Visualization and optimization

- Matplotlib
- Jupyter
- scipy.optimize.minimize

matplotlib

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.

```
pip install matplotlib
```

matplotlib.org

Plot

pyplot module ≈ MATLAB-like plotting framework

matplotlib-simple.py

```python
import matplotlib.pyplot as plt

plt.plot([1, 2, 3], [5, 2, 7], 'bo:')

plt.show()
```

add plot to figure

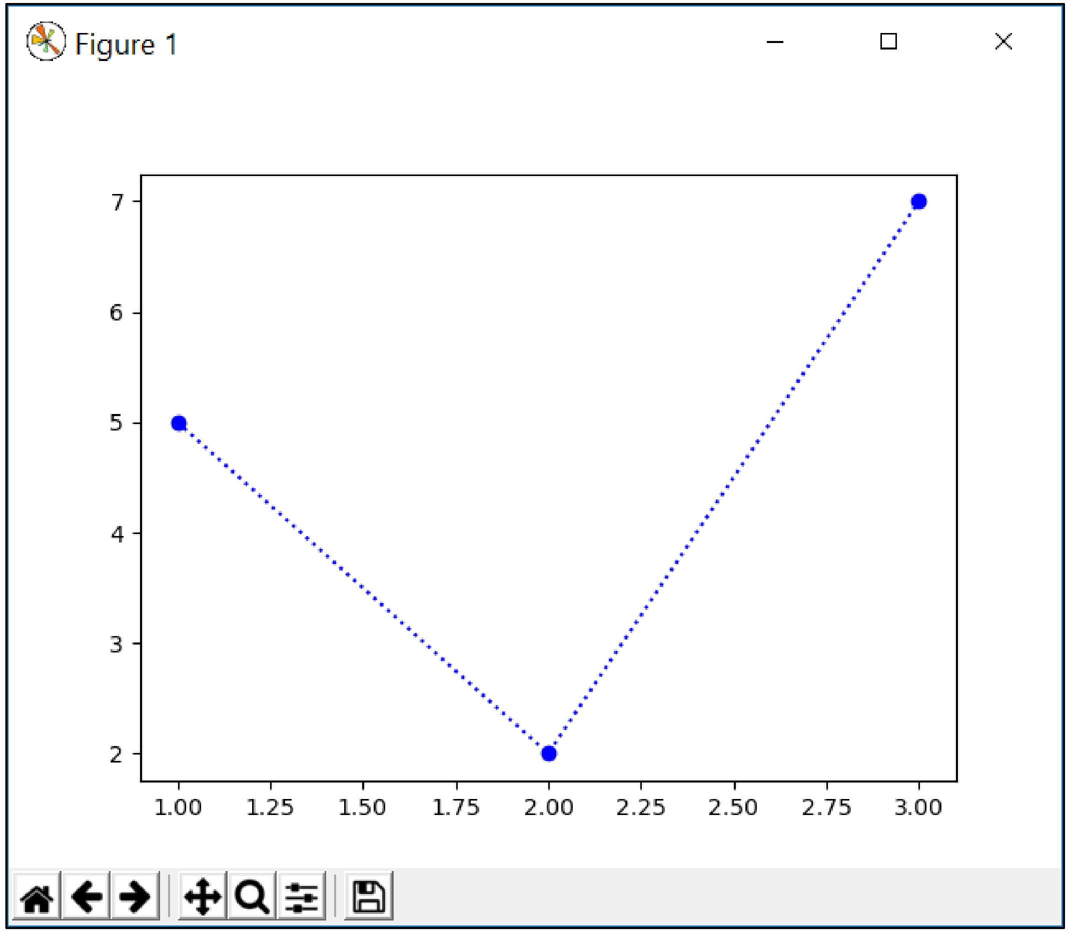
figure is first shown when show is called

x coordinates

y coordinates

format string

Colors		Line styles		Marker styles					
b	🟦	-	———	.	·	2	⋏	+	+
g	🟩	--	– – – –	,	·	3	≺	x	×
r	🟥	-.	—·—·	o	●	4	≻	D	◆
c	🟦	:	········	v	▼	s	■	d	♦
m	🟪			^	▲	p	⬟	|	|
y	🟨			<	◀	*	★	_	–
k	⬛			>	▶	h	⬢		
w	⬜			1	⋎	H	⬣		



save current view as picture

adjust margins

zoom rectangle

pan and zoom

navigate view history

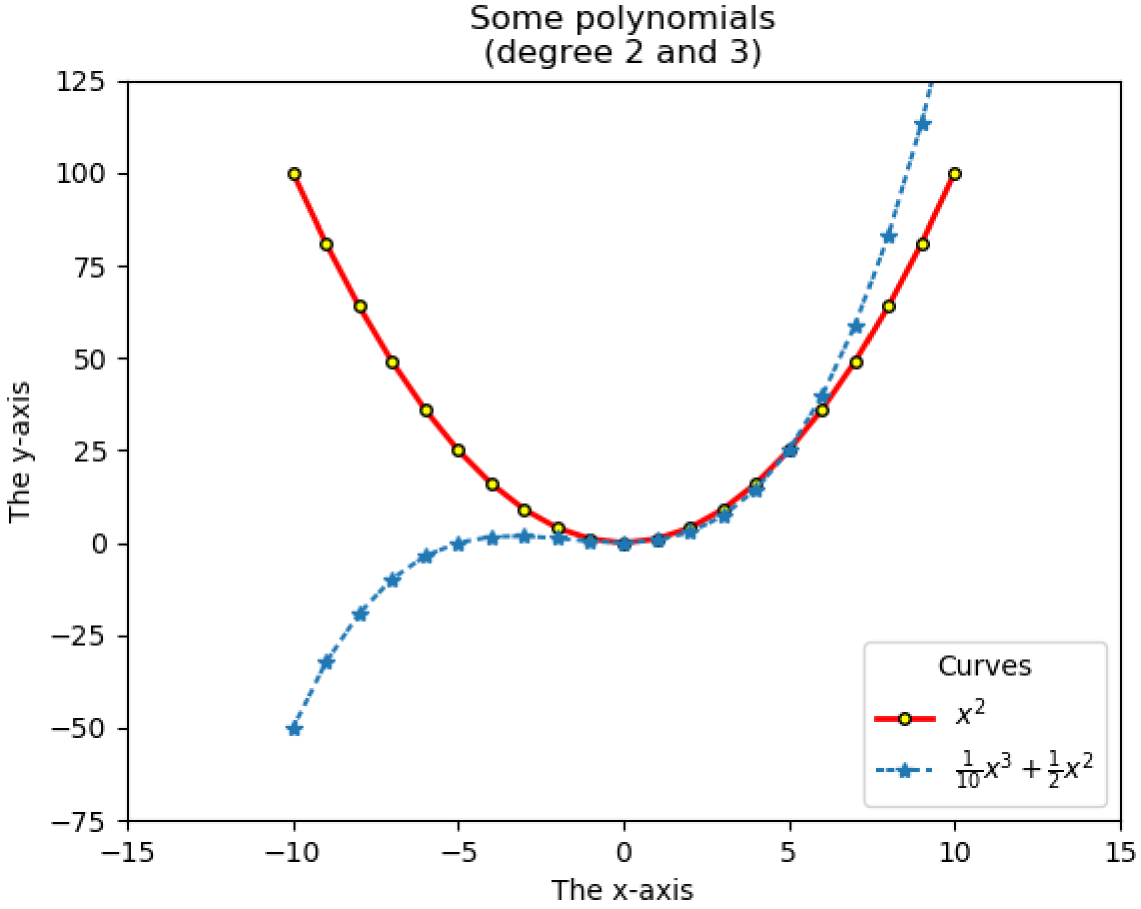
reset view

Plot – some keyword arguments

matplotlib-plot.py

```
import matplotlib.pyplot as plt

X = range(-10, 11)
Y1 = [x ** 2 for x in X]
Y2 = [x ** 3 / 10 + x ** 2 / 2 for x in X]

plt.plot(X, Y1, color='red', label='$x^2$',
    linestyle='-', linewidth=2,
    marker='o', markersize=4,
    markeredgewidth=1,
    markeredgecolor='black',
    markerfacecolor='yellow')

plt.plot(X, Y2, '*', dashes=(2, 0.5, 2, 1.5),
    label=r'$\frac{1}{10}x^3+\frac{1}{2}x^2$')

plt.xlim(-15, 15)
plt.ylim(-75, 125)
plt.title('Some polynomials\n(degree 2 and 3)')

plt.xlabel('The x-axis')
plt.ylabel('The y-axis')
plt.legend(title='Curves')

plt.show()  # finally show figure
```

LaTeX



matplotlib.org/api/_as_gen/matplotlib.pyplot.plot.html

Colors: matplotlib.org/gallery/color/named_colors.html

Scatter (points with individual size and color)

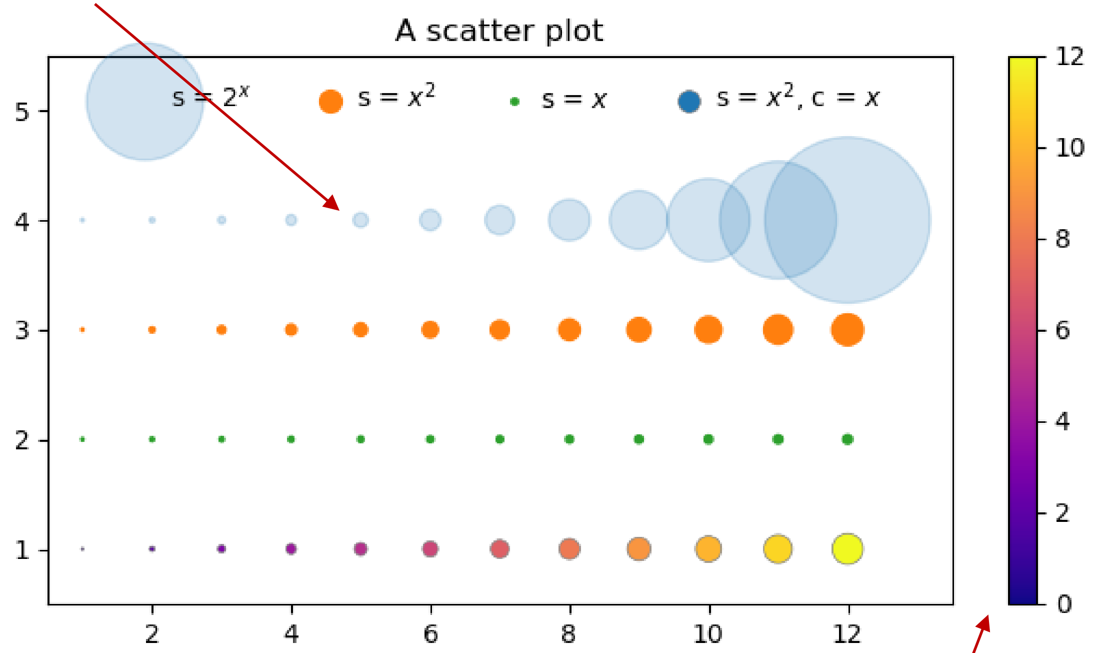
matplotlib-scatter.py

```
import matplotlib.pyplot as plt
n = 13
X = range(n)
S = [x ** 2 for x in X]
E = [2 ** x for x in X]
plt.scatter(X, [4] * n, s=E, label='s = $2^x$', alpha=.2)
plt.scatter(X, [3] * n, s=S, label='s = $x^2$')
plt.scatter(X, [2] * n, s=X, label='s = $x$')
plt.scatter(X, [1] * n, s=S, c=X, cmap='plasma',
    label='s = $x^2$, c = $x$',
    edgecolors='gray', linewidth=0.5)
plt.colorbar()
plt.ylim(0.5, 5.5)
plt.xlim(0.5, 13.5)
plt.title('A scatter plot')
plt.legend(loc='upper center', frameon=False, ncol=4,
           handletextpad=0)
plt.show()
```

transparency

colormap (predefined)
color of each point
size ≈ area of each point
point boundary width
point boundary color

manual placement of legend box (default automatic); remove frame; place legends in 4 columns (default 1); reduce space between marks and label



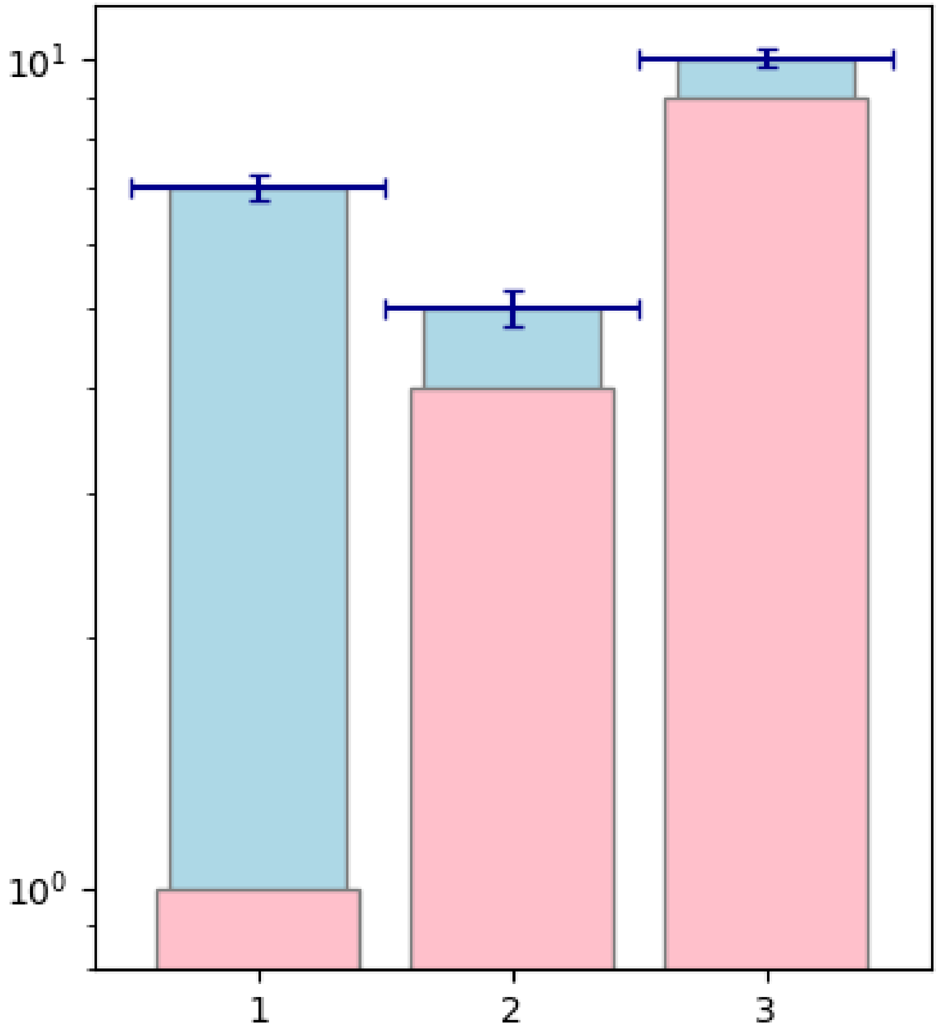
colorbar
(of most recently used colormap)

matplotlib.org/api/_as_gen/matplotlib.pyplot.scatter.html
matplotlib.org/tutorials/colors/colormaps.html

Bars

matplotlib-bars.py

```
import matplotlib.pyplot as plt
x = [1, 2, 3]
y = [7, 5, 10]
plt.bar(x, y,
        color='lightblue',   # bar background color
        linewidth=1,         # bar boundary width
        edgecolor='gray',    # bar boundary color
        tick_label=x,        # ticks on x-axis
        width=0.7,           # width, default 0.8
        yerr=0.25,           # Error bar: y length
        xerr=0.5,            #   x length
        capsize=3,           #   capsize in points
        ecolor='darkblue',   #   error bar color
        log=True)            # y-axis log scale
plt.bar(x, [v**2 for v in x],
        color='pink',
        linewidth=1,
        edgecolor='gray')
plt.show()
```

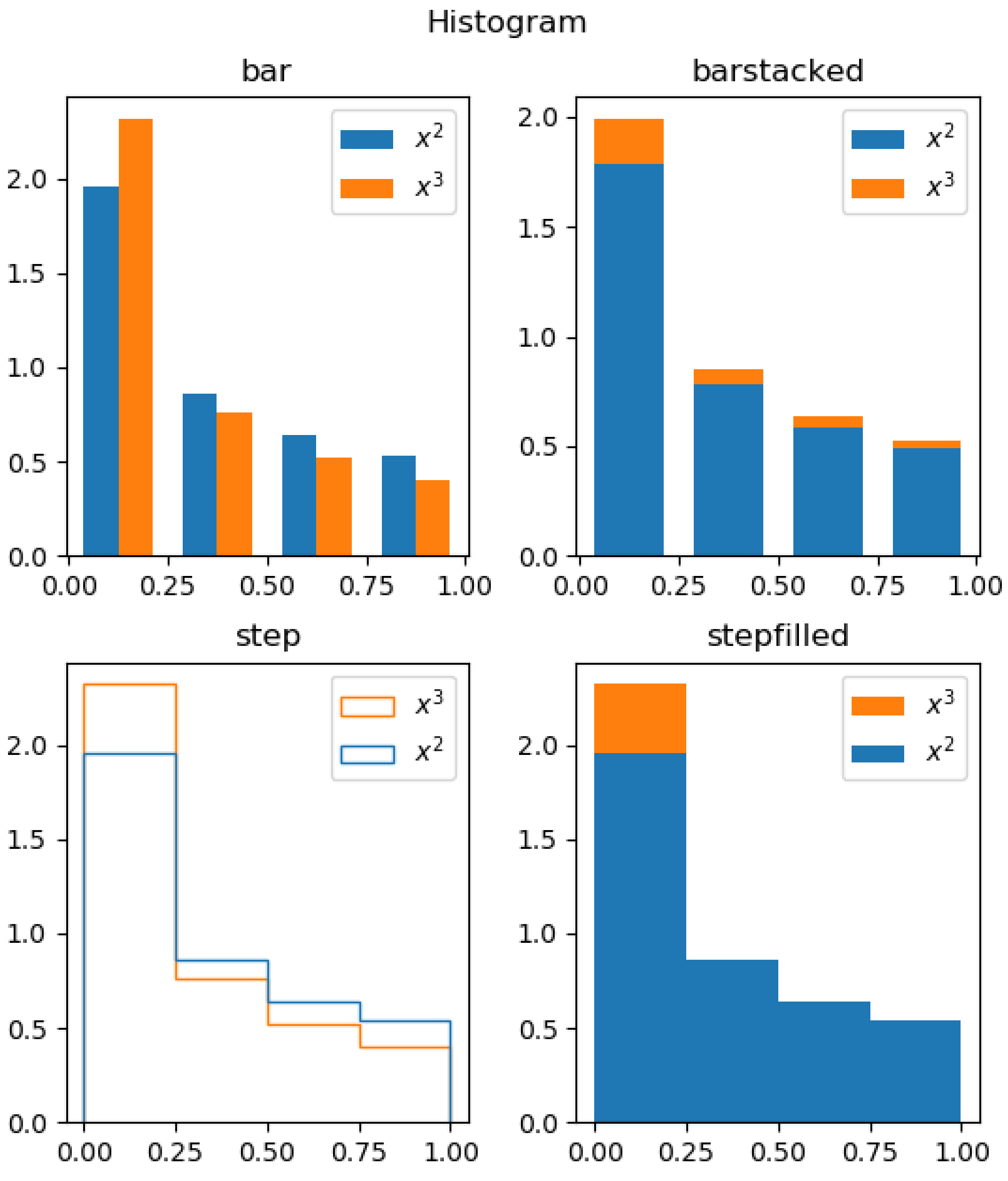


matplotlib.org/api/_as_gen/matplotlib.pyplot.bar.html

Histogram

matplotlib-histogram.py

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

values1 = [random()**2 for _ in range(1000)]
values2 = [random()**3 for _ in range(100)]

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

for i, ht in enumerate(
        ['bar', 'barstacked', 'step', 'stepfilled'],
        start=1):
    plt.subplot(2, 2, i)  # start new plot
    plt.hist([values1, values2],  # data sets
             bins,          # bucket boundaries
             histtype=ht,   # default ht='bar'
             rwidth=0.7,    # fraction of bucket width
             label=['$x^2$', '$x^3$'],  # labels
             density=True)   # norm. prob. density
    plt.title(ht)          # plot title
    plt.xticks(bins)       # ticks on x-axis
    plt.legend()

plt.suptitle('Histogram') # figure title
plt.show()
```

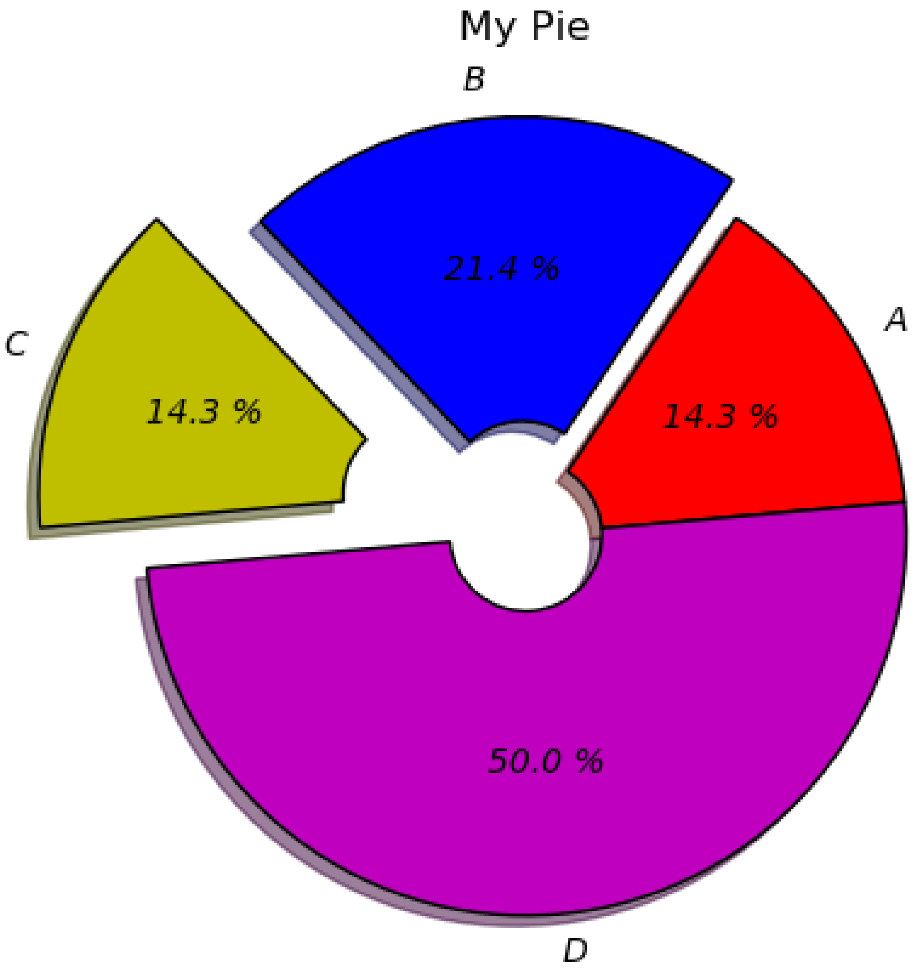


matplotlib.org/api/_as_gen/matplotlib.pyplot.hist.html

Pie

matplotlib-pie.py

```
import matplotlib.pyplot as plt

plt.title('My Pie')
plt.pie([2, 3, 2, 7],         # relative wedge sizes
        labels=['A','B','C','D'],
        colors=['r', 'b', 'y', 'm'],
        explode=(0, 0.1, 0.3, 0),   # radius fraction
        startangle=5,         # angle above horizontal
        counterclock=True,    # default True
        rotatelabels=False,   # default False
        shadow=True,          # default False
        textprops=dict(       # text properties, dict
            color='black',    # text color
            style='italic'),  # text style
        wedgeprops=dict(      # wedge properties, dict
            width=0.8,        # width (missing center)
            linewidth=1,      # wedge boundary width
            edgecolor='black'),  # boundary color
        autopct='%1.1f %%')   # percent formatting
plt.show()
```



matplotlib.org/api/_as_gen/matplotlib.pyplot.pie.html

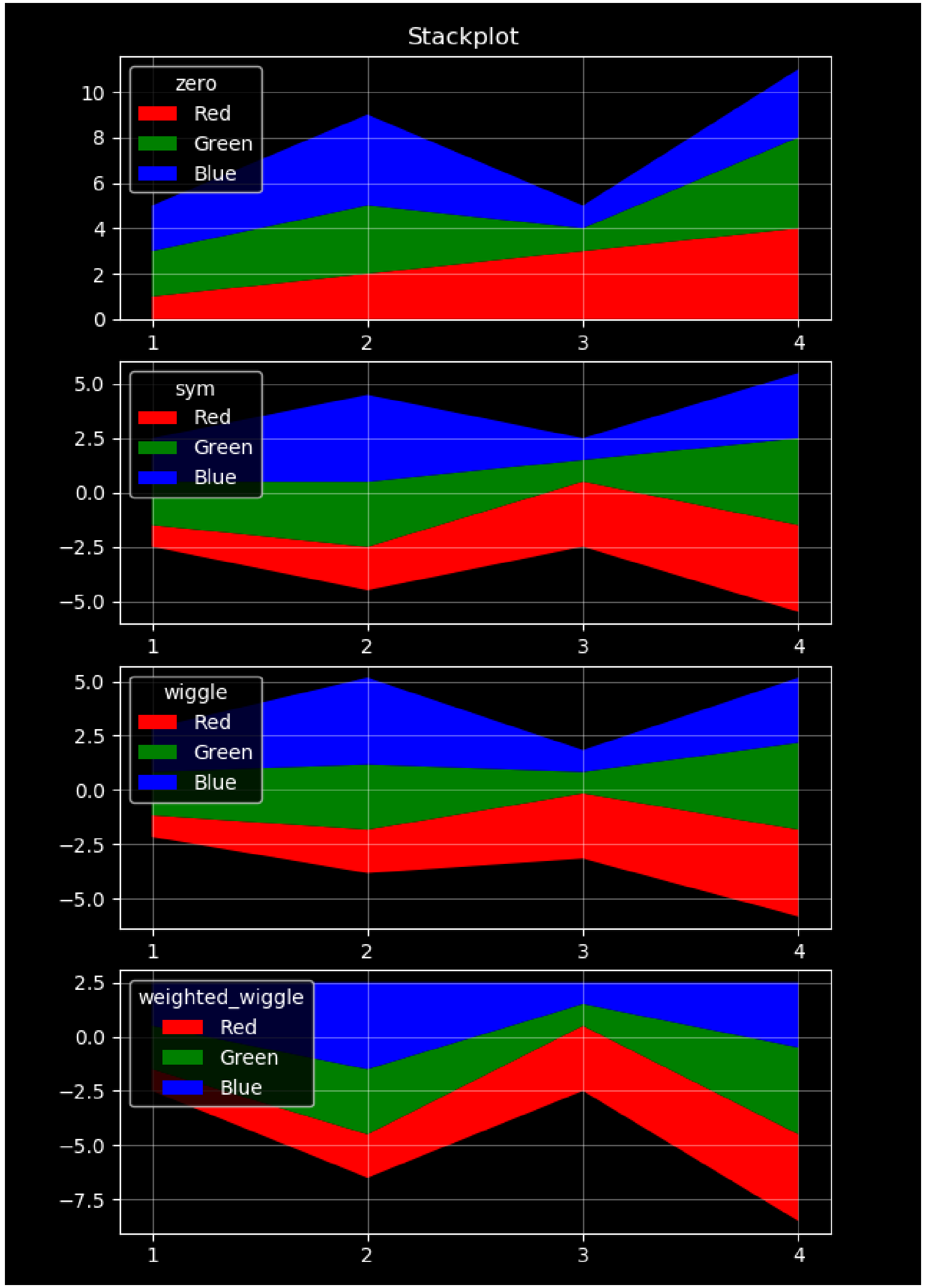
Stackplot

matplotlib-stackplot.py

```python
import matplotlib.pyplot as plt

x = [1, 2, 3, 4]

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

plt.style.use('dark_background')
for i, base in enumerate(
        ['zero', 'sym', 'wiggle','weighted_wiggle'],
        start=1):
    plt.subplot(4, 1, i)
    plt.stackplot(x, y1, y2, y3,
                  colors=['r', 'g', 'b'],
                  labels=['Red', 'Green', 'Blue'],
                  baseline=base)
    plt.grid(axis='both',  # 'x', 'y', or 'both'
        linewidth=0.5, linestyle='-', alpha=0.5)
    plt.legend(title=base, loc='upper left')
    plt.xticks(x)  # a tick for each value in x

plt.suptitle('Stackplot')
plt.show()
```

Stacked Graphs – Geometry & Aesthetics
Lee Byron & Martin Wattenberg, 2008

To list all available styles:
`print(plt.style.available)`

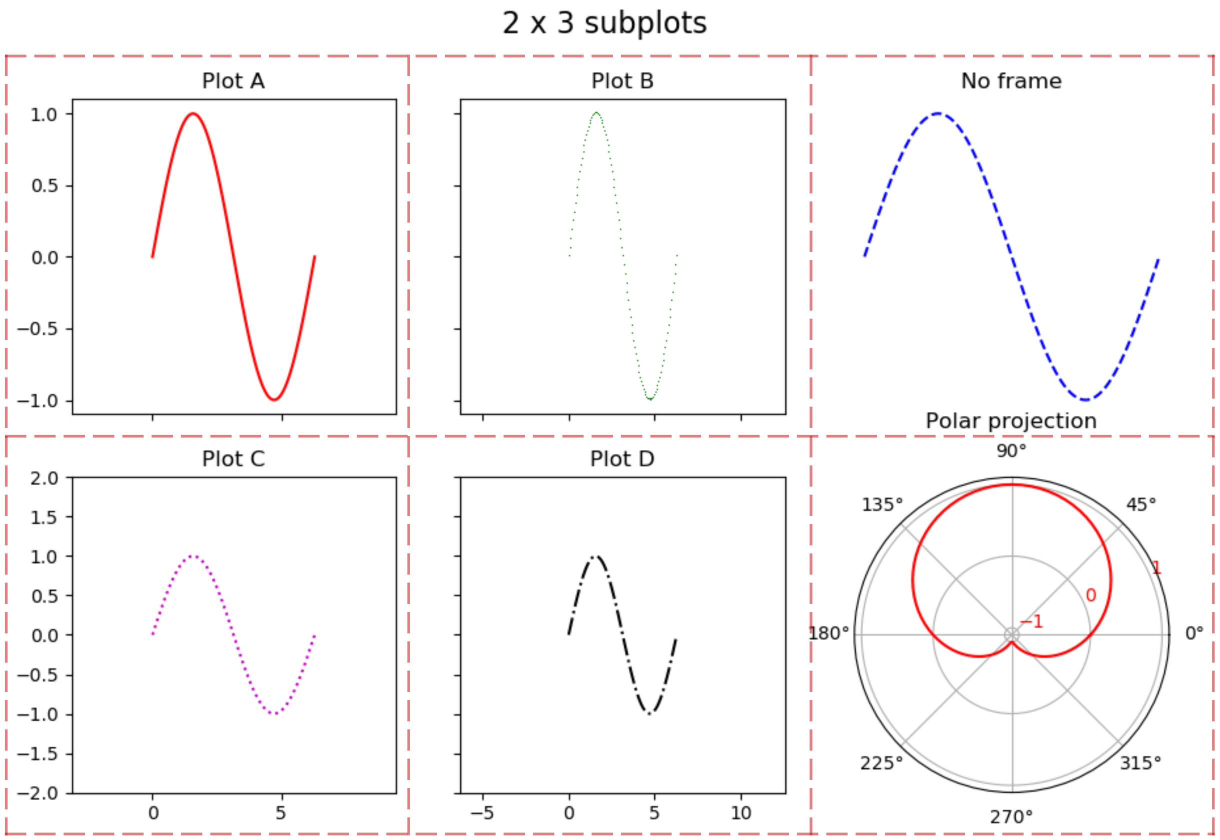


matplotlib.org/api/_as_gen/matplotlib.pyplot.stackplot.html matplotlib-subplot.py

```python
import matplotlib.pyplot as plt
from math import pi, sin
x_min, x_max, n = 0, 2 * pi, 100
x = [x_min + (x_max - x_min) * i / n for i in range(n + 1)]
y = [sin(v) for v in x]
ax1 = plt.subplot(2, 3, 1)  # 2 rows, 3 columns
ax1.label_outer()           # removes x-axis labels
plt.xlim(-pi, 3 * pi)       # increase x-axis range
plt.plot(x, y, 'r-')
plt.title('Plot A')
ax2 = plt.subplot(2, 3, 2)
ax2.label_outer()           # removes x- and y-axis labels
plt.xlim(-2 * pi, 4 * pi)   # increase x-axis range
plt.plot(x, y, 'g,')
plt.title('Plot B')
ax3 = plt.subplot(2, 3, 3, frameon=False)  # remove frame
ax3.set_xticks([])          # remove x-axis ticks & labels
ax3.set_yticks([])          # remove x-axis ticks & labels
plt.plot(x, y, 'b--')
plt.title('No frame')
ax4 = plt.subplot(2, 3, 4, sharex=ax1)  # share x-axis range
plt.ylim(-2, 2)             # increase y-axis range
plt.plot(x, y, 'm:')
plt.title('Plot C')
ax5 = plt.subplot(2, 3, 5, sharex=ax2, sharey=ax4) # share ranges
ax5.set_xticks(range(-5, 15, 5))  # specific x-ticks & x-labels
ax5.label_outer()           # removes y-axis labels
plt.plot(x, y, 'k-.')
plt.title('Plot D')
ax6 = plt.subplot(2, 3, 6, projection='polar')  # polar projection
ax6.set_yticks([-1, 0, 1])                       # y-labels
ax6.tick_params(axis='y', labelcolor='red')     # color of y-labels
plt.plot(x, y, 'r')
plt.title('Polar projection\n')  # \n to avoid overlap with 90°
plt.suptitle('2 x 3 subplots', fontsize=16)
plt.show()
```

Subplot

(2 rows, 3 columns)



- Subplots are numbered 1..6 row-by-row, starting top-left
- subplot returns an axes to access the plot in the figure

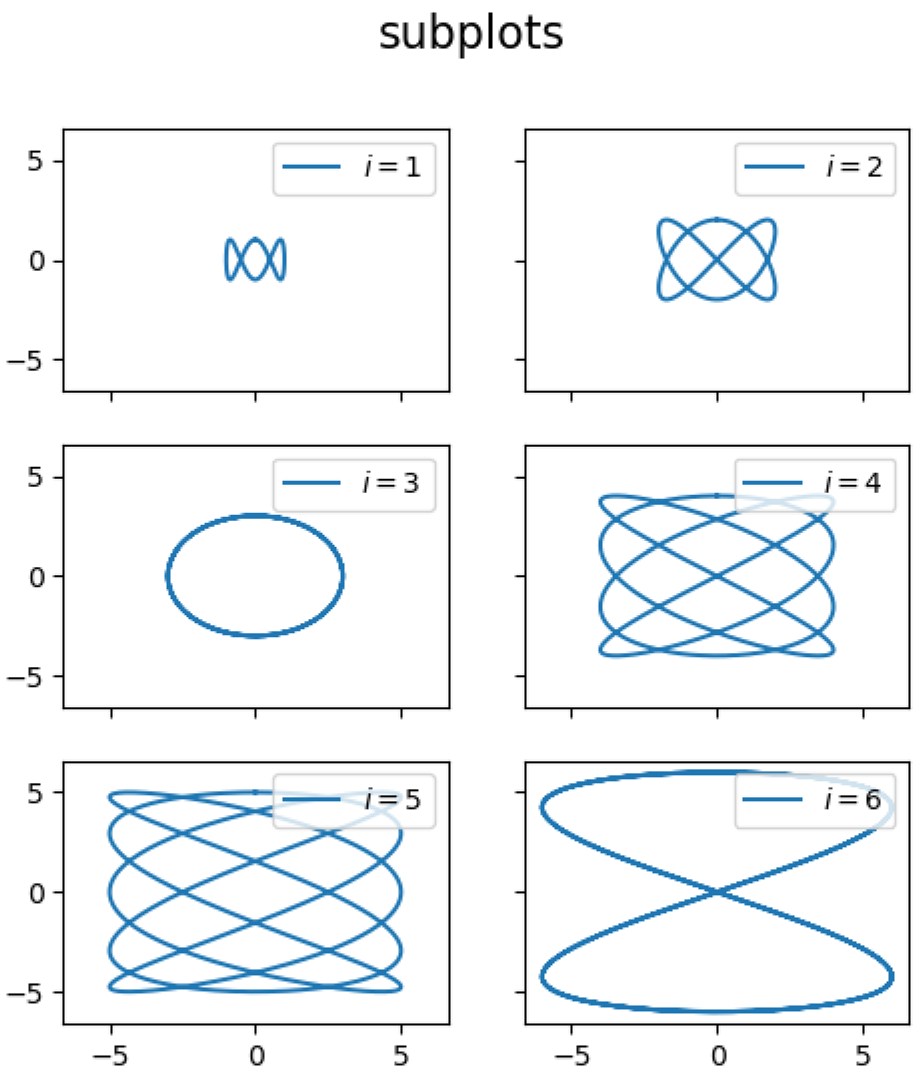
matplotlib.org/api/_as_gen/matplotlib.pyplot.subplot.html

Subplots

matplotlib-subplots.py

```
import matplotlib.pyplot as plt
from math import pi, sin, cos
times = [2 * pi * t / 1000 for t in range(1001)]

fig, ((ax1, ax2), (ax3, ax4), (ax5, ax6)) = \
    plt.subplots(3, 2, sharex=True, sharey=True)

for i, ax in enumerate([ax1, ax2, ax3, ax4, ax5, ax6],
                       start=1):
    x = [i * sin(i * t) for t in times]
    y = [i * cos(3 * t) for t in times]
    ax.plot(x, y, label=f'$i = {i}$')  # plot to axes
    ax.legend(loc='upper right')       # axes legend
fig.suptitle('subplots', fontsize=16)  # figure title
plt.show()
```

create 6 axes in 3 rows with 2 colums
share the x- and y-axis ranges (automatically
applies label_outer to created axes)
returns a pair (figure, axes)



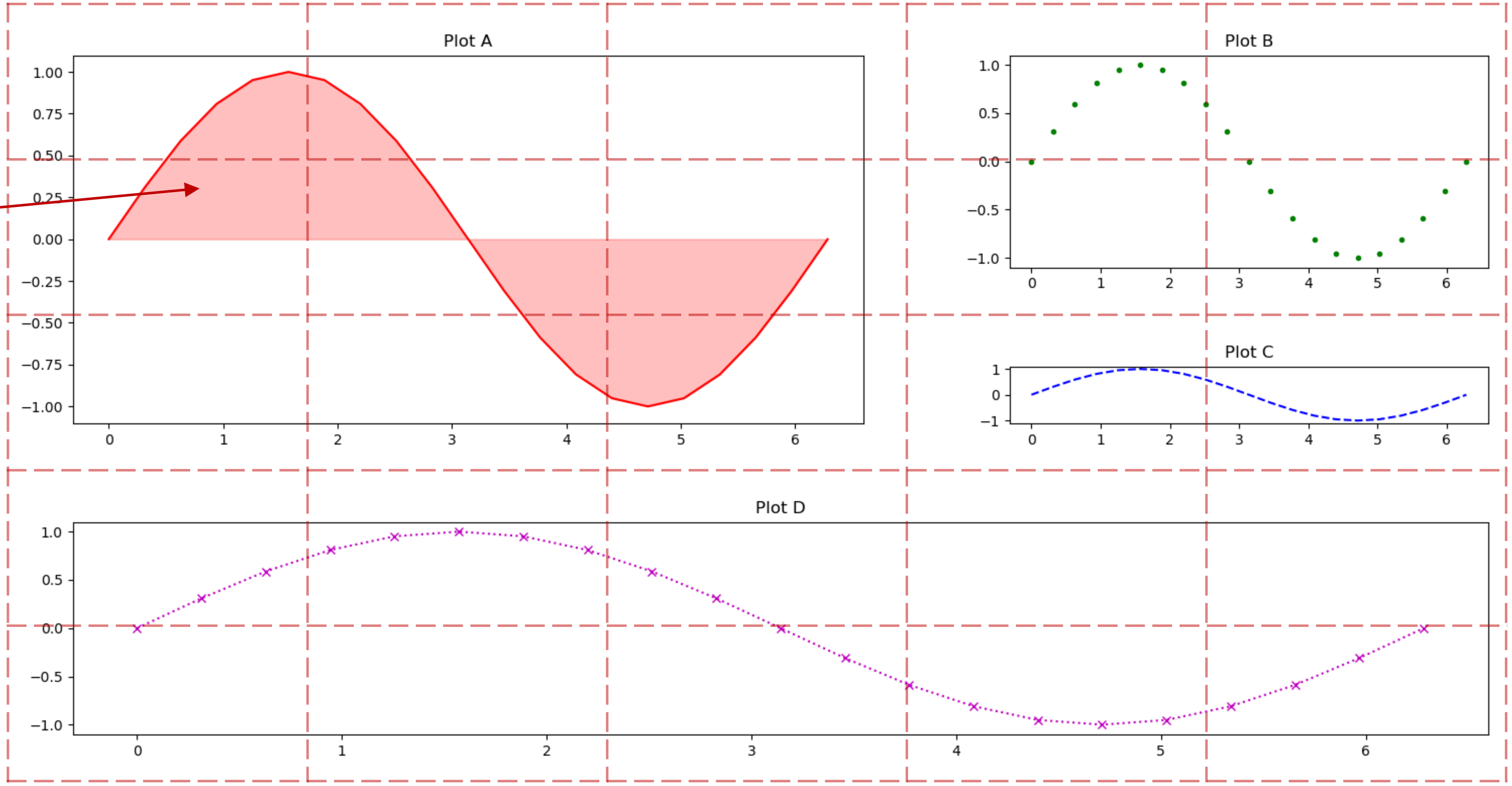
matplotlib.org/api/_as_gen/matplotlib.pyplot.subplots.html

subplot2grid (5 x 5)

matplotlib-subplot2grid.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.fill_between(x, 0.0, y,
                          alpha=0.25, color='r')
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()  # adjust padding
plt.show()
```

upper left corner (row, column)

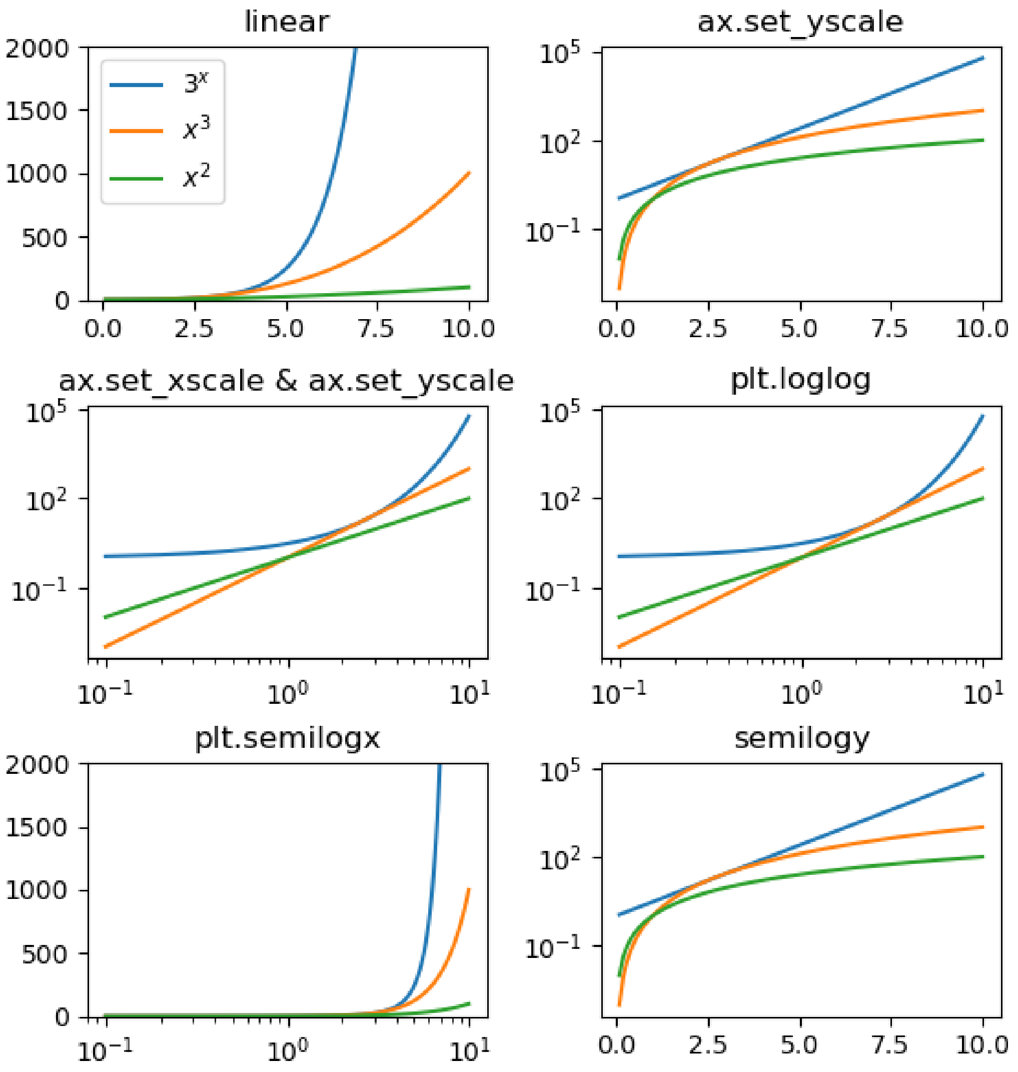


matplotlib.org/api/_as_gen/matplotlib.pyplot.subplot2grid.html

log scales

matplotlib-log.py

```
import matplotlib.pyplot as plt
x = [i / 10 for i in range(1, 101)]
y1 = [i ** 2 for i in x]
y2 = [i ** 3 for i in x]
y3 = [3 ** i for i in x]
for i in range(1, 7):
    ax = plt.subplot(3, 2, i)
    plt.plot(x, y3, label='$3^x$')
    plt.plot(x, y2, label='$x^3$')
    plt.plot(x, y1, label='$x^2$')
    if i == 1:
        plt.ylim(0, 2000)
        plt.xscale('linear')  # default
        plt.yscale('linear')  # default
        plt.legend()
        plt.title('linear')
    if i == 2:
        plt.yscale('log')
        plt.title('ax.yscale')
    if i == 3:
        ax.set_xscale('log')
        ax.set_yscale('log')
        plt.title('ax.set_xscale & ax.set_yscale')
    if i == 4:
        plt.loglog()
        plt.title('plt.loglog')
    if i == 5:
        plt.ylim(0, 2000)
        plt.semilogx()
        plt.title('plt.semilogx')
    if i == 6:
        plt.semilogy()
        plt.title('semilogy')
plt.show()
```

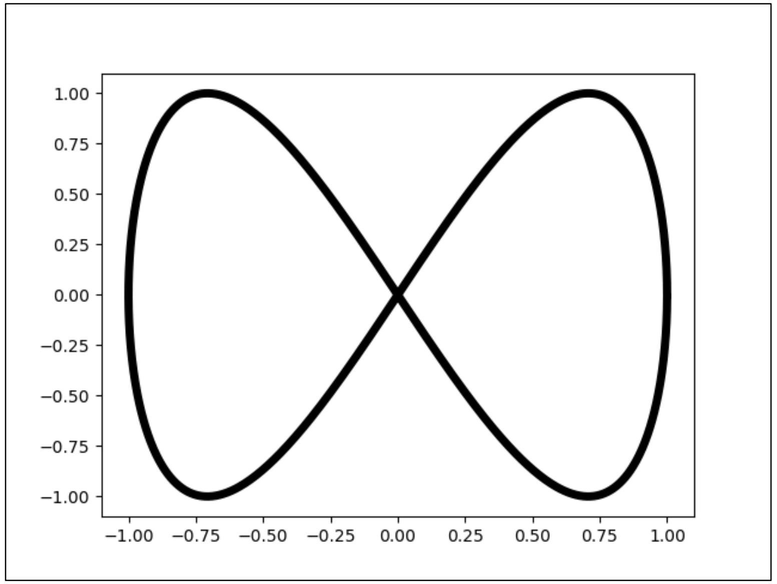


- There are many ways to make the x- and/or y-axis logarithmic with pyplot

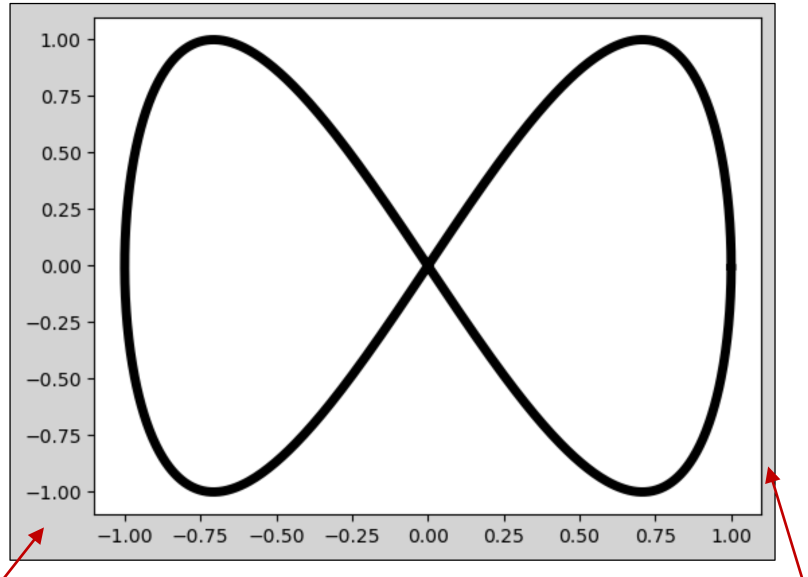
Saving figures

matplotlib-savefig.py

```python
import matplotlib.pyplot as plt
from math import pi, sin, cos
n = 1000
points = [(cos(2 * pi * i / n),
           sin(4 * pi * i / n)) for i in range(n)]
x, y = zip(*points)
plt.plot(x, y, 'k-', linewidth=5)
plt.savefig('butterfly.png')  # save plot as PNG
plt.savefig('butterfly-grey.png',
    dpi=100,                  # dots per inch
    bbox_inches='tight',      # crop to bounding box
    pad_inches=0.1,           # space around figure
    facecolor='lightgrey',    # background color
    format='png')             # optional if file extension
plt.savefig('butterfly.pdf')  # save plot as PDF
plt.show()                    # interactive viewer
```



butterfly.png



butterfly-grey.png

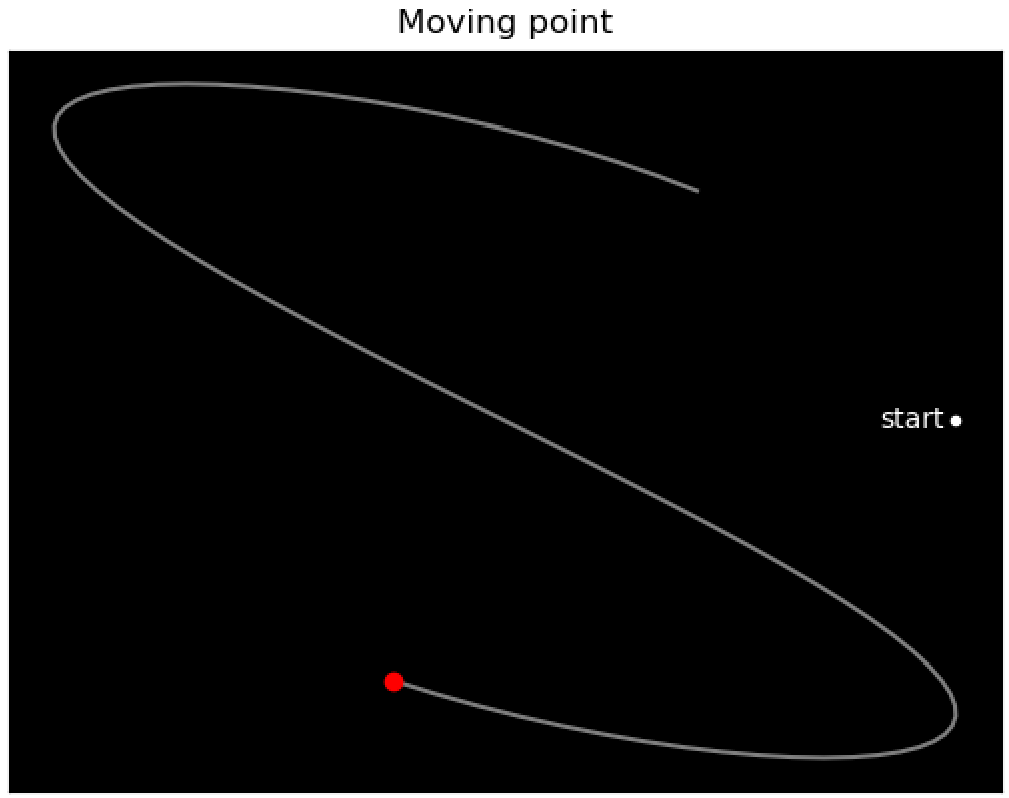
facecolor

pad_inches

matplotlib.org/api/_as_gen/matplotlib.pyplot.savefig.html matplotlib-animation.py

```python
import matplotlib.pyplot as plt
from matplotlib.animation import FuncAnimation
from math import pi, cos, sin

n, tail_length = 200, 75
points = []                # tail_length recent poins

def point(i):
    t = 2 * pi * i / n
    return (cos(3 * t), sin(2 * t))

fig = plt.figure()         # new figure
ax = plt.gca()             # get current axes
ax.set_facecolor('black')  # set background color
plt.xlim(-1.1, 1.1)        # set x-axis range
plt.ylim(-1.1, 1.1)        # set y-axis range
plt.xticks([])             # remove x-ticks & labels
plt.yticks([])             # remove y-ticks & labels
plt.title('Moving point')  # plot title

x, y = point(0)
plt.plot(x, y, 'w.')       # start point
plt.text(x - 0.025, y, 'start', color='w', # text label
    ha='right', va='center')                # alignment
tail, = plt.plot([], [], 'w-', alpha=0.5)  # init. tail
head, = plt.plot([], [], 'ro')      # init. current point

def move(frame):      # frame = value from frames
    points.append(point(frame))
    del points[:-tail_length]       # limit tail
    tail.set_data(*zip(*points))    # update tail points
    head.set_data(*points[-1])      # update head point

animation = FuncAnimation(fig,      # figure to animate
    func=move,        # function called for each frame
    frames=range(n),  # array like to iterate over
    interval=25,      # milliseconds between frames
    repeat=True,      # repeat frames when done
    repeat_delay=0)   # wait milliseconds before repeat

plt.show()
```

matplotlib.animation.FuncAnimation



- **plot** returns "Line2D" objects representing the plotted data
- "Line2D" objects can be updated using **set_data**
- To make an animation you need to repeatedly update the "line2D" objects
- **FuncAnimation** repeatedly calls func in regular intervals interval, each time with the next value from frames (if frames is None, then the frame values provided to func will be the infinite sequence 0,1,2,3,...)

matplotlib.org/api/_as_gen/matplotlib.animation.FuncAnimation.html

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.

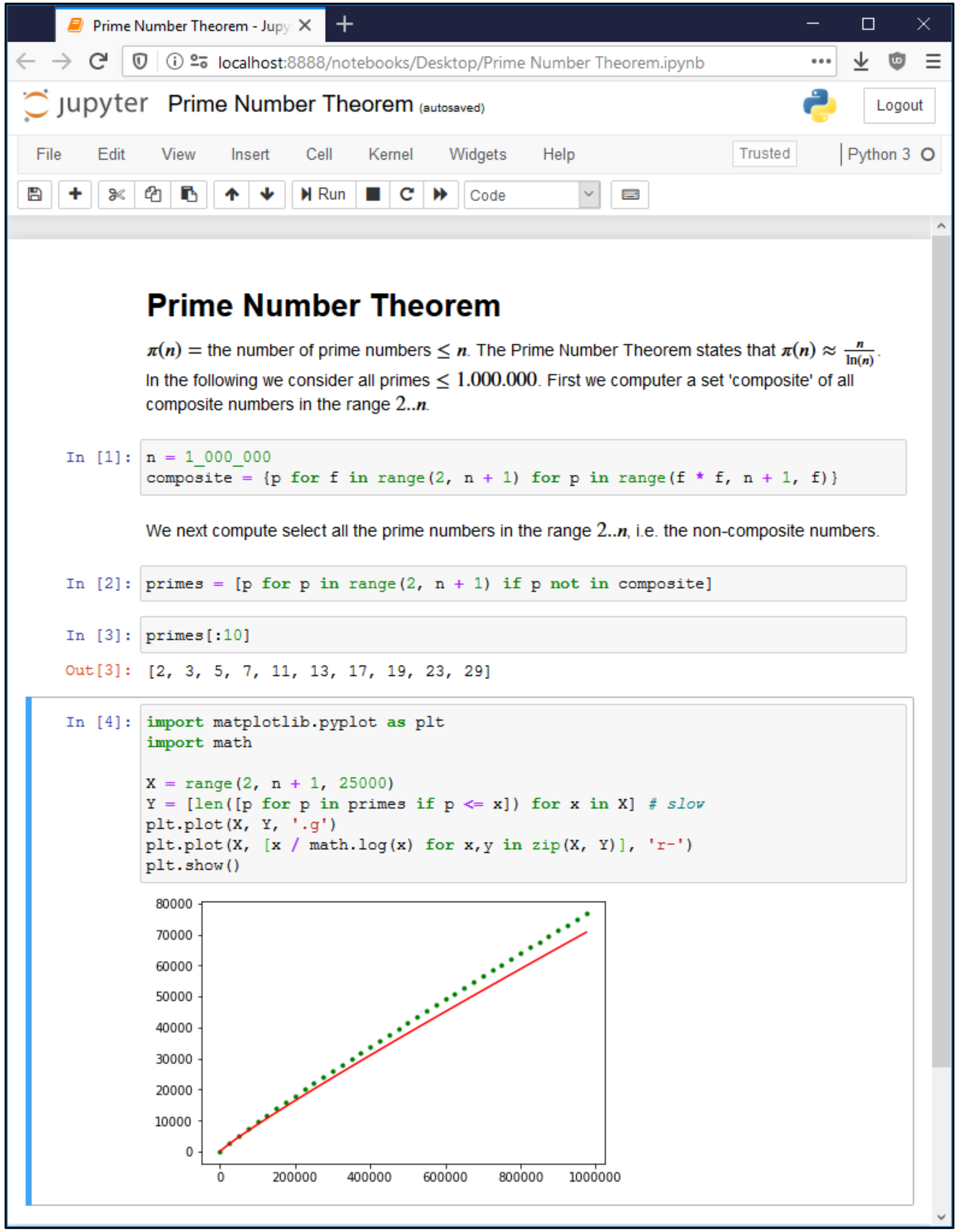
jupyter.org

python

IP[y]:
IPython

jupyter

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


Prime Number Theorem - Jupy
localhost:8888/notebooks/Desktop/Prime Number Theorem.ipynb
jupyter
Prime Number Theorem (autosaved)
Logout
File
Edit
View
Insert
Cell
Kernel
Widgets
Help
Trusted
Python 3
Run
Code

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 set 'composite' of all composite numbers in the range $2..n$.

```
In [1]: n = 1_000_000
        composite = {p for f in range(2, n + 1) for p in range(f * f, n + 1, f)}
```

We next compute select all the prime numbers in the range $2..n$, i.e. the non-composite numbers.

```
In [2]: primes = [p for p in range(2, n + 1) if p not in composite]
```

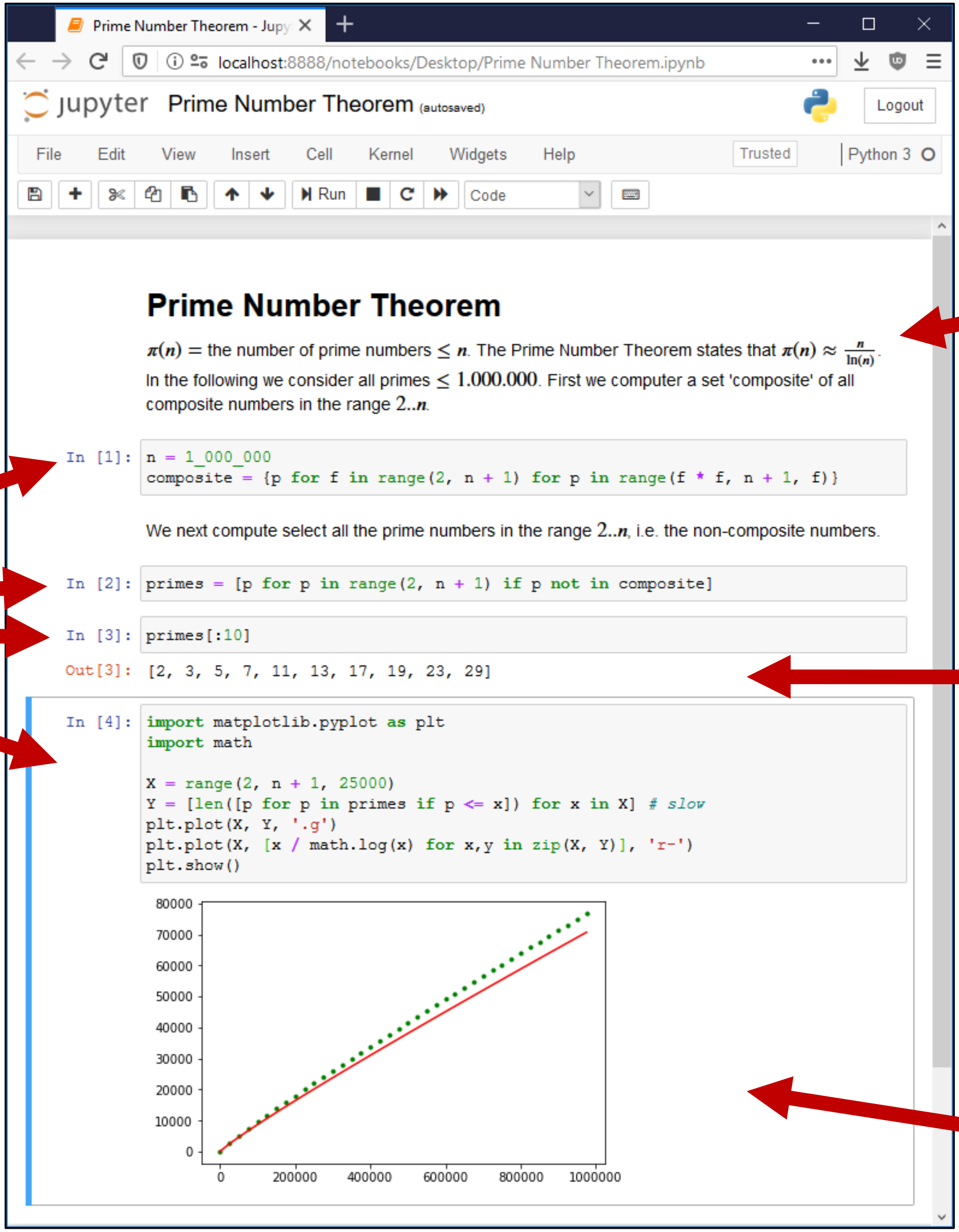
```
In [3]: primes[:10]
Out[3]: [2, 3, 5, 7, 11, 13, 17, 19, 23, 29]
```

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

        X = range(2, n + 1, 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()
```

Web Browser

User

cells



Prime Number Theorem

$\pi(n)$ = the number of prime numbers $\leq n$. The Prime Number Theorem states that $\pi(n) \approx \frac{n}{\ln(n)}$.

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```
In [1]: n = 1_000_000
        composite = {p for f in range(2, n + 1) for p in range(f * f, n + 1, f)}
```

We next compute select all the prime numbers in the range $2..n$, i.e. the non-composite numbers.

```
In [2]: primes = [p for p in range(2, n + 1) if p not in composite]
```

```
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

        X = range(2, n + 1, 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()
```

python code

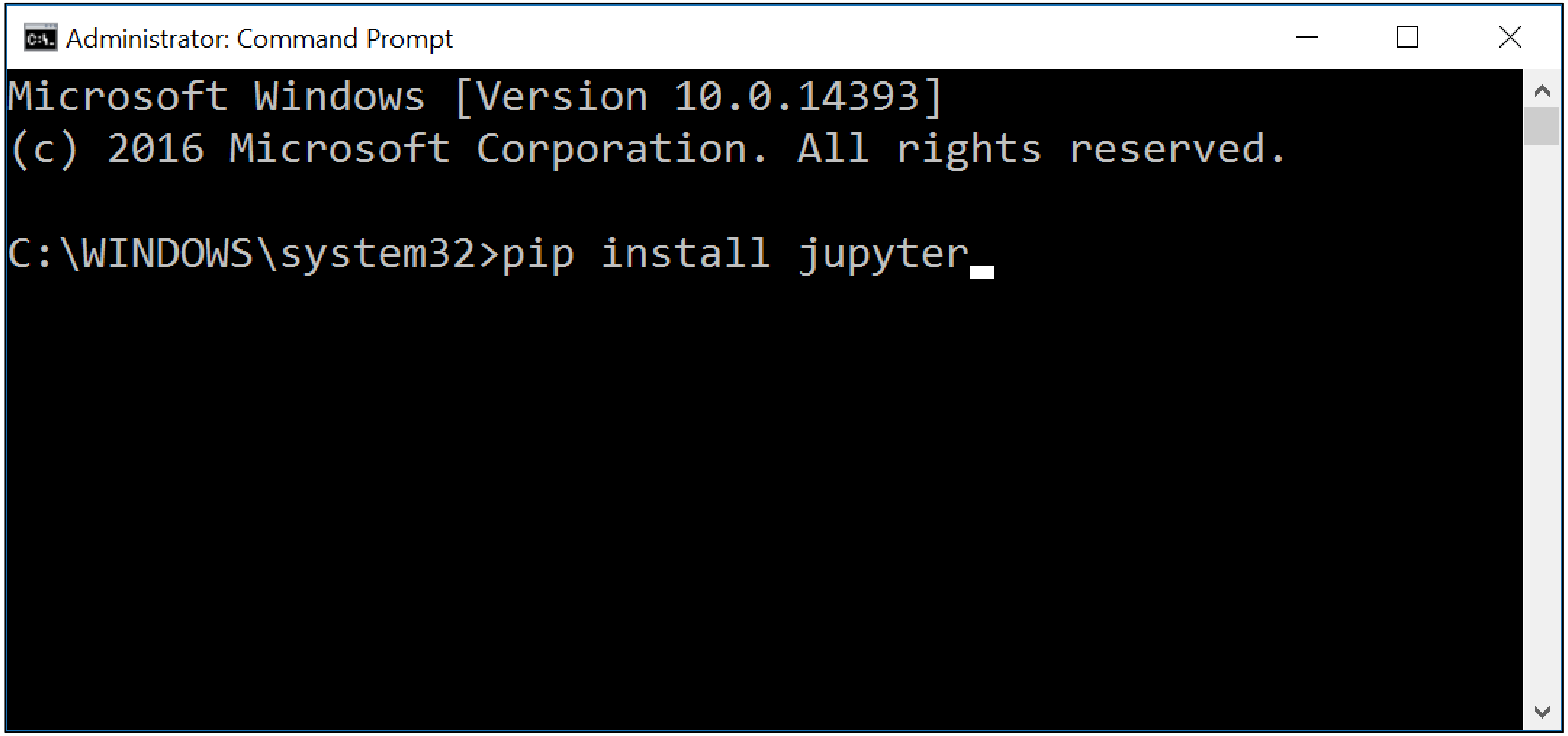
formatted text: Markdown / LaTeX / HTML / ...

python shell output

matplotlib / numpy / ... output

Jupyter - installing

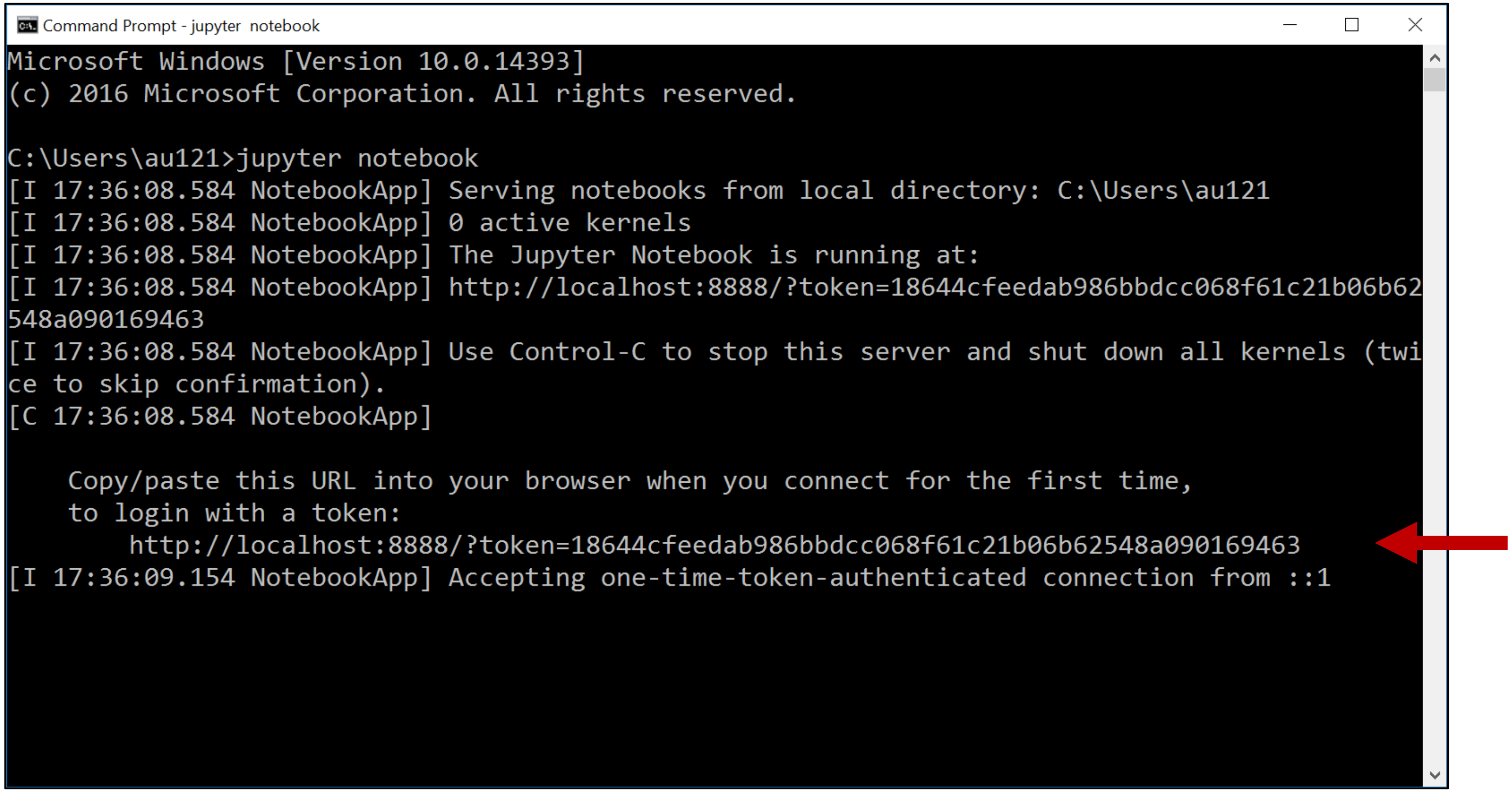
- Open a windows shell and run: `pip install jupyter`



```
Microsoft Windows [Version 10.0.14393]
(c) 2016 Microsoft Corporation. All rights reserved.

C:\WINDOWS\system32>pip install jupyter
```

Jupyter – launching the jupyter server

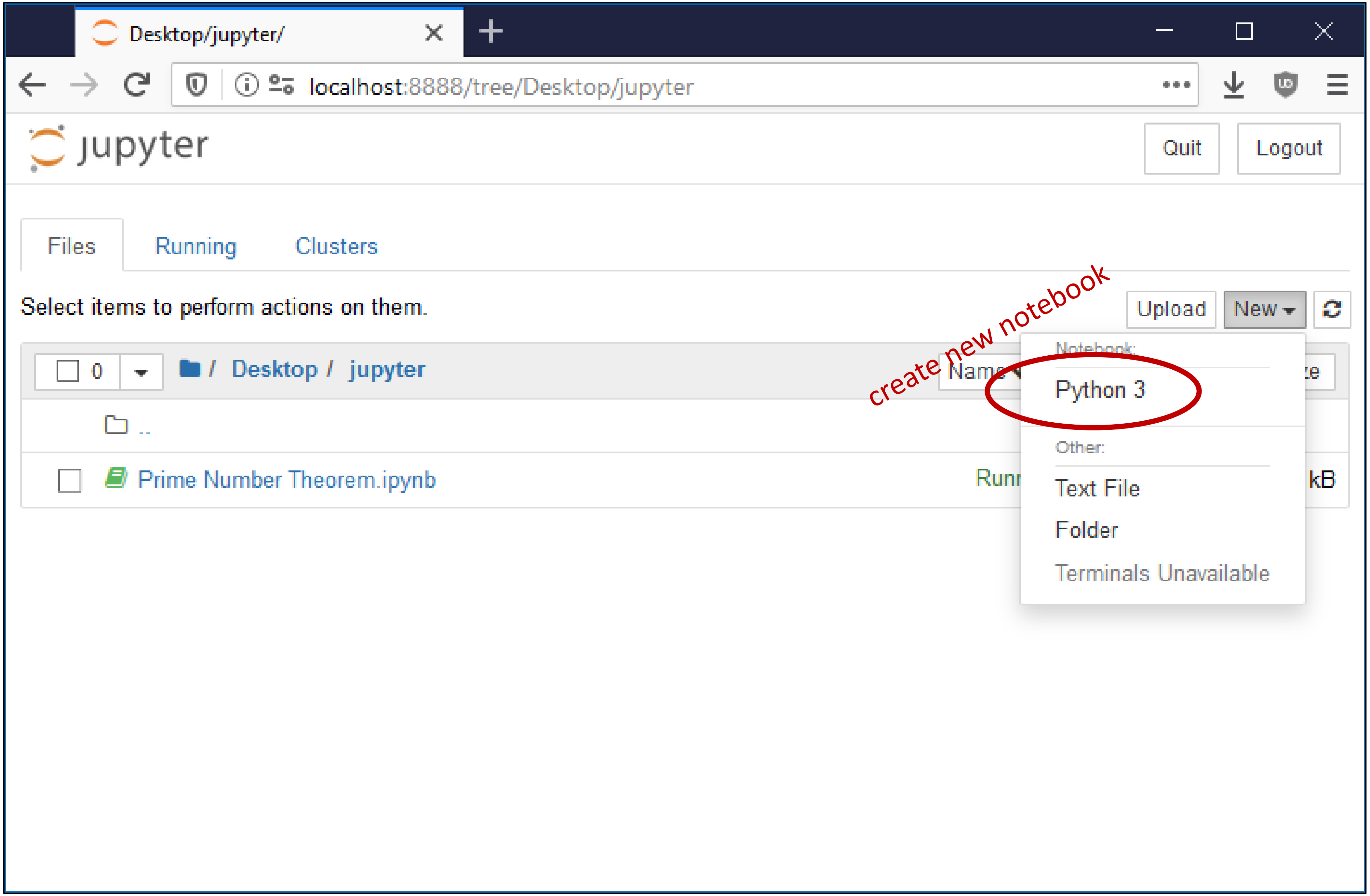
- Open a windows shell and run: `jupyter notebook`



```
Microsoft Windows [Version 10.0.14393]
(c) 2016 Microsoft Corporation. All rights reserved.

C:\Users\au121>jupyter notebook
[I 17:36:08.584 NotebookApp] Serving notebooks from local directory: C:\Users\au121
[I 17:36:08.584 NotebookApp] 0 active kernels
[I 17:36:08.584 NotebookApp] The Jupyter Notebook is running at:
[I 17:36:08.584 NotebookApp] http://localhost:8888/?token=18644cfeedab986bbdcc068f61c21b06b62
548a090169463
[I 17:36:08.584 NotebookApp] Use Control-C to stop this server and shut down all kernels (twi
ce to skip confirmation).
[C 17:36:08.584 NotebookApp]

    Copy/paste this URL into your browser when you connect for the first time,
    to login with a token:
        http://localhost:8888/?token=18644cfeedab986bbdcc068f61c21b06b62548a090169463
[I 17:36:09.154 NotebookApp] Accepting one-time-token-authenticated connection from ::1
```

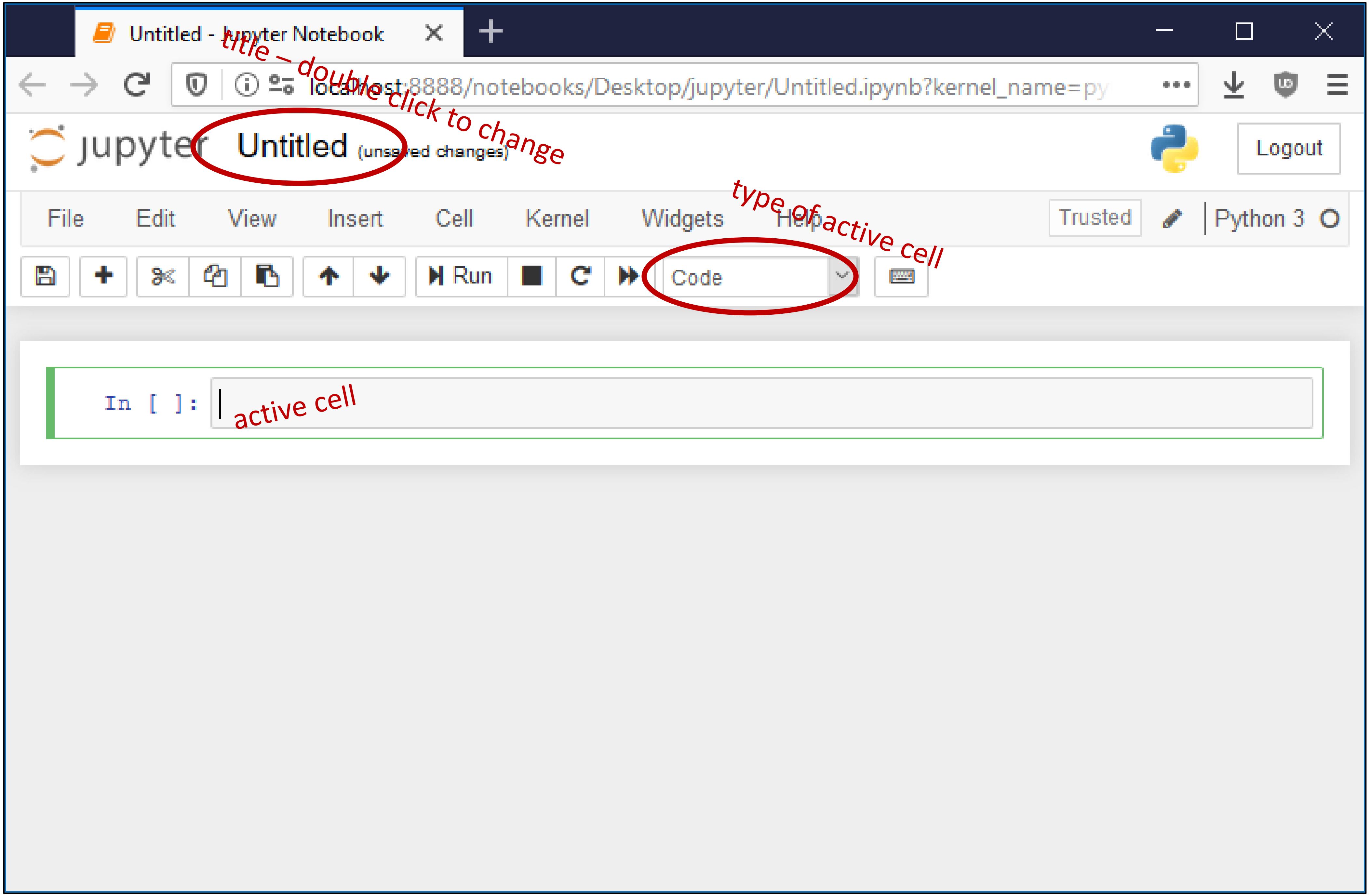
url

- If this does not work, then try `python -m notebook`



Select items to perform actions on them.

create new notebook

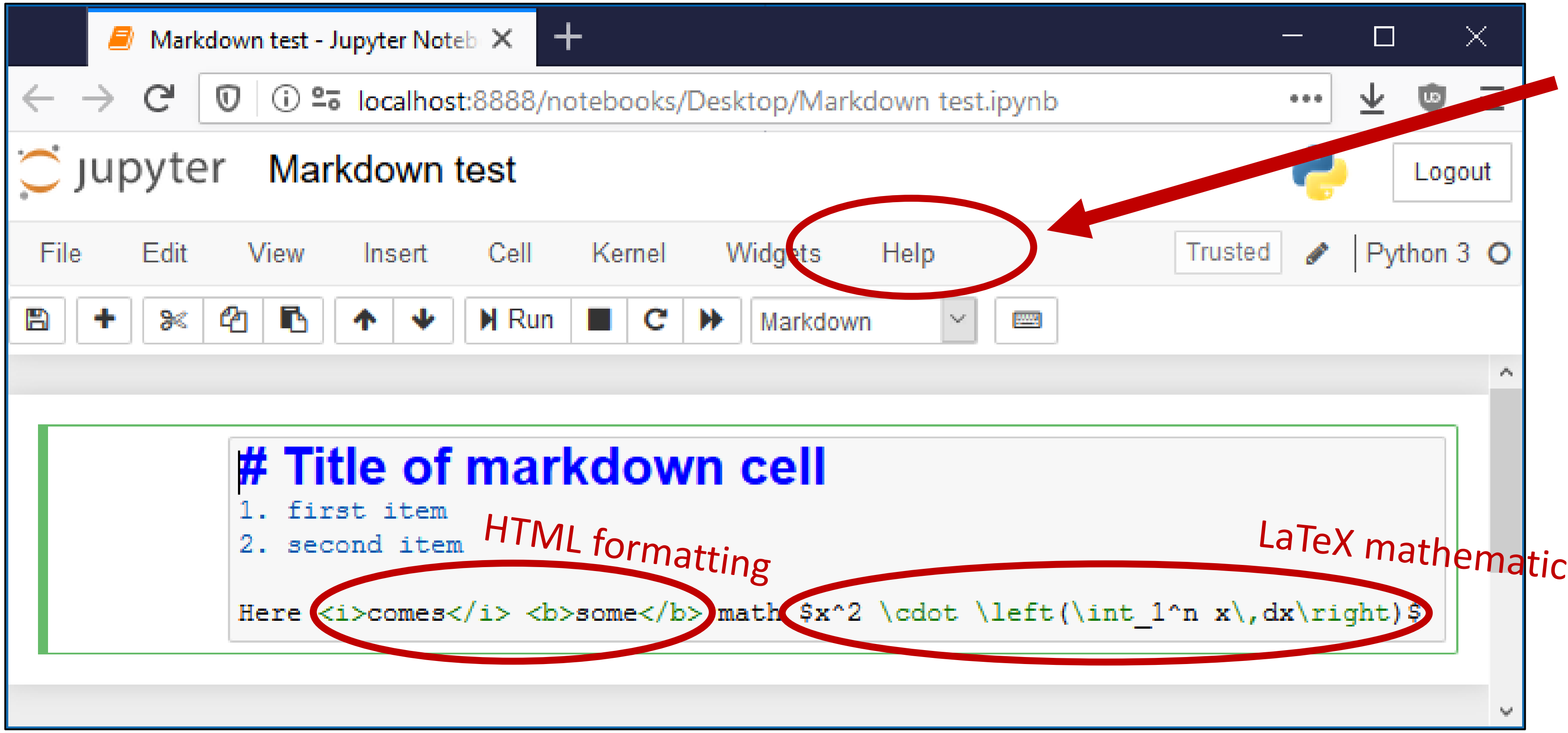


title – double click to change

type of active cell

active cell

Untitled - Jupyter Notebook
localhost:8888/notebooks/Desktop/jupyter/Untitled.ipynb?kernel_name=py
jupyter
Untitled (unsaved changes)
Logout
File
Edit
View
Insert
Cell
Kernel
Widgets
Help
Trusted
Python 3
Run
Code
In [ ]:



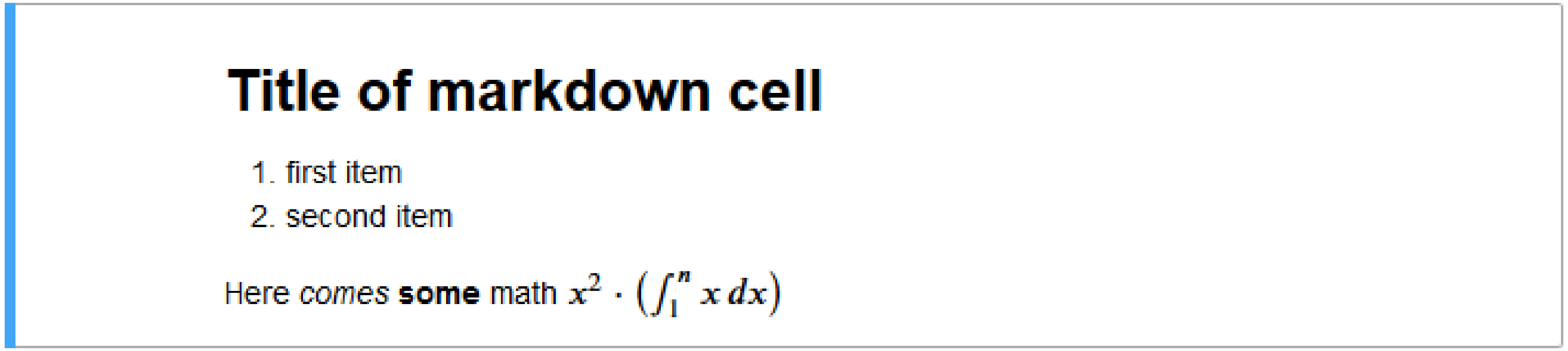
```
# Title of markdown cell
1. first item
2. second item

Here <i>comes</i> <b>some</b> math $x^2 \cdot \left(\int_1^n x\,dx\right)$
```

HTML formatting

LaTeX mathematics

Try:
Help > User Interface Tour
Help > Markdown

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



Title of markdown cell

1. first item
2. second item

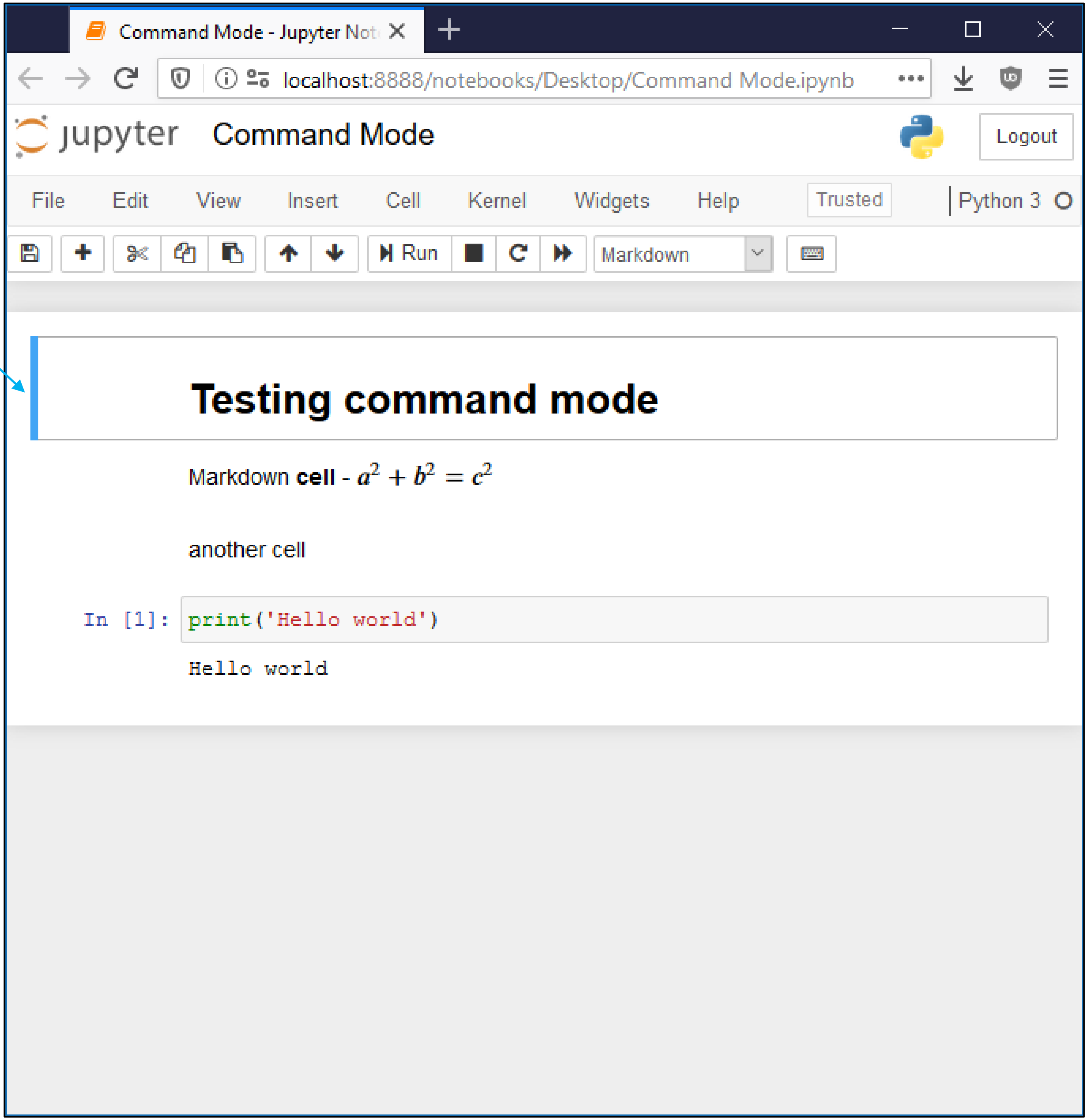
Here *comes* **some** math $x^2 \cdot \left(\int_1^n x\,dx\right)$

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

Command Mode

- Used to naviagte between cells
- Current cell is marked with blue bar
- Keyboard shortcuts

h	show keyboard shortcuts
enter	enter Edit Mode on current cell
shift-enter	run cell + select below
ctrl-enter	run selected cells
alt-enter	run cell and insert below
Y M R	change cell type (code, markdown, raw text)
1 2 3 4 5 6	change heading level
ctrl-A	select all cells
down up	move to next/previous cell
space shift-space	scroll down/up
shift-up shift-down	extend selected cells
A B	insert cell above/below
X C V shift-V Z DD	cut, copy, paste below/above, undo, delete cells
shift-L	toggle line numbers in cells
shift-M	merge selected cells (or with cell below)
O	toggle output of selected cells
shift-O	toggle scrollbar on selected cells (long output)



Testing command mode

Markdown **cell** - $a^2 + b^2 = c^2$

another cell

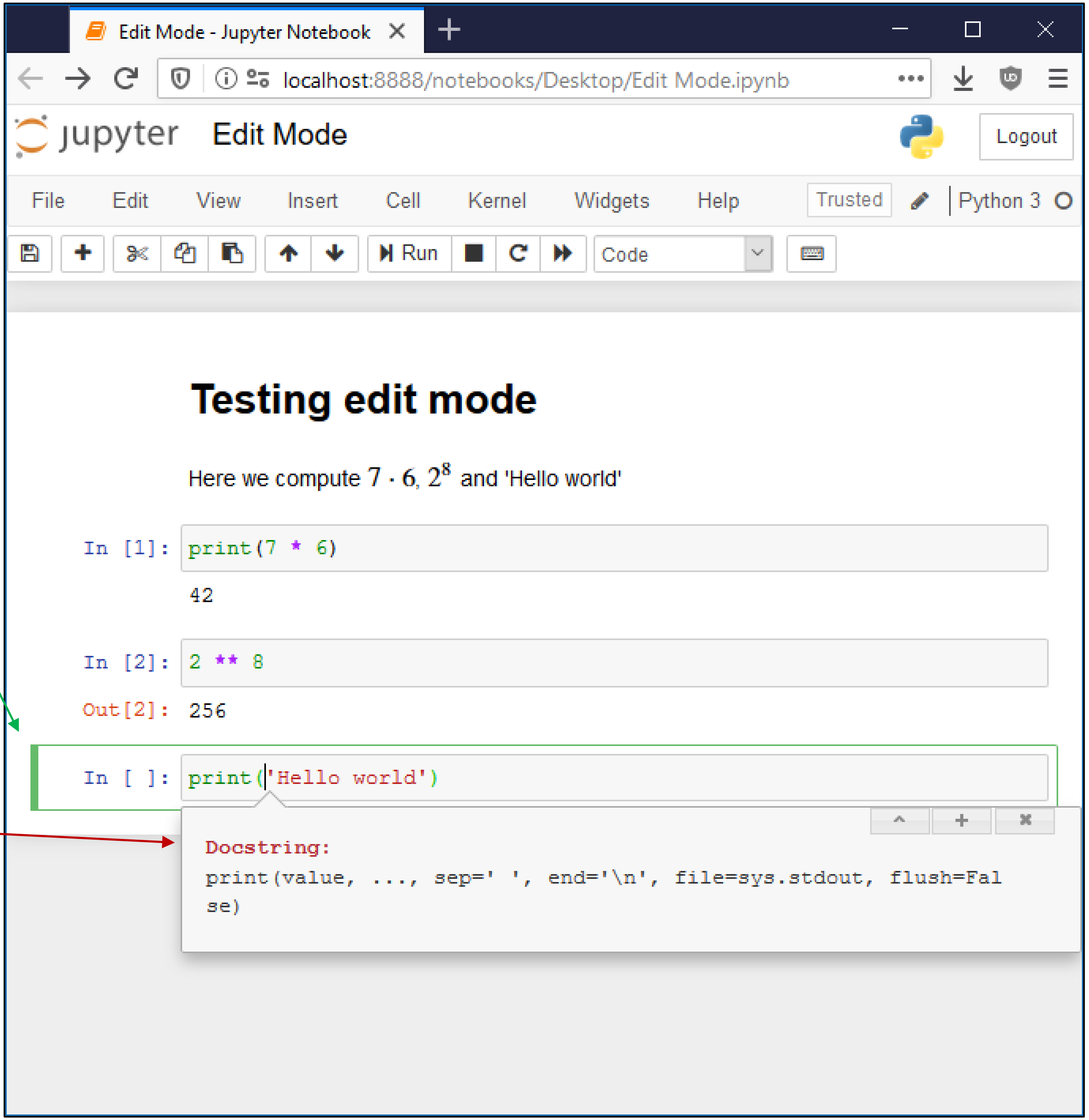
```
In [1]: print('Hello world')
```

```
Hello world
```

Edit Mode

- Used to edit current cell
- Current cell is marked with green bar
- Keyboard shortcuts

esc	enter Command Mode
shift-enter	run cell + select below
ctrl-enter	run selected cells
alt-enter	run cell and insert below
ctrl-shift- -	split cell at cursor
ctrl-shift-f	command palette
tab	indent or code completion
shift-tab	show docstring
ctrl-a -x -c -v -z -y	select all, cut, copy, paste, undo, redo
ctrl-d	delete line



Testing edit mode

Here we compute $7 \cdot 6$, 2^8 and 'Hello world'

```
In [1]: print(7 * 6)

42

In [2]: 2 ** 8

Out[2]: 256

In [ ]: print('Hello world')
```

```
Docstring:
print(value, ..., sep=' ', end='\n', file=sys.stdout, flush=Fal
se)
```

Evaluating cells

- To evaluate cell

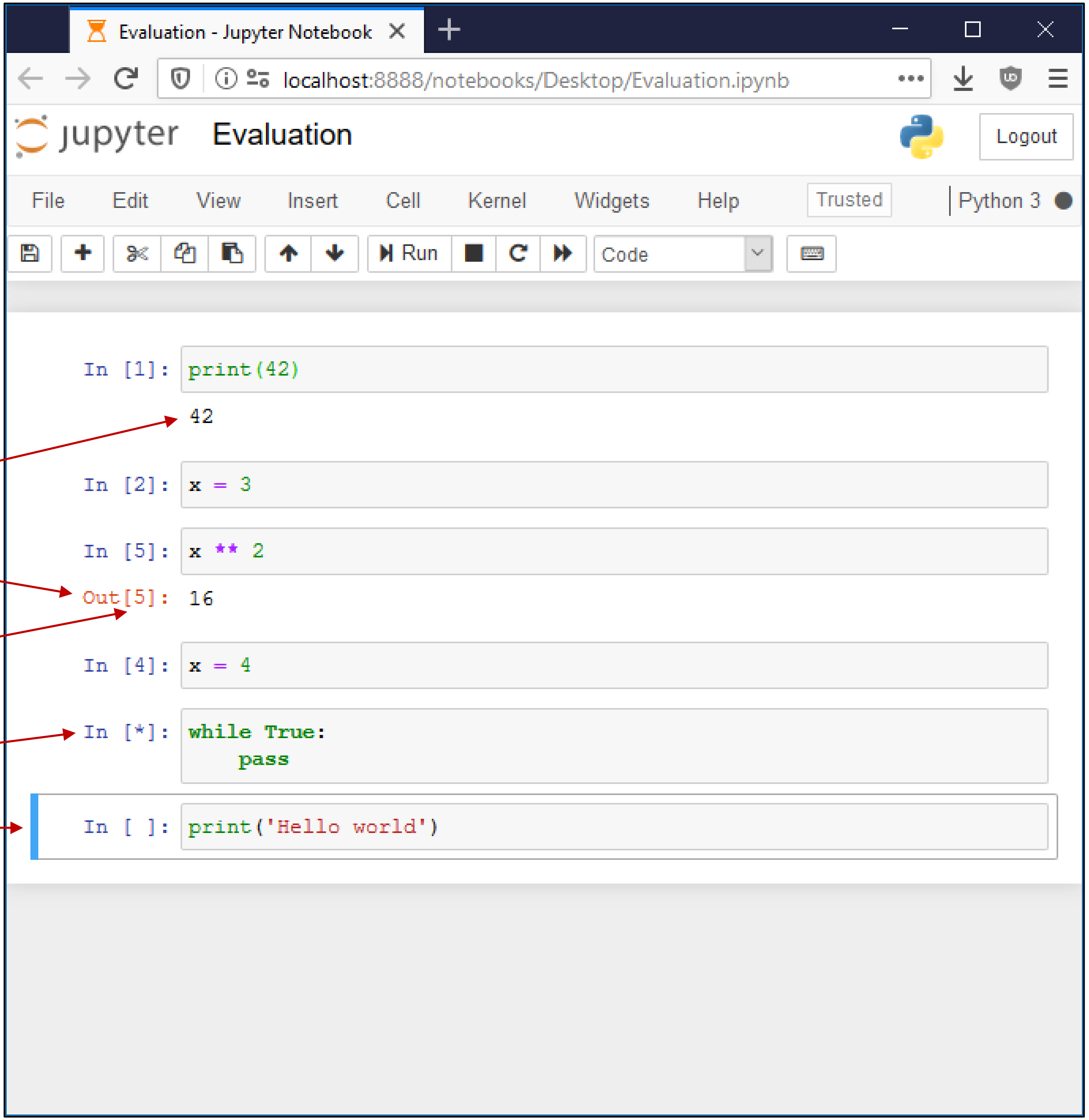
  ctrl-enter, alt-enter, shift-enter

- Output from program shown below cell
- Result of last evaluated line
- Order of code cells evaluated

  Note ”x ** 2” computed after ”x = 4”

- [*] are cells being evaluated / waiting
- [ ] not yet evaluated
- Recompute all cells top-down

  ⏩ or Kernel > Restart & Run all

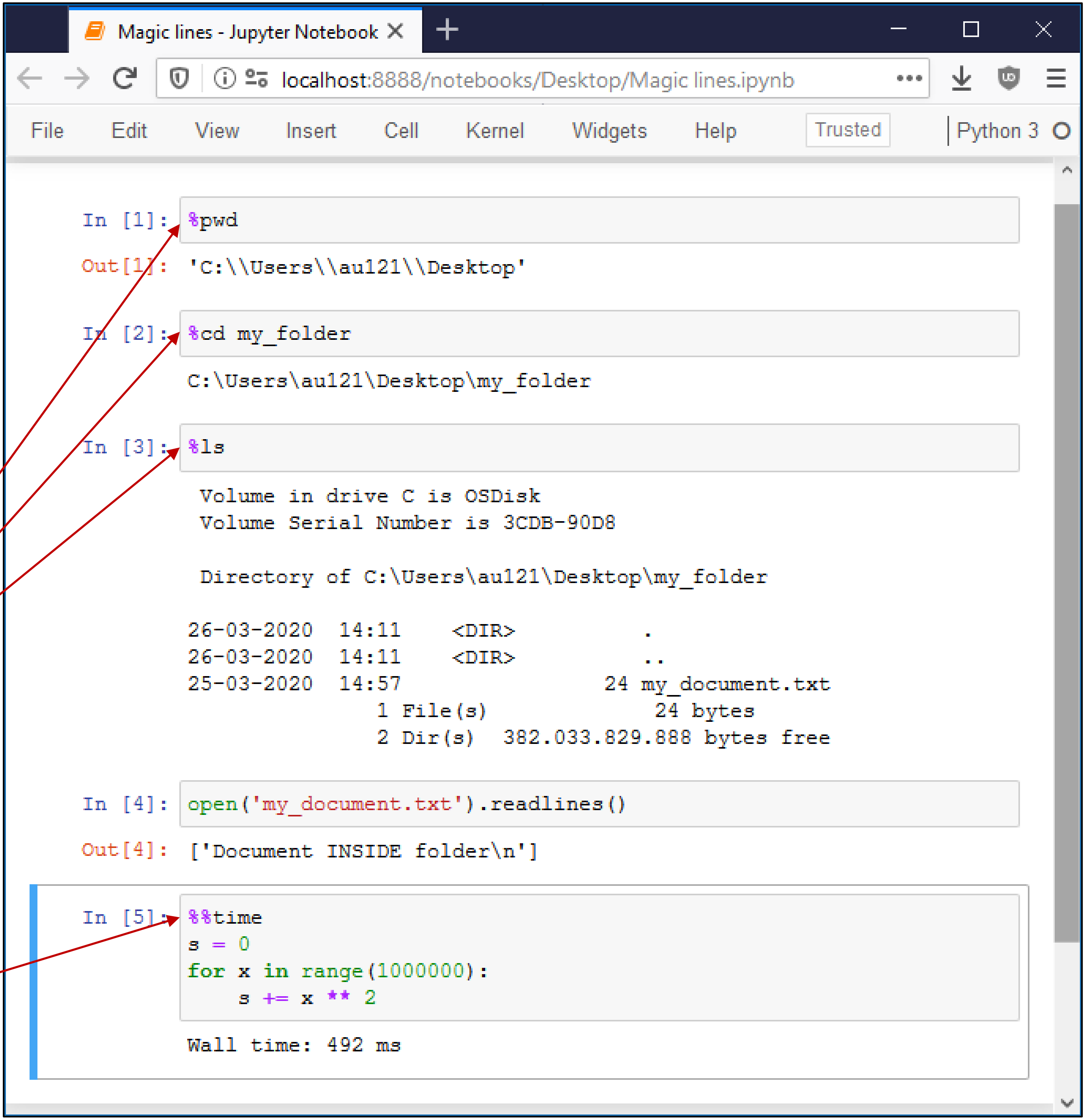


```
In [1]: print(42)
        42

In [2]: x = 3

In [5]: x ** 2
Out[5]: 16

In [4]: x = 4

In [*]: while True:
            pass

In [ ]: print('Hello world')
```

Magic lines

- Jupyter code cells support *magic commands* (actually it is IPython)
- % is a *line magic*
- %% is a *cell magic*

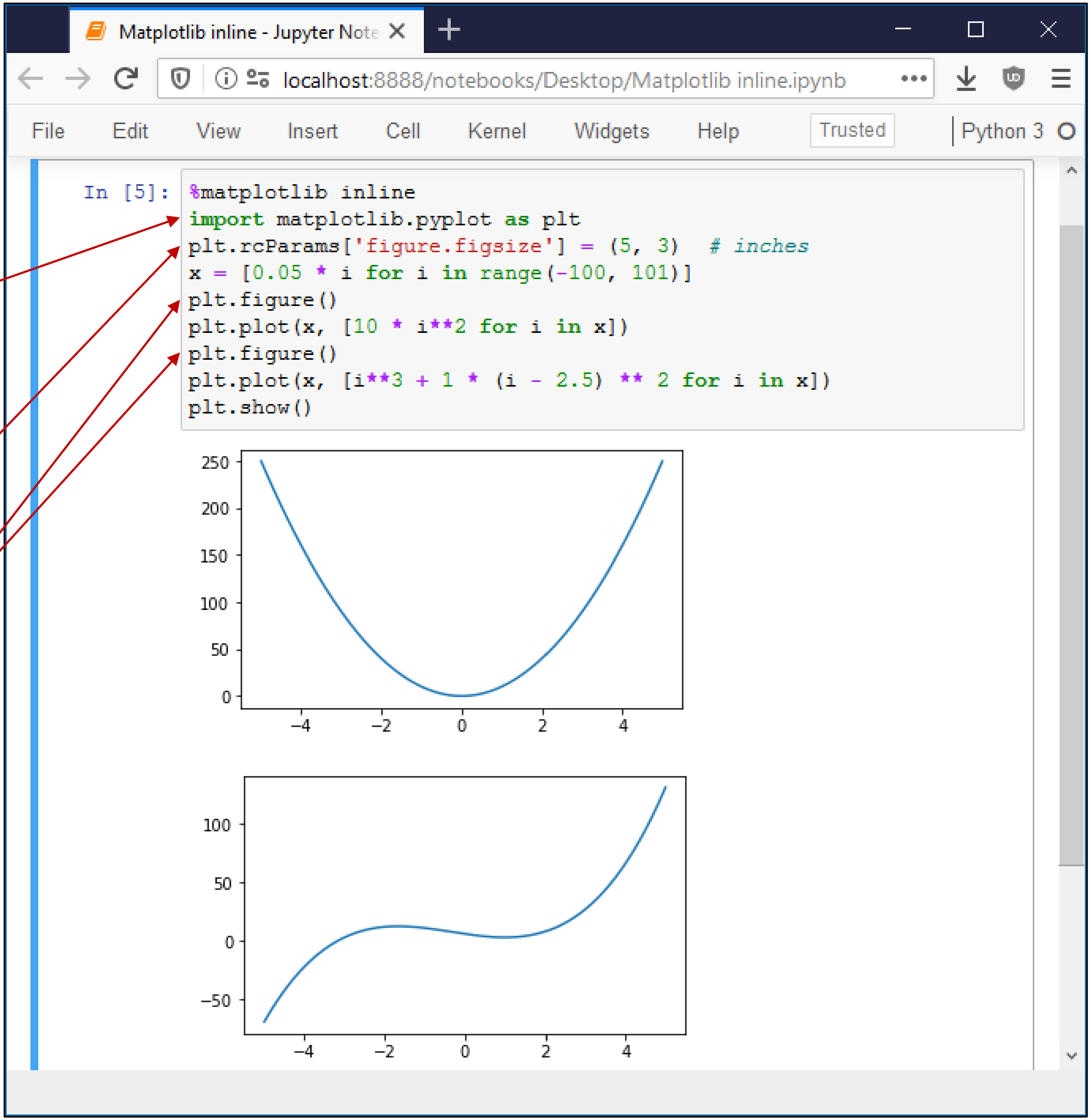
%lsmagic	list magic commands
%quickref	quick reference sheet to IPython
%pwd	print working directory (current folder)
%cd *directory*	change directory (absolut or relative)
%ls	list content of current directory
%pip *or* %conda	run pip or conda from jupyter
%load *script*	insert external script into cell
%run *program*	run external program and show output
%automagic	toggle if %-prefix is required
%matplotlib inline	no zoom & resize, allows multiple plots
%matplotlib notebook	a single plot can be zoomed & resized
%%writefile *file*	write content of cell to a file
%%time	measure time for cell execution
%timeit *expression*	time for simple expression


Magic lines - Jupyter Notebook
localhost:8888/notebooks/Desktop/Magic lines.ipynb
File
Edit
View
Insert
Cell
Kernel
Widgets
Help
Trusted
Python 3

```
In [1]: %pwd
Out[1]: 'C:\\Users\\au121\\Desktop'

In [2]: %cd my_folder
        C:\Users\au121\Desktop\my_folder

In [3]: %ls
         Volume in drive C is OSDisk
         Volume Serial Number is 3CDB-90D8

         Directory of C:\Users\au121\Desktop\my_folder

        26-03-2020  14:11    <DIR>          .
        26-03-2020  14:11    <DIR>          ..
        25-03-2020  14:57                24 my_document.txt
                       1 File(s)             24 bytes
                       2 Dir(s)  382.033.829.888 bytes free

In [4]: open('my_document.txt').readlines()
Out[4]: ['Document INSIDE folder\n']

In [5]: %%time
        s = 0
        for x in range(1000000):
            s += x ** 2

        Wall time: 492 ms
```

Jupyter
and matplotlib

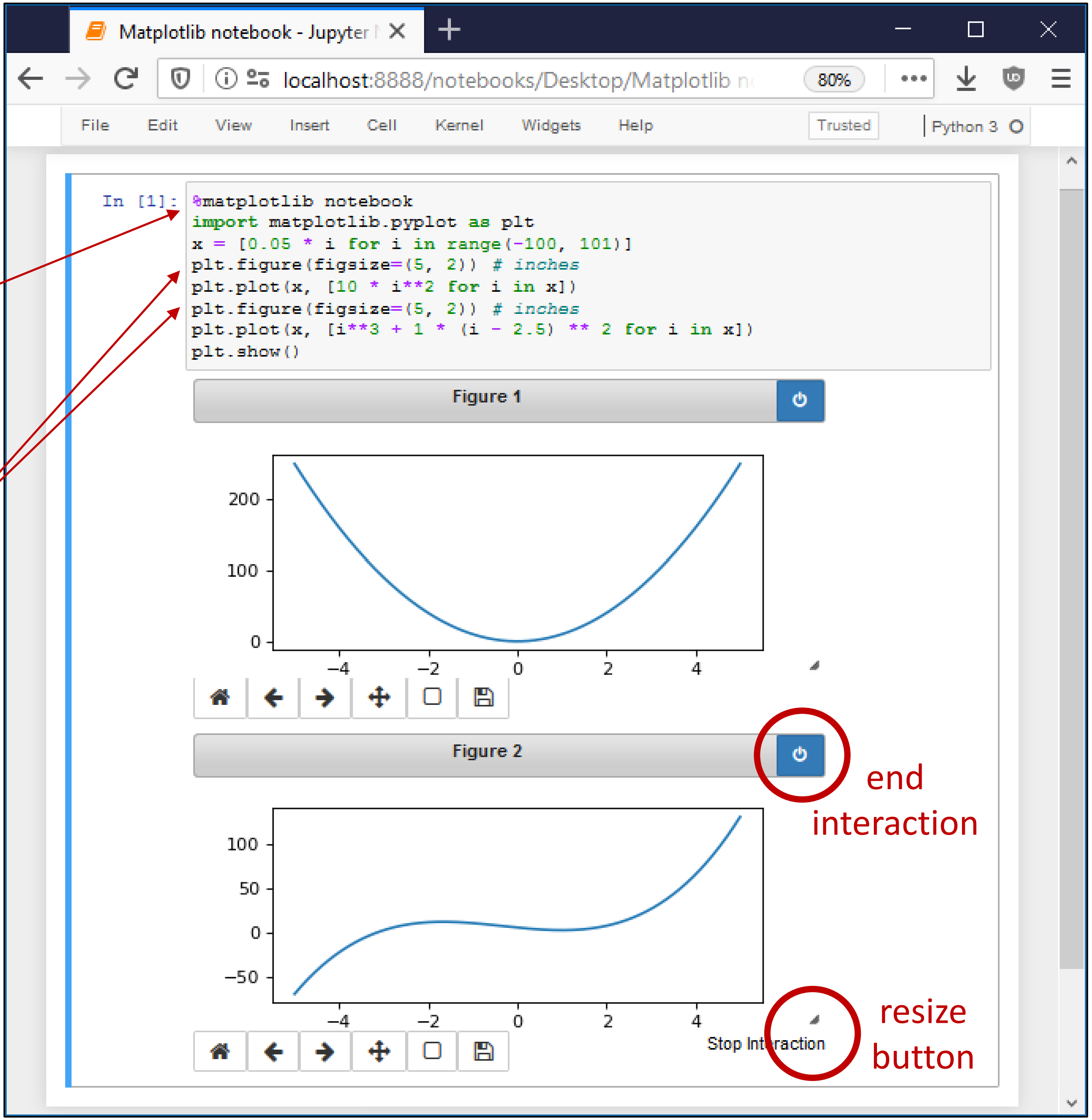
- `%matplotlib inline`
  pyplot figures are shown *without* interactive zoom and pan (default)
- Consider changing default figure size
  `plt.rcParams['figure.figsize']`
- Start each figure with `plt.figure`
- Final call to `show` can be omitted



In [5]:
```
%matplotlib inline
import matplotlib.pyplot as plt
plt.rcParams['figure.figsize'] = (5, 3)  # inches
x = [0.05 * i for i in range(-100, 101)]
plt.figure()
plt.plot(x, [10 * i**2 for i in x])
plt.figure()
plt.plot(x, [i**3 + 1 * (i - 2.5) ** 2 for i in x])
plt.show()
```

Jupyter and matplotlib

- `%matplotlib notebook` pyplot figures are shown *with* interactive zoom and pan
- Start each figure with `plt.figure` (also allows setting figure size)
- Final call to `show` can be omitted



```
In [1]: %matplotlib notebook
        import matplotlib.pyplot as plt
        x = [0.05 * i for i in range(-100, 101)]
        plt.figure(figsize=(5, 2)) # inches
        plt.plot(x, [10 * i**2 for i in x])
        plt.figure(figsize=(5, 2)) # inches
        plt.plot(x, [i**3 + 1 * (i - 2.5) ** 2 for i in x])
        plt.show()
```

end interaction

resize button

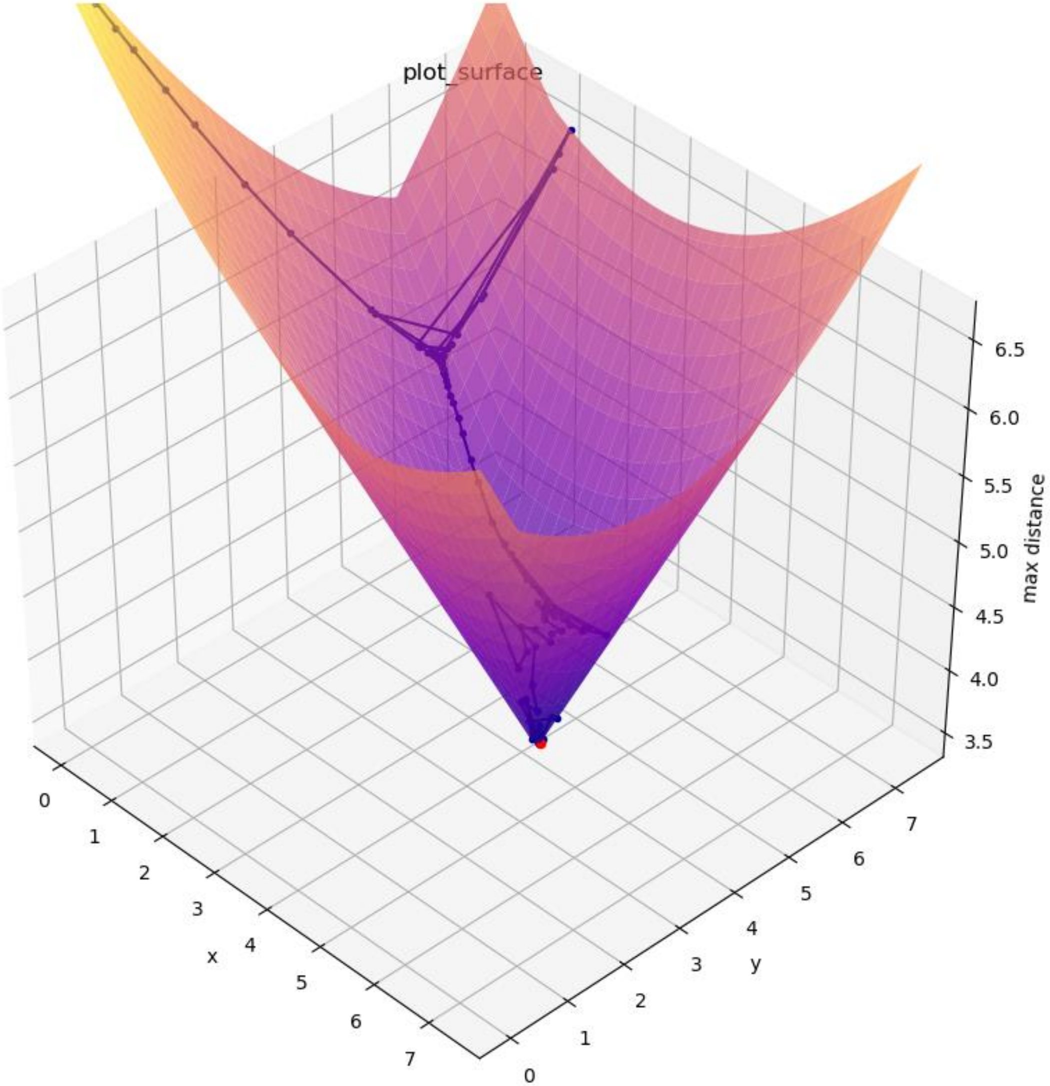
- Widespread tool used for data science applications
- Documentation, code for data analysis, and resulting visualizations are stored in one common format
- Easy to update visualizations
- Works with about 100 different programming languages (not only Python 3), many special features, ...
- Easy to share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

- *Many online tutorials and examples are available*

https://www.youtube.com/results?search_query=jupyter+python

scipy.optimize.minimize

- Find point p minimizing function f
- Supports 13 algorithms – but no guarantee that result is 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 when used as a black box



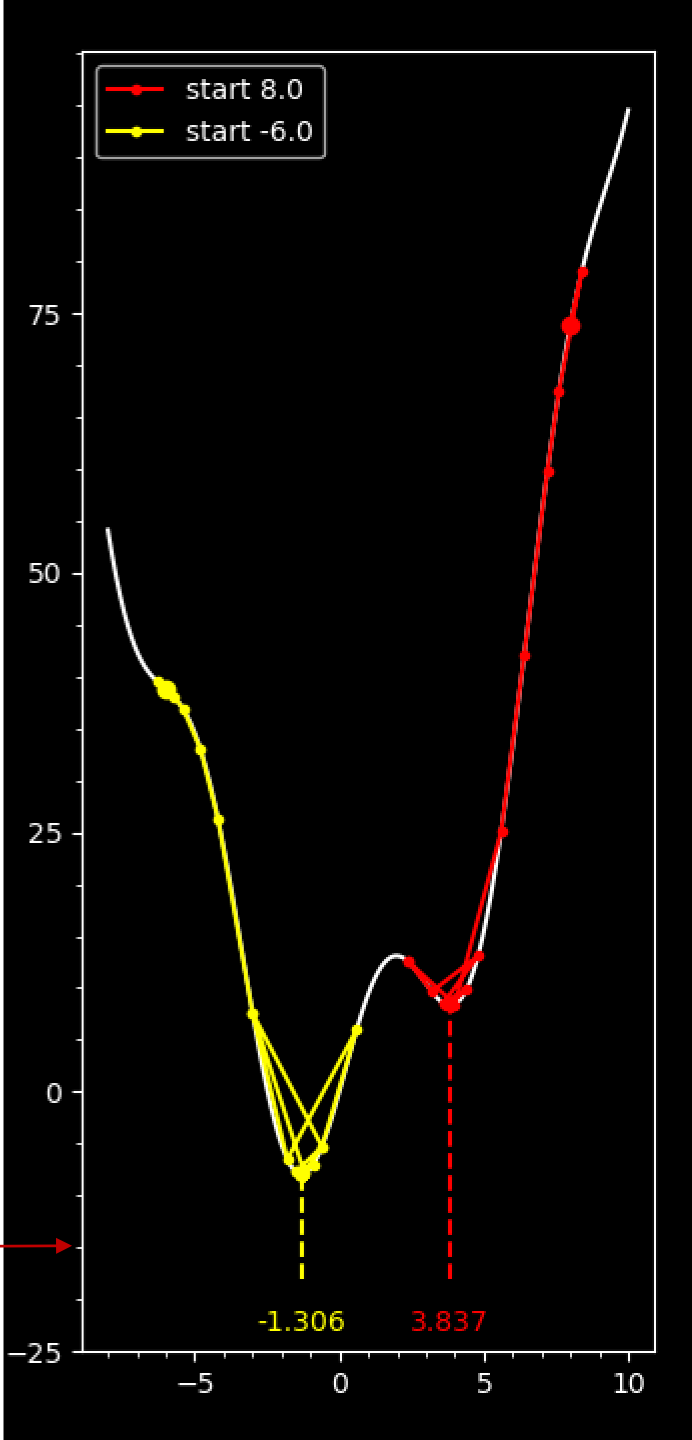
pip install scipy

docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.minimize.html minimize.py

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

trace = []  # remember calls to f

def f(x):
    value = x ** 2 + 10 * sin(x)
    trace.append((x, value))
    return value

X = [-8 + 18 * i / 9999 for i in range(1000)]
Y = [f(x) for x in X]

plt.style.use('dark_background')
plt.plot(X, Y, 'w-')
for start, color in [(8, 'red'), (-6, 'yellow')]:
    trace = []

    solution = minimize(f, [start], method='nelder-mead')

    x, y = solution.x[0], solution.fun
    plt.plot(*zip(*trace), '.-', c=color, label=f'start {start:.1f}') # trace
    plt.plot(*trace[0], 'o', c=color)                             # first trace point
    plt.text(x, -23, f'{x:.3f}', c=color, ha='center')            # show minimum x
    plt.plot([x, x], [-18, y], '--', c=color)                     # dash to minimum
plt.xticks(range(-5, 15, 5))
plt.yticks(range(-25, 100, 25))
plt.minorticks_on()
plt.legend()
plt.show()
```

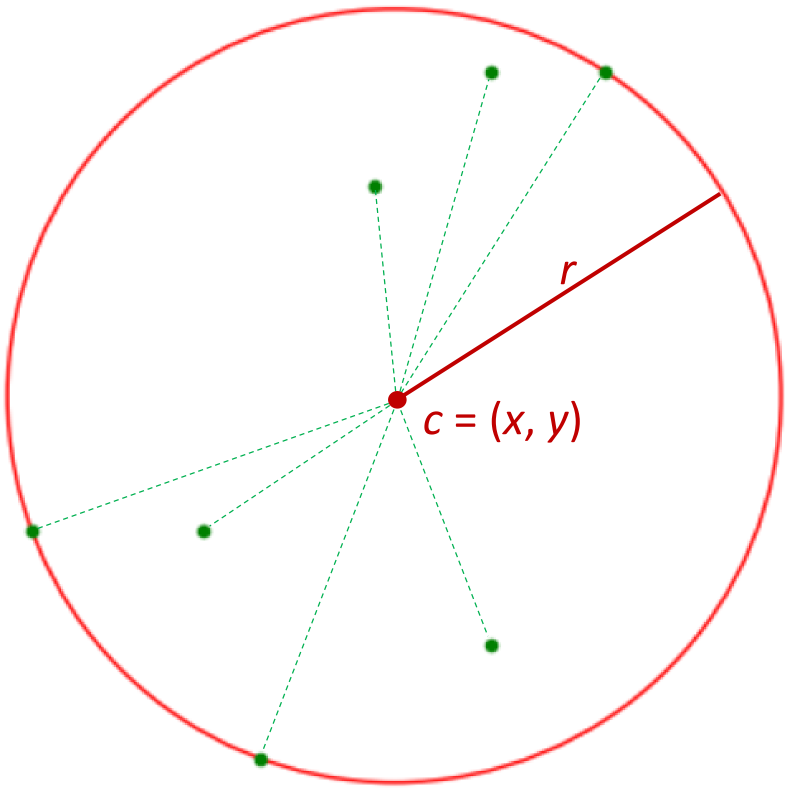
Python shell

```
> print(solution)
| final_simplex: (array([[-1.3064209 ],
|    [-1.30649414]]), array([-7.94582337, -7.94582336]))
|           fun: -7.94582337348758
|       message: 'Optimization terminated successfully.'
|          nfev: 38
|           nit: 19
|        status: 0
|       success: True
|             x: array([-1.3064209])
```



minimize tries to find a local minimum for **f** by repeatedly evaluating **f** for different **x** values

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

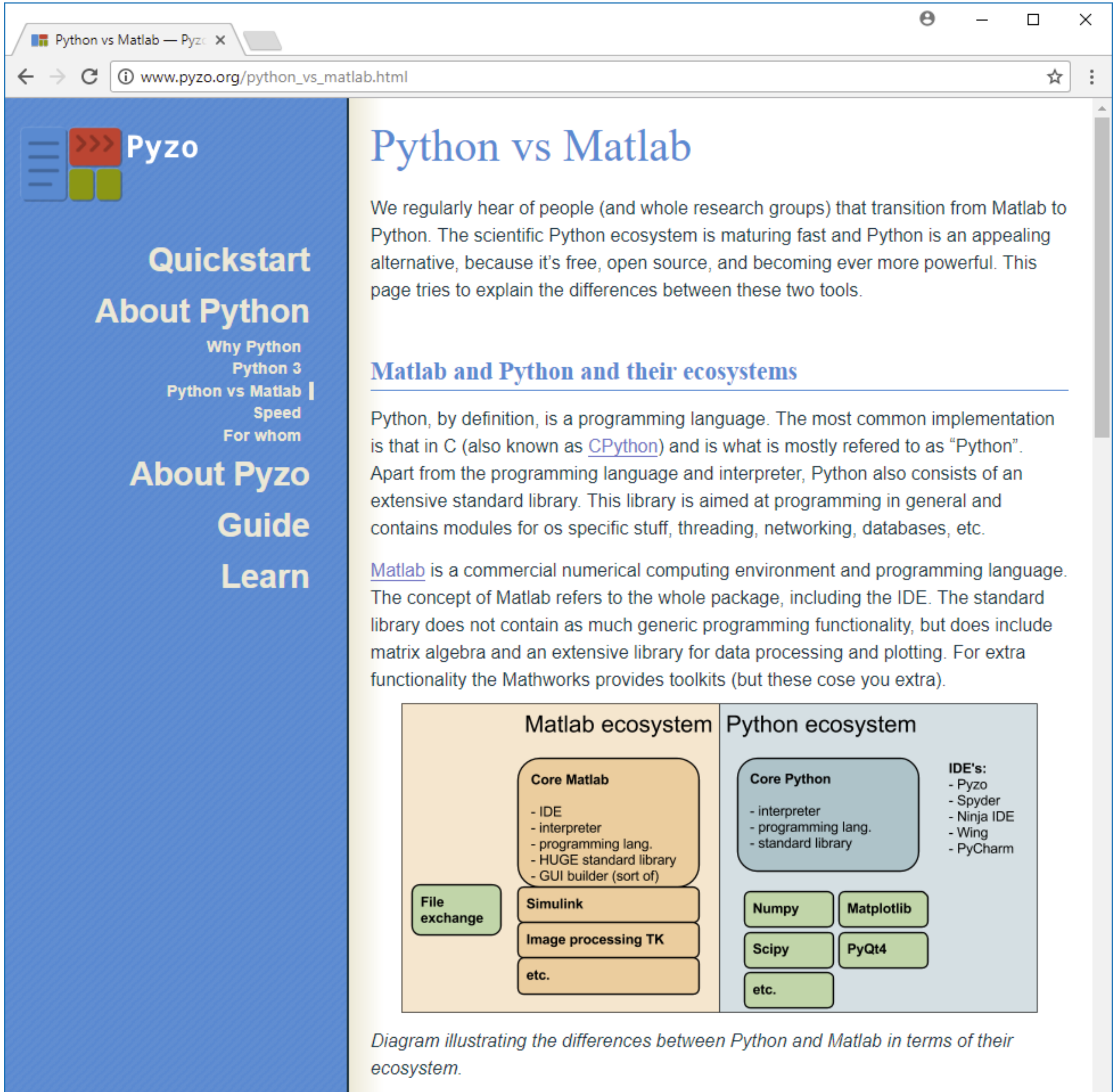
- ⚠ Computation involves max and $\sqrt{x}$, which can be hard for numeric optimization solvers

Python/scipy
vs MATLAB

Some basic differences

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

like R, Mathematica, Julia, AWK, Smalltalk, ...



Python vs Matlab

We regularly hear of people (and whole research groups) that transition from Matlab to Python. The scientific Python ecosystem is maturing fast and Python is an appealing alternative, because it's free, open source, and becoming ever more powerful. This page tries to explain the differences between these two tools.

Matlab and Python and their ecosystems

Python, by definition, is a programming language. The most common implementation is that in C (also known as CPython) and is what is mostly refered to as "Python". Apart from the programming language and interpreter, Python also consists of an extensive standard library. This library is aimed at programming in general and contains modules for os specific stuff, threading, networking, databases, etc.

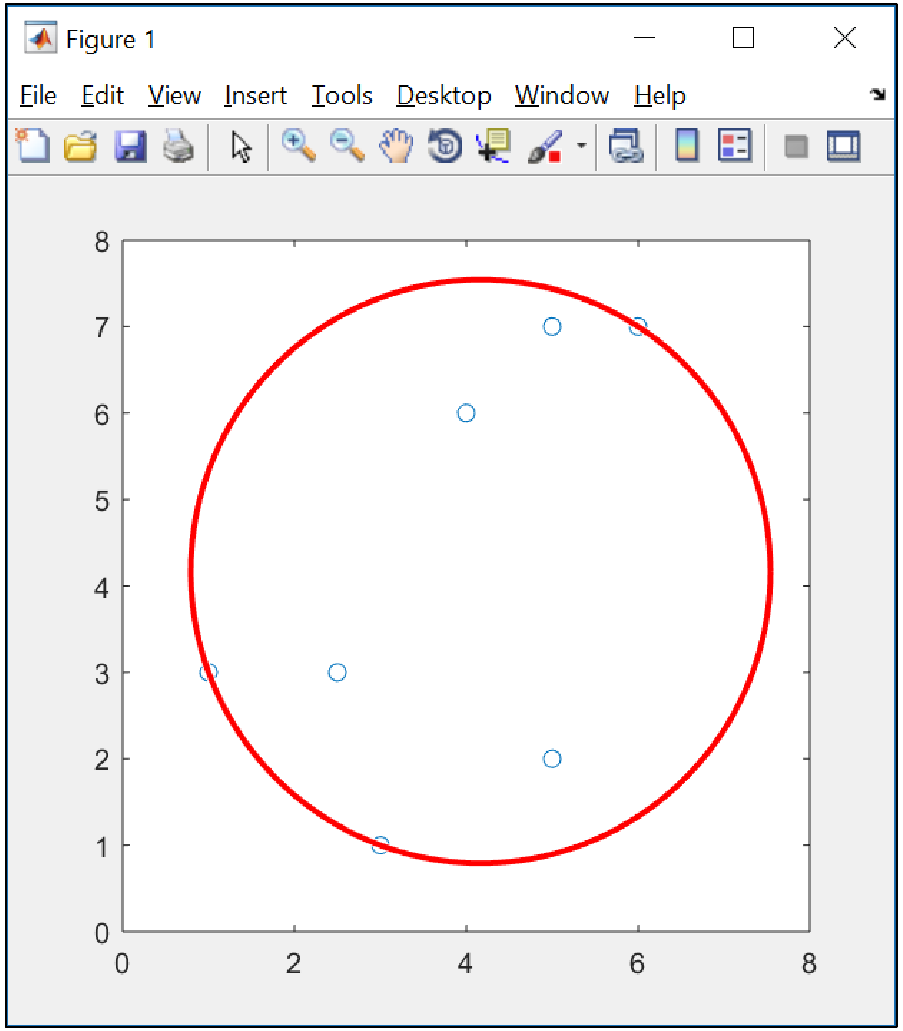
Matlab is a commercial numerical computing environment and programming language. The concept of Matlab refers to the whole package, including the IDE. The standard library does not contain as much generic programming functionality, but does include matrix algebra and an extensive library for data processing and plotting. For extra functionality the Mathworks provides toolkits (but these cose you extra).

Diagram illustrating the differences between Python and Matlab in terms of their ecosystem.

Minimum enclosing circle in MATLAB

enclosing_circle.m

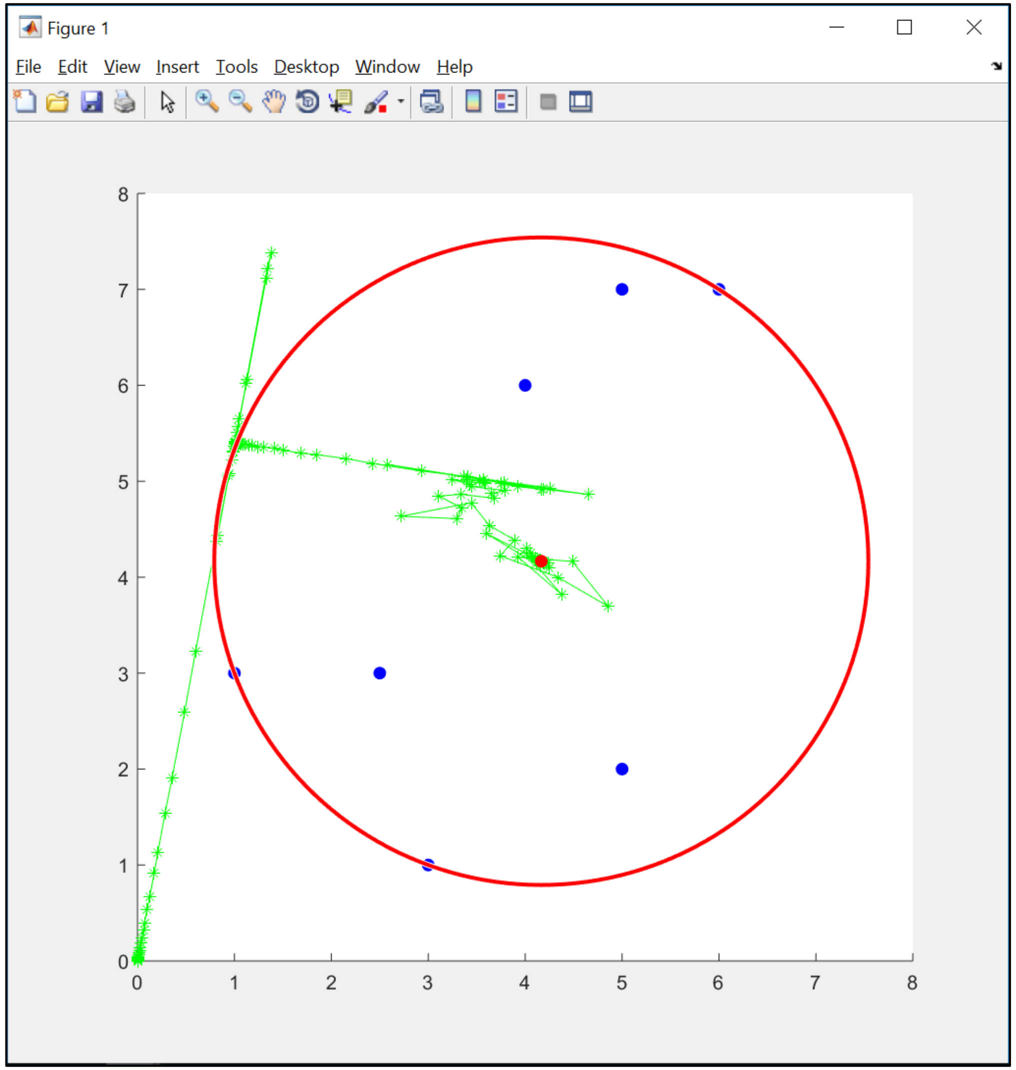
```
% Minimum enclosing circle of a point set
% fminsearch uses the Nelder-Mead algorithm

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

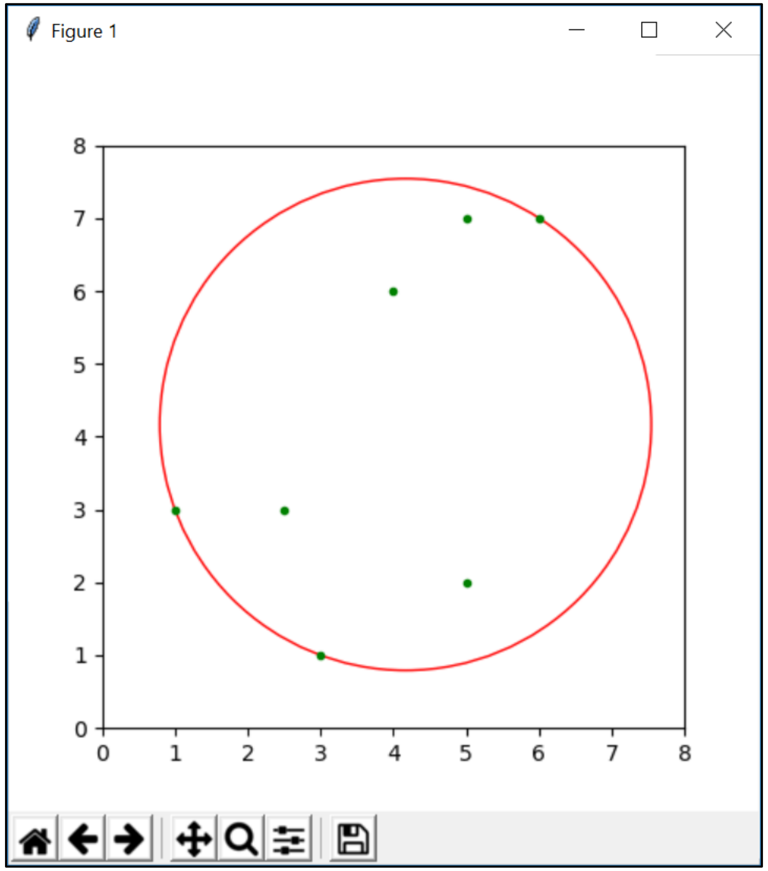
enclosing_circle.py

```python
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

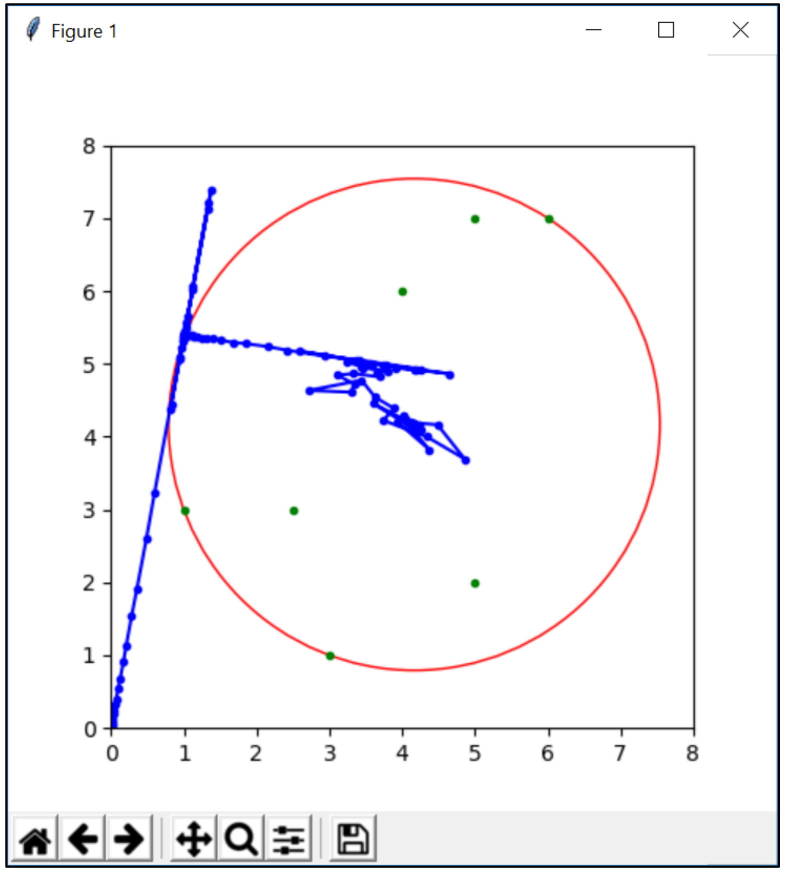
manually set axis (force circle inside plot)



Minimum enclosing circle in Python (trace)

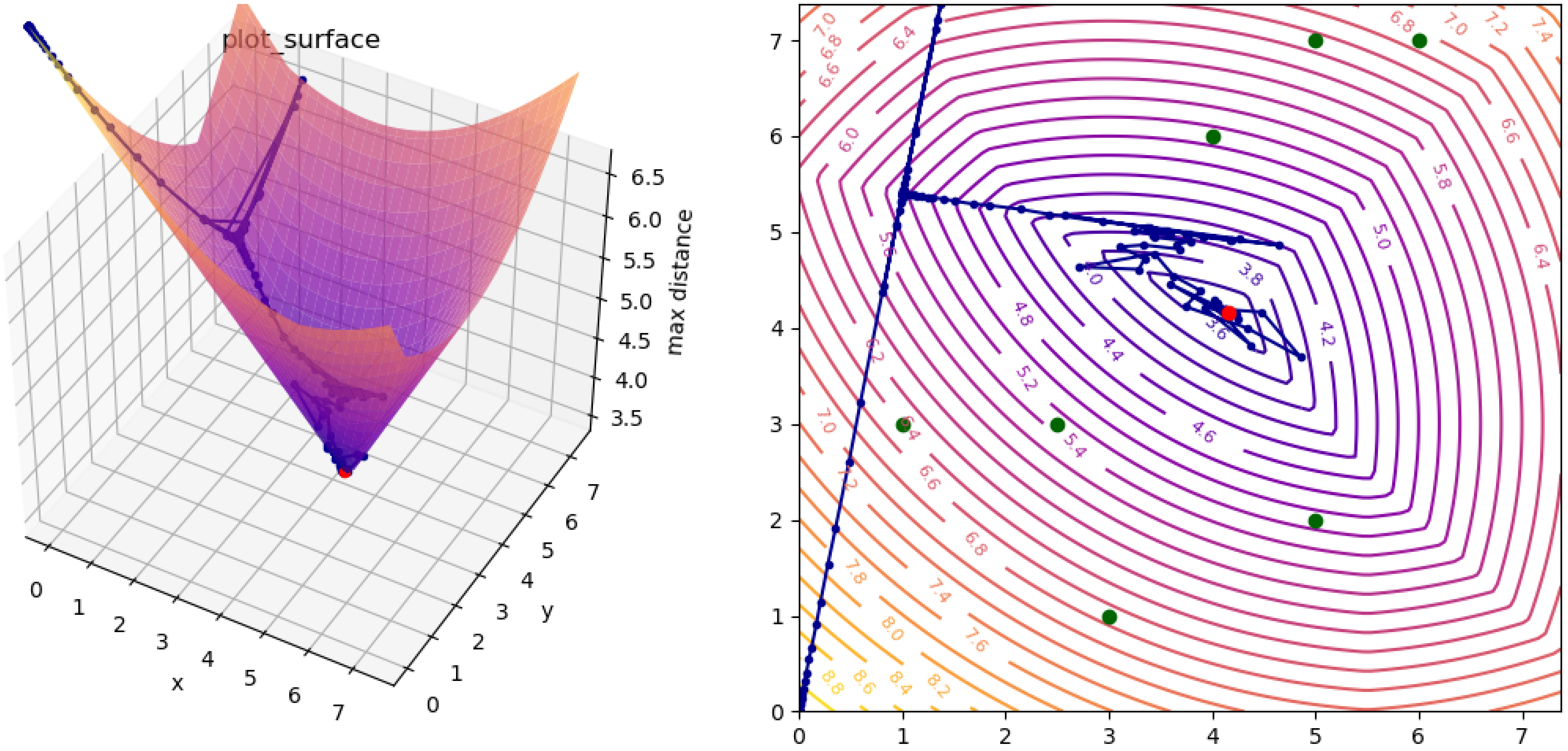
enclosing_circle_trace.py

```
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

Maximum distance to an input point



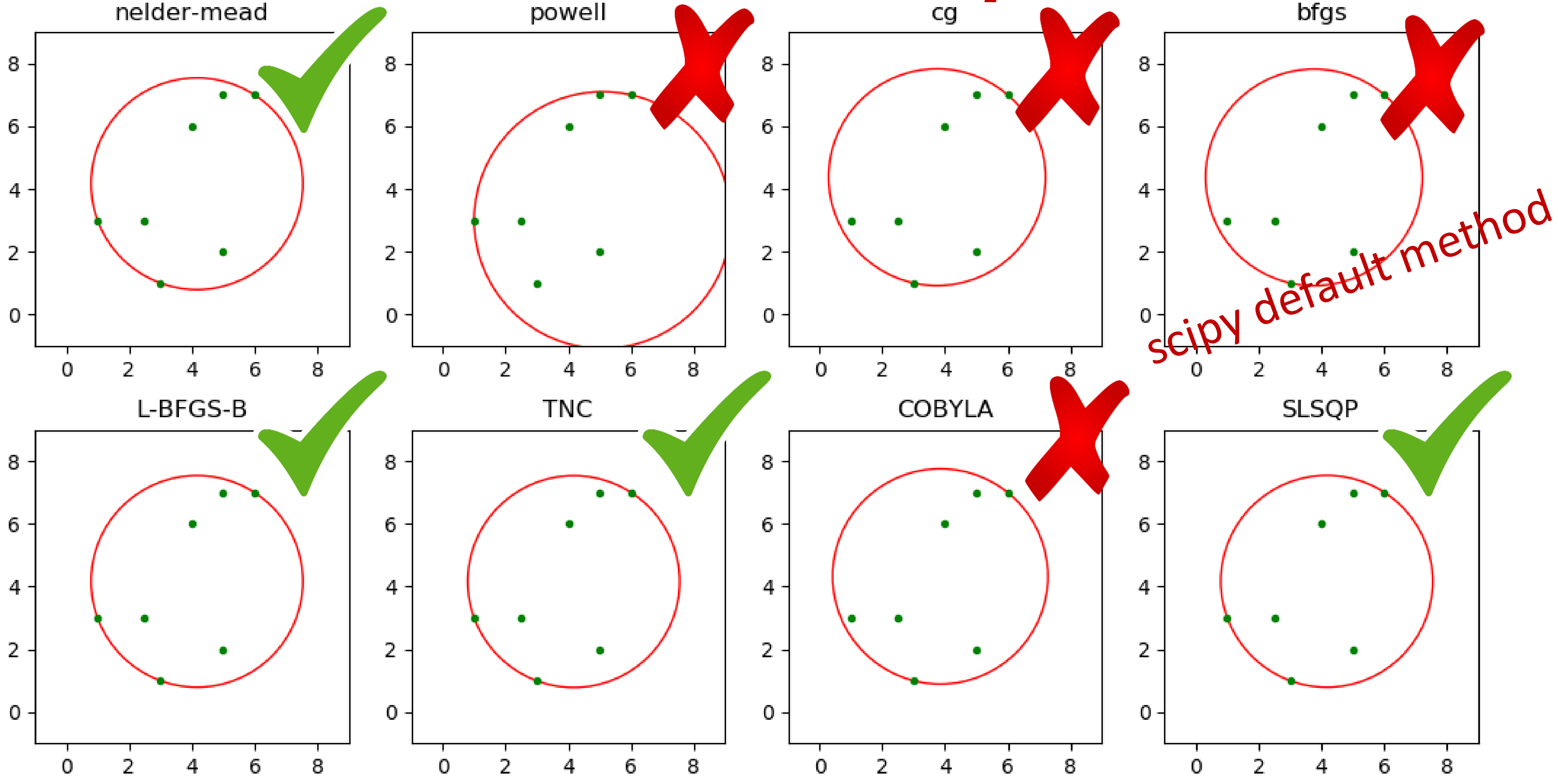
enclosing_circle_search_space.py (previous slide)

```python
from math import sqrt
from scipy.optimize import minimize
import matplotlib.pyplot as plt
import numpy as np
from mpl_toolkits.mplot3d import Axes3D

points = [(1.0, 3.0), (3.0, 1.0), (2.5, 3.0),
  (4.0, 6.0), (5.0, 7.0), (6.0, 7.0), (5.0, 2.0)]

#  Minimum enclosing circle solver

trace = []

def distance(p, q):
    return sqrt((p[0]-q[0])**2 + (p[1]-q[1])**2)

def distance_max(q):
    dist = max(distance(p, q) for p in points)
    trace.append((*q, dist))
    return dist

solution = minimize(distance_max, [0.0, 0.0],
                    method='nelder-mead')
center = solution.x
radius = solution.fun

#  unzip point coordinates

points_x, points_y = zip(*points)
trace_x, trace_y, trace_z = zip(*trace)

#  Bounding box [x_min, x_max] x [y_min, y_max]

xs, ys = points_x + trace_x, points_y + trace_y
x_min, x_max = min(xs), max(xs)
y_min, y_max = min(ys), max(ys)
# enforce apsect ratio
x_max = max(x_max, x_min + y_max - y_min)
y_max = max(y_max, y_min + x_max - x_min)
```

```python
#  Minimum enclosing circle - 3D surface plot
#  (plot_surface requires X, Y, Z are 2D numpy.arrays)

X, Y = np.meshgrid(np.linspace(x_min, x_max, 100),
                   np.linspace(y_min, y_max, 100))
Z = np.zeros(X.shape)
for px, py in points:
    Z = np.maximum(Z, (X - px)**2 + (Y - py)**2)
Z = np.sqrt(Z)

ax = plt.subplot(1, 2, 1, projection='3d')
ax.plot_surface(X, Y, Z, cmap='plasma', alpha=0.7)
ax.plot(trace_x, trace_y, trace_z, '.-', c='darkblue')
ax.scatter(*center, radius, 'o', c='red')
ax.set_xlabel('x')
ax.set_ylabel('y')
ax.set_zlabel('max distance')
ax.set_title('plot_surface')

#  Minimum enclosing circle - contour plot

plt.subplot(1, 2, 2)
plt.title('pyplot.contour')
plt.plot(trace_x, trace_y, '.-', color='darkblue')
plt.plot(points_x, points_y, 'o', color='darkgreen')
plt.plot(*center, 'o', c='red')
qcs = plt.contour(X, Y, Z, levels=30, cmap='plasma')
plt.clabel(qcs, inline=1, fontsize=8, fmt='%.1f')

plt.suptitle('Maximum distance to an input point')
plt.tight_layout()
plt.show()
```

⚠ numpy arrays

scipy.minimize $f(c) = \max_{p} |p - c|$

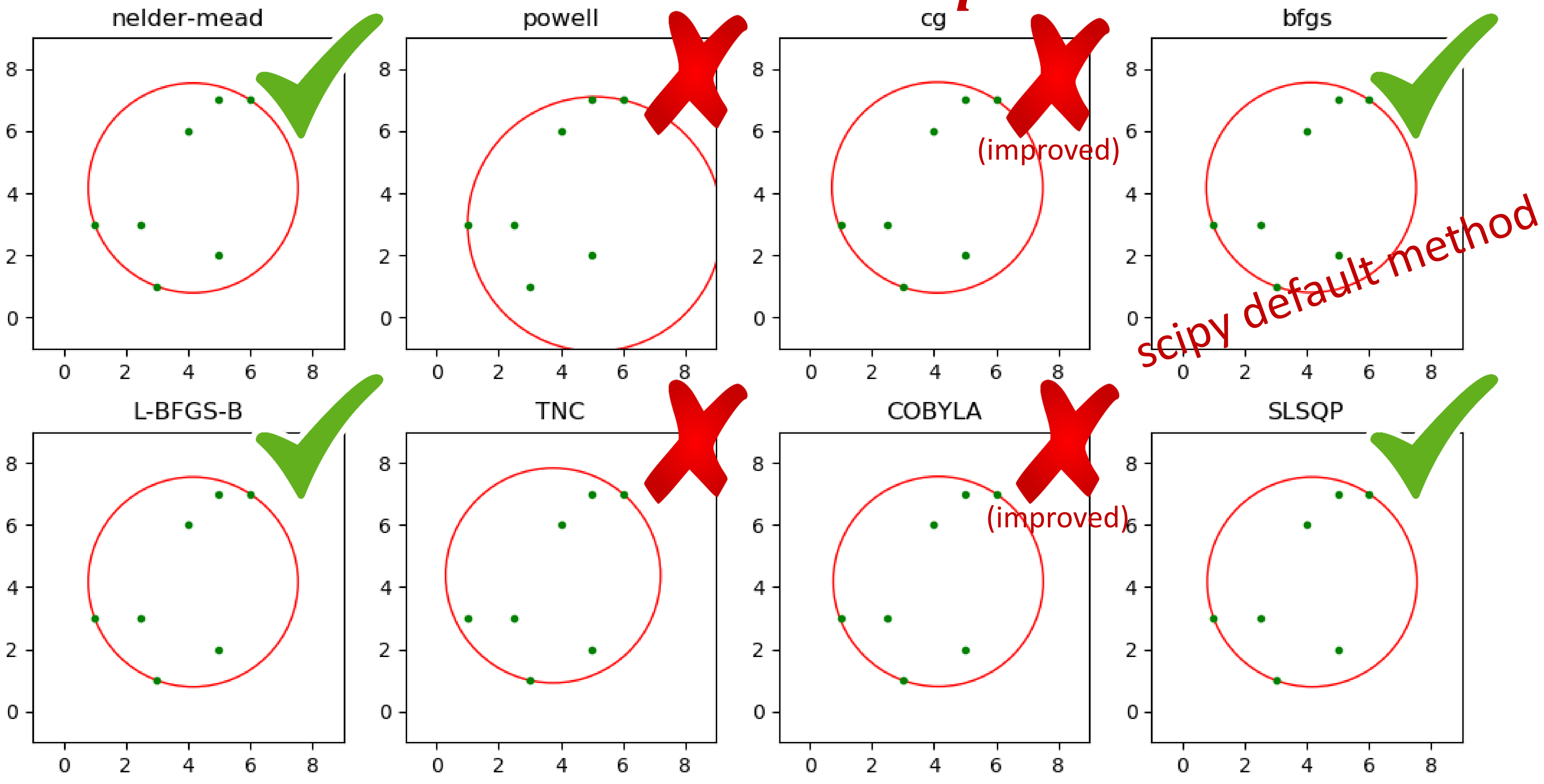


scipy default method

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

scipy.minimize $f(c) = \max_{p} |p - c|^2$

avoids $\sqrt{}$



(improved)

(improved)

scipy default method