

Lecture 18

Jupyter + plotting



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Lecture 18 outline

Last time: BioPython

This time: plotting

- Jupyter
- matplotlib



<https://jupyter.org>

Jupyter is a framework for creating interactive computational ***notebooks***

Jupyter notebooks are organized into a series of ***cells***

Each cell can contain executable code, richly formatted text, and more

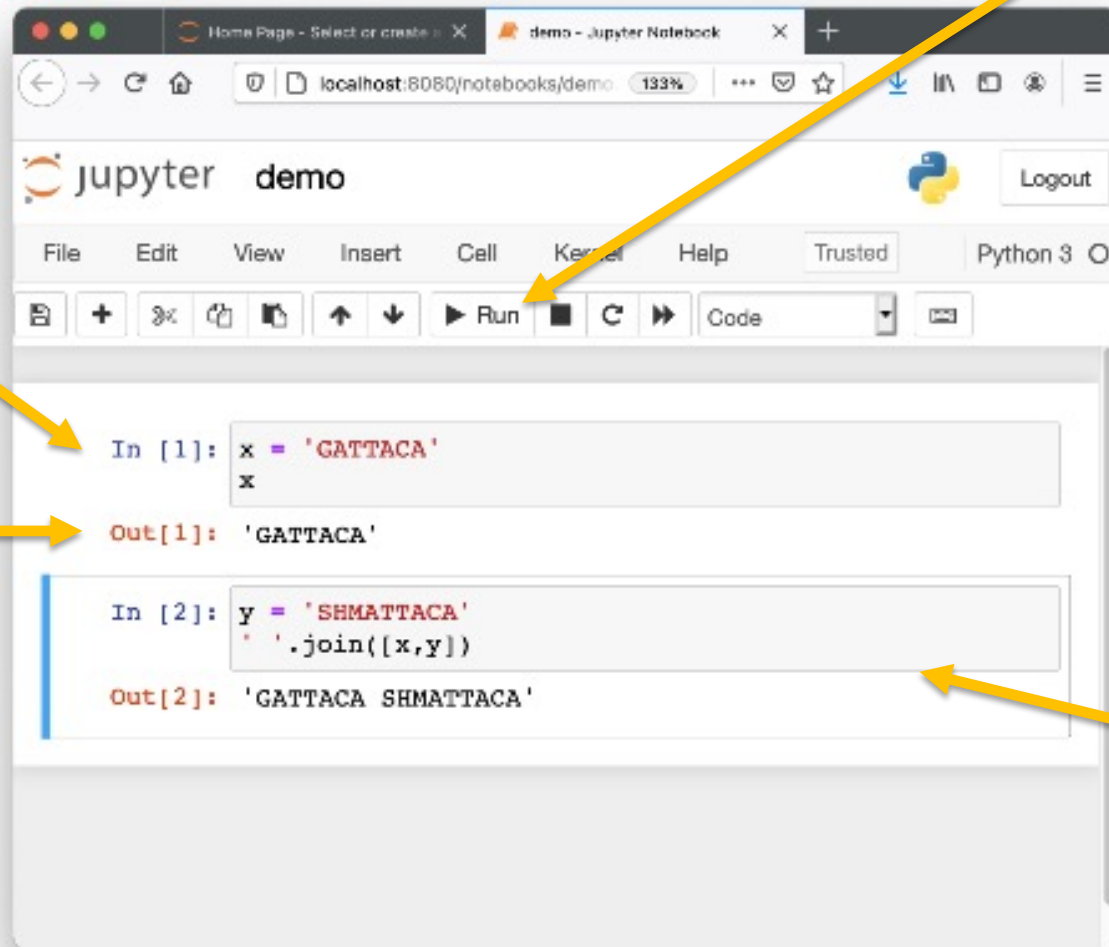
Promising platform for open and reproducible science

Jupyter notebook

execute code
in active cell

code from
cell #1

output from
cell #1



The screenshot shows a Jupyter Notebook interface in a web browser. The browser's address bar displays 'localhost:8080/notebooks/demo'. The notebook's title bar reads 'demo - Jupyter Notebook'. The main interface includes a menu bar (File, Edit, View, Insert, Cell, Kernel, Help) and a toolbar with icons for file operations and execution. The 'Run' button is highlighted with a yellow arrow pointing to it from the text 'execute code in active cell'. Below the menu bar, there are two code cells. The first cell, labeled 'In [1]:', contains the code `x = 'GATTACA'` followed by `x` on the next line. Its output, 'Out[1]: 'GATTACA'', is displayed below. The second cell, labeled 'In [2]:', contains the code `y = 'SHMATTACA'` followed by `print(''.join([x,y]))` on the next line. Its output, 'Out[2]: 'GATTACA SHMATTACA'', is displayed below. A yellow arrow points from the text 'code from cell #1' to the code in the first cell. Another yellow arrow points from the text 'output from cell #1' to the output of the first cell. A third yellow arrow points from the text 'cell #2 is active (blue)' to the second cell, which is highlighted with a blue border. The text 'cell #2 is active (blue)' is written in blue.

```
In [1]: x = 'GATTACA'
        x
Out[1]: 'GATTACA'

In [2]: y = 'SHMATTACA'
        print(''.join([x,y]))
Out[2]: 'GATTACA SHMATTACA'
```

cell #2
is active
(blue)

Using Jupyter with SSH (will cover in lab)

Remote computer (Jupyter host)

1. Connect to VPN
2. SSH into remote computer
3. Launch Jupyter server:

jupyter notebook --no-browser --port=8080

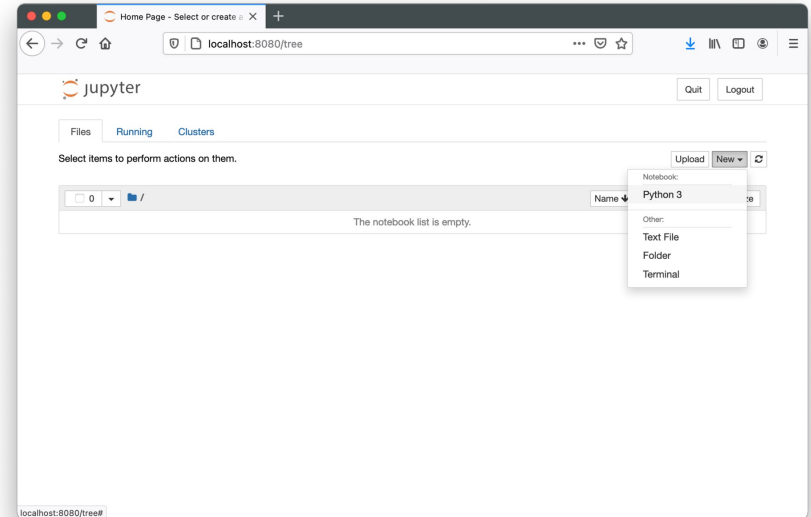
Local computer (Jupyter client)

4. Create SSH tunnel from port 8080 on remote machine into port 8080 on local workstation:

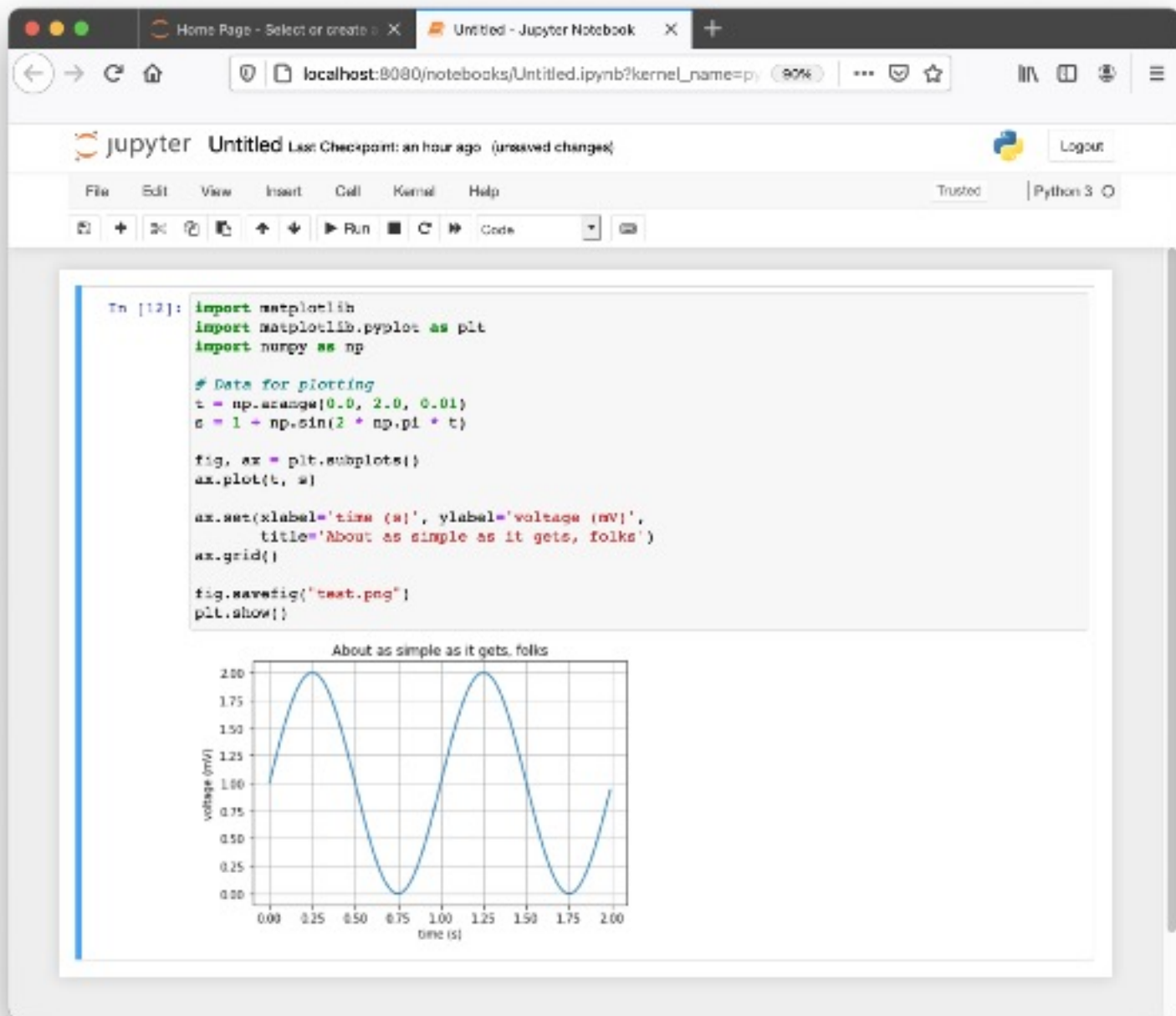
ssh -N -L 8080:localhost:8080 snoopy@12.34.56.78

5. Access Jupyter browser page with "token":

<https://localhost:8080?token=xxxxxxxxxxxxxxxxxxxxxxxxxxxx>



Jupyter browser

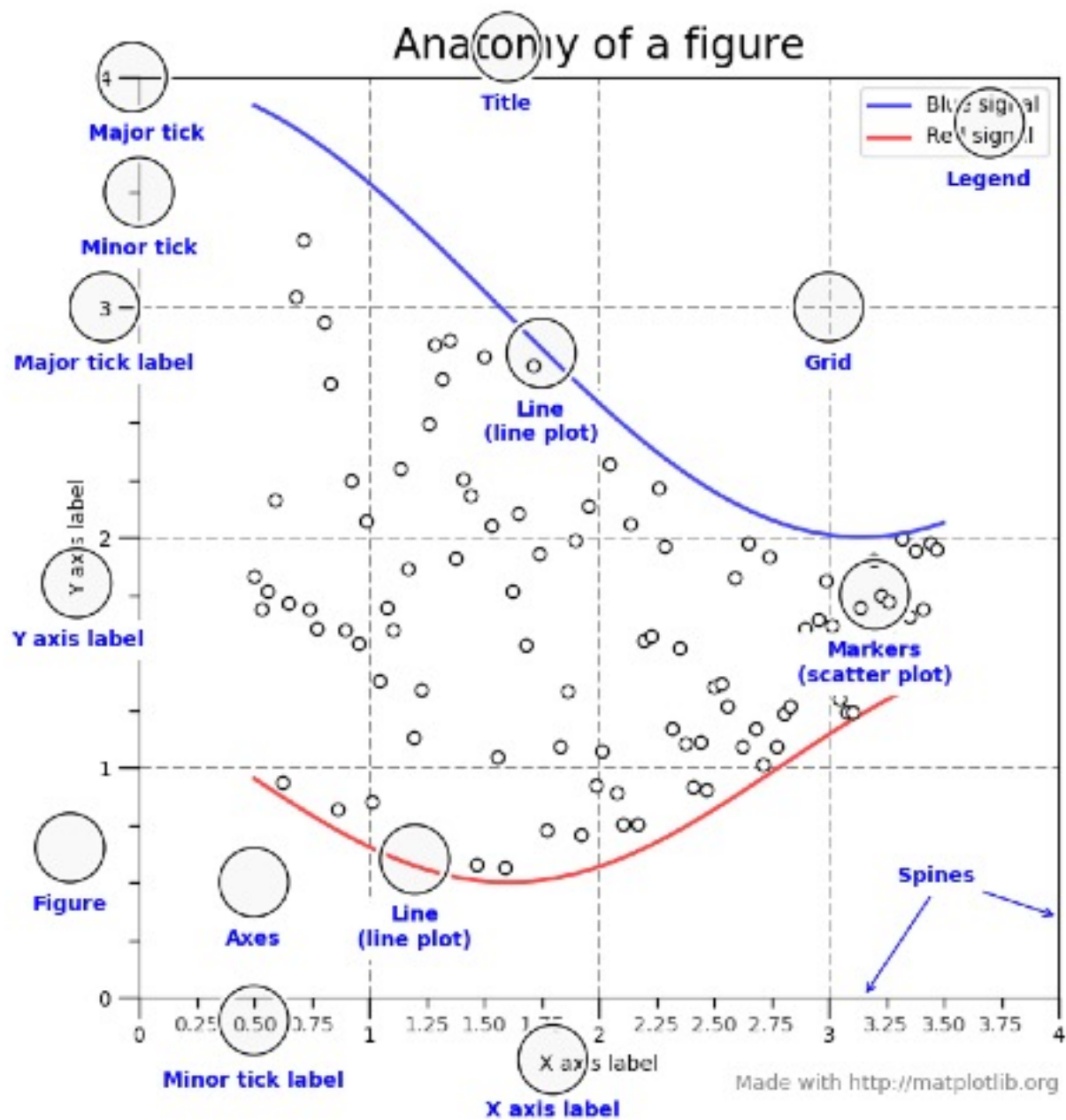




Matplotlib is a library for visualizing data

Supports a wide range of customizable plots from simpler scatterplots, to contoured heatmaps, to interactive 3D plots

Detailed examples for how to use Matplotlib are published through the [user guide](#) and [gallery](#)



matplotlib drawing interfaces

Explicit interface

- verbose
- allows customization

```
# import plot interface
import matplotlib.pyplot as plt
# make figure object from plot
fig = plt.figure()
# make axis object from figure
ax = fig.subplots()
# plot data within axis object
ax.plot([1, 2, 3, 4], [0, 0.5, 1, 0.2])
```

Implicit interface:

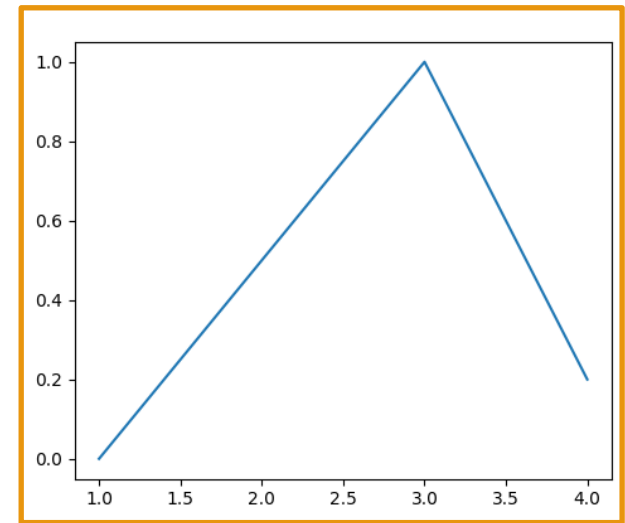
- simpler
- no customization

```
# import matplotlib
import matplotlib.pyplot as plt
# draw directly through plot interface
# (internally handles figure and axis)
plt.plot([1, 2, 3, 4], [0, 0.5, 1, 0.2])
```

Plot interface

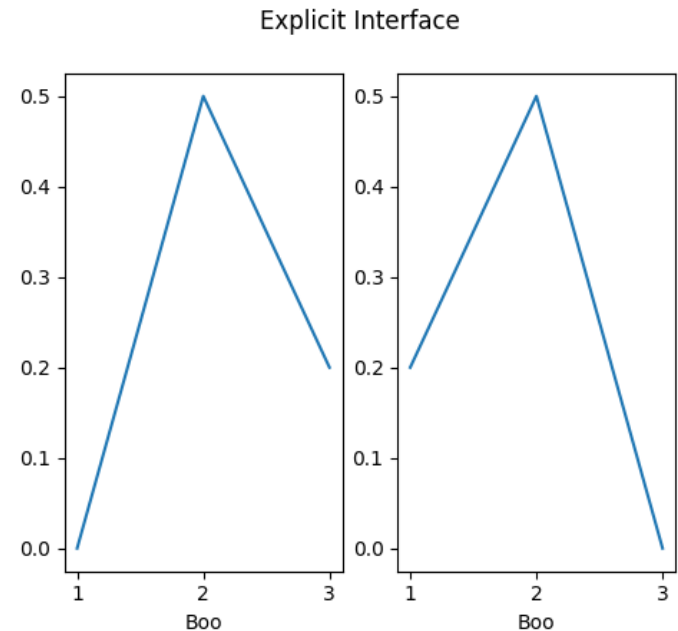
Figure interface

Axes interface



Gallery example: multiple panels

```
# import matplotlib
import matplotlib.pyplot as plt
# construct a matrix of (1,2) subplots
# save figure and axes (list) interfaces
fig, axs = plt.subplots(1, 2)
# create lineplot in the 0th axis interface
axs[0].plot([1, 2, 3], [0, 0.5, 0.2])
# create lineplot in the 1st axis interface
axs[1].plot([3, 2, 1], [0, 0.5, 0.2])
# customize title for the figure interface that
# contains both axis interfaces
fig.suptitle('Explicit Interface')
# customize x-axis label for each axis interface
for i in range(2):
    axs[i].set_xlabel('Boo')
```



Gallery example: lineplot

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

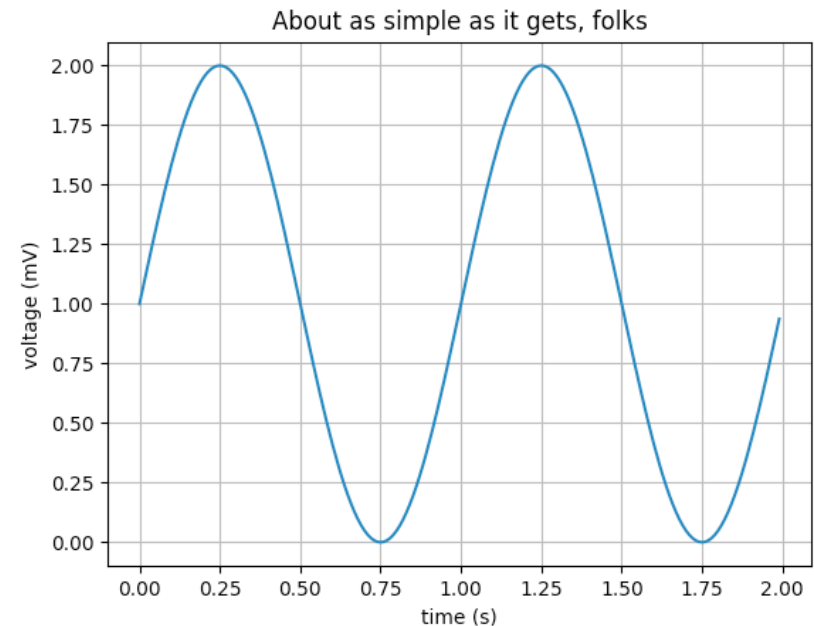
# Data for plotting
t = np.arange(0.0, 2.0, 0.01)
s = 1 + np.sin(2 * np.pi * t)

fig, ax = plt.subplots()
ax.plot(t, s)

ax.set(xlabel='time (s)',
       ylabel='voltage (mV)',
       title='About as simple as it gets,
            folks')

ax.grid()

fig.savefig("test.png")
plt.show()
```



Gallery example: barplot

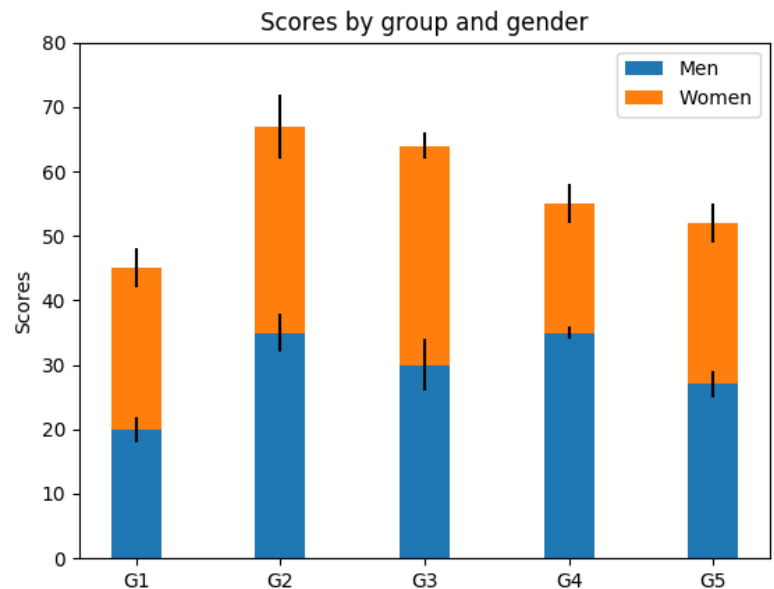
```
import numpy as np
import matplotlib.pyplot as plt

N = 5
menMeans = (20, 35, 30, 35, 27)
womenMeans = (25, 32, 34, 20, 25)
menStd = (2, 3, 4, 1, 2)
womenStd = (3, 5, 2, 3, 3)
ind = np.arange(N) # x-locations for groups
width = 0.35 # the width of the bars:

p1 = plt.bar(ind, menMeans, width, yerr=menStd)
p2 = plt.bar(ind, womenMeans, width,
bottom=menMeans, yerr=womenStd)

plt.ylabel('Scores')
plt.title('Scores by group and gender')
plt.xticks(ind, ('G1', 'G2', 'G3', 'G4', 'G5'))
plt.yticks(np.arange(0, 81, 10))
plt.legend((p1[0], p2[0]), ('Men', 'Women'))

plt.show()
```



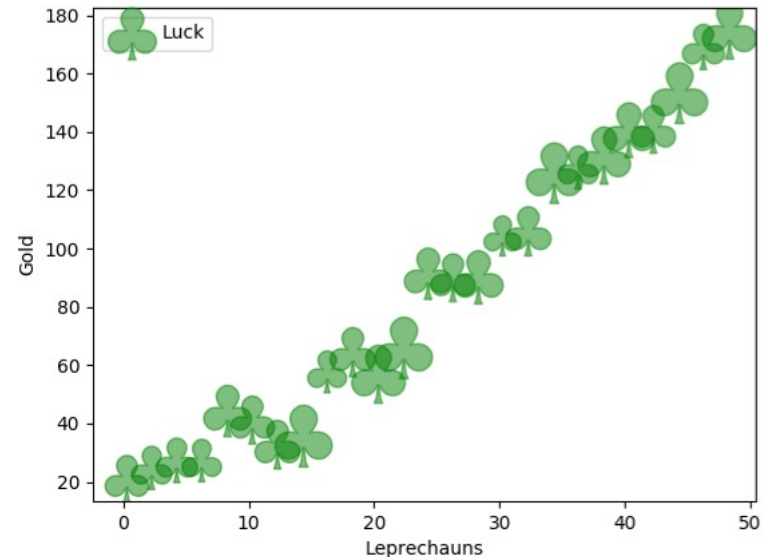
Gallery example: scatterplot

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

# Fixing random state for reproducibility
np.random.seed(19680801)

x = np.arange(0.0, 50.0, 2.0)
y = x ** 1.3 + np.random.rand(*x.shape) * 30.0
s = np.random.rand(*x.shape) * 800 + 500

plt.scatter(x, y, s, c="g",
            alpha=0.5,
            marker=r'$\clubsuit$',
            label="Luck")
plt.xlabel("Leprechauns")
plt.ylabel("Gold")
plt.legend(loc='upper left')
plt.show()
```



Gallery example: histogram

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

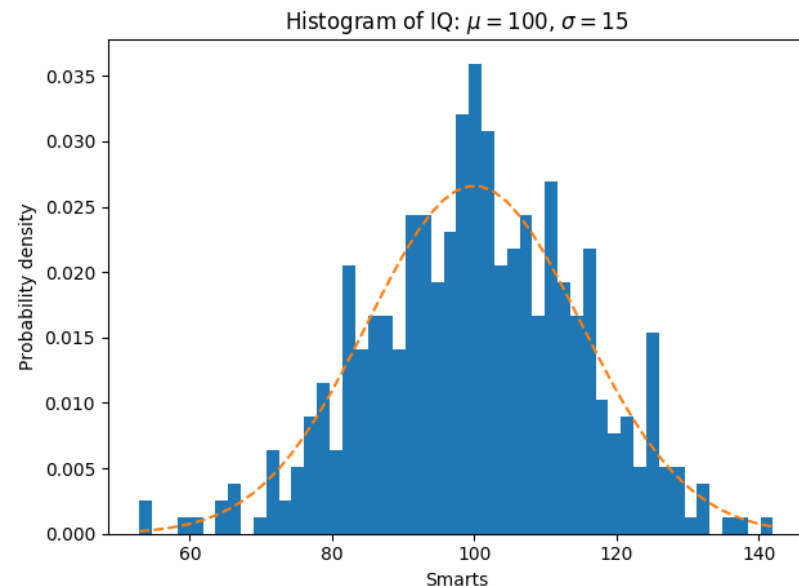
np.random.seed(19680801)

# example data
mu = 100 # mean of distribution
sigma = 15 # standard deviation of distribution
x = mu + sigma * np.random.randn(437)
num_bins = 50

# the histogram of the data
fig, ax = plt.subplots()
n, bins, patches = ax.hist(x, num_bins, density=1)

# add a 'best fit' line
y = ((1 / (np.sqrt(2 * np.pi) * sigma)) *
      np.exp(-0.5 * (1 / sigma * (bins - mu))**2))
ax.plot(bins, y, '--')
ax.set_xlabel('Smarts')
ax.set_ylabel('Probability density')
title=r'Histogram of IQ: $\mu=100$, $\sigma=15$'
ax.set_title(title)

# Tweak spacing to prevent clipping of ylabel
fig.tight_layout()
plt.show()
```



Gallery example: heatmap

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

# Define numbers of data points and bins per axis.
N_numbers = 100000
N_bins = 100

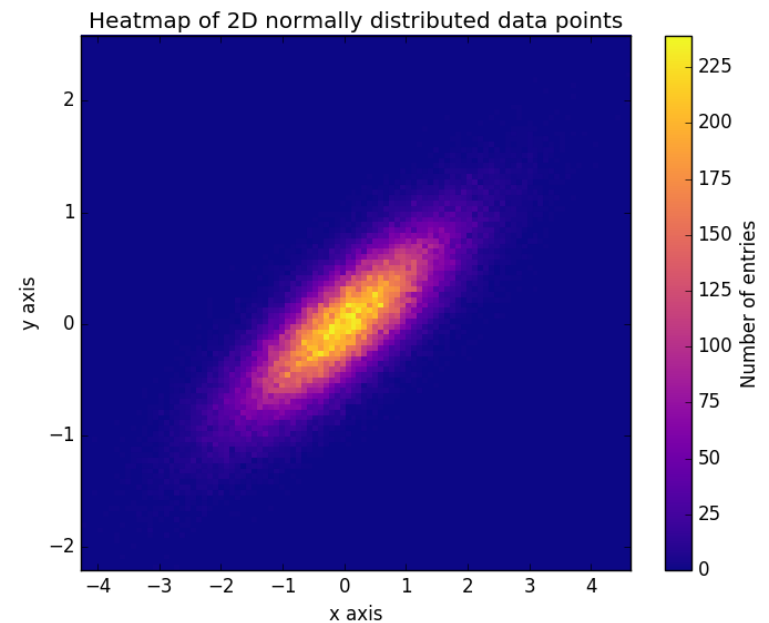
# set random seed
np.random.seed(0)

# Generate 2D normally distributed numbers.
x, y = np.random.multivariate_normal(
    mean=[0.0, 0.0], # mean
    cov=[[1.0, 0.4],
         [0.4, 0.25]], # covariance matrix
    size=N_numbers).T # transpose into columns

# Construct 2D histogram using the 'plasma' colormap
plt.hist2d(x, y, bins=N_bins, cmap='plasma')

# Plot a colorbar with label.
cb = plt.colorbar()
cb.set_label('Number of entries')

# Add title and labels to plot.
title='Heatmap of 2D normally distributed data points'
plt.title(title)
plt.xlabel('x axis')
plt.ylabel('y axis')
plt.show()
```





Ten Simple Rules for Better Figures

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Paper linked in course schedule:

1. Know your audience
2. Identify your message
3. Adapt figure to support medium
4. Captions are not optional
5. Do not trust the defaults
6. Use color effectively
7. Do not mislead the reader
8. Avoid "chart junk"
9. Message trumps beauty
10. Get the right [plotting] tool

Overview for Lab 18