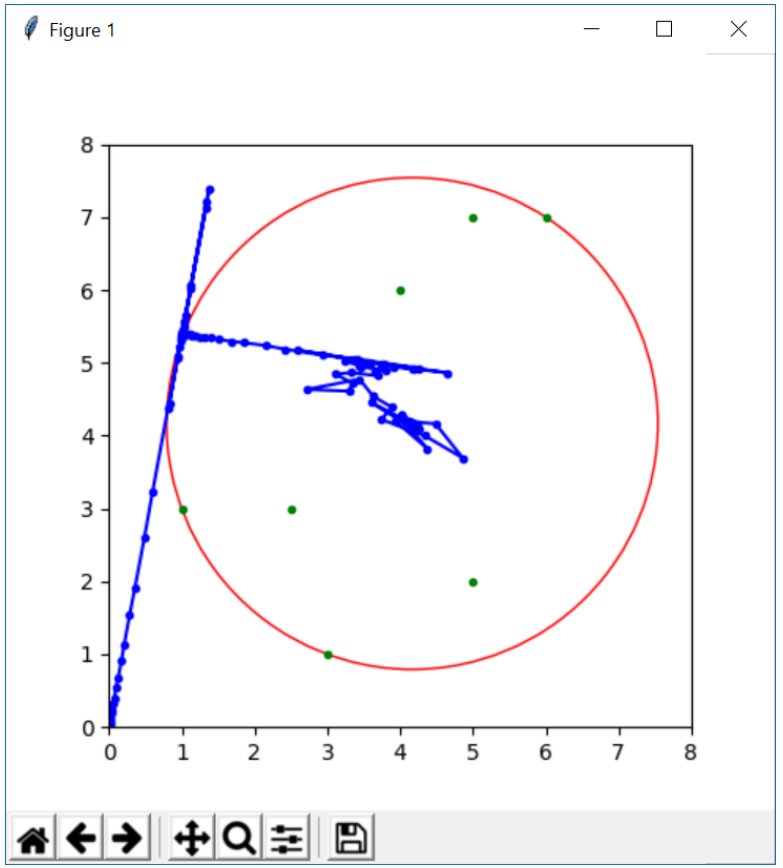
manually set axis (force circle inside plot)



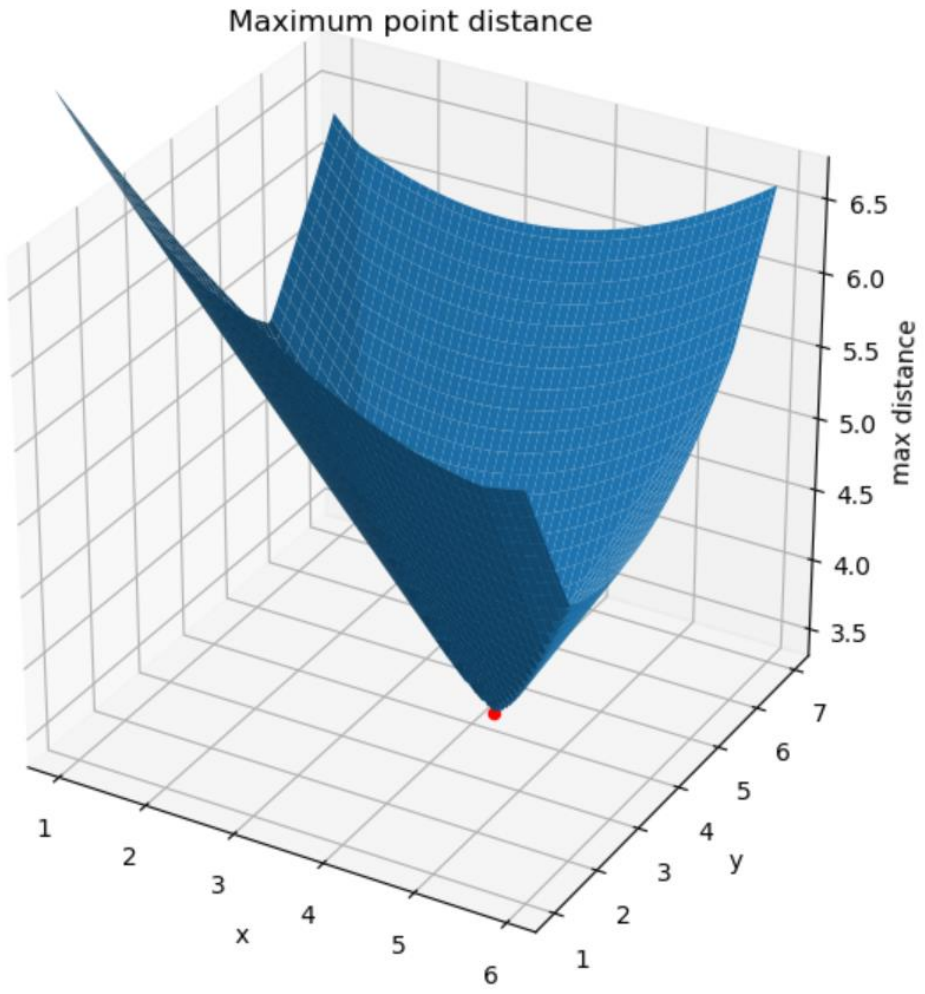
Minimum enclosing circle in Python (trace)

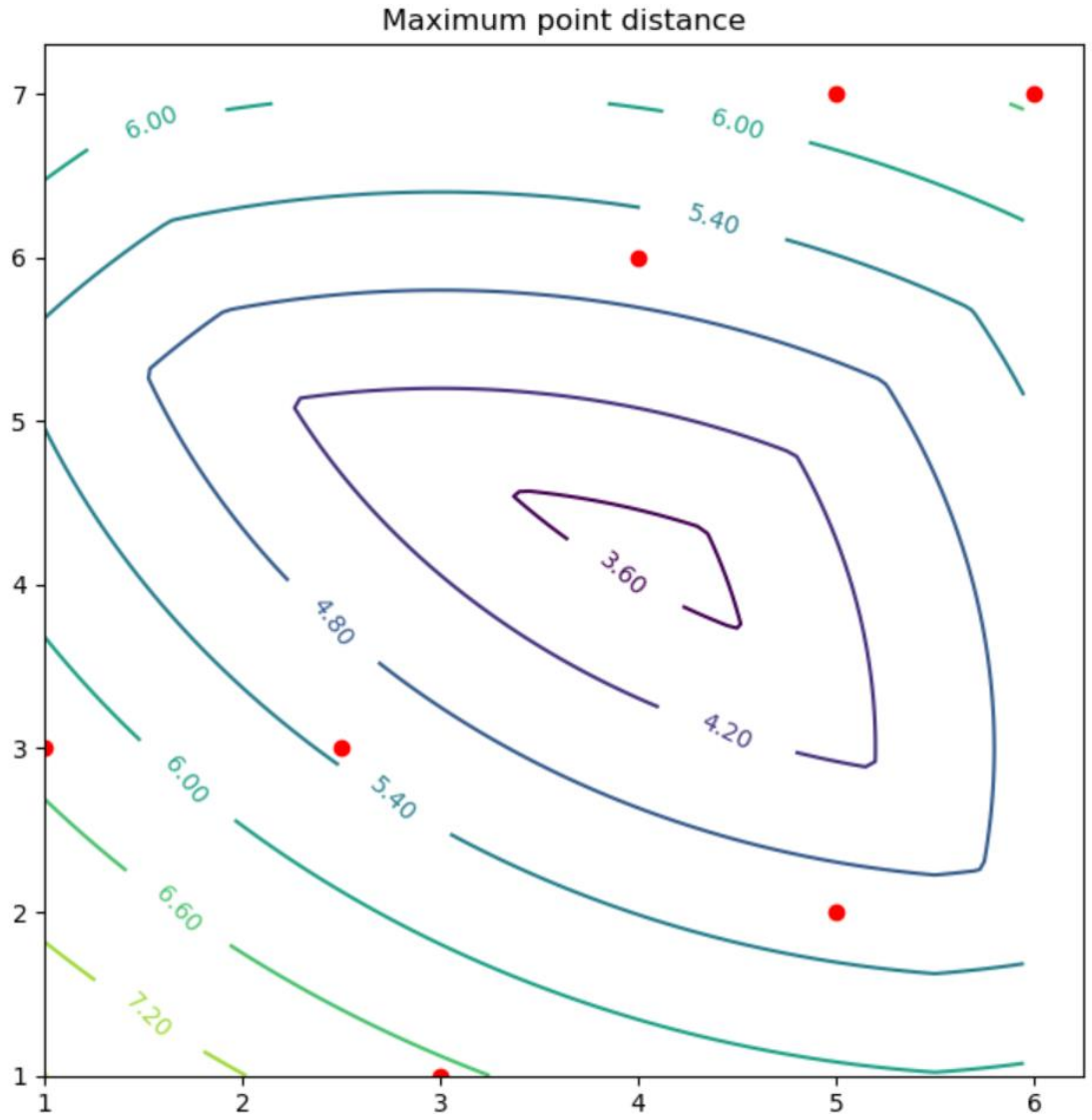
enclosing_circle_trace.py

```
from math import sqrt
from scipy.optimize import minimize
import matplotlib.pyplot as plt

x = [1.0, 3.0, 2.5, 4.0, 5.0, 6.0, 5.0]
y = [3.0, 1.0, 3.0, 6.0, 7.0, 7.0, 2.0]
trace = []

def dist(p, q):
    return sqrt((p[0]-q[0])**2 + (p[1]-q[1])**2)
def max_distance(c):
    trace.append(c)
    return max([dist(p, c) for p in zip(x, y)])

c = minimize(max_distance, [0.0, 0.0],
             method="nelder-mead").x
ax = plt.gca()
ax.set_xlim((0, 8))
ax.set_ylim((0, 8))
ax.set_aspect("equal")
plt.plot(x, y, "g.")
plt.plot(*zip(*trace), "b.-")
ax.add_artist(plt.Circle(c, max_distance(c),
                         color="r", fill=False))
plt.show()
```

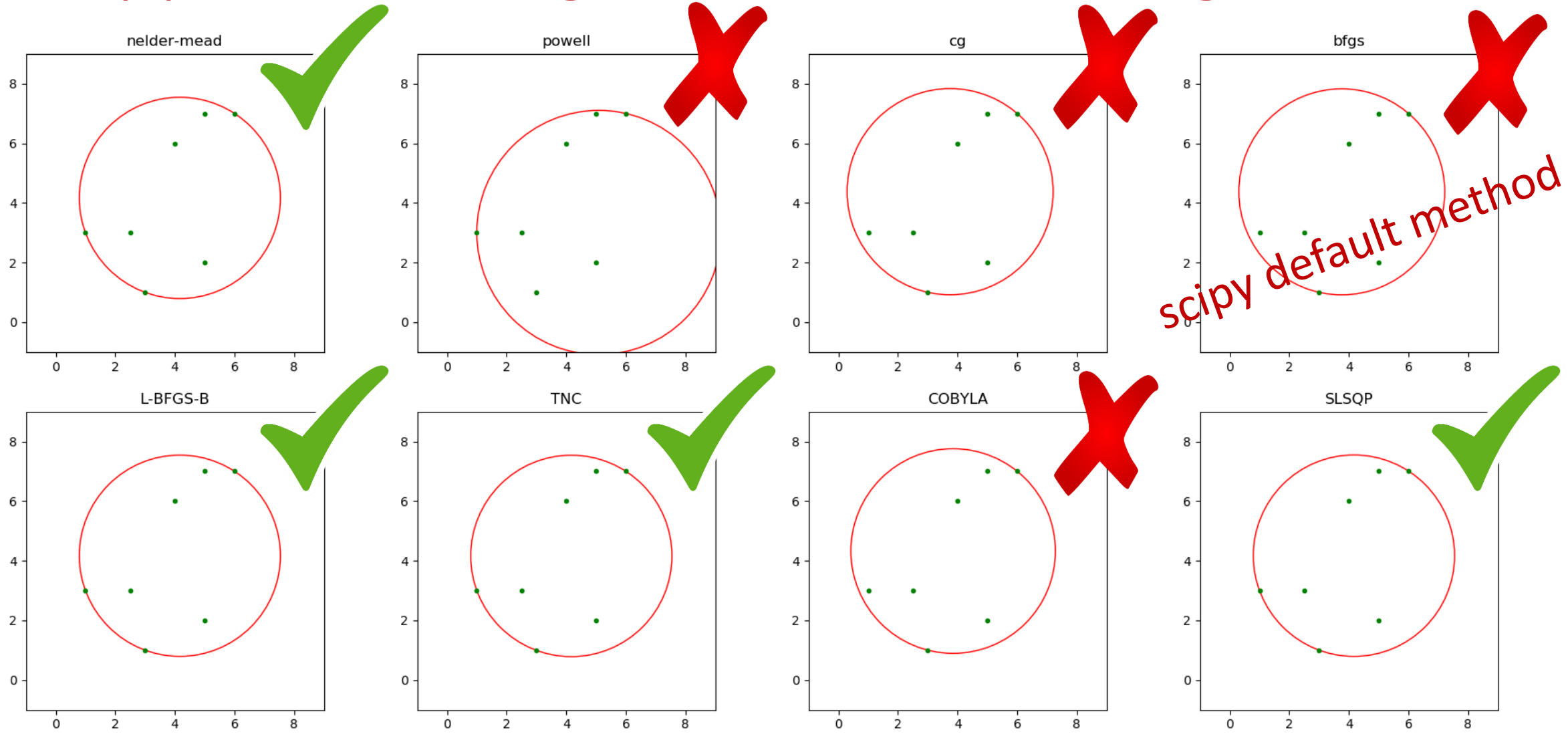


Minimum enclosing circle – search space





scipy.minimize algorithms (without arguments)



https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.minimize.html