University of Zurich[UZH]

Department of Physics

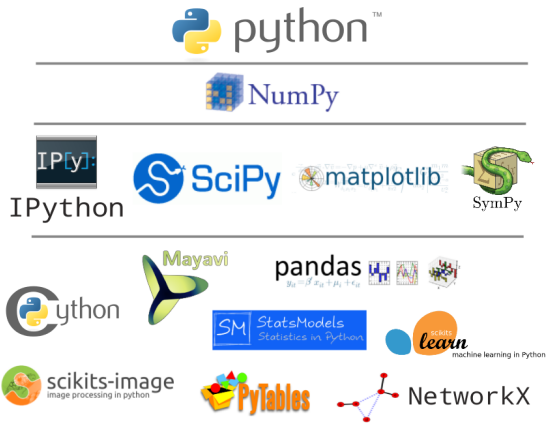
Data Visualization and more

Scientific Programming with Python

Jonas Eschle

Based partially on a talk by Stéfan van der Walt and modified by Andreas Weiden

The Ecosystem of Homo Python Scientificus

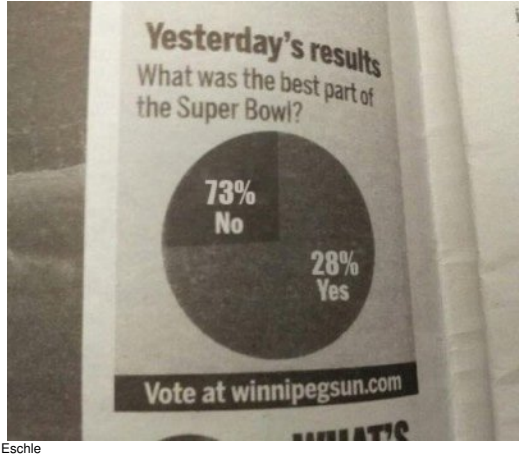


[Ondřej Čertík/LANL]

Table of Contents

Visualisation

Visualization as well as Content Matters



Visualization Options in Python

Matplotlib

- Started as emulation for MATLAB
- Basic plotting also in more than one dimension

Seaborn

- Collection of more complex plots
- Based on Matplotlib

bokeh

- Web publishable graphics
- Large variety of usable interactions

Folium

- Python interface to leaflet (maps)
- Plotting of geo data

Color

Color is a double-edged sword:

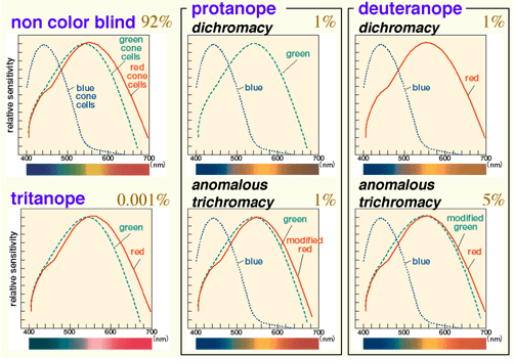
- Color can convey a lot of information
- But there are many forms of Color-blindness
- Many people will print your paper in black & white (for many reasons)

monolens is a package that allows you to see your plots simulated colorblind or in black and white.
Two (non-exclusive) ways to deal with this:

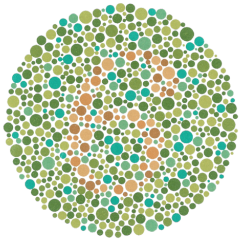
- Use Colors that are differentiable for all people and also in black & and white

Colorblindness

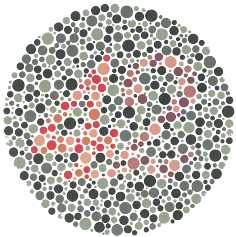
Colorblindness is not a total loss of color vision. Colorblind people can recognize a wide ranges of colors. But certain ranges of colors are hard to distinguish.



Colorblindness



6

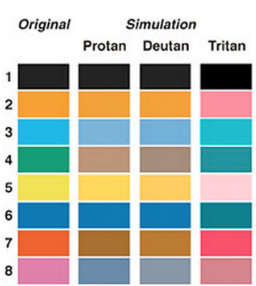


42

8% of Caucasian, 5% of Asian, and (4%) of African males are so-called "red-green" Colorblind. Chance to have at least one Colorblind reviewer out of three is up to $1 - (1 - 0.92)^3 = 22\%$!

Colorblindness

The way to deal with Colorblindess is to use redundant encoding of information
Most Colorblind people might not be able to distinguish certain colors, but are usually able to distinguish different brightness



	Hue	for Photoshop, Illustrator, Freehand, etc. C,M,Y,K (%)	for Photoshop, Illustrator, Freehand, etc. R,G,B (0-255)	for Word, Power Point, Canvas, etc. R,G,B (%)	Hex (0-f)
Black	– °	(0,0,0,100)	(0,0,0)	(0,0,0)	#000000
Orange	41°	(0,50,100,0)	(230,159,0)	(90,60,0)	#e69f00
Sky Blue	202°	(80,0,0,0)	(86,180,233)	(35,70,90)	#56b4e9
bluish Green	164°	(97,0,75,0)	(0,158,115)	(0,60,50)	#009e73
Yellow	56°	(10,5,90,0)	(240,228,66)	(95,90,25)	#f0e442
Blue	202°	(100,50,0,0)	(0,114,178)	(0,45,70)	#0072b2
Vermilion	27°	(0,80,100,0)	(213,94,0)	(80,40,0)	#d55e00
reddish Purple	326°	(10,70,0,0)	(204,121,167)	(80,60,70)	#cc799c

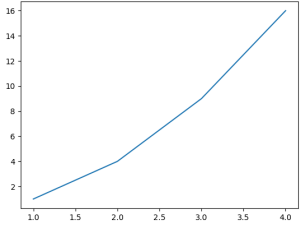
Use a color-palette taking advantage of this (either built-in or self-defined)

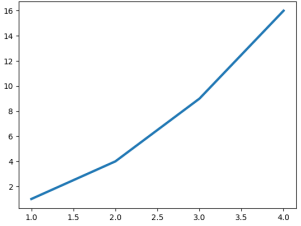
Texture

Use redundant coding. Not only Color, but also texture/patterns:

- Different markers
- Different line-styles
- Different filling-styles

Make plots visible enough using thick enough lines:

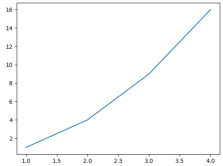




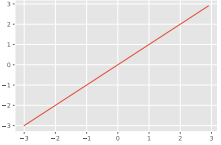
Custom styles

Matplotlib allows changing the style globally using an `.mplstyle` file or in the code with `mpl.rcParams[some_config] = ...`.
Some libraries offer pre-configured styles, e.g. mplhep `mplhep.style.use(hep.style.ATLAS)`.
In this file you can define almost everything, from frame line width, fonts, background color and grid, up to default figure size:

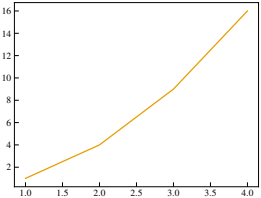
Default style



ggplot



custom style for LHCb



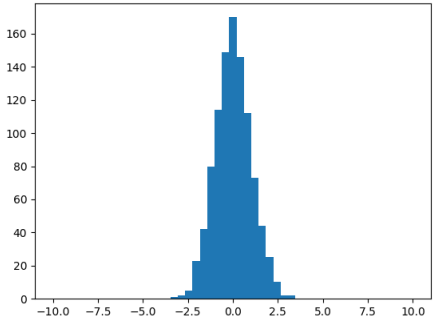
An example file with all options can be found on the matplotlib page
https://matplotlib.org/tutorials/introductory/customizing.html

1D data

Histograms

```
import matplotlib.pyplot as plt
import numpy as np
x = np.random.randn(1000)
bins = np.linspace(-10, 10)
plt.hist(x, bins=bins)
plt.show()
```

- See the distribution of a variable
- Can pass number of bins, range of bins or bin edges
- Set `density=True` for normalization

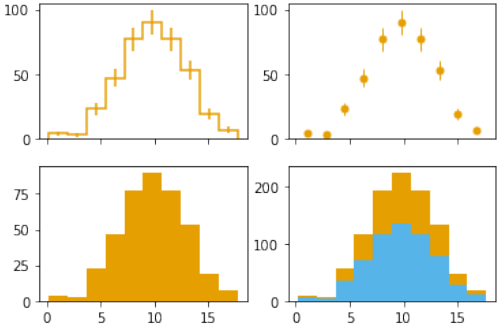


Histograms from HEP

Prebinned histograms

```
import mplhep
h, bins = np.histogram(np.random.normal(10, 3, 400),
                       bins=10)
axs = plt.subplots(2, 2, sharex=True)[1].flatten()

mplhep.histplot(h, bins, yerr=True, ax=axs[0])
mplhep.histplot(h, bins, yerr=np.sqrt(h),
                histtype='errorbar', ax=axs[1])
mplhep.histplot(h, bins, histtype='fill', ax=axs[2])
mplhep.histplot([1.5 * h, h], bins, histtype="fill",
                stack=True, ax=axs[3])
```



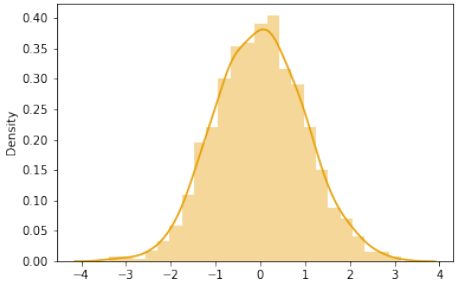
- Prebinned histograms: mplhep (matplotlib can't do this out-of-the-box)
- Takes yerr, weights (and weights error)

1D data

Kernel Density Estimation

```
import seaborn as sns
sns.distplot(x)
```

- Smooth estimation of a distribution
- Processes each datapoint as a gaussian centered at the point with given width (called bandwidth)
- Use `sns.kdeplot` for only the KDE
- `kdeplot` can take `cumulative=True`



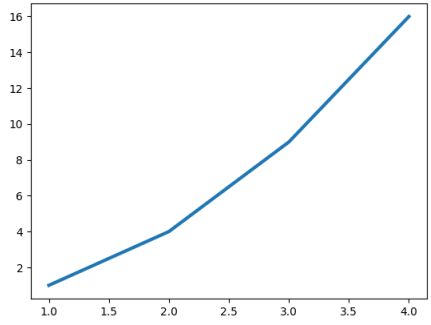
2D data

Line plots

```
x = np.array([1, 2, 3, 4])
y = x**2
plt.plot(x, y, linewidth=3)

import pandas as pd
df = pd.DataFrame({"x": x, "y":y})
df.plot("x", "y")
```

- Basic drawing command
- Can also be directly called from `pandas`

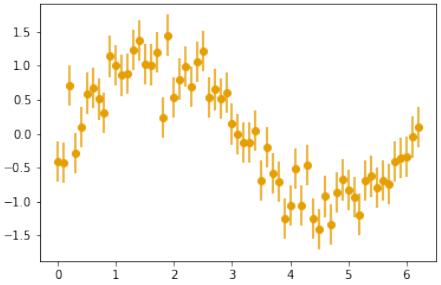


2D data

Error bars

```
x = np.arange(0, 2*np.pi, 0.1)
yerr = 0.3
noise = yerr * np.random.randn(*x.shape)
y = np.sin(x) + noise
plt.errorbar(x, y, yerr=yerr, fmt="o")
```

- Uncertainties are very important in science
- Can optionally take `xerr` and `yerr`
- `yerr` can be an array or a 2-tuple of arrays for asymmetric uncertainties

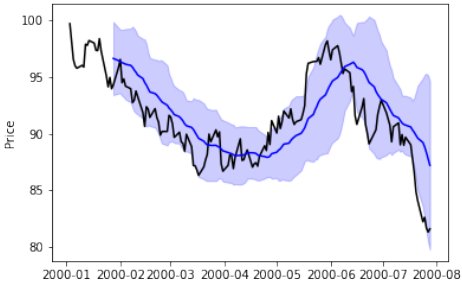


2D data

Filling areas

```
from numpy.random import randn

t = pd.date_range("2000-1-1", periods=150,
                  freq="B")
price = pd.Series(100+randn(150).cumsum(),
                  index=t)
avg = price.rolling(20).mean()
std = price.rolling(20).std()
plt.plot(price.index, price, "k")
plt.plot(avg.index, avg, "b")
plt.fill_between(std.index, avg-2*std,
                 avg+2*std, color="b",
                 alpha=0.2)
plt.ylabel("Price")
```



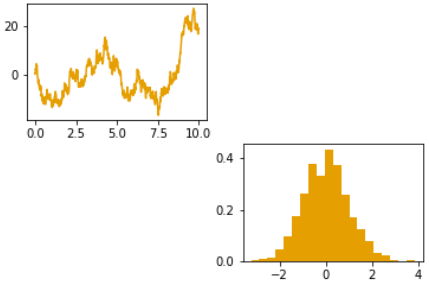
- Useful for errorbands

Intermezzo - Multiple graphs

Subplot

```
np.random.seed(42)
x = np.arange(0, 10, 0.01)
y = np.random.randn(len(x)).cumsum()
d = np.diff(y)

plt.subplot(2, 2, 1)
plt.plot(x, y)
plt.subplot(224)
plt.hist(d, bins=20, density=True)
```



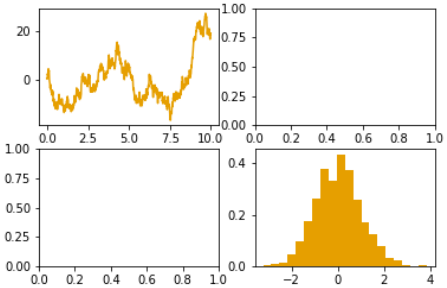
- Useful for independent plots
- Use `sharex` and `sharey` if neccessary

Intermezzo - Multiple graphs

Subplots

```
fig, axes = plt.subplots(2, 2)
axes[0,0].plot(x, y)
axes[1,1].hist(d, bins=20, density=True)
```

- Useful for grid of plots
- Use `sharex` and `sharey` if neccessary
- Access the axes as a `numpy` array

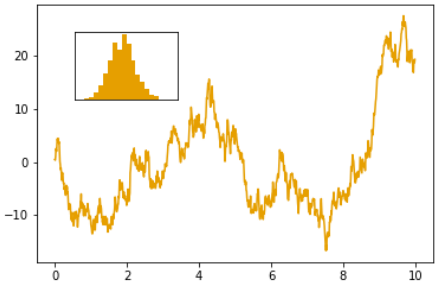


Intermezzo - Multiple graphs

Plot-in-plot

```
plt.plot(x, y)
plt.axes([0.2, .6, .2, .2])
plt.hist(d, bins=20, density=True)
plt.xticks([])
plt.yticks([])
```

- Ideal for summary plot or zoomed version
- Can turn off the axes
- Freely placeable

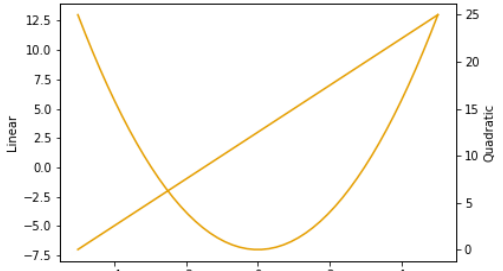


Intermezzo - Multiple graphs

Twin axes

```
plt.figure()
x = np.linspace(-5, 5)
y = 2*x + 3
y2 = x**2

ax1 = plt.gca()
ax1.plot(x, y)
ax1.set_ylabel("Linear")
ax2 = ax1.twinx()
ax2.plot(x, y2)
ax2.set_ylabel("Quadratic")
```



- Two completely independent axes
- Use `plt.twiny` for an additional x-axis
- Have to build legend manually

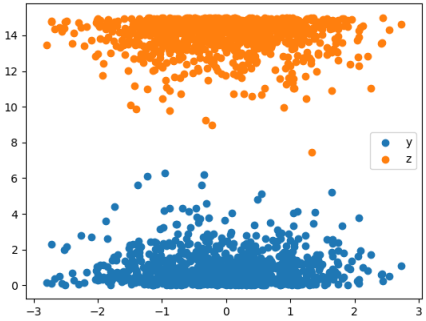
2D data

Scatter

```
from numpy.random import normal
from numpy.random import exponential

x = randn(1000)
y = exponential(1, 1000)
z = 15 - exponential(1, 1000)
plt.scatter(x, y, label="y")
plt.scatter(x, z, label="z")
plt.legend()
plt.savefig("figs/plt_scatter.png")
```

- Good at getting a feel for the data
- Bad for many datapoints

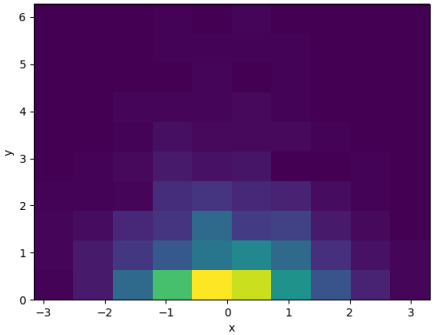


2D data

2D histogram

```
x = randn(1000)
y = exponential(size=1000)
plt.hist2d(x, y)
plt.xlabel("x")
plt.ylabel("y")
```

- Can take arbitrary binning like in 1D
- Also works for lots of data

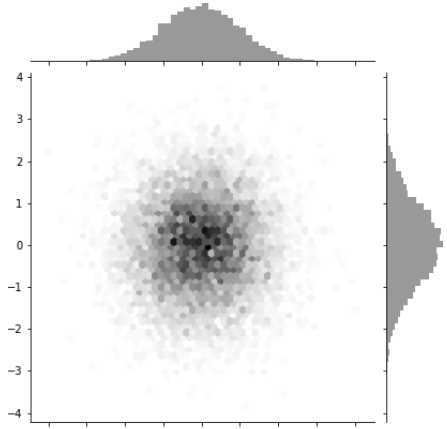


2D data

2D hexagonal histogram

```
x, y = randn(2, 1000)
sns.jointplot(x, y, kind="hex", color="k")
```

- Sometimes nicer to look at than square bins
- Has marginal distributions by default
- `matplotlib` also has a simpler version, `plt.hexbin`

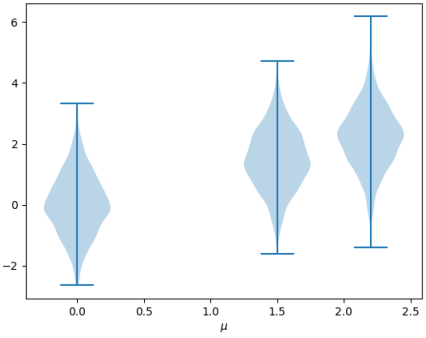


2D data

Violin plots

```
mus = 0, 1.5, 2.2
data = [normal(mu, 1, 1000) for mu in mus]
plt.violinplot(data, positions=mus)
plt.xlabel(r"$\mu$")
```

- More information than just plotting mean vs μ
- Can add plotting of individual data points, quantiles, etc



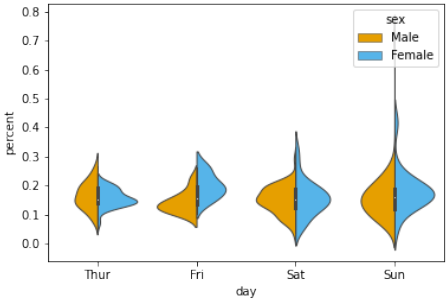
(2+1)D data

Split violin plots

```
import seaborn as sns
tips = sns.load_dataset("tips")

tips["percent"] = tips.tip/tips.total_bill
sns.violinplot("day", "percent", "sex",
               data=tips, split=True)
```

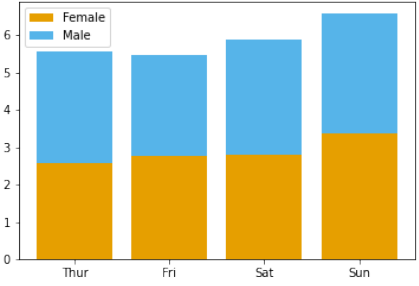
- Allows one more distinction via the two halves or more by putting them next to each other
- Good for additional category with few states



2D data

(Stacked) bar charts

```
bottom = 0
for sex, df in tips.groupby("sex"):
    df = df.groupby("day").tip.mean()\
           .reset_index()
    plt.bar(df["day"], df["tip"], 0.8,
            bottom, label=sex)
    bottom = df["tip"]
plt.legend()
```



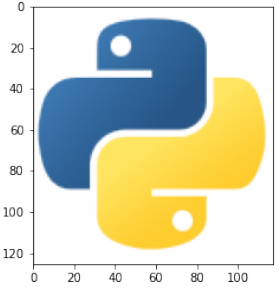
- Good for one or two categories also with multiple states
- Shows the composition well, but not the development of each component

2D data

Images

```
path = "figs/python.png"
img = plt.imread(path)
fig1 = plt.imshow(img)
```

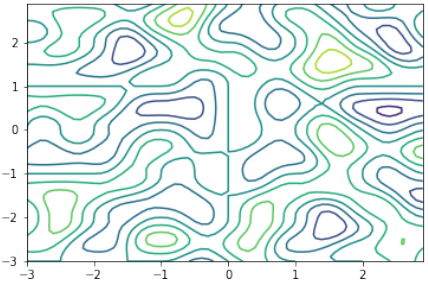
- `scipy.ndimage.imread` now deprecated
- Internally stored as a (2+1)D `numpy` array, so you can use fancy indexing on/with it



3D data

Contour plots

```
import noise
pnoise2 = np.vectorize(noise.pnoise2)
x = np.arange(-3, 3, 0.1)
y = np.arange(-3, 3, 0.1)
X, Y = np.meshgrid(x, y)
z = pnoise2(X, Y)
plt.contour(X, Y, z)
```



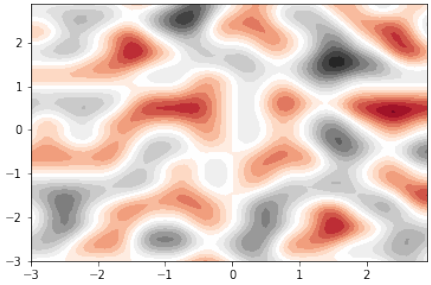
- Lines show fixed values, encoding in color
- Suitable for printing (no fancy gradients)

3D data

Filled contours

```
plt.contourf(X, Y, z, 20, cmap='RdGy')
```

- Contains more information than height lines
- Can use any colormap

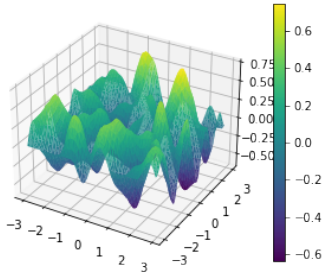


3D data

Surface plots

```
from mpl_toolkits.mplot3d import Axes3D
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')

cmap = plt.cm.viridis
x, y, z = X.flatten(), Y.flatten(), z.flatten()
surf = ax.plot_trisurf(x, y, z, cmap=cmap)
plt.colorbar(surf)
```

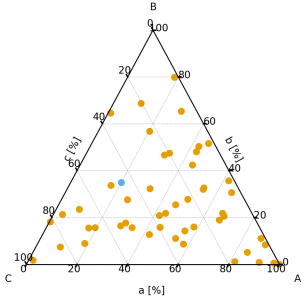


- Easy to immediately grasp
- Can zoom/rotate in interactive environments

3D data

Ternary plots

```
import ternary
fig, tax = ternary.figure(scale=100)
fig.set_size_inches(5, 5)
a=100*rand(50);b=(100-a)*rand(50);c=100-a-b
tax.scatter(np.array([[a, b, c]]))
tax.scatter([[20, 35, 45]])
tax.right_corner_label("A")
tax.top_corner_label("B")
tax.left_corner_label("C")
tax.bottom_axis_label("a [%]")
...
tax.gridlines(multiple=20, color="gray")
tax.ticks(axis='lbr', multiple=20)
tax.boundary(linewidth=1)
tax.get_axes().axis('off')
```

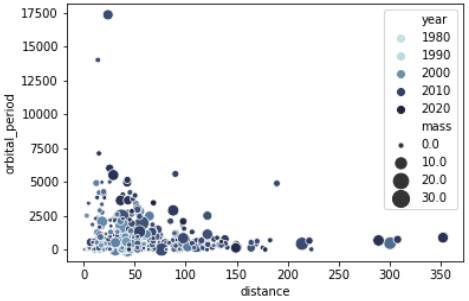


- For analyzing composition with three components that sum to a constant
- Need `python-ternary` for this

4D data

Enhanced scatter plot

```
planets = sns.load_dataset("planets")
cmap = sns.cubehelix_palette(rot=-.2,
                             as_cmap=True)
ax = sns.scatterplot(x="distance",
                     y="orbital_period",
                     hue="year",
                     size="mass",
                     palette=cmap,
                     sizes=(10, 200),
                     data=planets)
```



- Sometimes you can encode information in color and size of markers

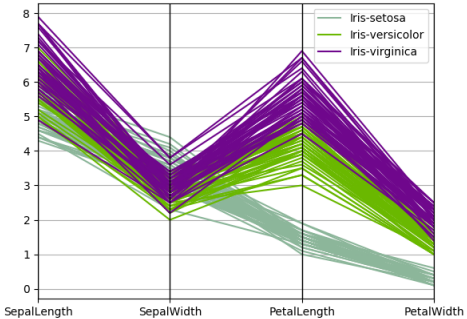
ND data

Parallel coordinates

```
from pandas.plotting import parallel_coordinates

iris = pd.read_csv("data/iris.csv")
parallel_coordinates(data, "Name")
```

- Works for an arbitrary number of dimensions
- Results may vary according to order of dimensions
- Can only see broad features
- Best for distinguishing groups in multiple dimensions



ND data

Radar plot

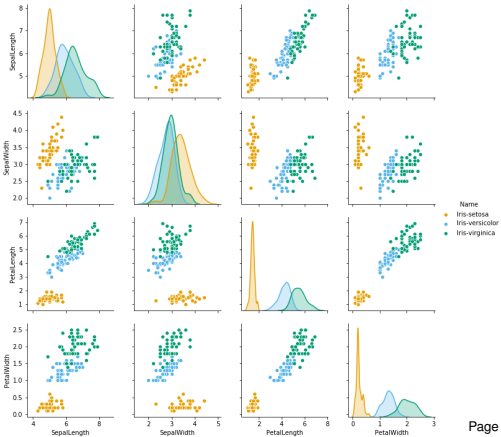
- Can be used to compare few examples in many dimensions
- No easy implementation available
- Find this example here

ND data

Pairplot

```
sns.pairplot(iris, diag_kind="kde",
             hue="Name")
```

- Plots each variables correlation with each other variable
- Can be used to find correlations between two variables out of many
- Easy to find a simple cut for classification
- Can even add automatic linear regression

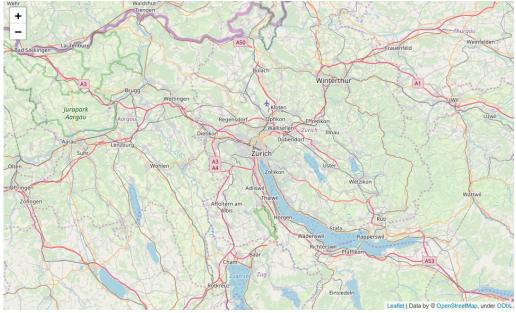


Geospatial data

Folium

```
import folium
m = folium.Map(location=[47.3686, 8.5391])
```

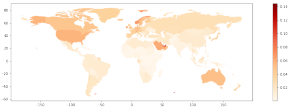
- Takes data from OpenStreetMap
- Interactive visualization via javascript in the browser
- No easy way to save the resulting map



Geospatial data

Geopandas

```
import geopandas
fig = plt.figure(figsize=(20, 5))
ax = fig.gca()
world = geopandas.read_file(
    geopandas.datasets.get_path(
        'naturalearth_lowres'))
world = world[(world.pop_est>0)
          & (world.name!="Antarctica")]
world['gdp_per_cap'] = world.gdp_md_est \
                       / world.pop_est
world.plot(column='gdp_per_cap', ax=ax,
           legend=True, cmap="OrRd")
```



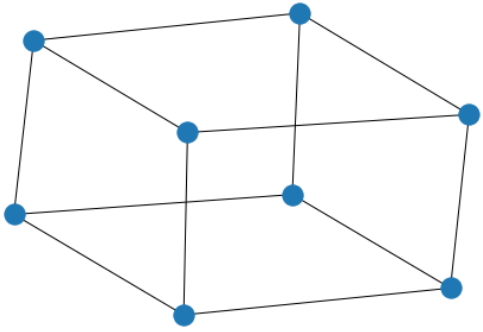
- Has a low-res version of all countries included
- Can read shapefiles in many common formats
- Combines them with `pandas` dataframes

Networks

Networkx

```
import networkx as nx
g = nx.cubical_graph()
nx.draw(g)
```

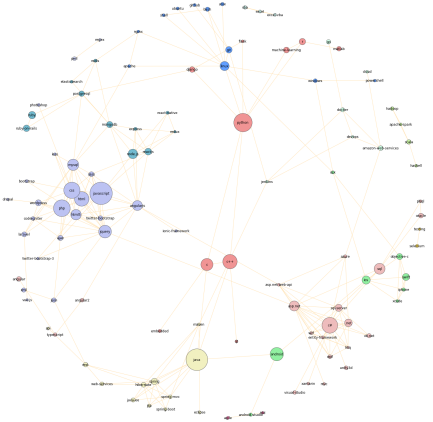
- Automatically positions the nodes according to the weights on the nodes
- Many common graphs included
- Many customizations possible



Networks

Networkx

- Automatically positions the nodes according to the weights on the nodes
- Useful for text analysis



Resources

- Pyplot tutorial: https://matplotlib.org/users/pyplot_tutorial.html
- Matplotlib documentation: https://matplotlib.org/api/pyplot_summary.html
- Custom style-sheets: https://matplotlib.org/users/customizing.html
- Pandas plotting documentation: https://pandas.pydata.org/pandas-docs/stable/visualization.html
- Seaborn documentation: https://seaborn.pydata.org/