Visualization and optimization

- Matplotlib
- Jupyter
- scipy.optimize.minimize

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

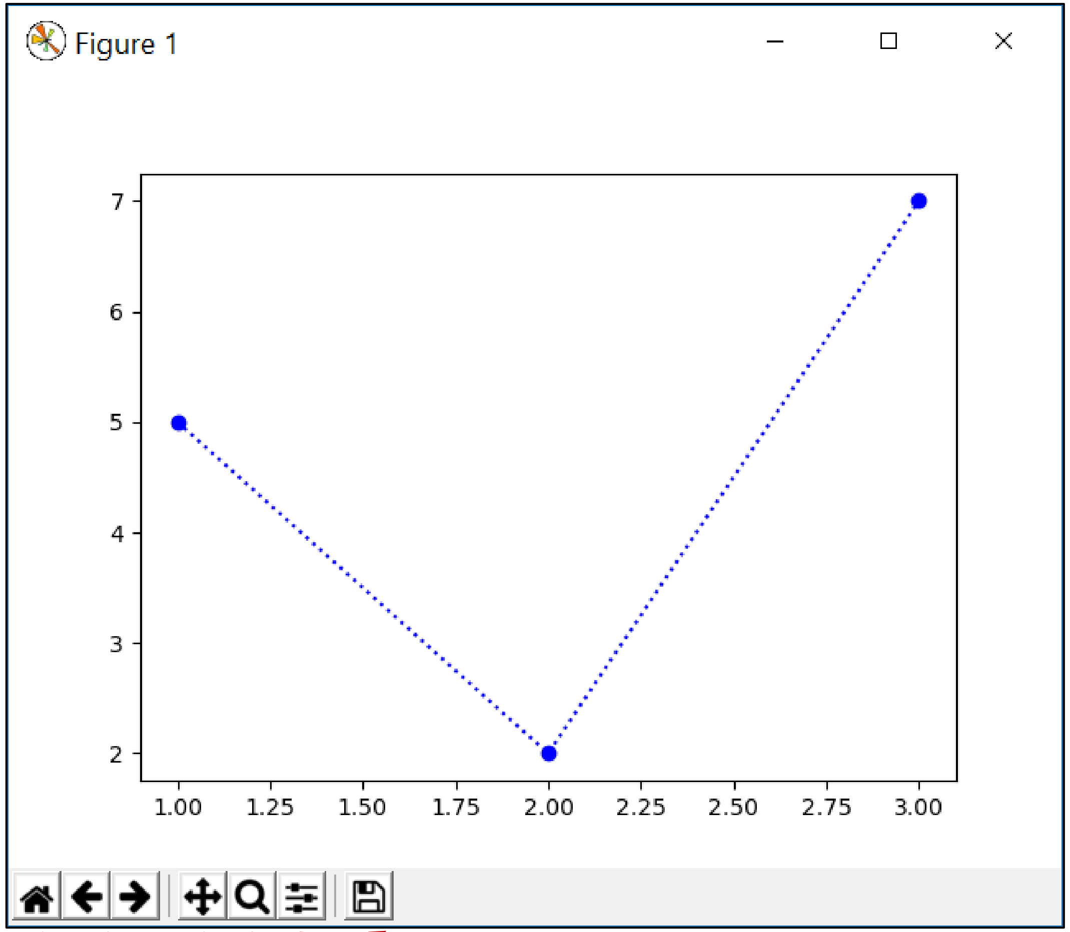
x coordinates

y coordinates

format string

figure is first shown when show is called

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

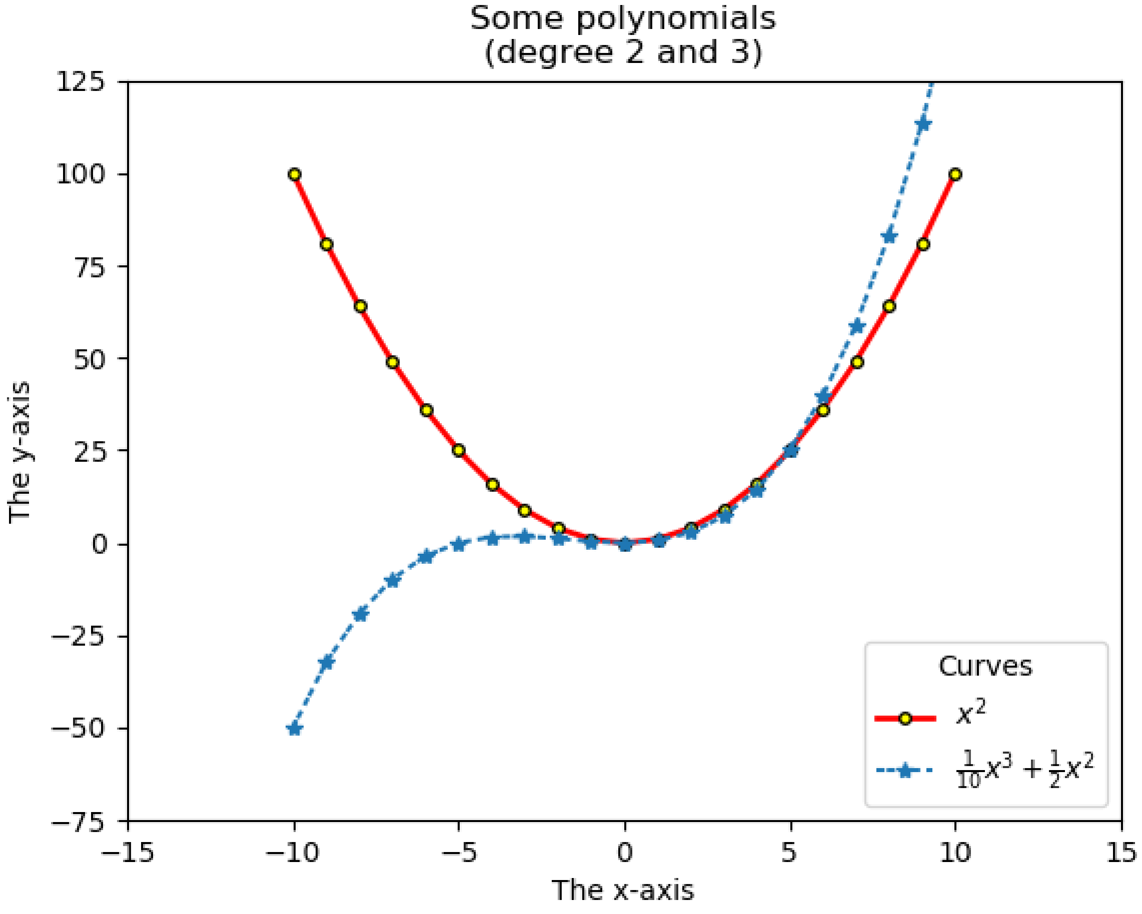
reset view

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)

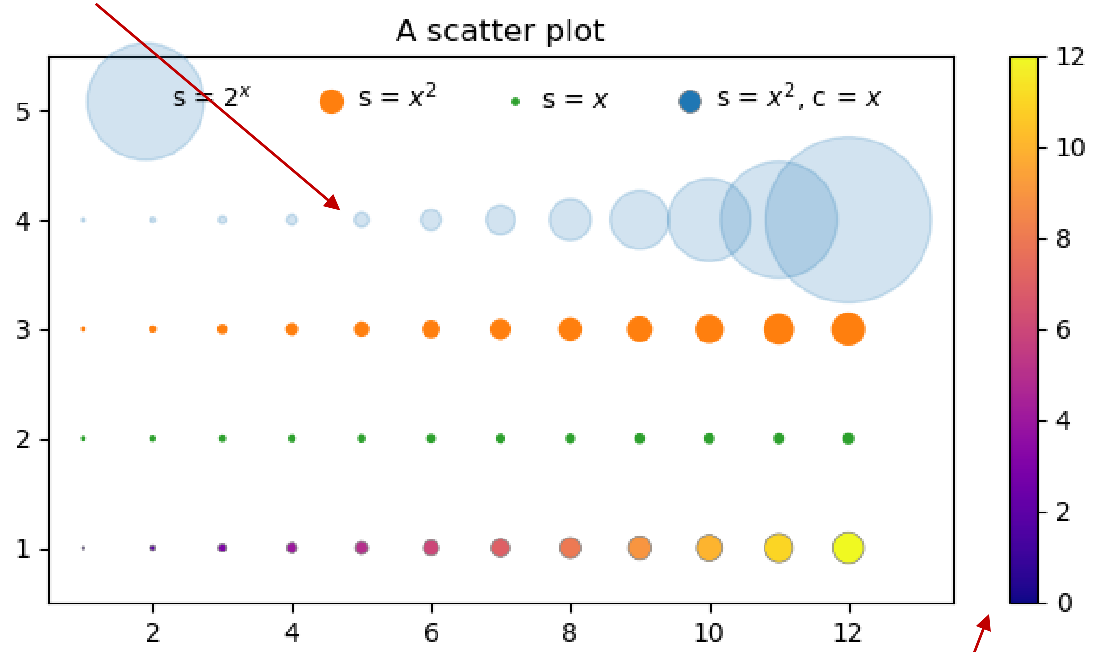
matplotlib-scatter.py

```python
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



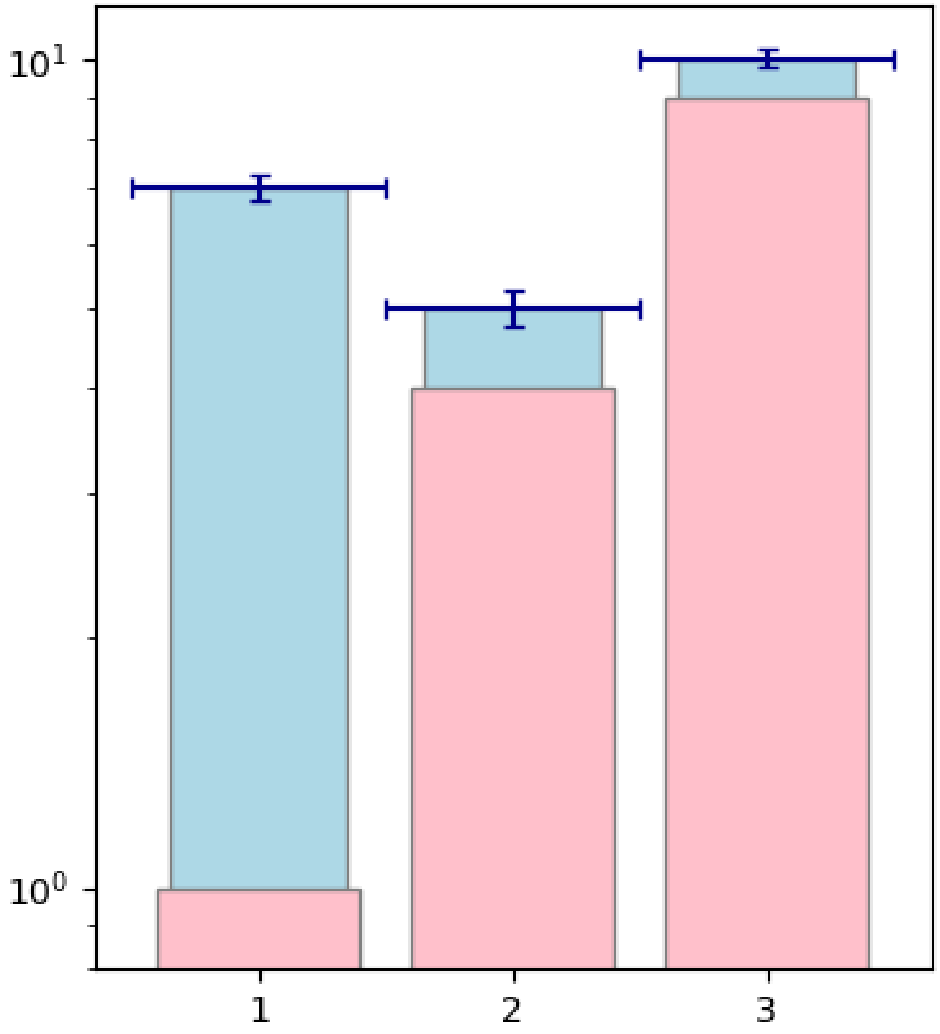
colorbar
(of most recently used colormap)

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()
```

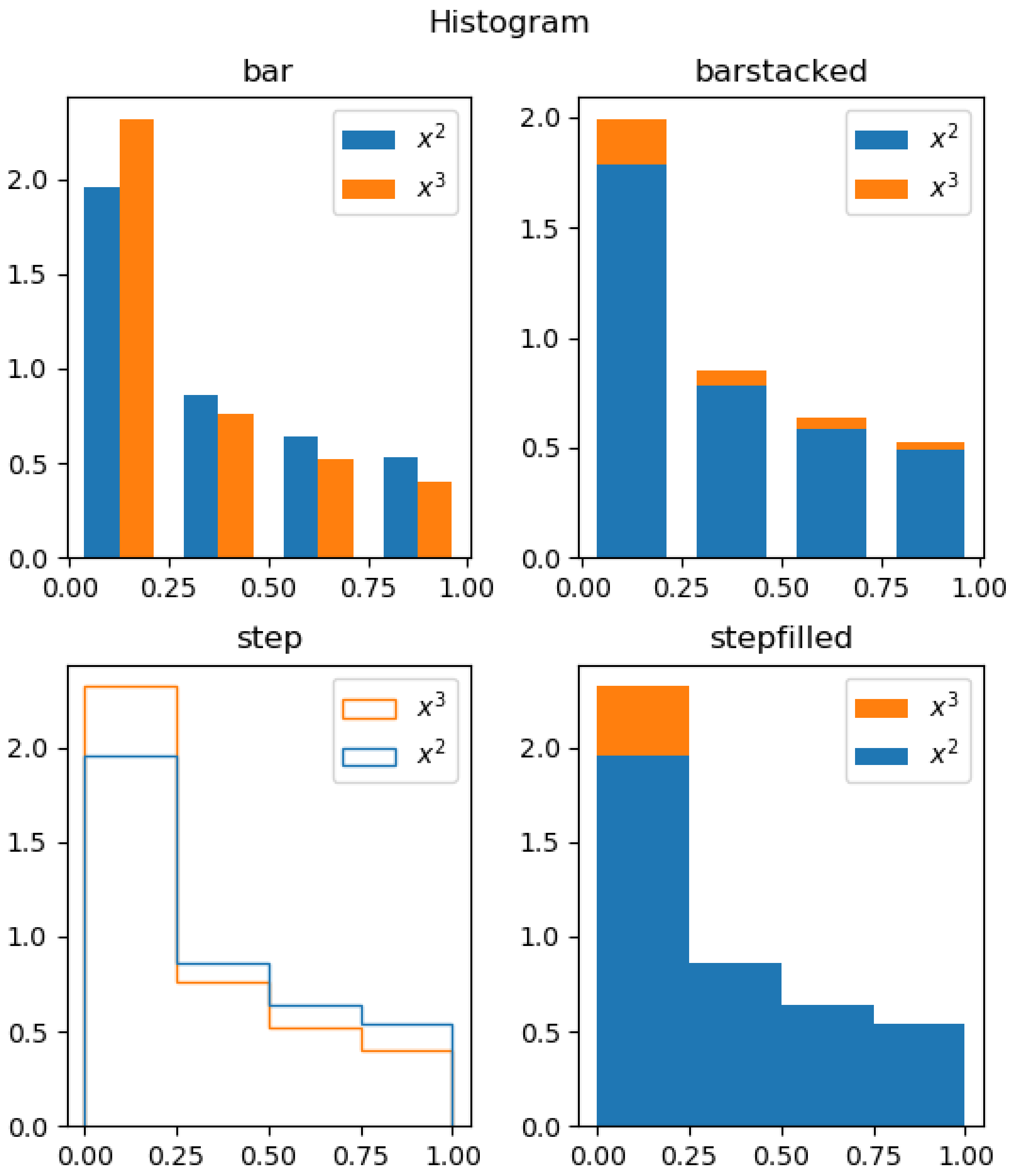


matplotlib.org/api/_as_gen/matplotlib.pyplot.bar.html

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()
```

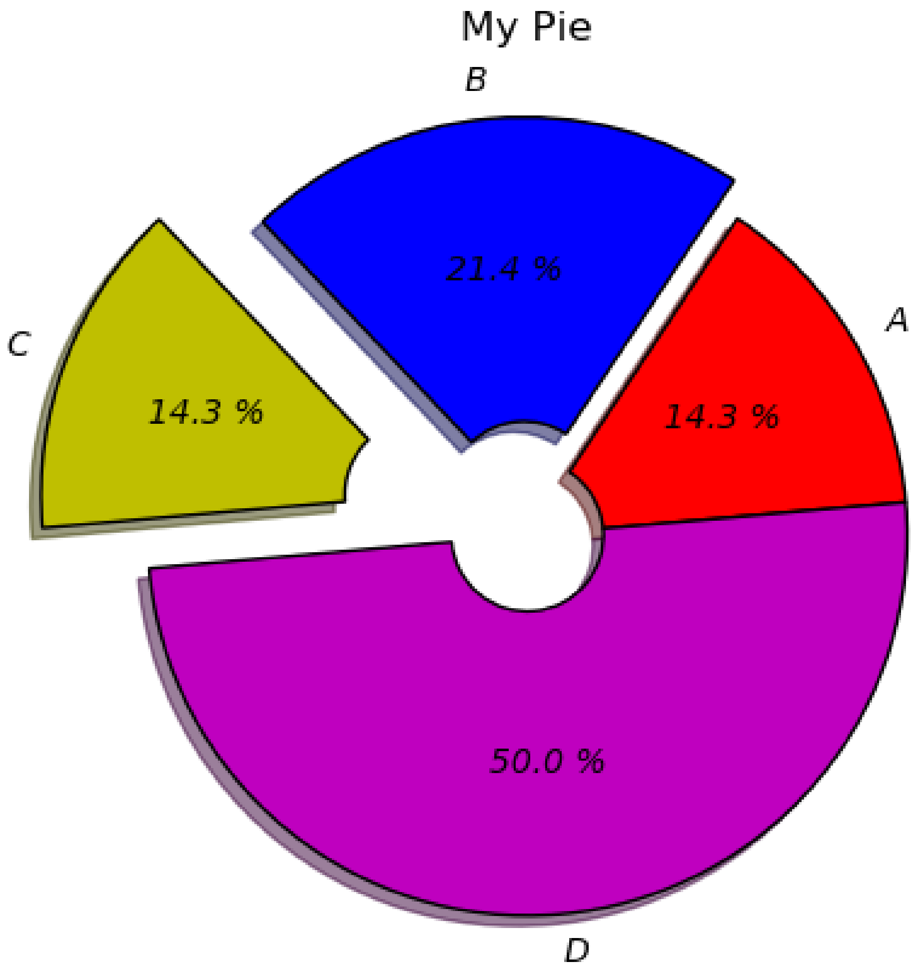


matplotlib.org/api/_as_gen/matplotlib.pyplot.hist.html

Pie

matplotlib-pie.py

```python
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

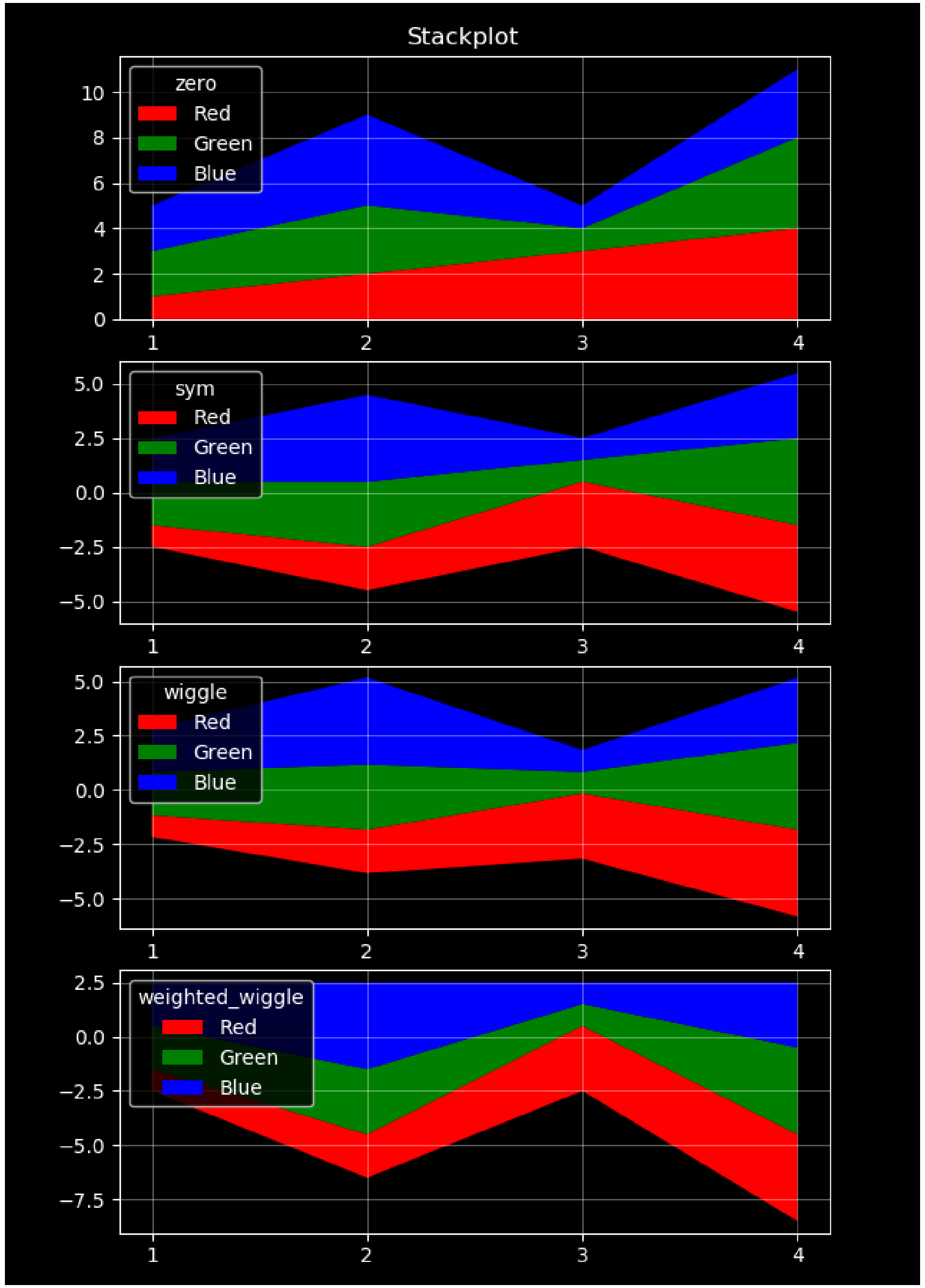
Stackplot

matplotlib-stackplot.py

```
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)`

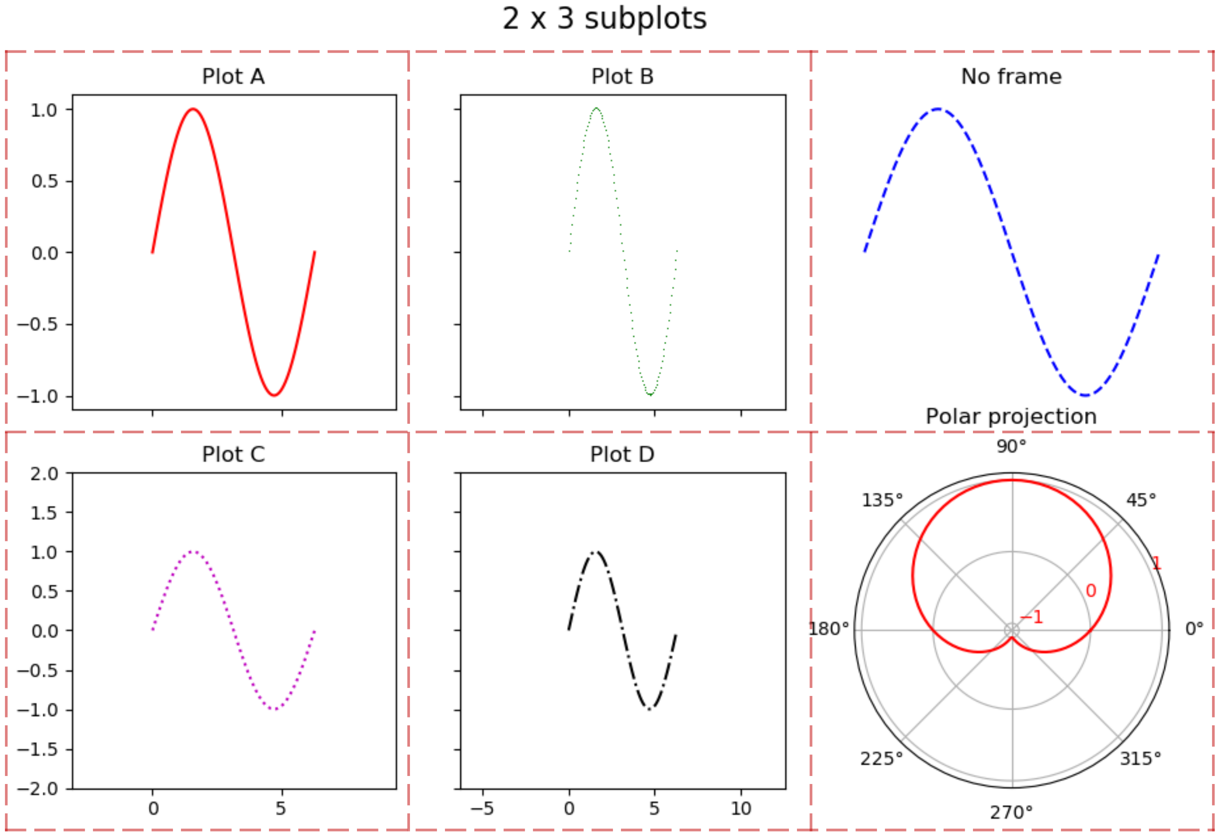


matplotlib.org/api/_as_gen/matplotlib.pyplot.stackplot.html matplotlib-subplot.py

```
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

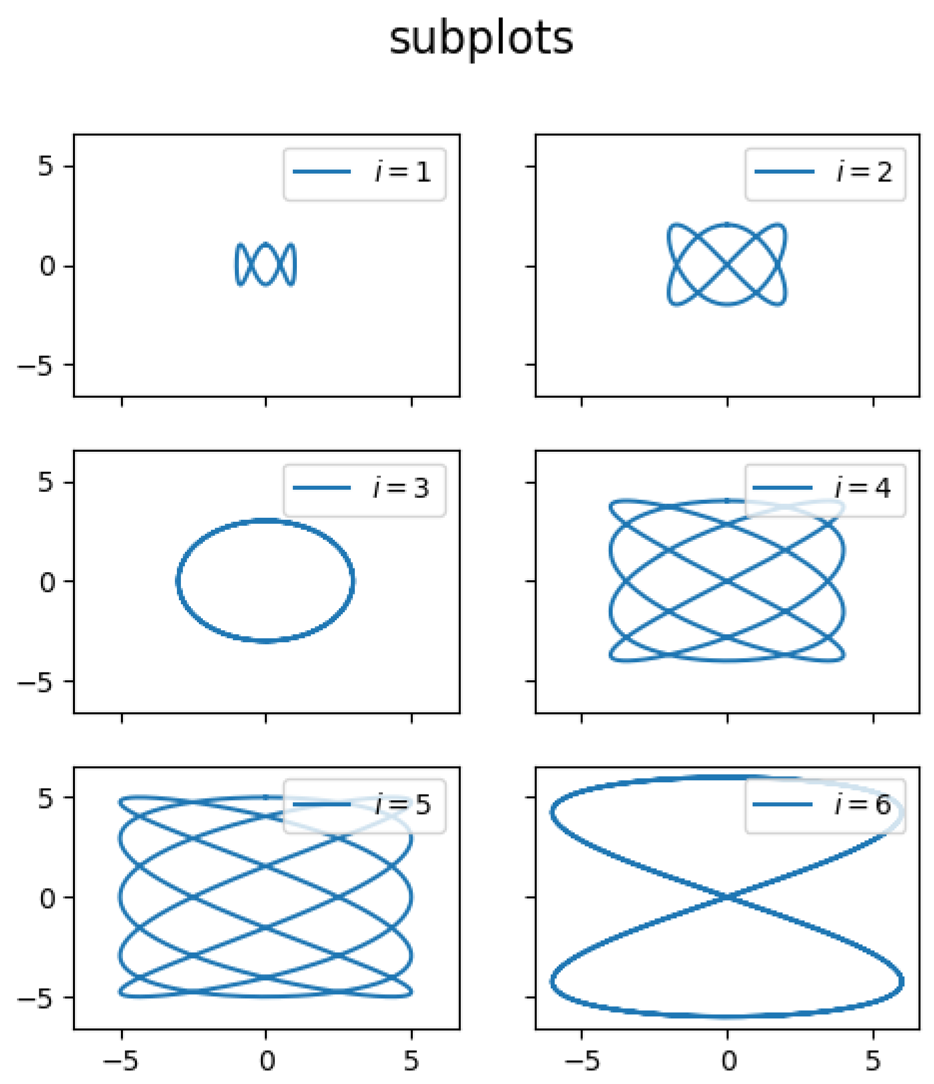
matplotlib.org/api/_as_gen/matplotlib.pyplot.subplot.html

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)



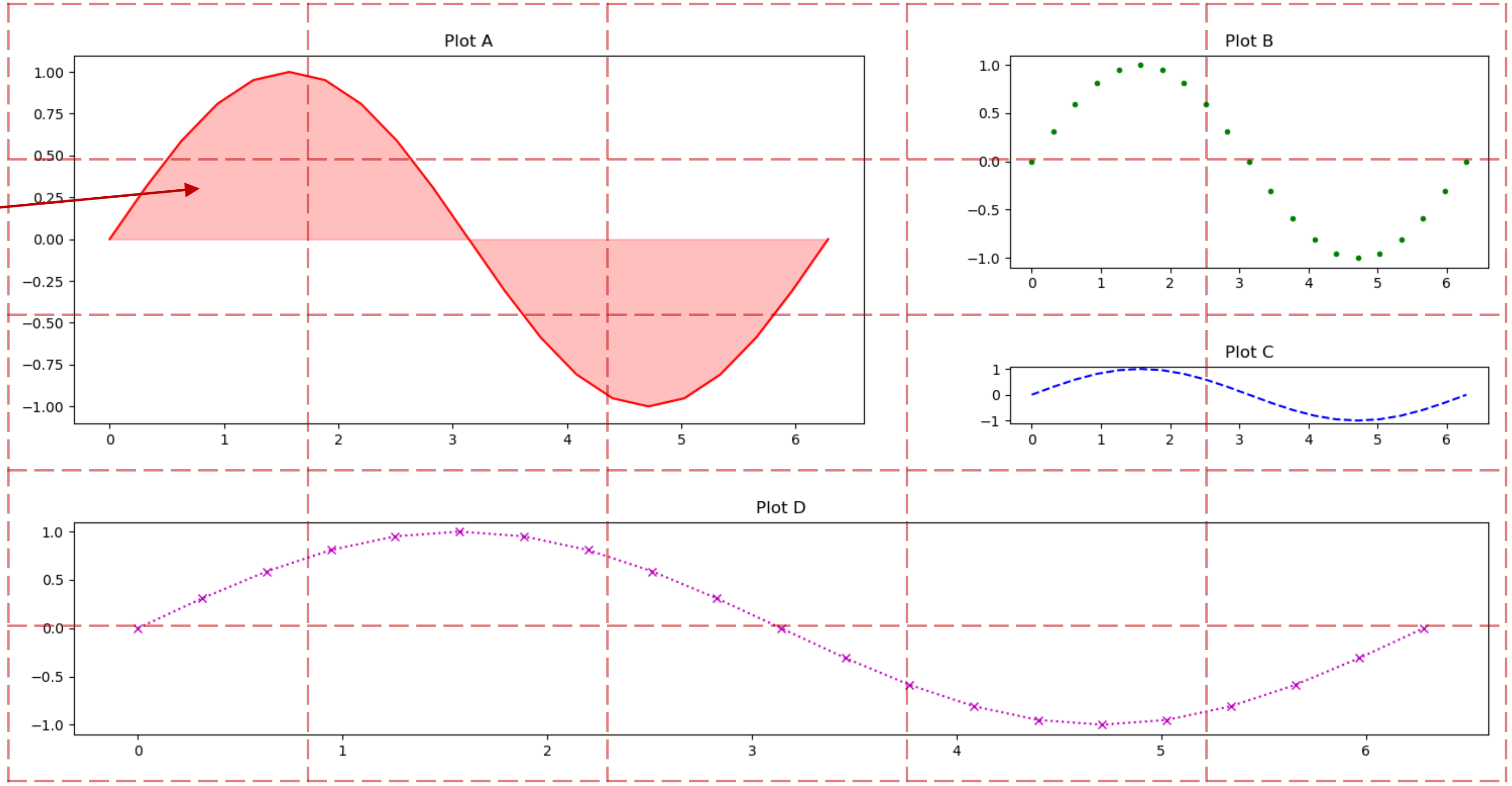
matplotlib.org/api/_as_gen/matplotlib.pyplot.subplots.html

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()
```

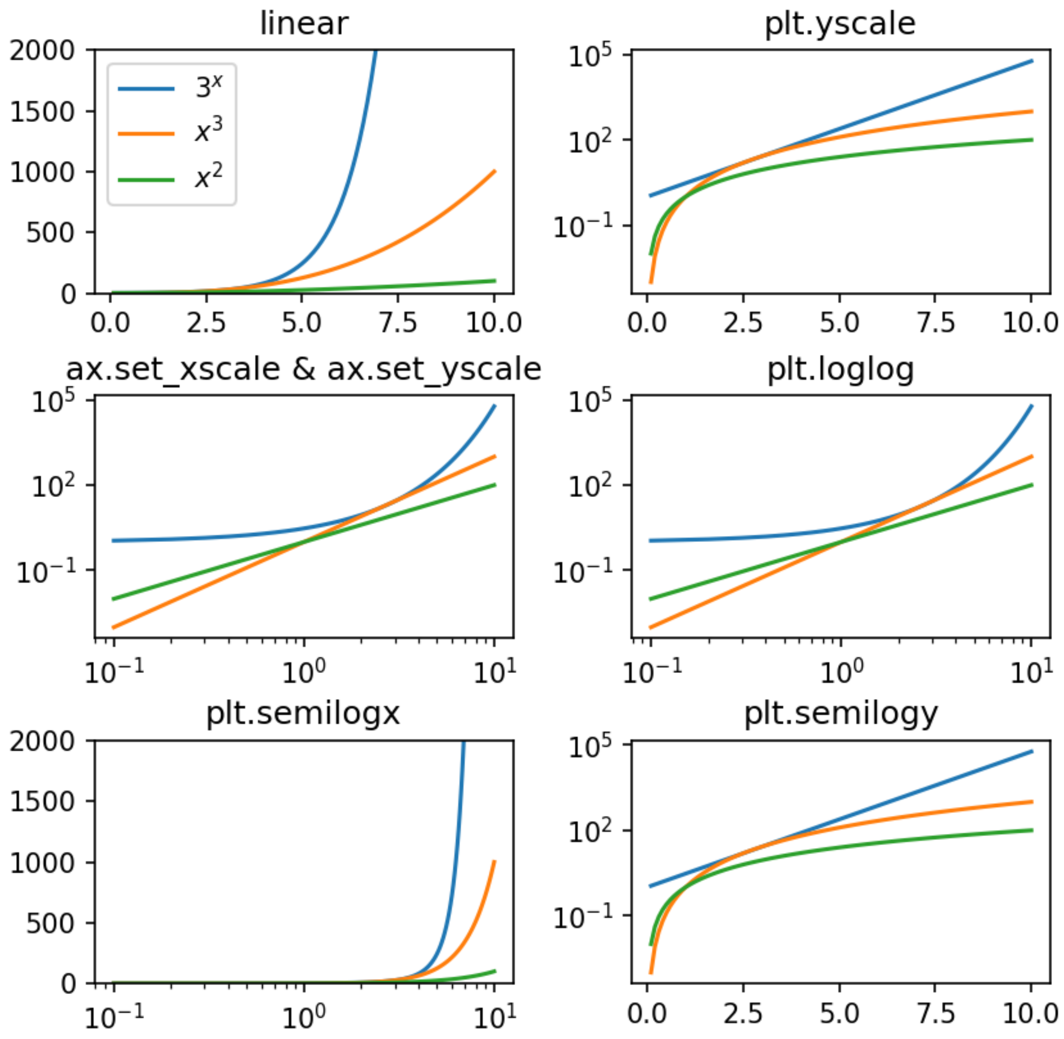
upper left corner (row, column)



matplotlib.org/api/_as_gen/matplotlib.pyplot.subplot2grid.html 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='$x^2$')
    match i:
      case 1:
        plt.ylim(0, 2000)
        plt.xscale('linear')  # default
        plt.yscale('linear')  # default
        plt.legend()
        plt.title('linear’)
      case 2:
        plt.yscale('log')
        plt.title('plt.yscale')
      case 3:
        ax.set_xscale('log')
        ax.set_yscale('log')
        plt.title('ax.set_xscale & ax.set_yscale')
      case 4:
        plt.loglog()
        plt.title('plt.loglog')
      case 5:
        plt.ylim(0, 2000)
        plt.semilogx()
        plt.title('plt.semilogx')
      case 6:
        plt.semilogy()
        plt.title('plt.semilogy')
plt.show()
```

log scales

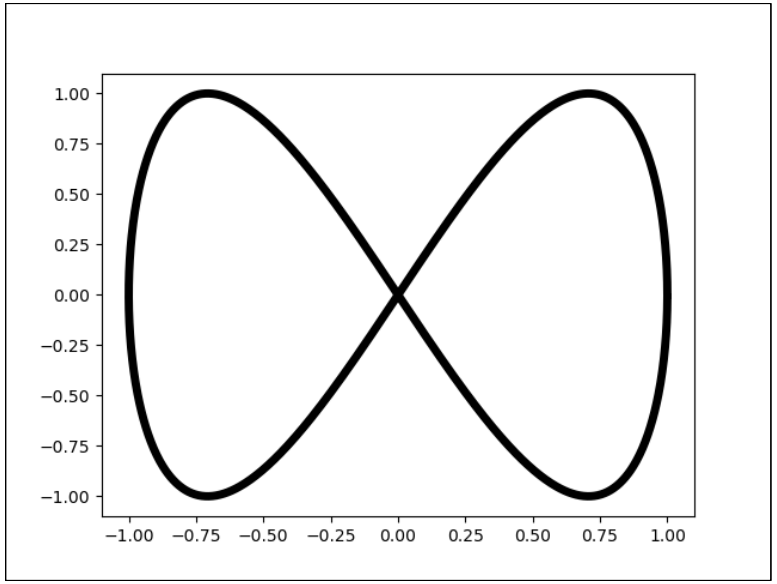


- There are many ways to make the x- and/or y-axis logarithmic with pyplot

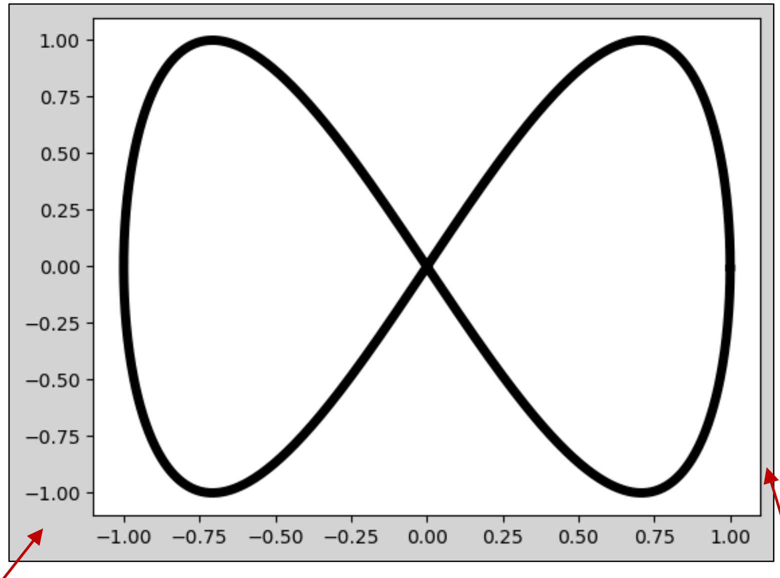
Saving figures

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

A crude animation

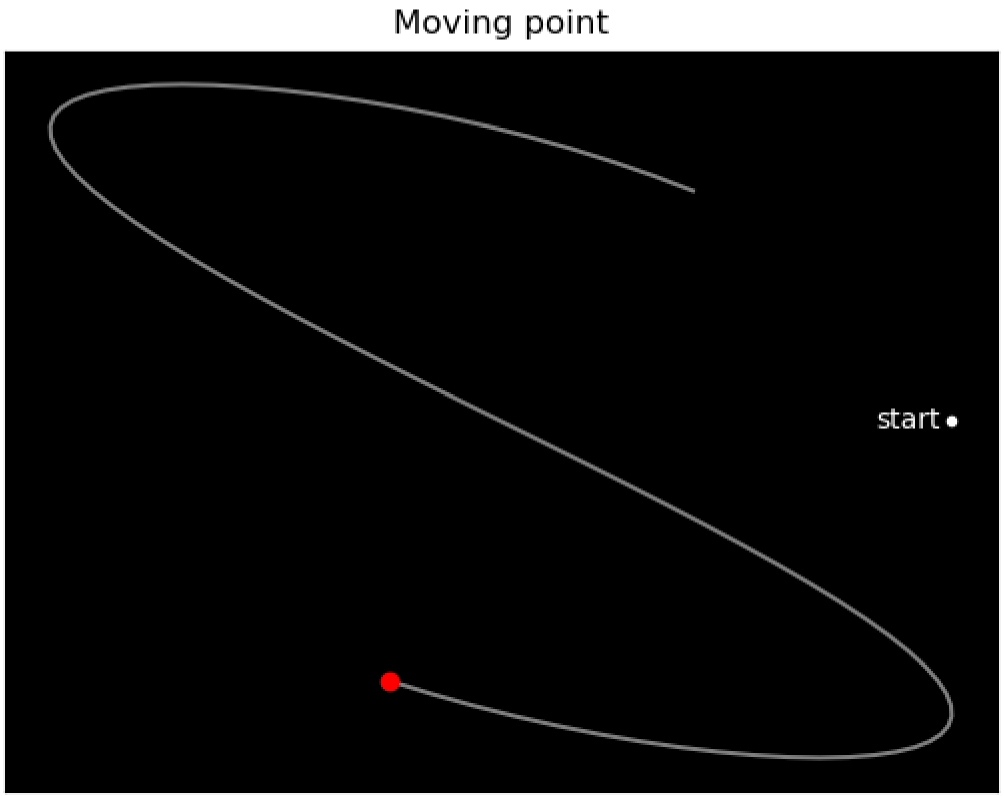
clock.py

```
import matplotlib.pyplot as plt
from math import pi, sin, cos
import datetime

def plot_clock(hour, minute, second):
    plt.axis('off')                   # hide x and y axes
    plt.gca().set_aspect('equal')  # don’t squeeze circle
    for i in range(60):               # show second marks
        angle = 2 * pi * i / 60
        x, y = cos(angle), sin(angle)
        start = 0.98 if i % 5 else .94  # every 5'th mark should be longer
        plt.plot([start * x, x], [start * y, y], c='black')  # mark
    for angle, length, style in [
        (second / 60, .90, dict(c='red',   lw=2, solid_capstyle='round')),
        (minute / 60, .85, dict(c='black', lw=3, solid_capstyle='round')),
        (hour   / 12, .50, dict(c='black', lw=8, solid_capstyle='round'))
    ]:
        angle = 2 * pi * (0.25 - angle)
        x, y = length * cos(angle), length * sin(angle)
        plt.plot([0, x], [0, y], **style)  # clock arm
    plt.plot(0, 0, 'o', ms=10, c='black')  # center dot

while True:
    now = datetime.datetime.now()  # UTZ
    plot_clock(now.hour, now.minute, now.second)
    plt.pause(1)  # show figure and pause 1 second
    plt.clf()     # clear figure
```

matplotlib.org/stable/api/_as_gen/matplotlib.pyplot.pause.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



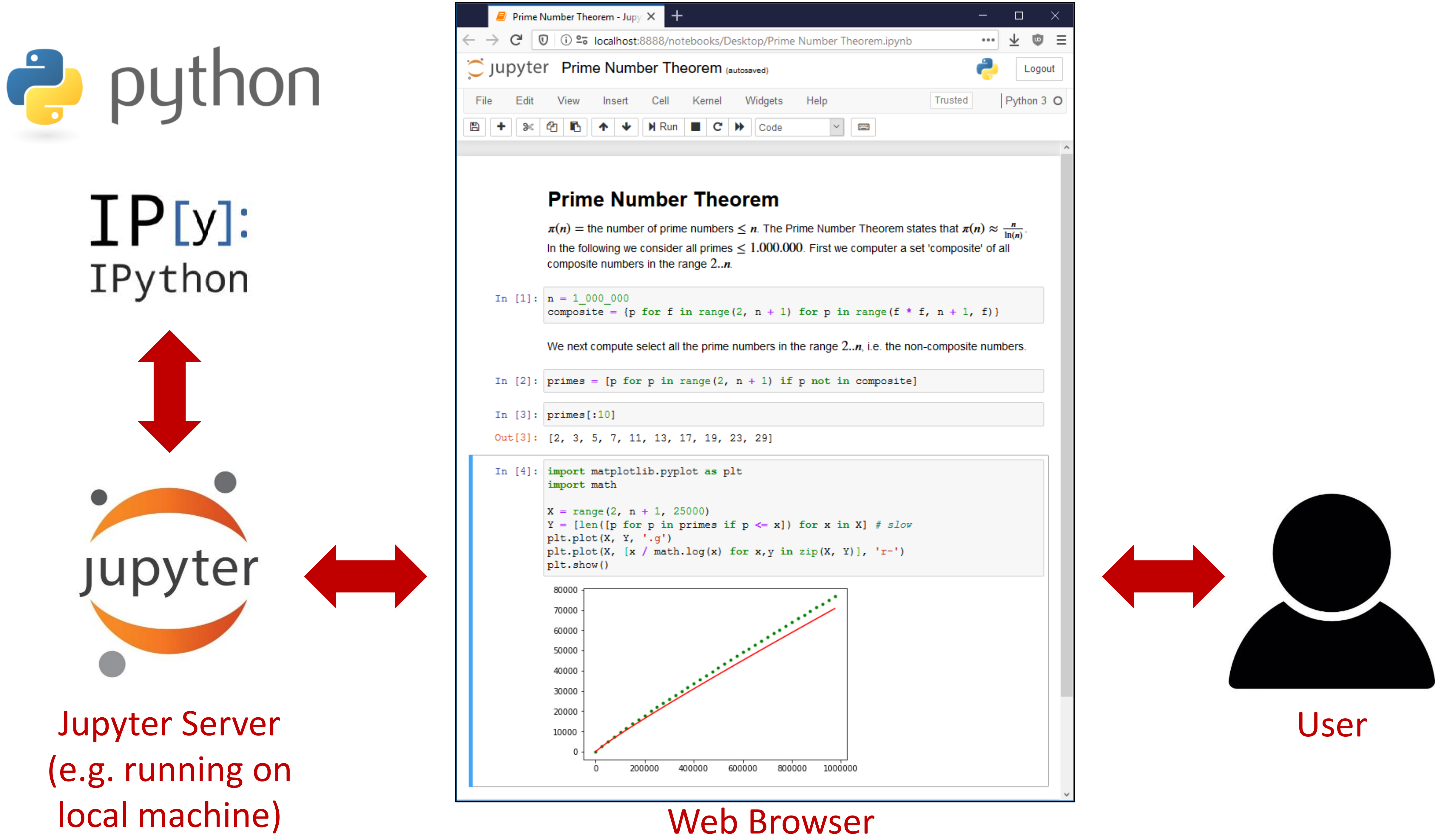
- **plot** returns "Line2D" objects representing the plotted data
- "Line2D" objects can be updated using **set_data**
- To make an animation you need to repeatedly update the "line2D" objects
- **FuncAnimation** repeatedly calls func in regular intervals interval, each time with the next value from 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.

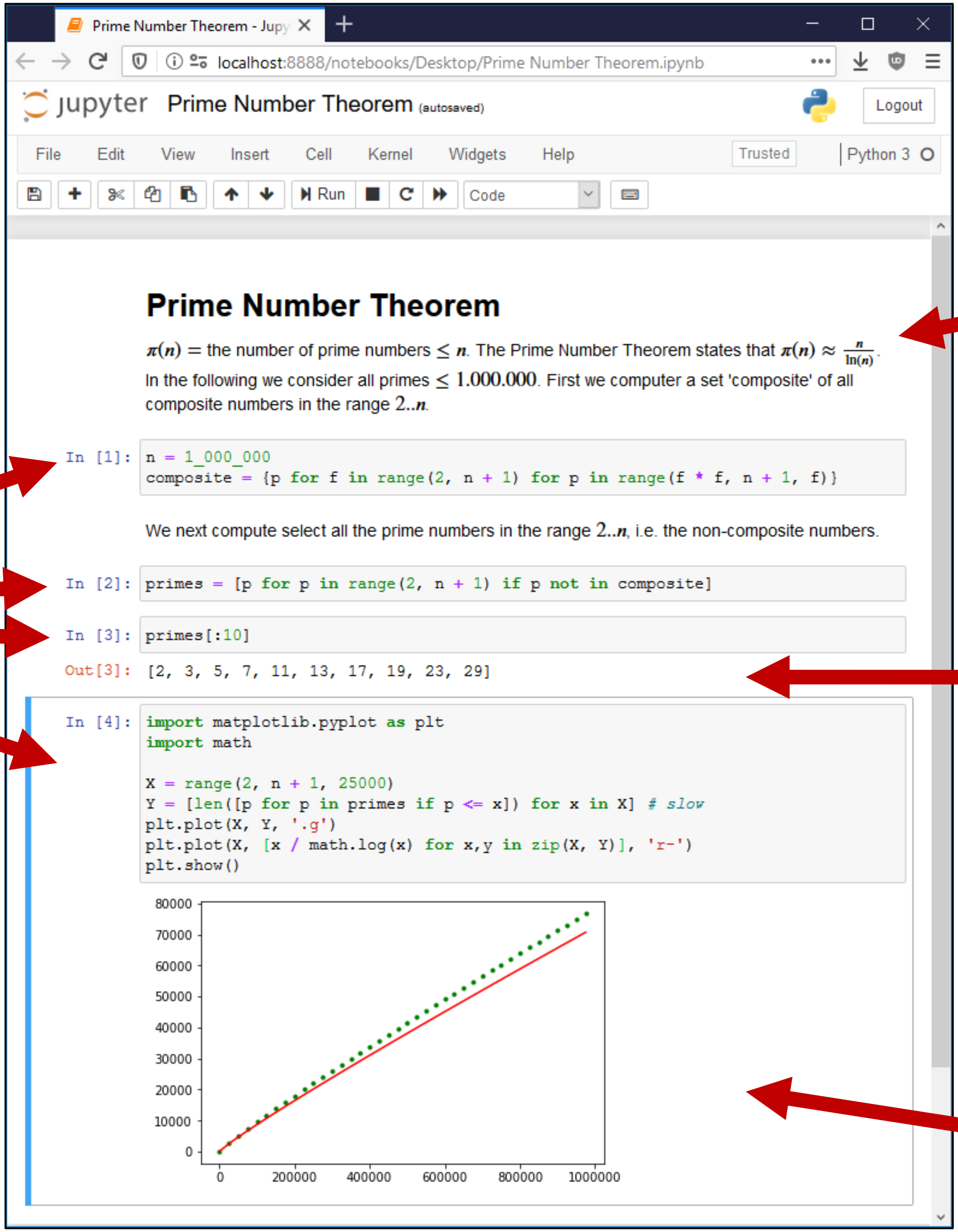
jupyter.org


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
π(n) = the number of prime numbers ≤ n. The Prime Number Theorem states that π(n) ≈ n/ln(n).
In the following we consider all primes ≤ 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()
80000
70000
60000
50000
40000
30000
20000
10000
0
0
200000
400000
600000
800000
1000000
Web Browser
User

cells

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

python code

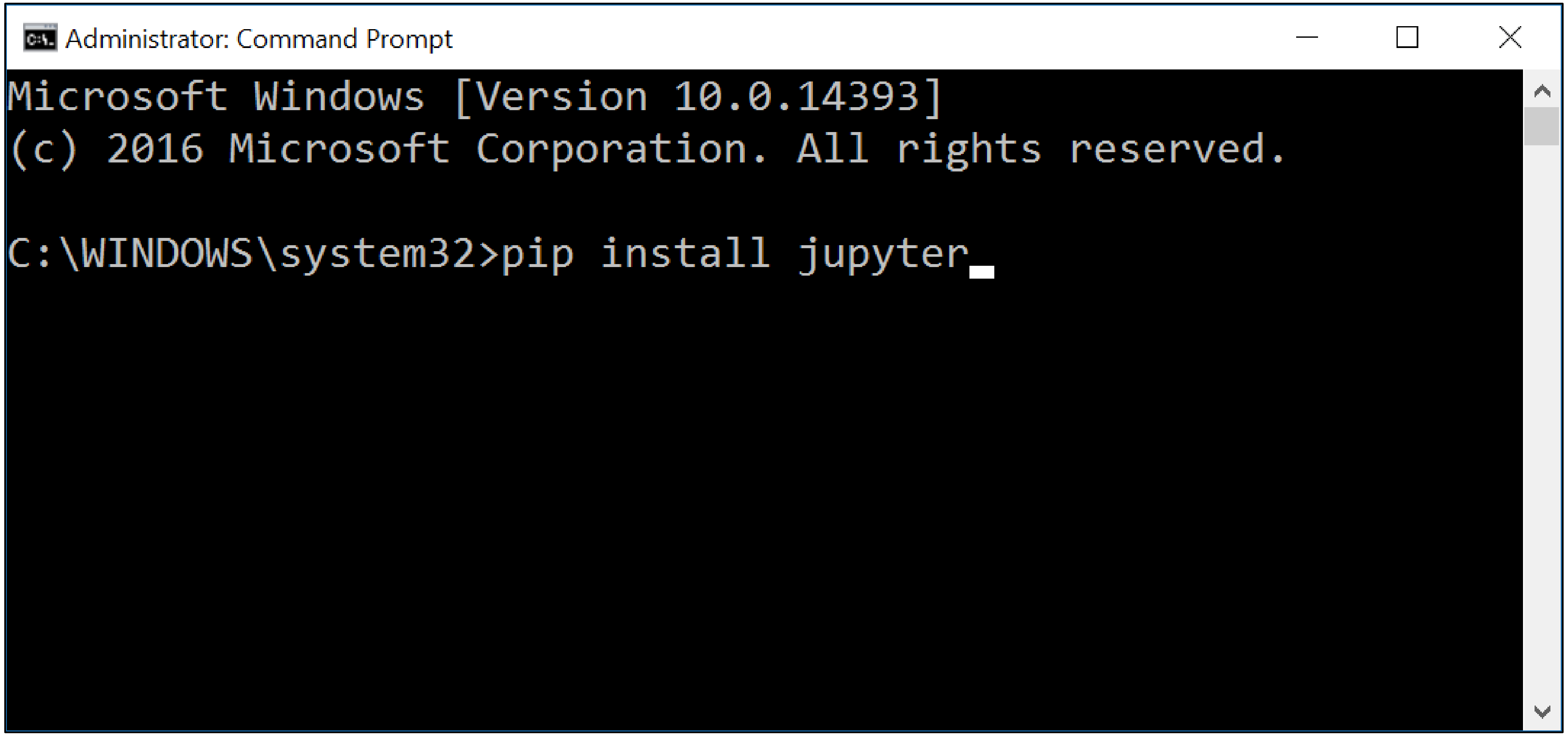


python shell output

matplotlib / numpy / ... output

Jupyter - installing

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



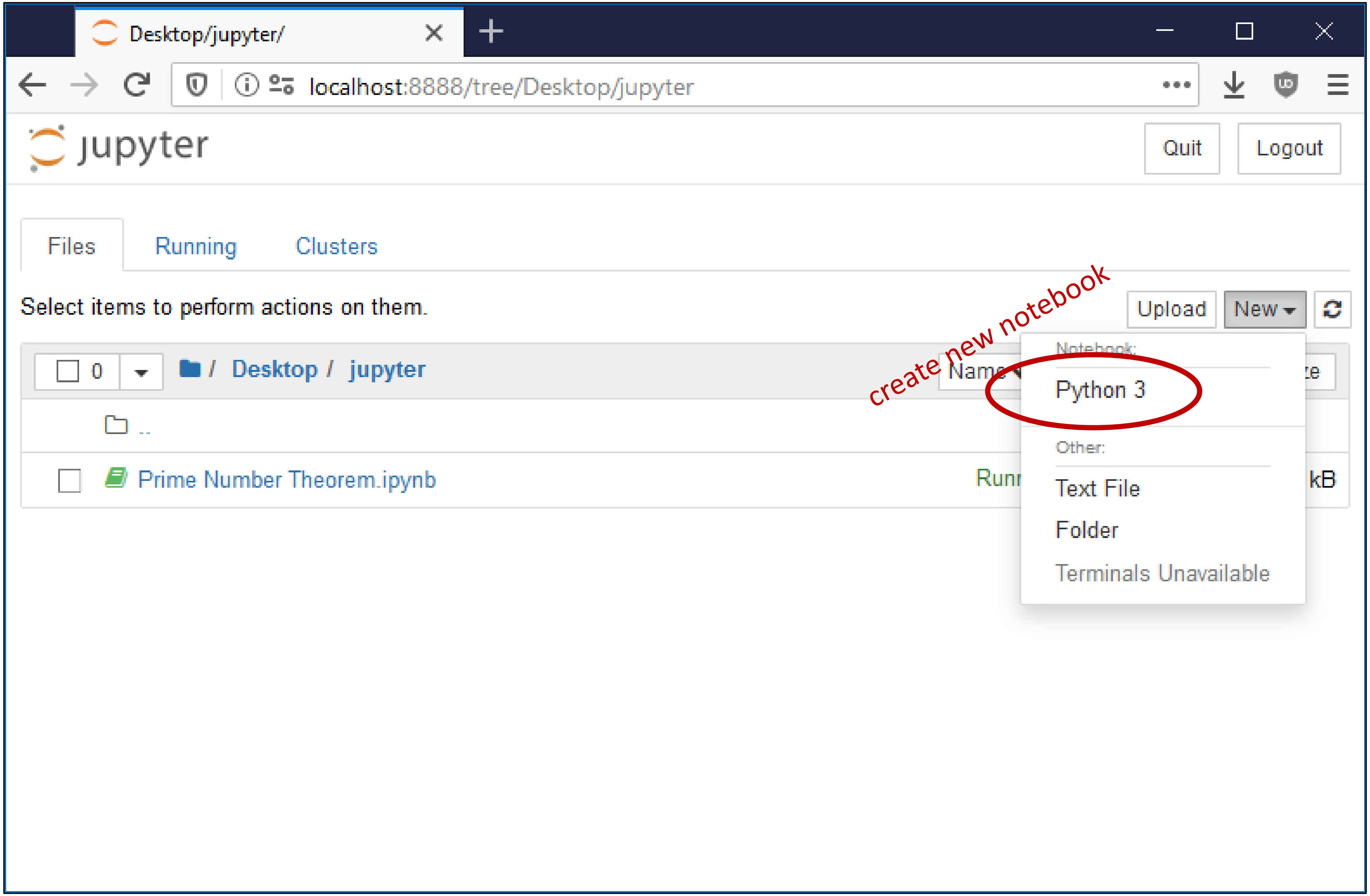
Jupyter – launching the jupyter server

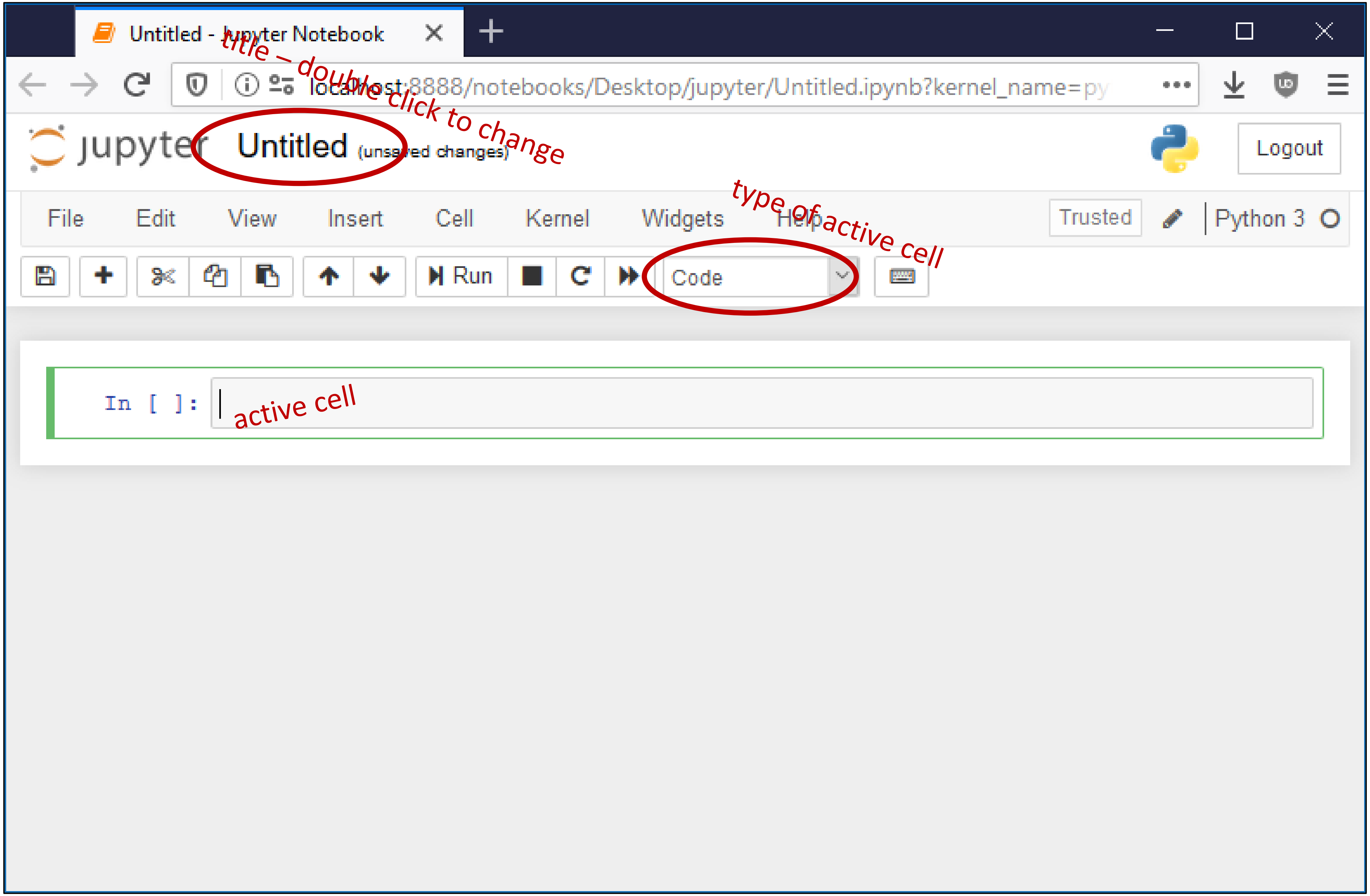
- Open a windows shell and run: `jupyter notebook`

```
Command Prompt - 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`

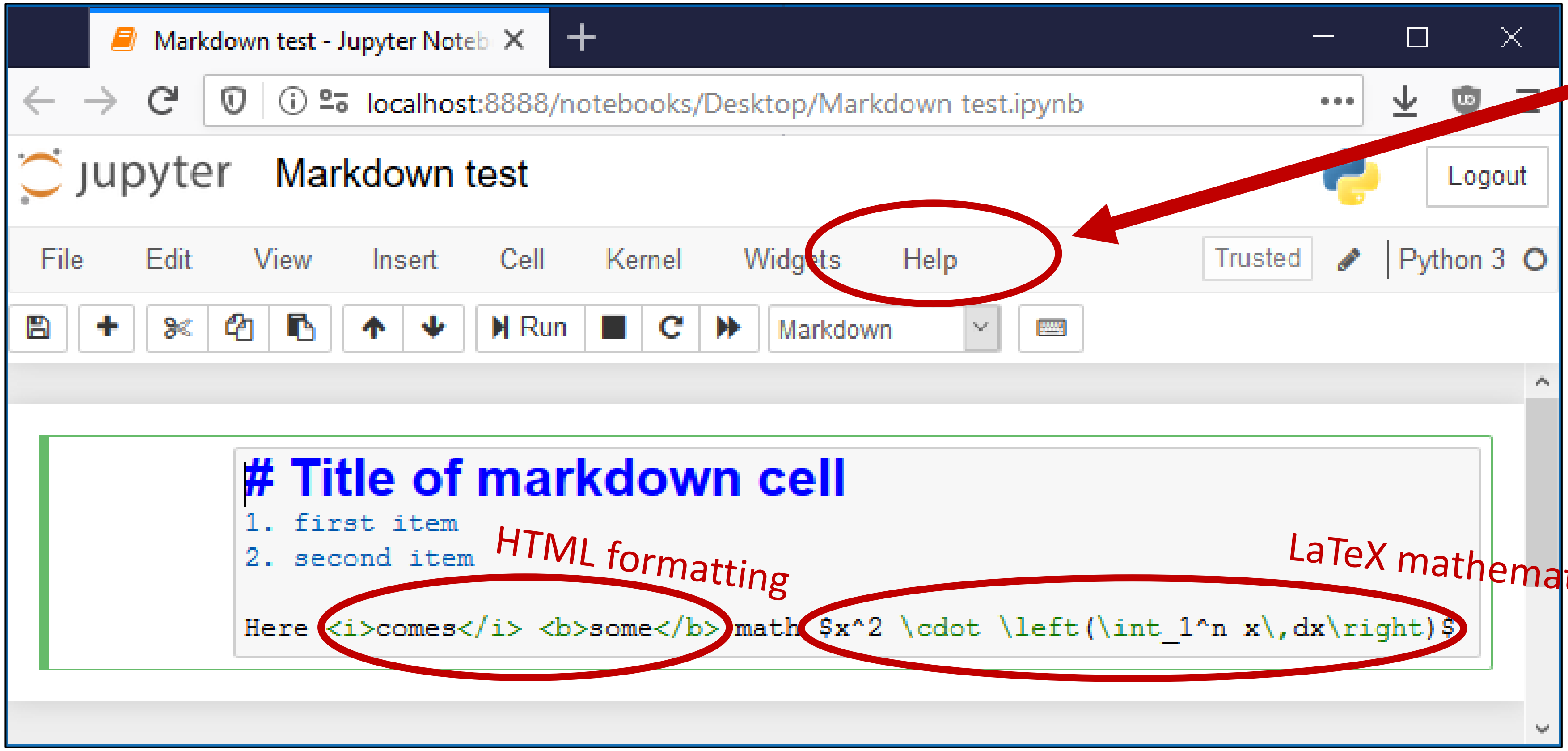

Desktop/jupyter/
localhost:8888/tree/Desktop/jupyter
jupyter
Quit
Logout
Files
Running
Clusters
Select items to perform actions on them.
Upload
New
create new notebook
Notebook:
Python 3
Other:
Text File
Folder
Terminals Unavailable
0
Desktop / jupyter
Prime Number Theorem.ipynb


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 – double click to change
type of active cell
active cell

Try:

Help > User Interface Tour

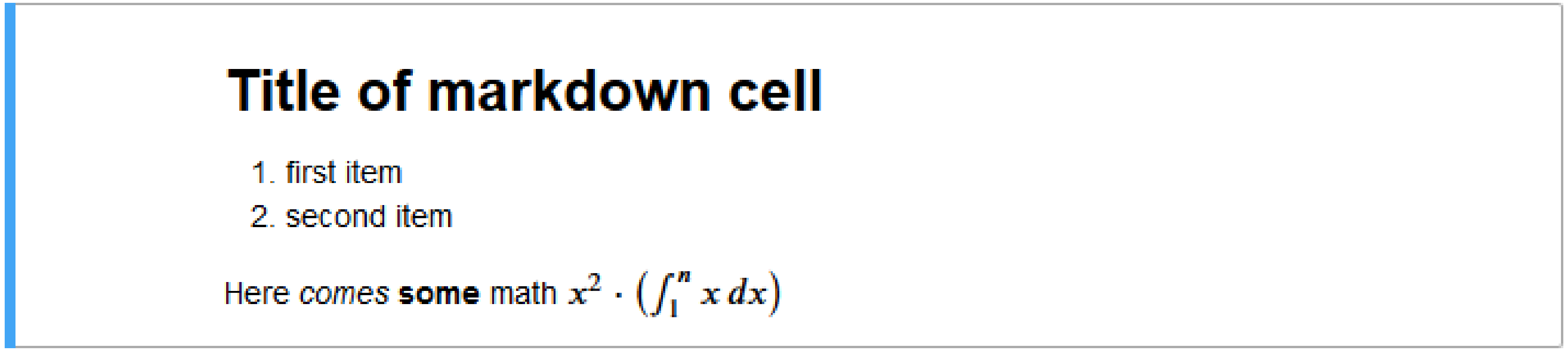
Help > Markdown



after pressing

Ctrl + Enter (evaluates)

Alt + Enter (evaluates + new cell)

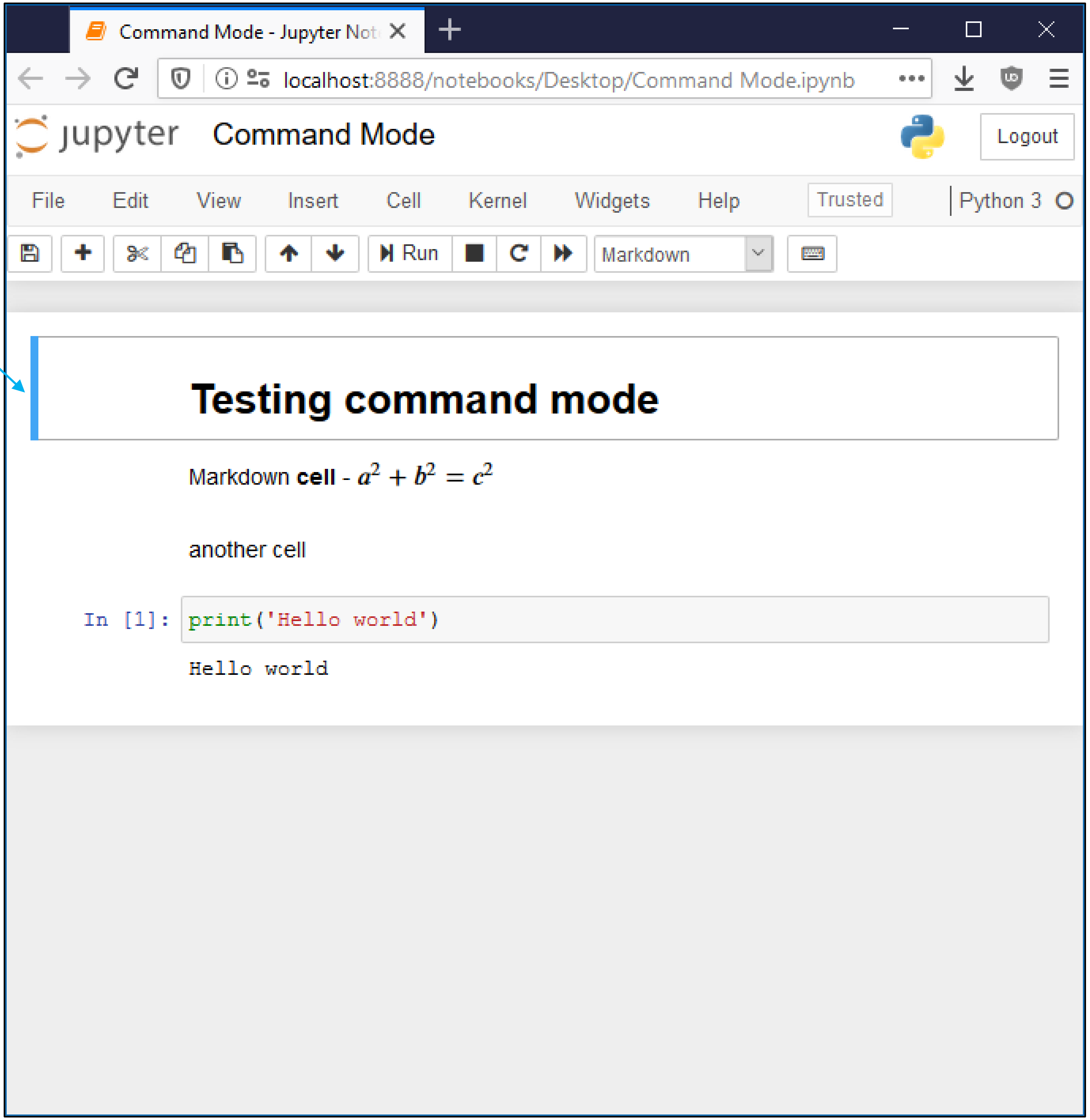


github.com/adam-p/markdown-here/wiki/Markdown-Cheatsheet

Command Mode

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

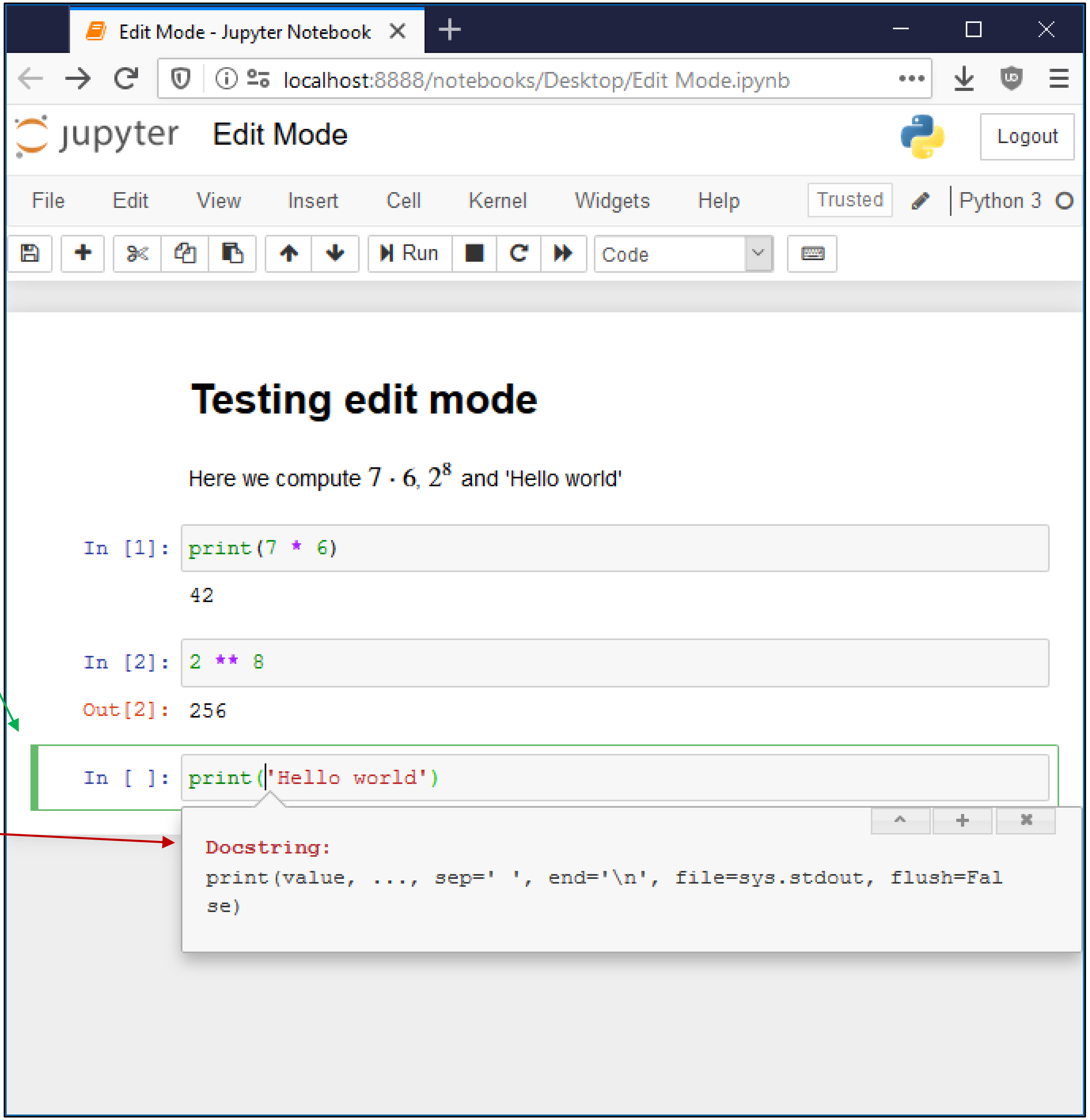
h	show keyboard shortcuts
enter	enter Edit Mode on current cell
shift-enter	run cell + select below
ctrl-enter	run selected cells
alt-enter	run cell and insert below
Y M R	change cell type (code, markdown, raw text)
1 2 3 4 5 6	change heading level
ctrl-A	select all cells
down up	move to next/previous 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)



Edit Mode

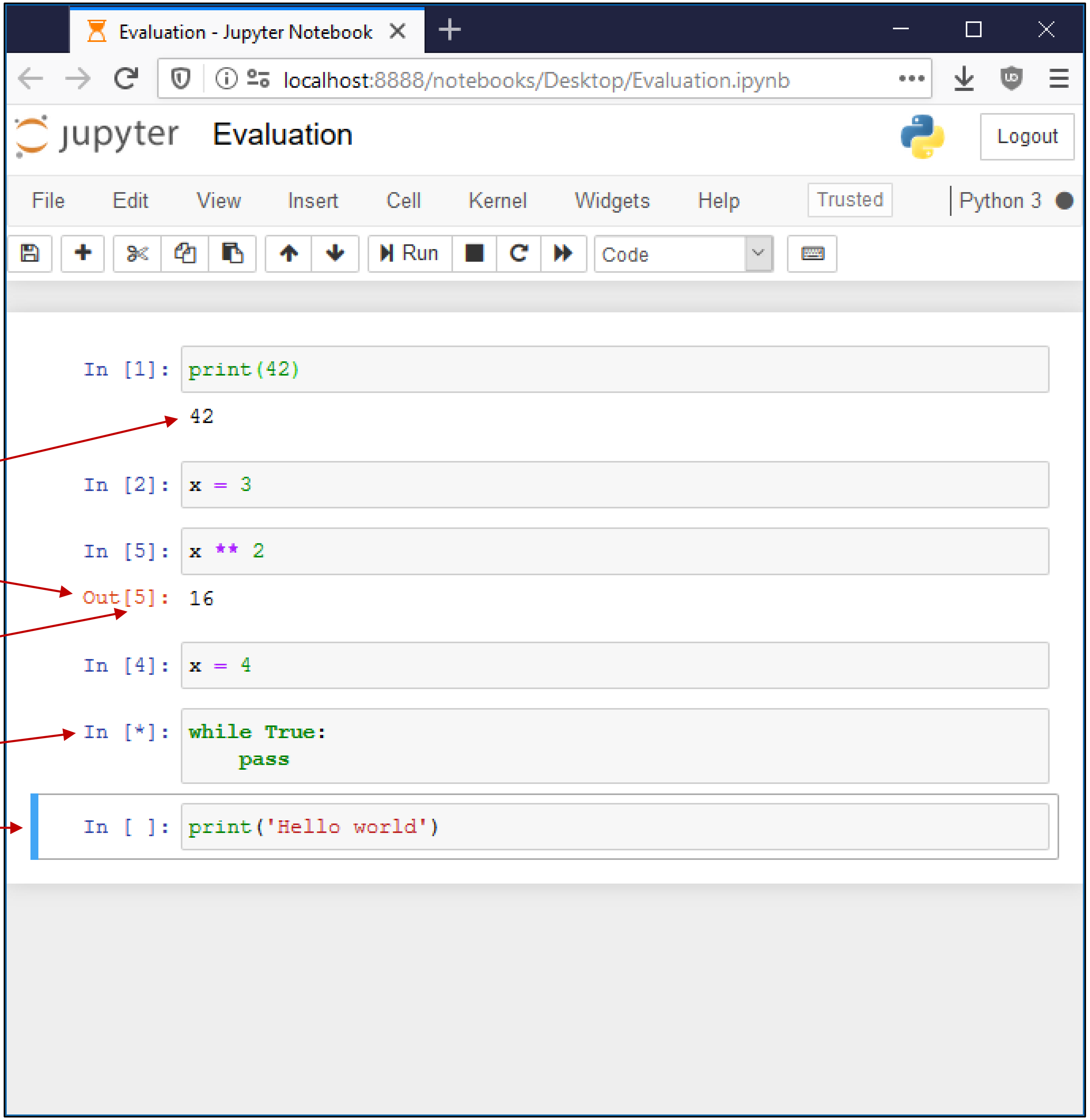
- Used to edit current cell
- Current cell is marked with green bar
- Keyboard shortcuts

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



Evaluating cells

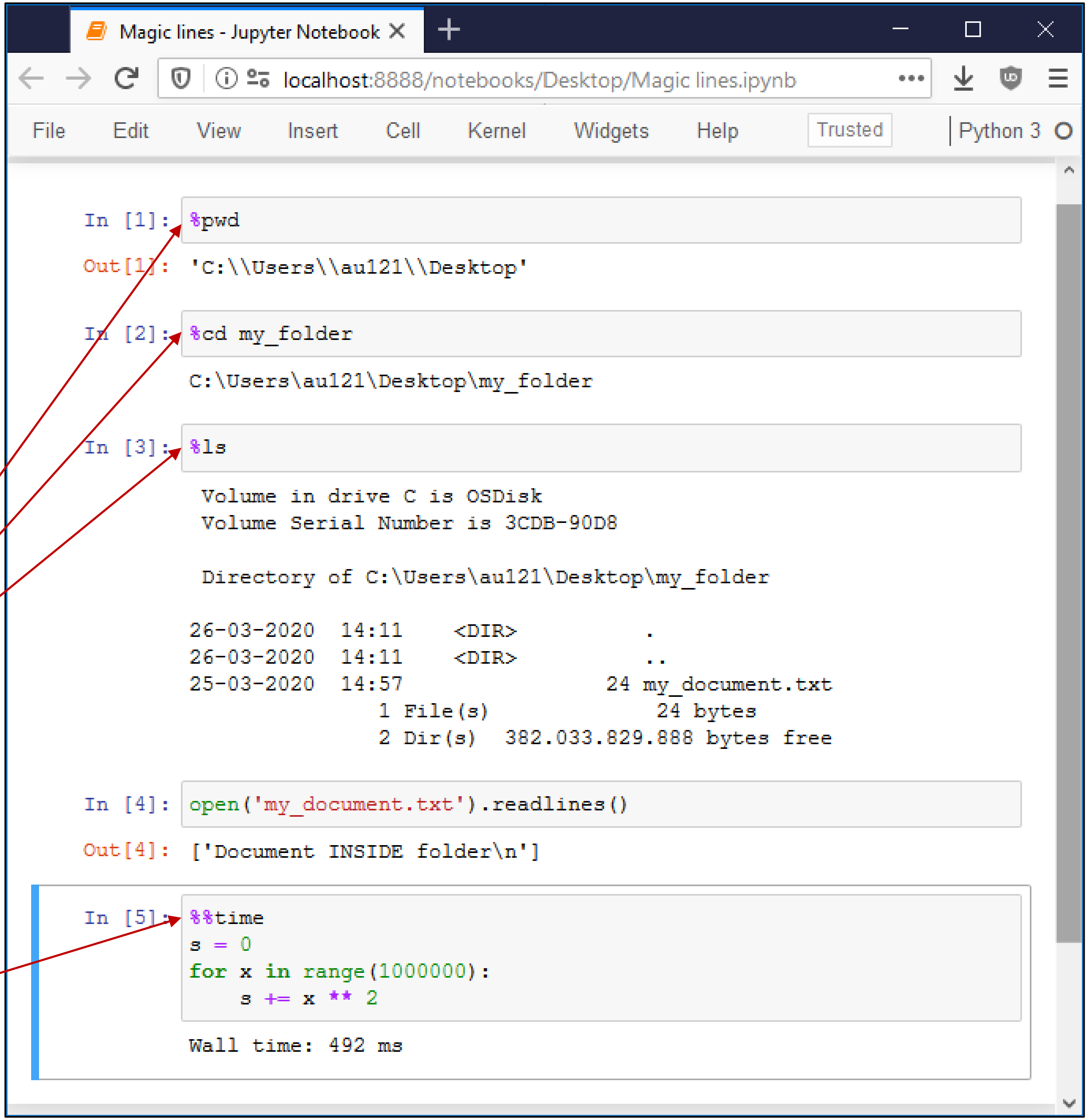
- To evaluate cell
  ctrl-enter, alt-enter, shift-enter
- Output from program shown below cell
- Result of last evaluated line
- Order of code cells evaluated
  Note ”x ** 2” computed after ”x = 4”
- [*] are cells being evaluated / waiting
- [ ] not yet evaluated
- Recompute all cells top-down
  or Kernel > Restart & Run all



Magic lines

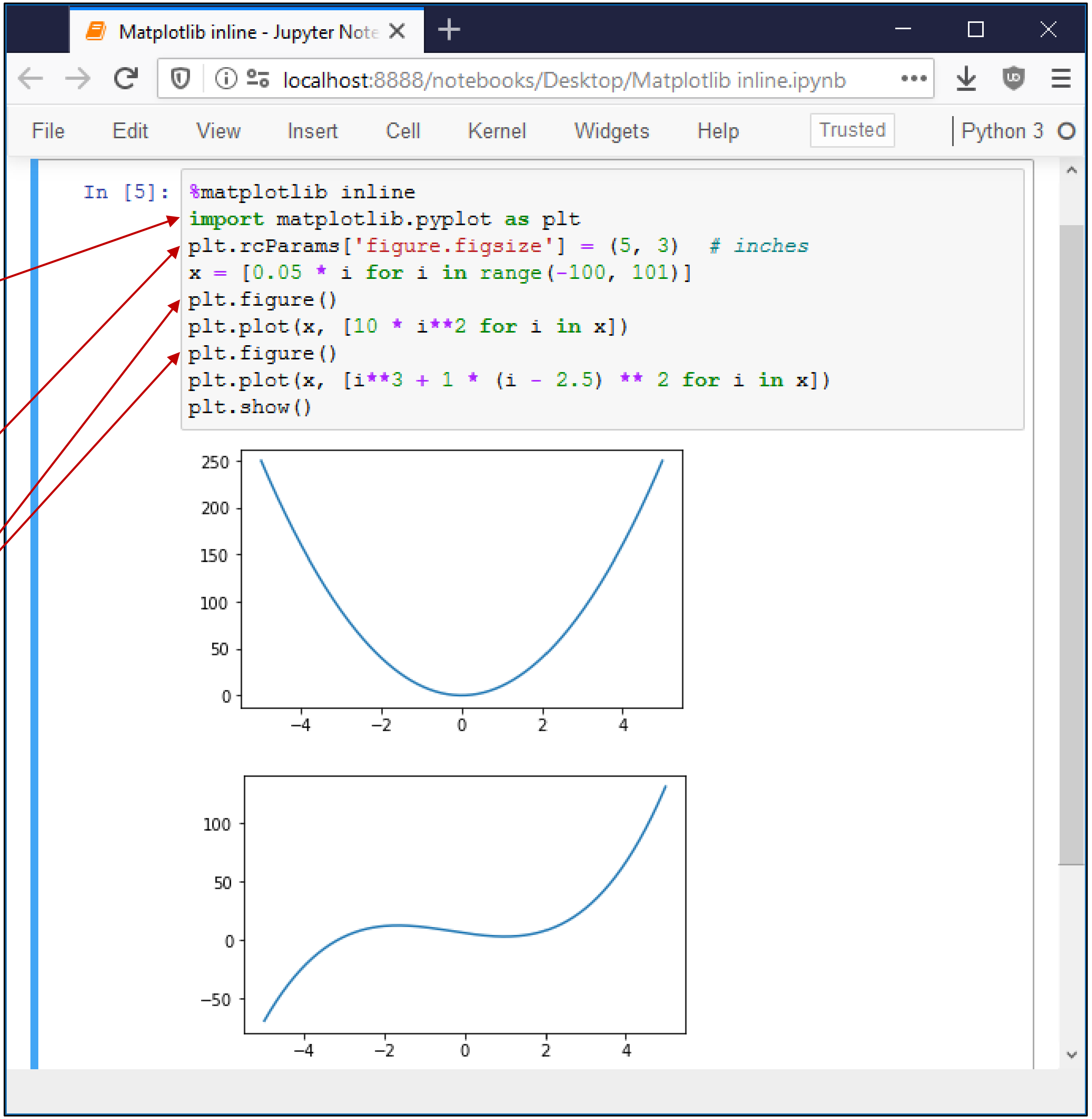
- Jupyter code cells support *magic commands* (actually it is IPython)
- % is a *line magic*
- %% is a *cell magic*

%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



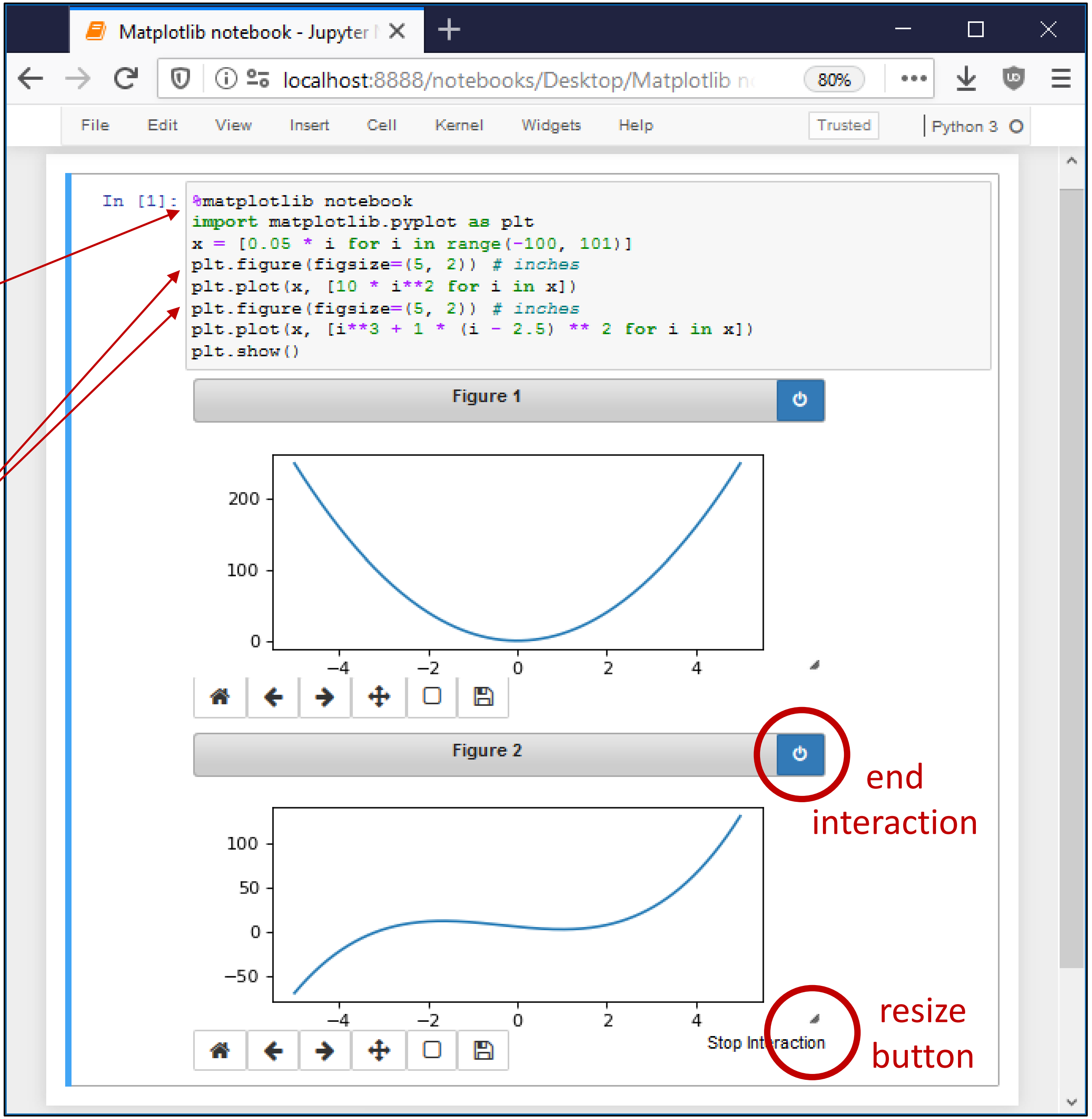
Jupyter and matplotlib

- `%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



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

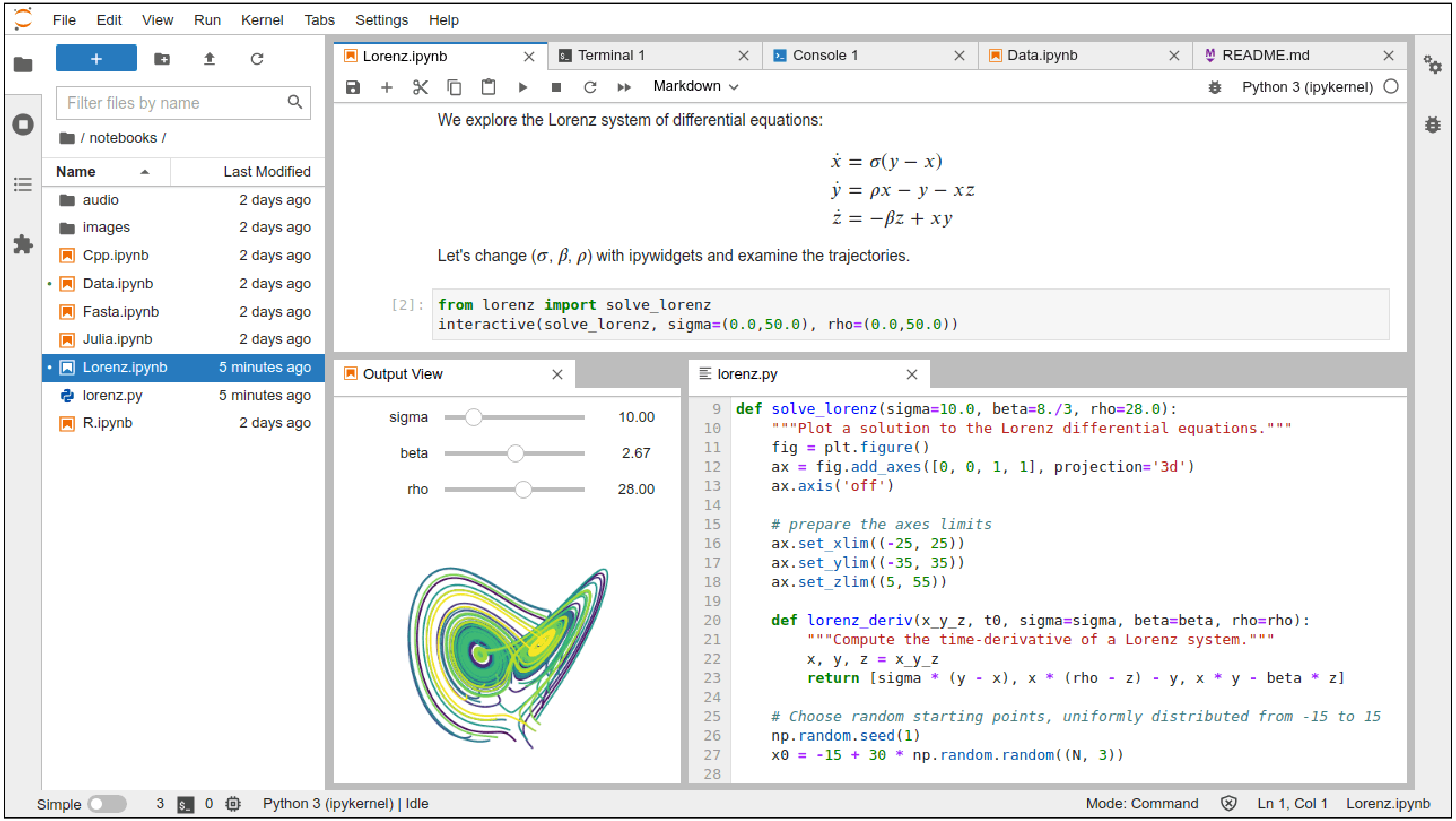


- Widespread tool used for data science applications
- Documentation, code for data analysis, and resulting visualizations are stored in one common format
- Easy to update visualizations
- Works with about 100 different programming languages (not only Python 3), many special features, ...
- Easy to share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

- *Many online tutorials and examples are available*

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

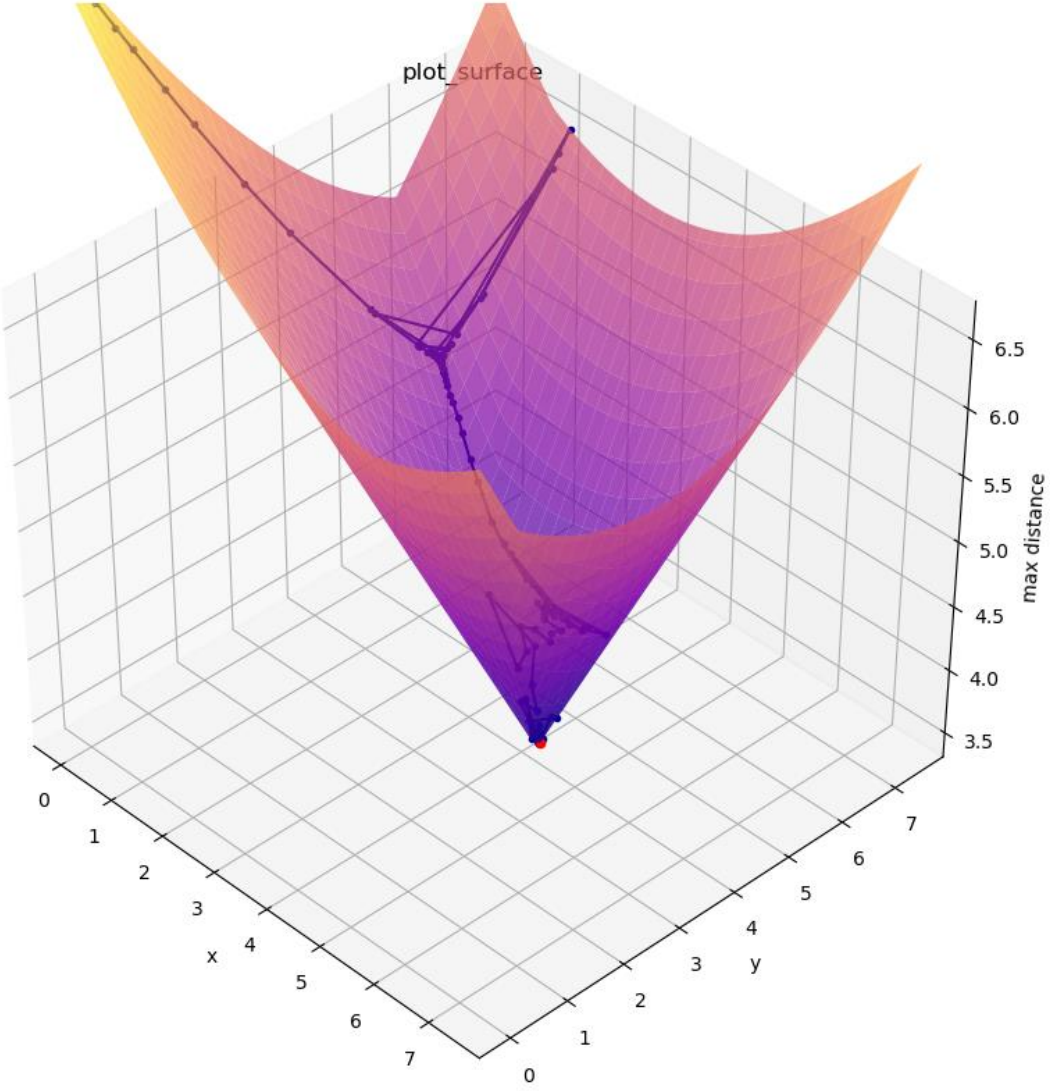
JupyterLab: A Next-Generation Notebook Interface



jupyter.org jupyterlab.readthedocs.io

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

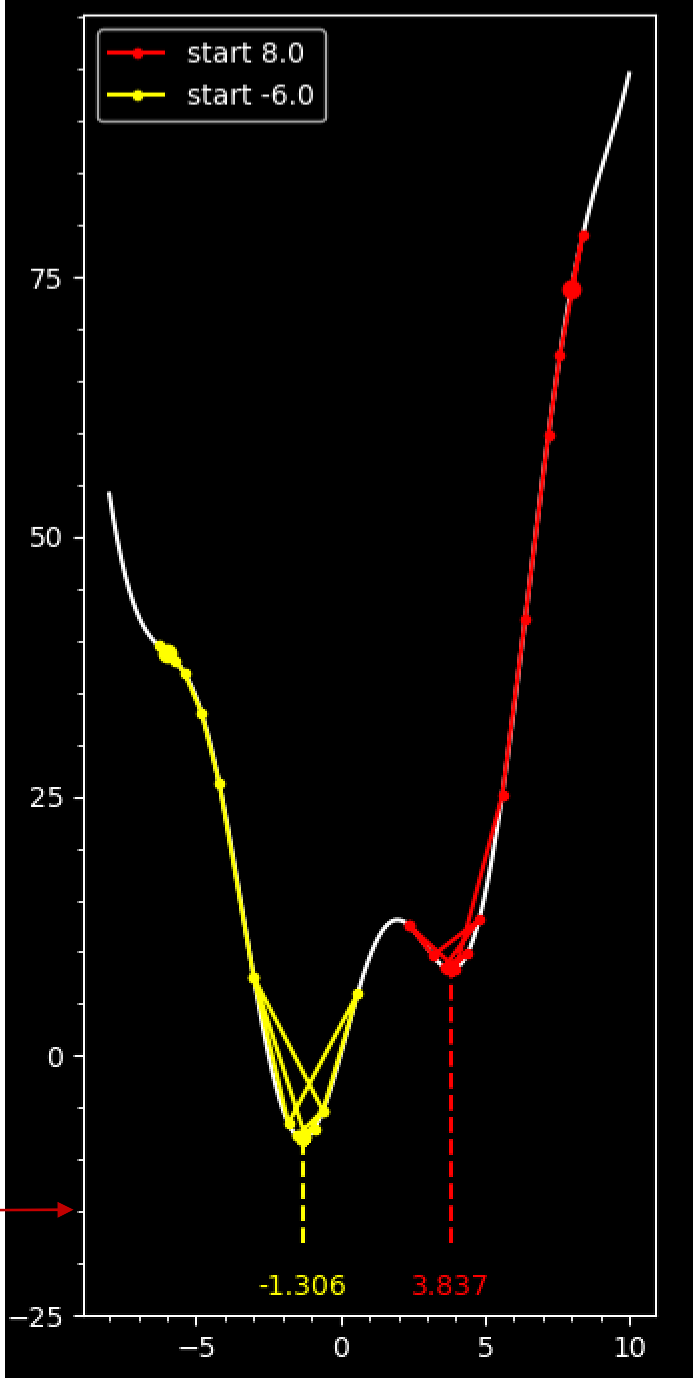
docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.minimize.html

minimize.py

```python
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()
```

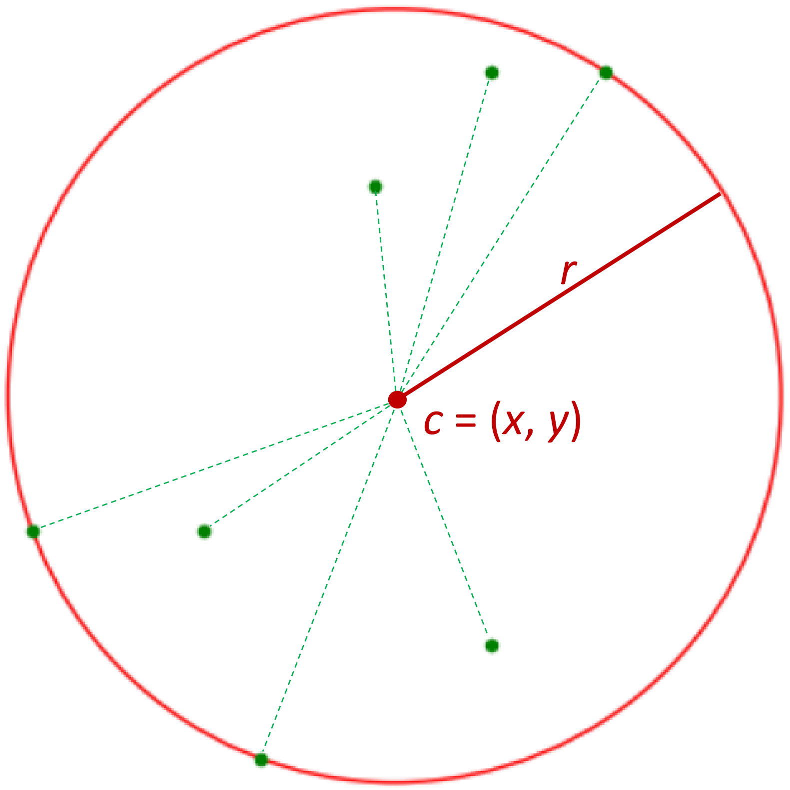
Python shell

```
> 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



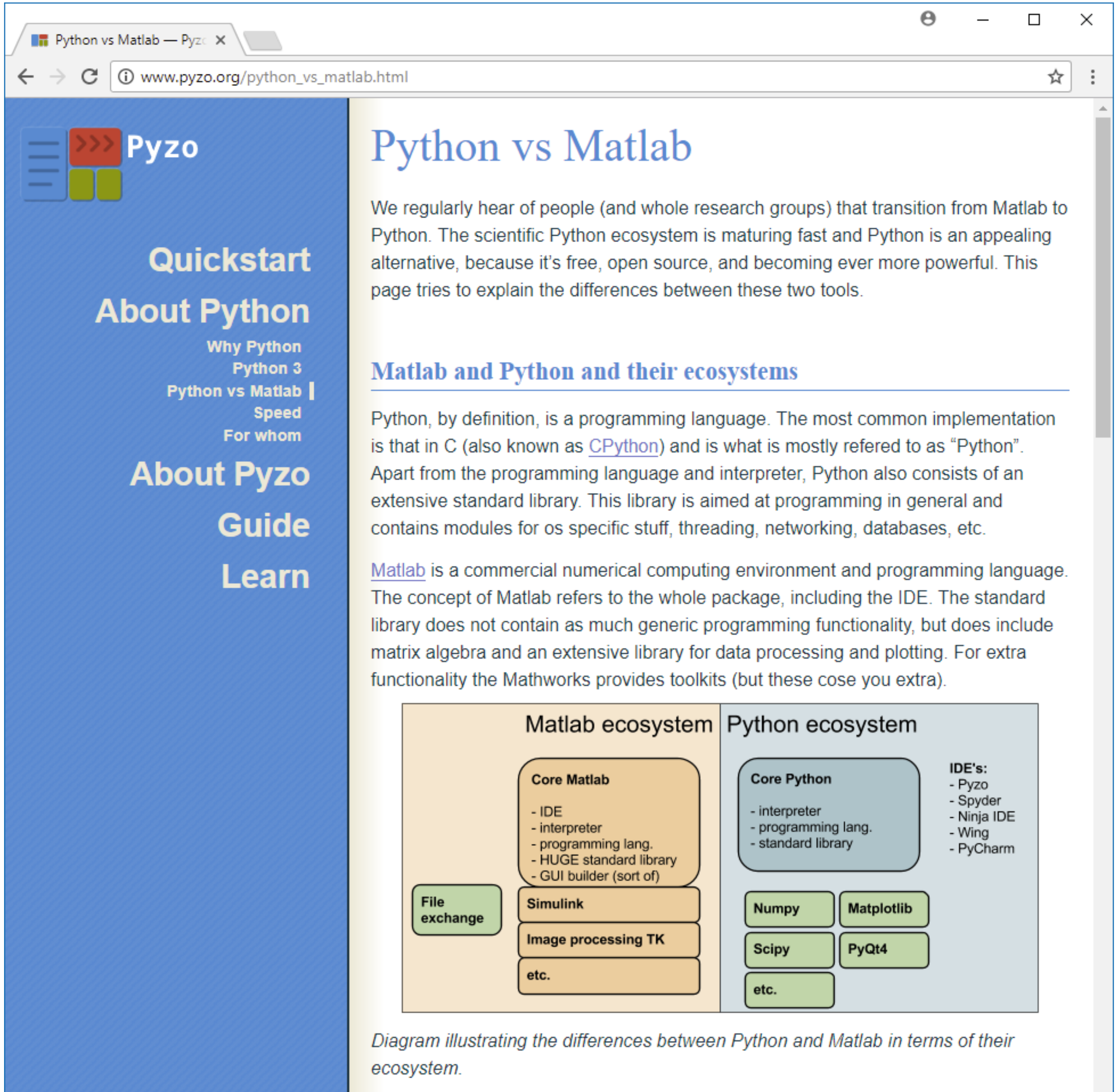
- Find c such that $r = \max_p |p - c|$ is minimized
- A solution is characterized by either
  1) three points on circle, where the triangle contains the circle center
  2) two opposite points on diagonal
- Try a standard numeric minimization solver
- ⚠ Computation involves max and $\sqrt{x}$, which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

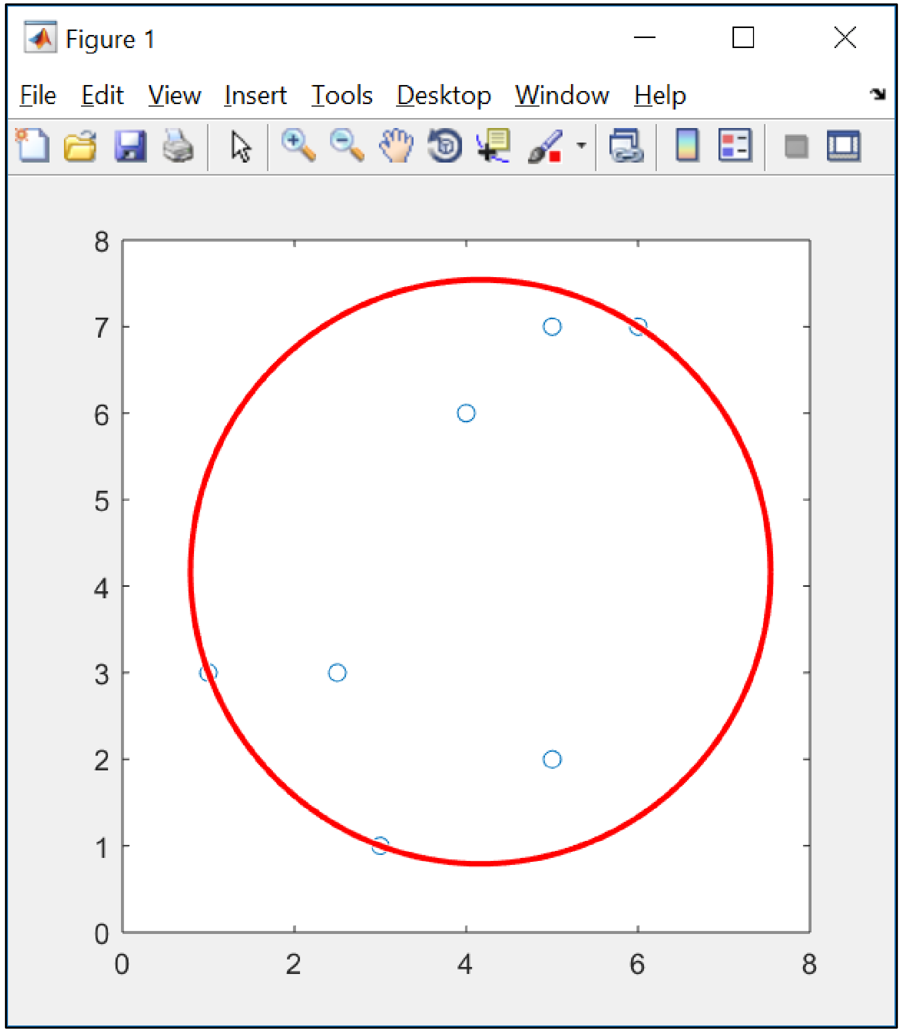
like R, Mathematica, Julia, AWK, Smalltalk, ...



Minimum enclosing circle in MATLAB

enclosing_circle.m

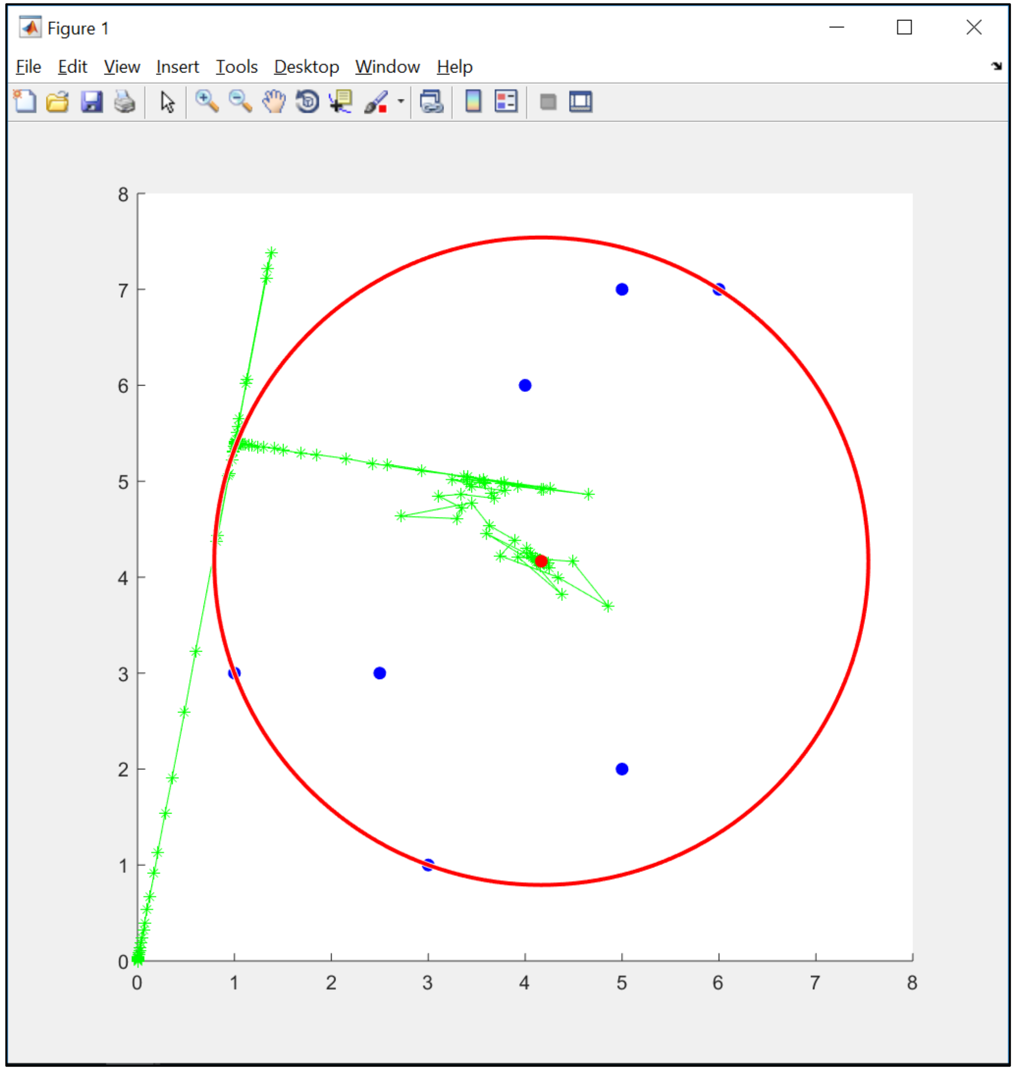
```
% Minimum enclosing circle of a point set
% fminsearch uses the Nelder-Mead algorithm

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

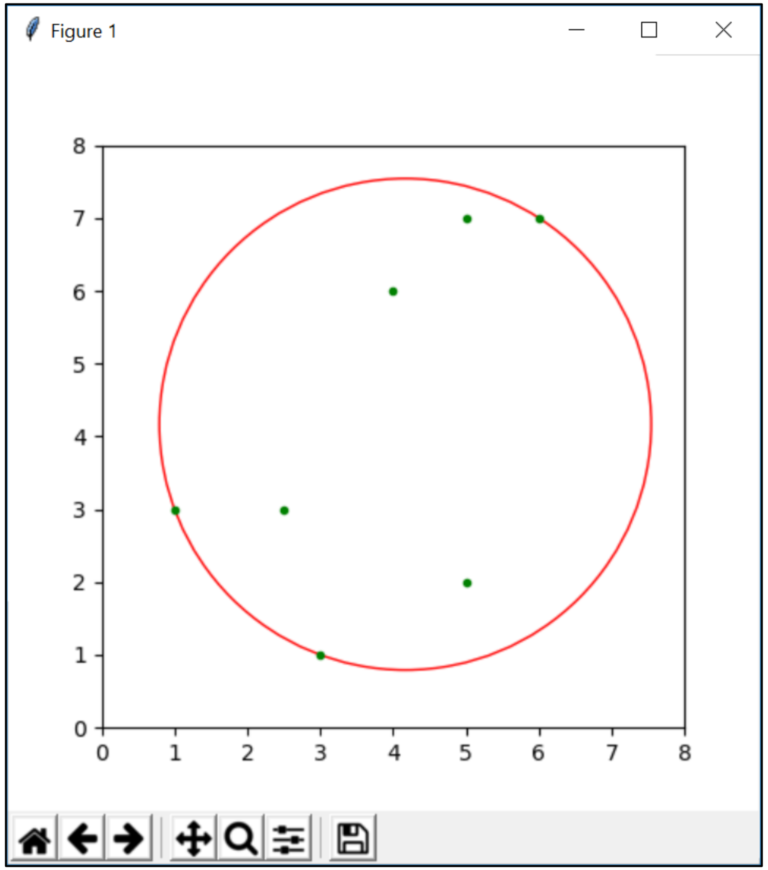
enclosing_circle.py

```
from 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 ((p[0] - q[0]) ** 2 + (p[1] - q[1]) ** 2)) ** 0.5
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

optimization method

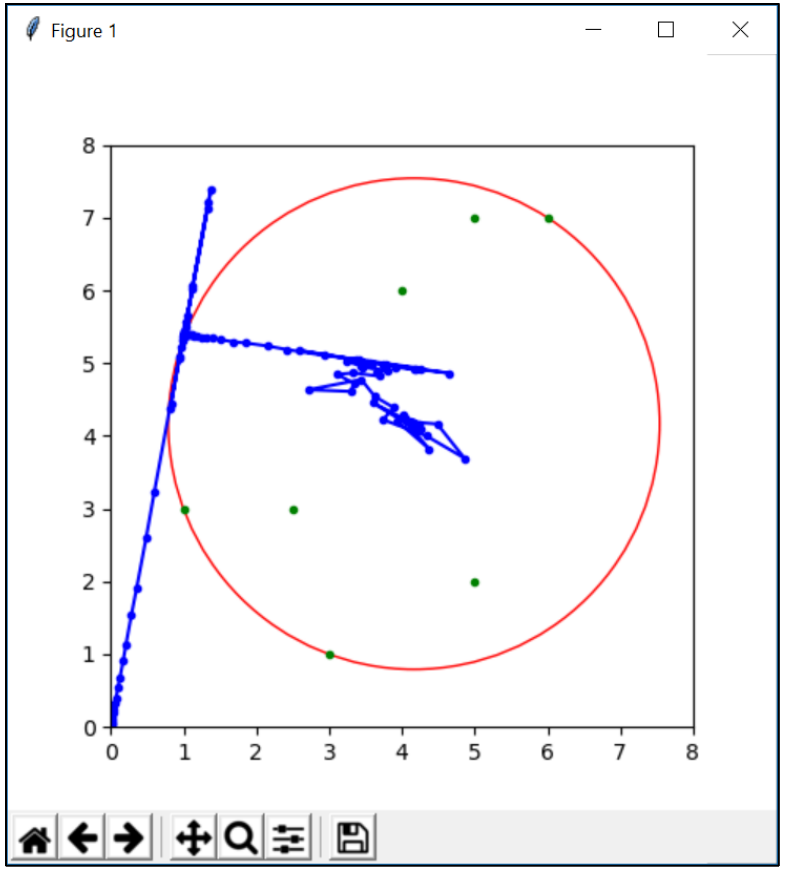
manually set axis (force circle inside plot)



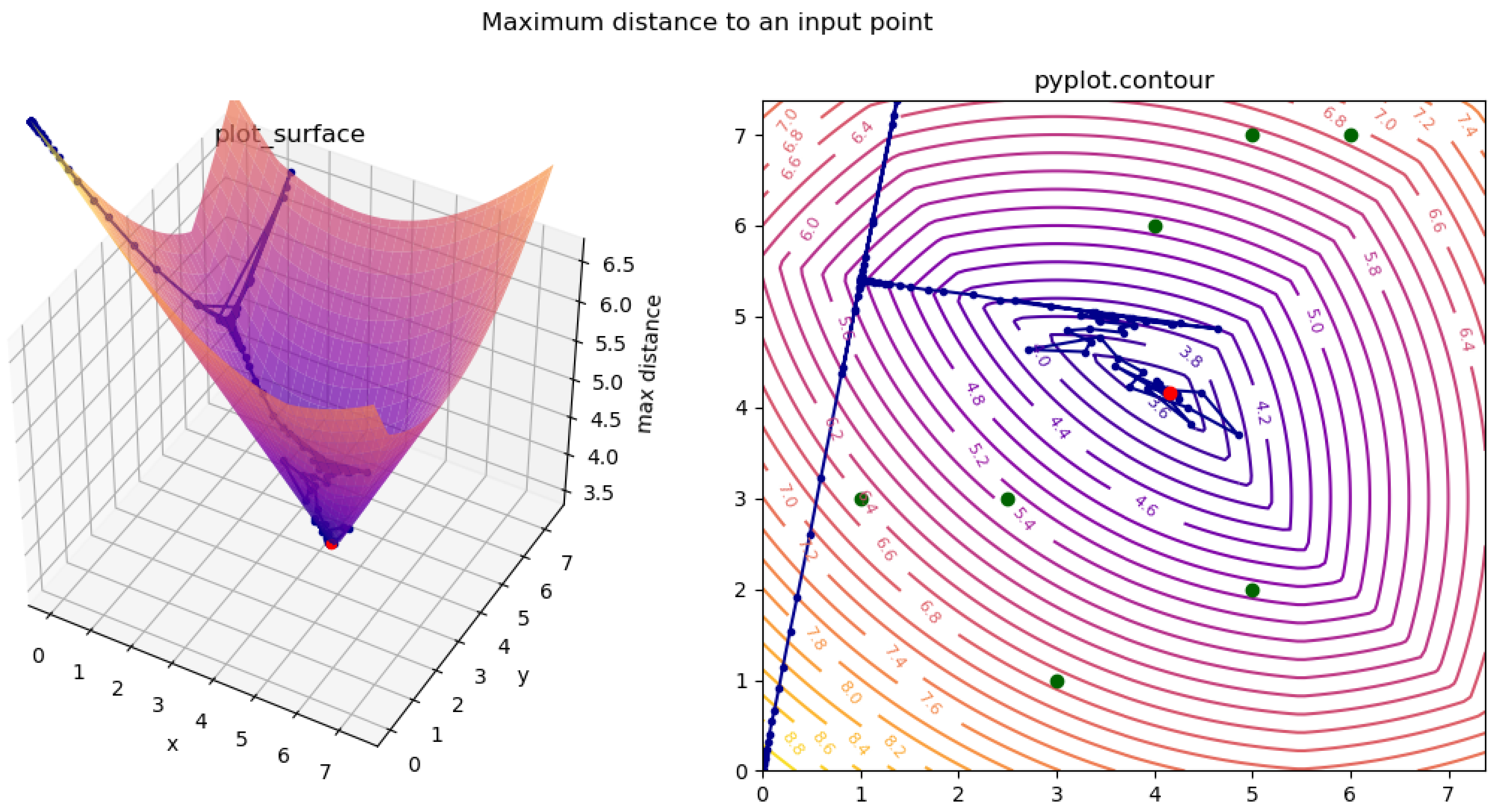
Minimum enclosing circle in Python (trace)

enclosing_circle_trace.py

```
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 ((p[0] - q[0]) ** 2 + (p[1] - q[1]) ** 2) ** 0.5
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



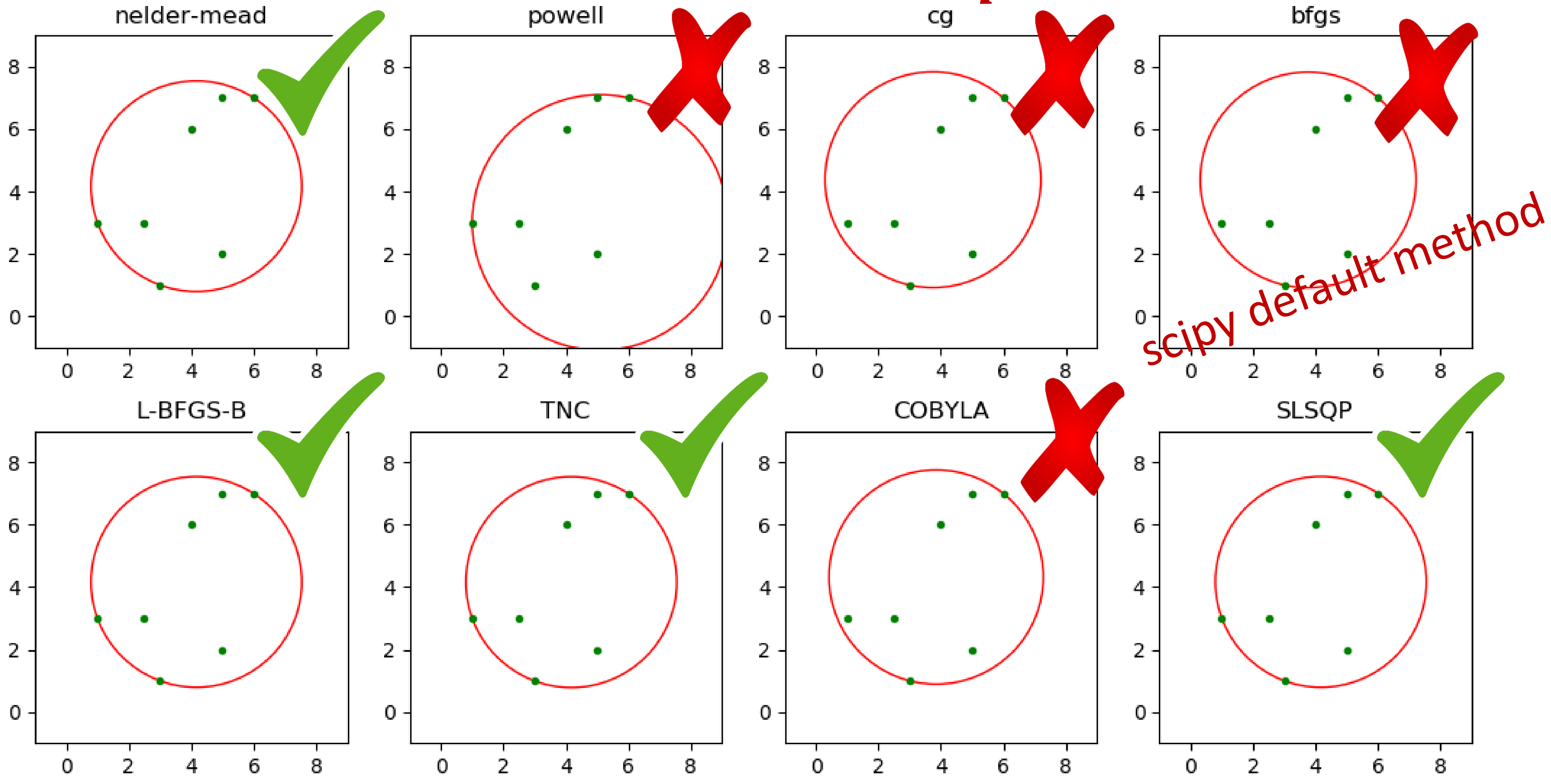
enclosing_circle_search_space.py (previous slide)

```
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 ((p[0]-q[0])**2 + (p[1]-q[1])**2)**0.5

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)
```

```
#  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 $f(c) = \max_{p} |p - c|$



docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.minimize.html avoids $\sqrt{}$

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