Mon, Nov 30

Lecture 12A:

Jupyter + Matplotlib

Practical Bioinformatics (Biol 4220)
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Lecture 12A outline

1. Jupyter Notebooks
2. Matplotlib
3. Lab 12A overview

https://jupyter.org

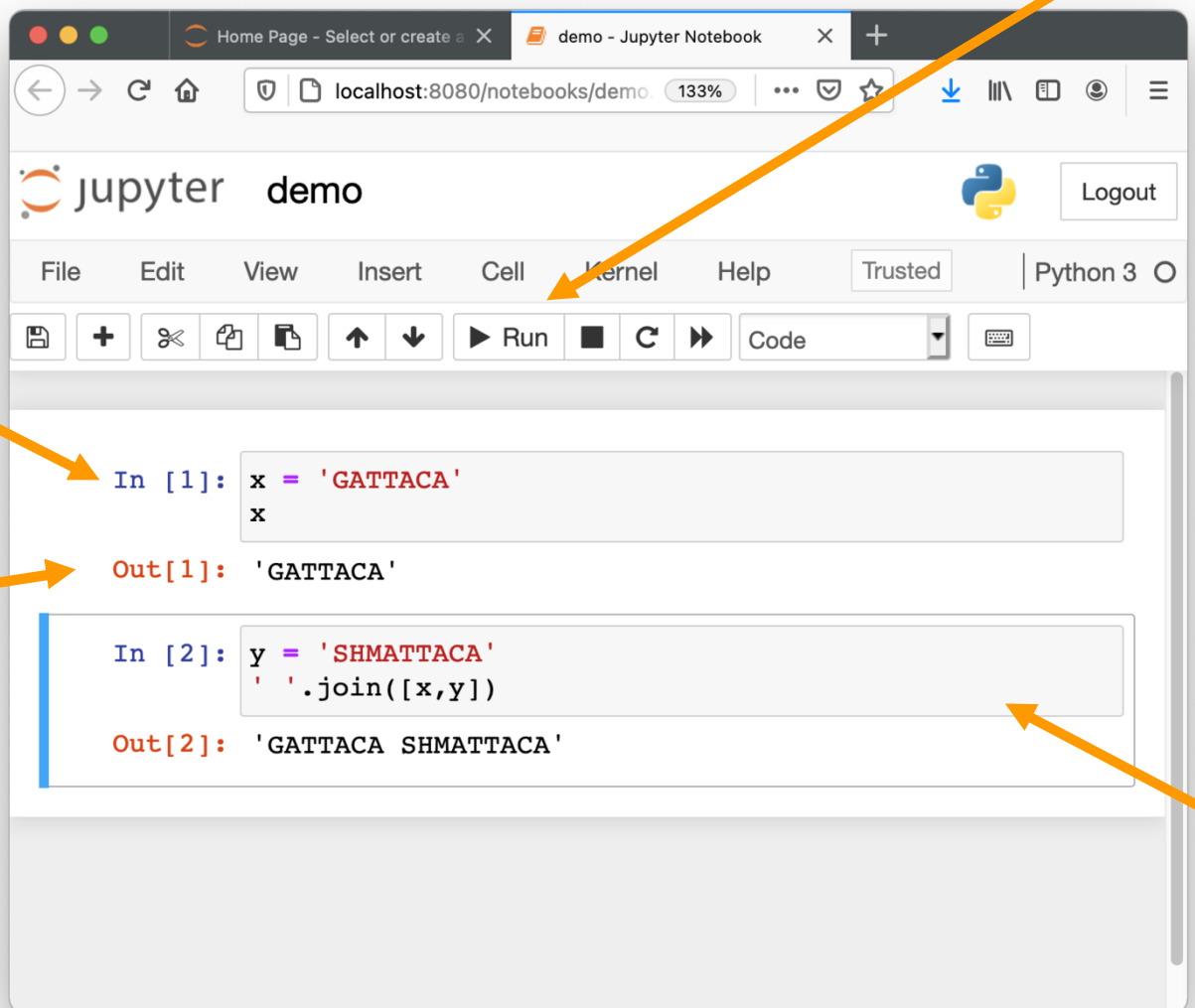
Jupyter is a framework for creating interactive and computational ***notebooks***

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

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

Promising framework for open science and reproducibility efforts

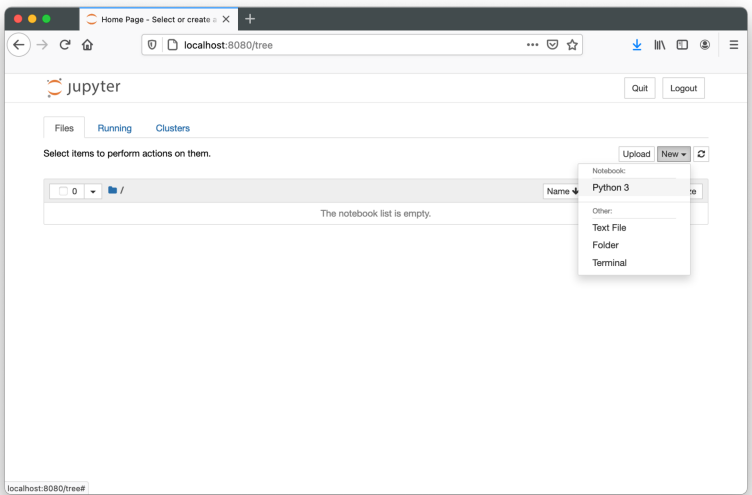
Jupyter notebook



Accessing Jupyter over 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



Jupyter browser

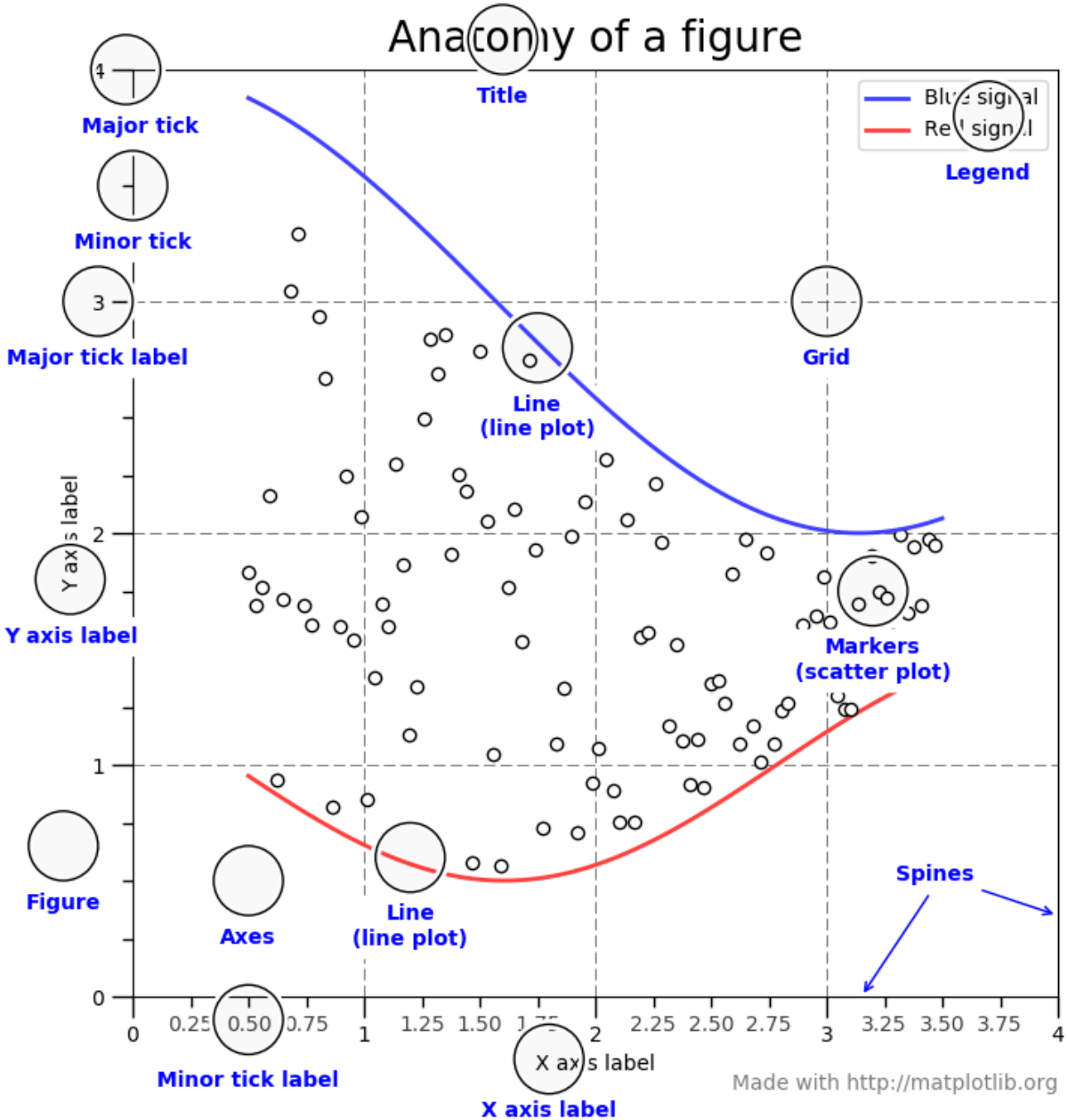
Local computer (Jupyter client)

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 (may require "token"):
   https://localhost:8080

Matplotlib is a library for visualizing data

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

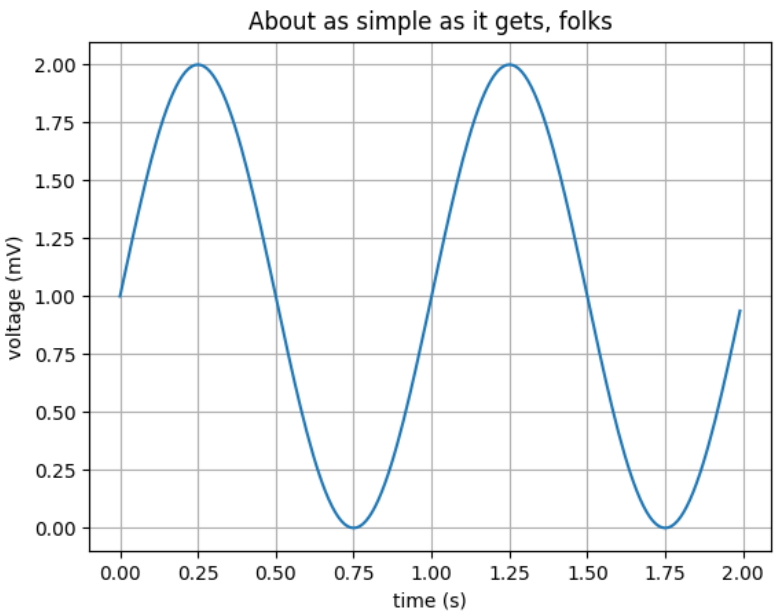
Detailed examples for how to use Matplotlib are published through the user guide and gallery



https://matplotlib.org/3.1.1/gallery/showcase/anatomy.html

Gallery example: lineplot

```
 1 import matplotlib
 2 import matplotlib.pyplot as plt
 3 import numpy as np
 4
 5 # Data for plotting
 6 t = np.arange(0.0, 2.0, 0.01)
 7 s = 1 + np.sin(2 * np.pi * t)
 8
 9 fig, ax = plt.subplots()
10 ax.plot(t, s)
11
12 ax.set(xlabel='time (s)', ylabel='voltage (mV)',
13        title='About as simple as it gets, folks')
14 ax.grid()
15
16 fig.savefig("test.png")
17 plt.show()
```



https://matplotlib.org/3.1.0/gallery/lines_bars_and_markers/simple_plot.html

Home Page - Select or create a | Untitled - Jupyter Notebook

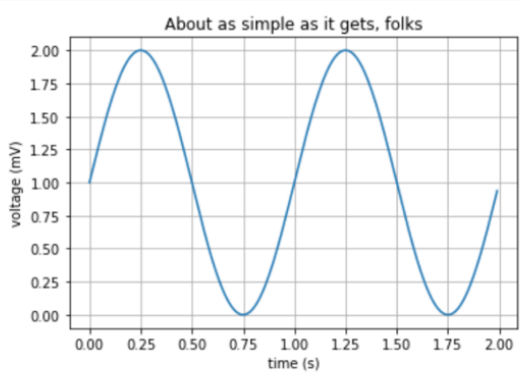
localhost:8080/notebooks/Untitled.ipynb?kernel_name=py 90%

jupyter **Untitled** Last Checkpoint: an hour ago (unsaved changes) Logout

File Edit View Insert Cell Kernel Help Trusted Python 3

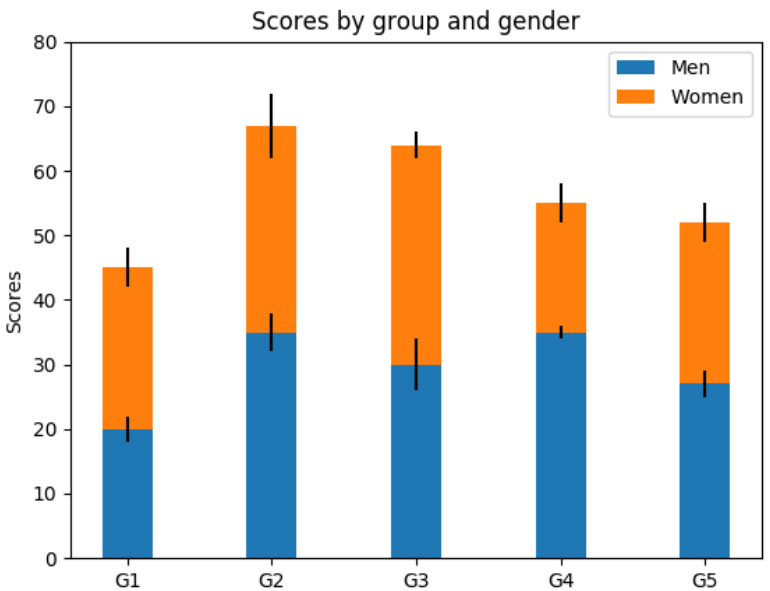
Run Code

In [12]:
```
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

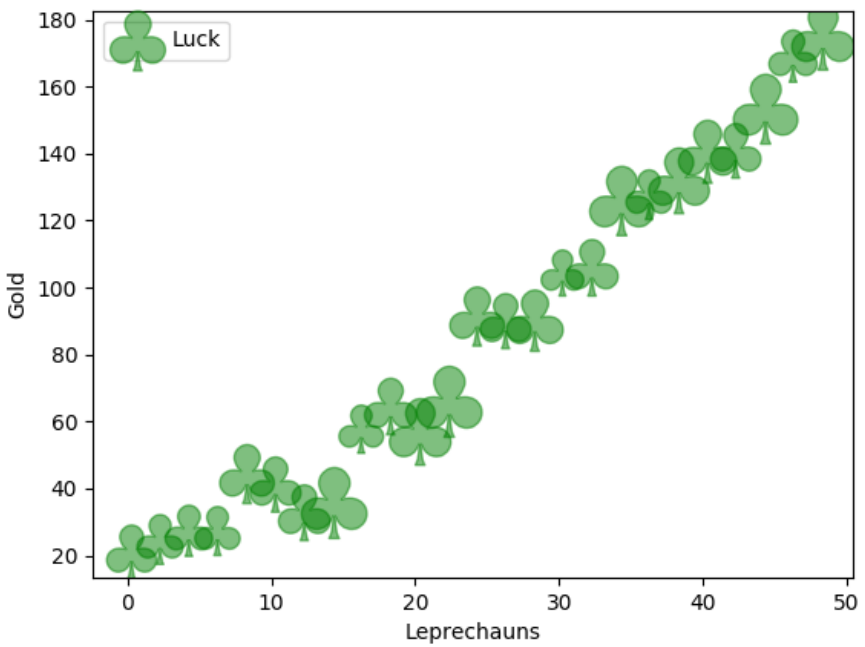
```python
import numpy as np
import matplotlib.pyplot as plt


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()
```



https://matplotlib.org/3.1.1/gallery/lines_bars_and_markers/bar_stacked.html

Gallery example: scatterplot

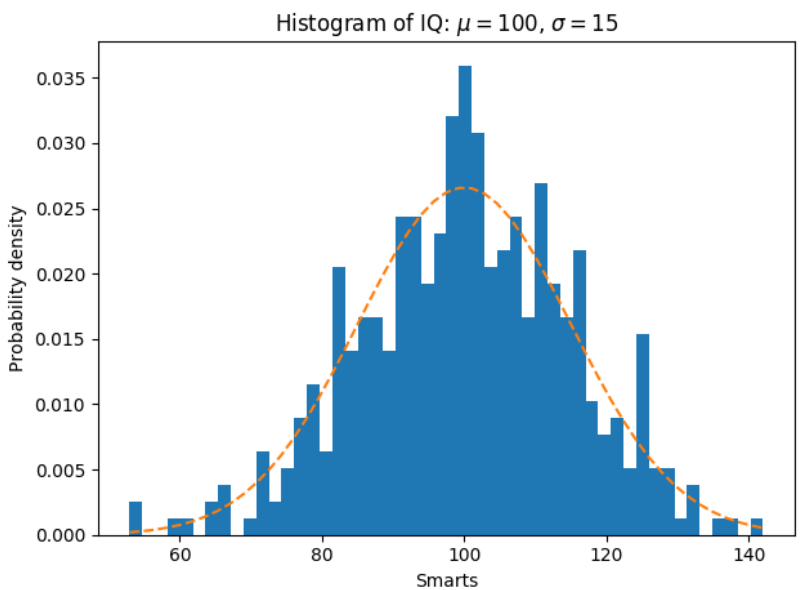
```python
import matplotlib.pyplot as plt
import numpy as np

# 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()
```



https://matplotlib.org/3.1.1/gallery/lines_bars_and_markers/scatter_symbol.html

Gallery example: histogram

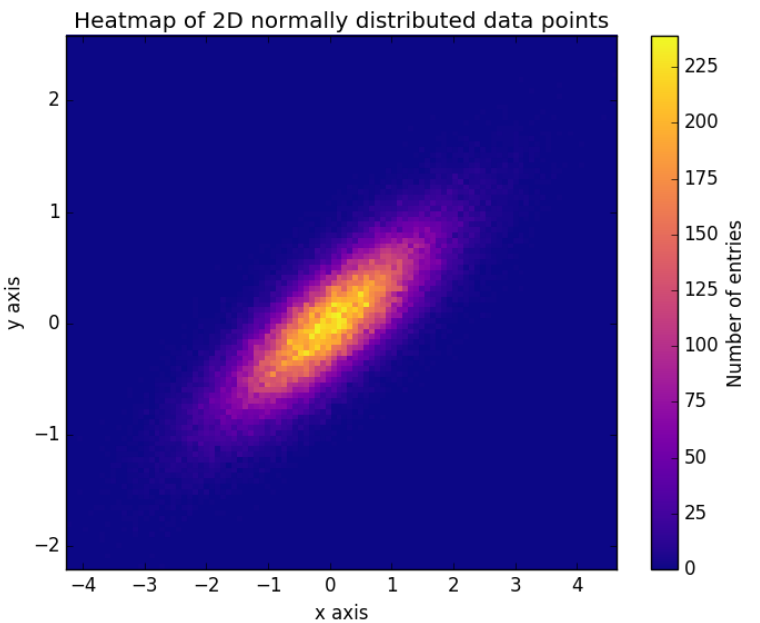
```python
import matplotlib
import numpy as np
import matplotlib.pyplot as plt

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

fig, ax = plt.subplots()

# the histogram of the data
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()
```



https://matplotlib.org/3.1.1/gallery/statistics/histogram_features.html

Gallery example: heatmap

```python
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()
plt.xlabel('x axis')
plt.ylabel('y axis')

# Show the plot.
plt.show()
```



https://riptutorial.com/matplotlib/example/17254/heatmap

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PLOS COMPUTATIONAL BIOLOGY

Editorial

Ten Simple Rules for Better Figures

Nicolas P. Rougier[1,2,3]*, Michael Droettboom[4], Philip E. Bourne[5]

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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

Lab 12A

github.com/WUSTL-Biol4220/home/labs/lab_12A.md