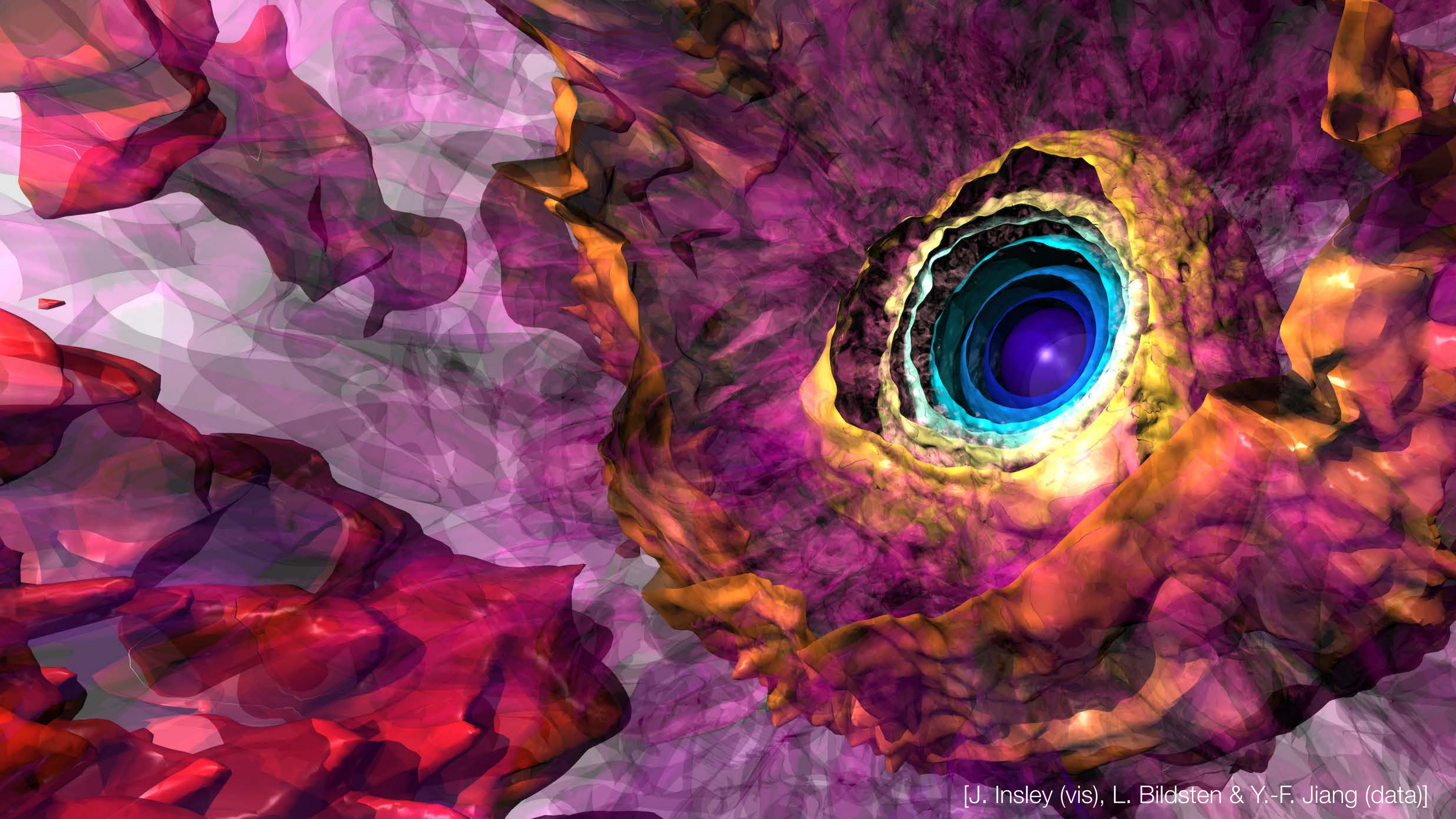
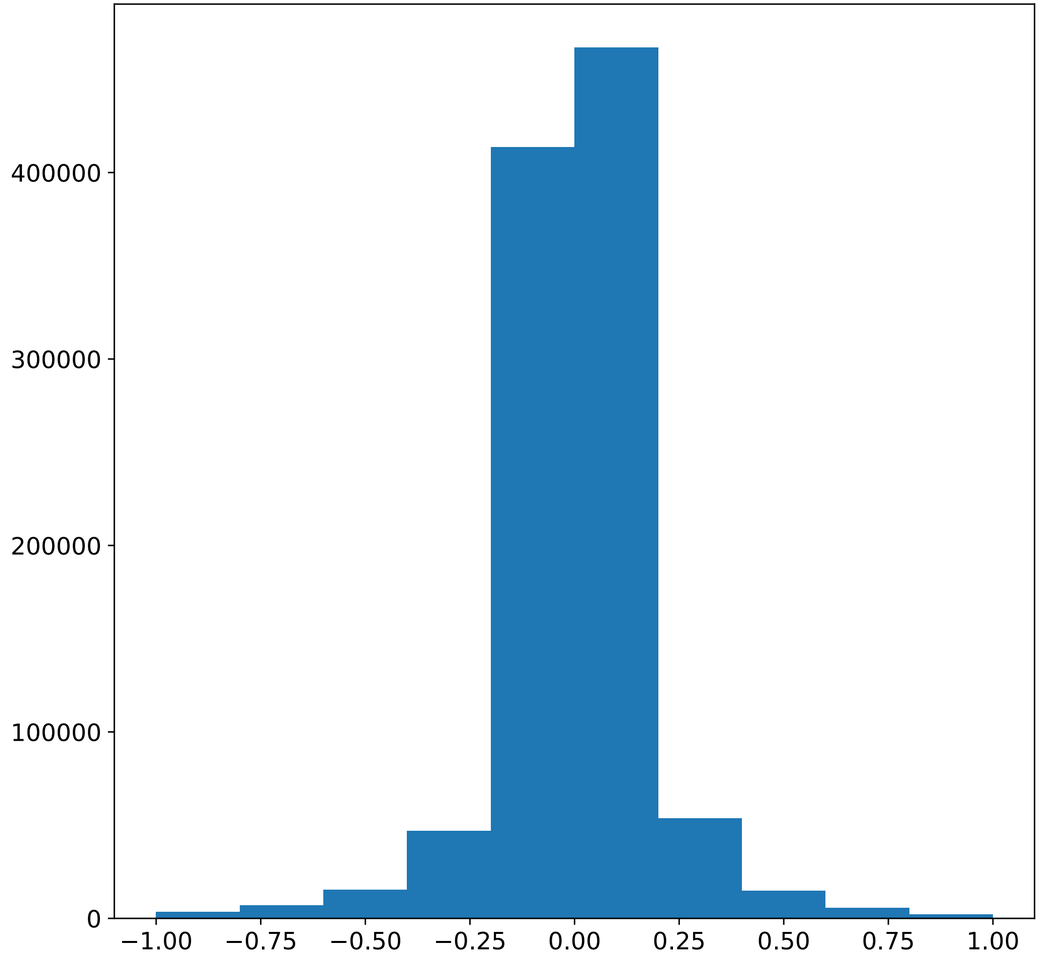
Data Visualization in Notebooks

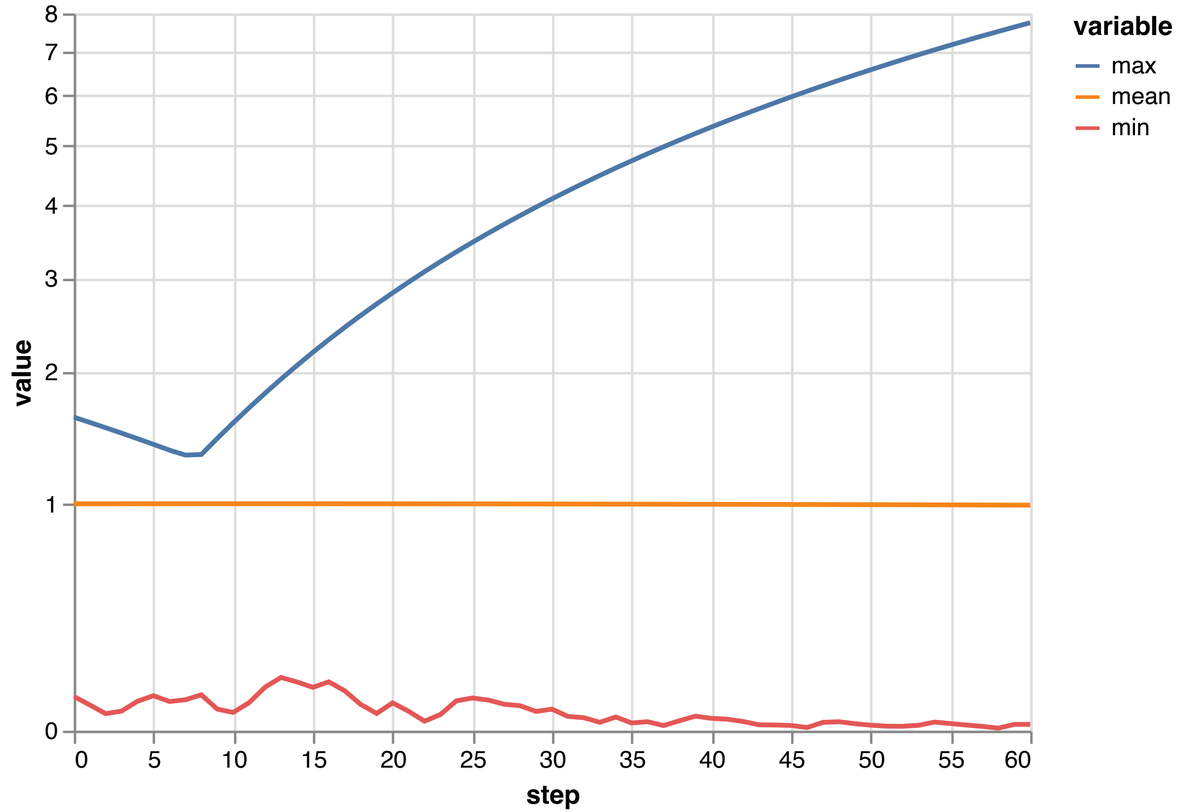
David Koop
Northern Illinois University



[J. Insley (vis), L. Bildsten & Y.-F. Jiang (data)]

Also Visualizations

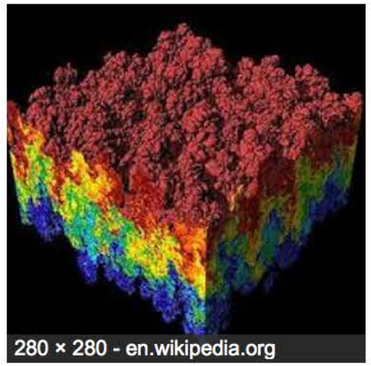


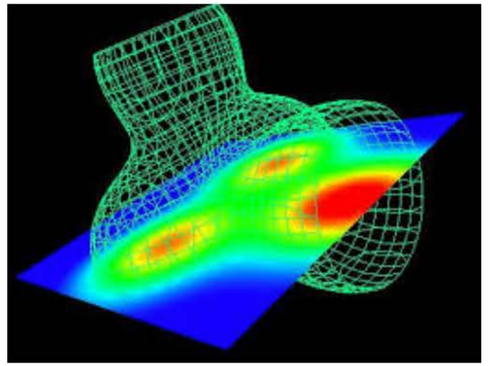


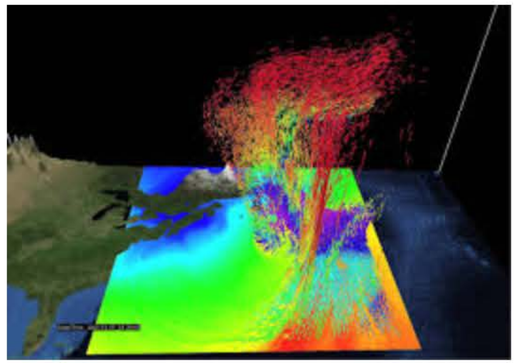
"Scientific" and "Information" Visualization

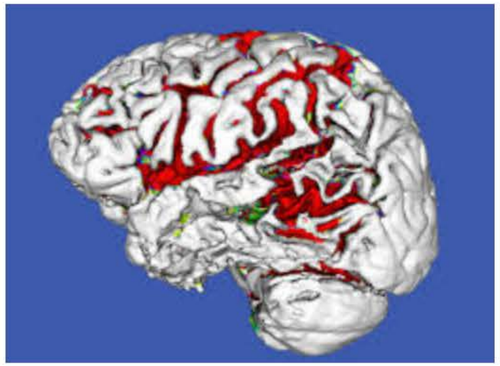
- Two subfields of visualization
- **Scientific visualization (SciVis)** deals with data where the spatial position is given with data
  - Usually continuous data
  - Often displaying physical phenonema
  - Techniques like isosurfacing, volume rendering, vector field vis
- **Information visualization (InfoVis)** deals with data that has no set spatial representation; the designer chooses how to visually represent data

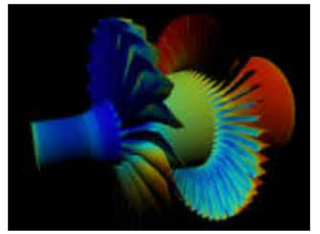
SciVis

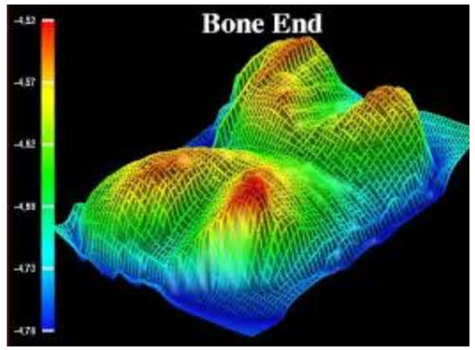

280 × 280 - en.wikipedia.org

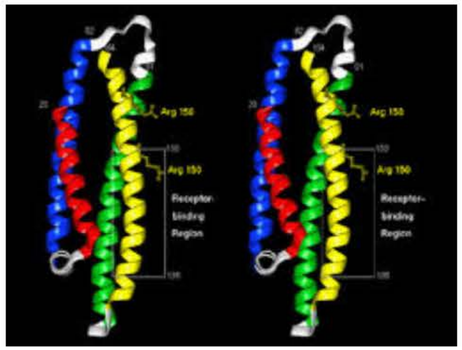


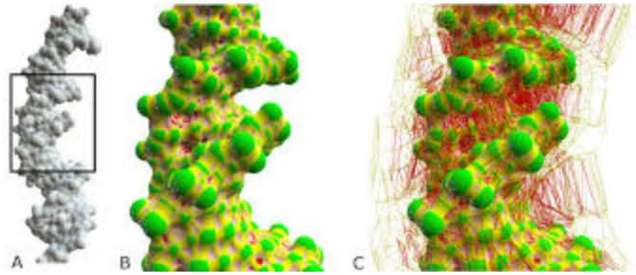


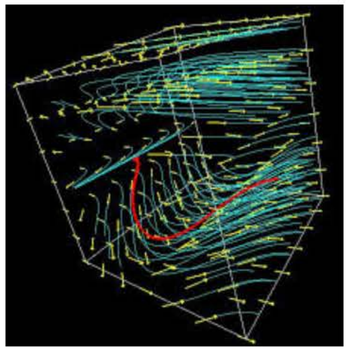


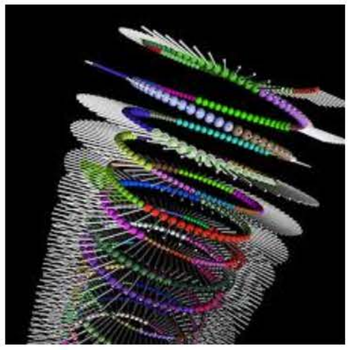


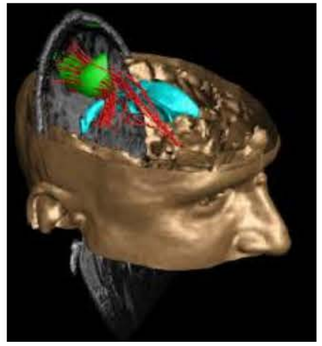

Bone End

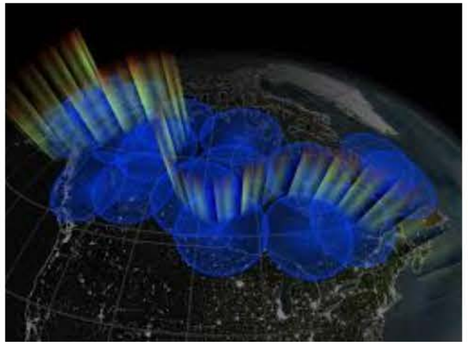

Arg 150
Arg 150
Receptor-
binding
Region
Arg 150
Arg 150
Receptor-
binding
Region

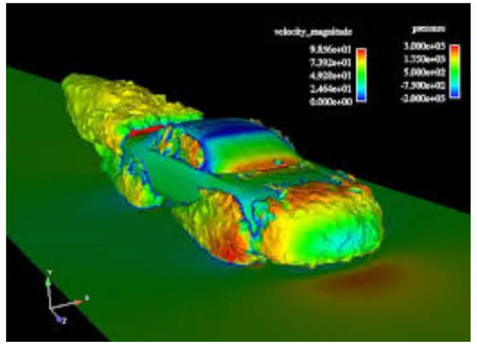

A
B
C










velocity_magnitude
9.856e+01
7.392e+01
4.928e+01
2.464e+01
0.000e+00
pressure
3.000e+03
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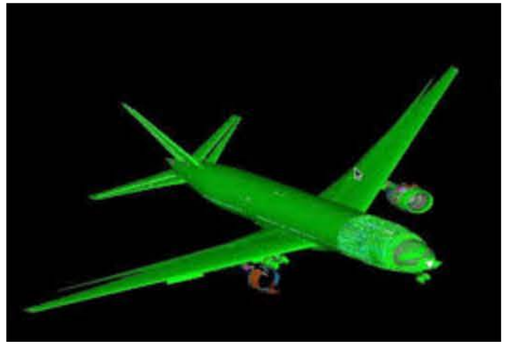
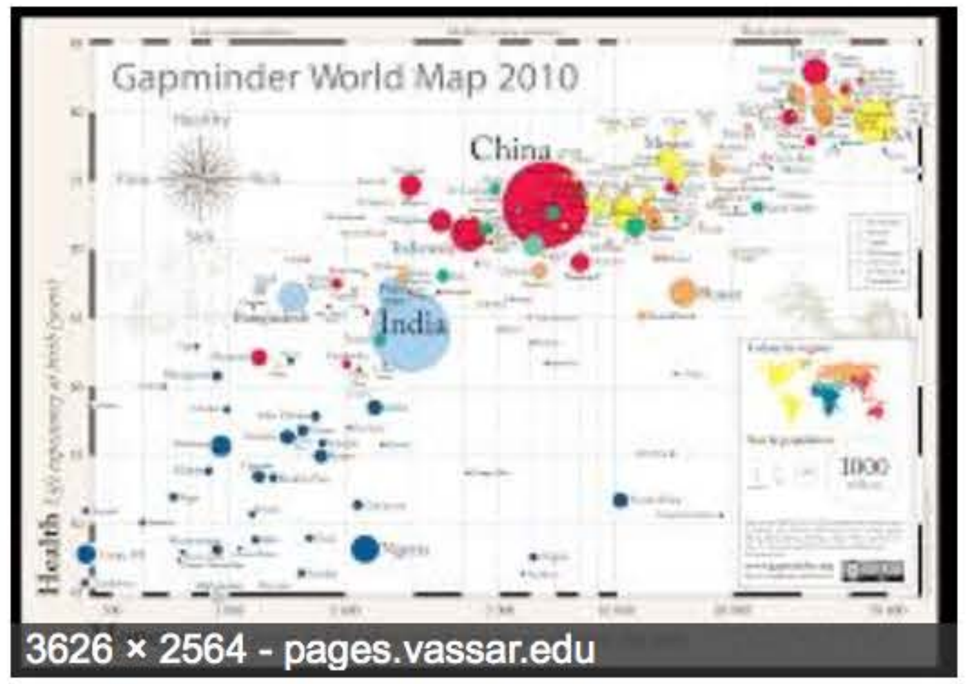
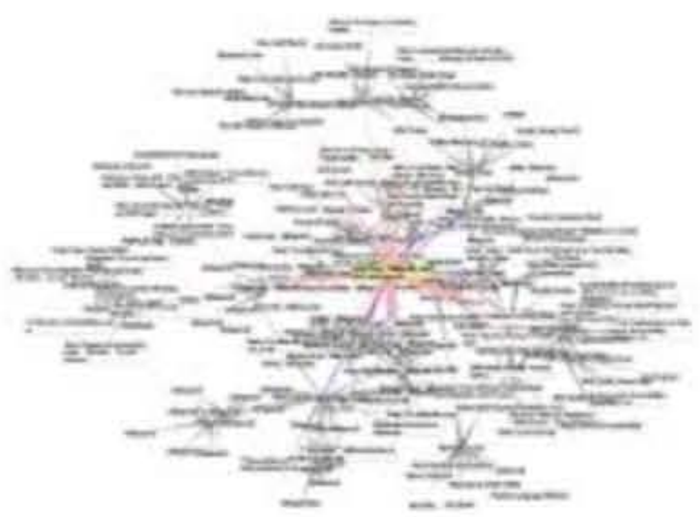
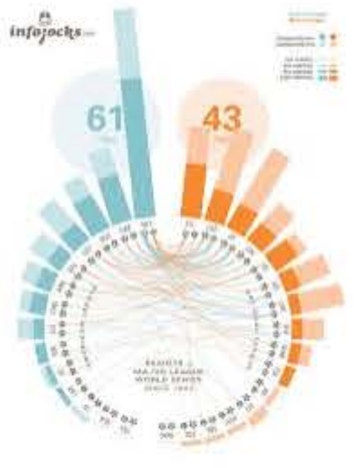
5.000e+02
-7.500e+02
-2.000e+03

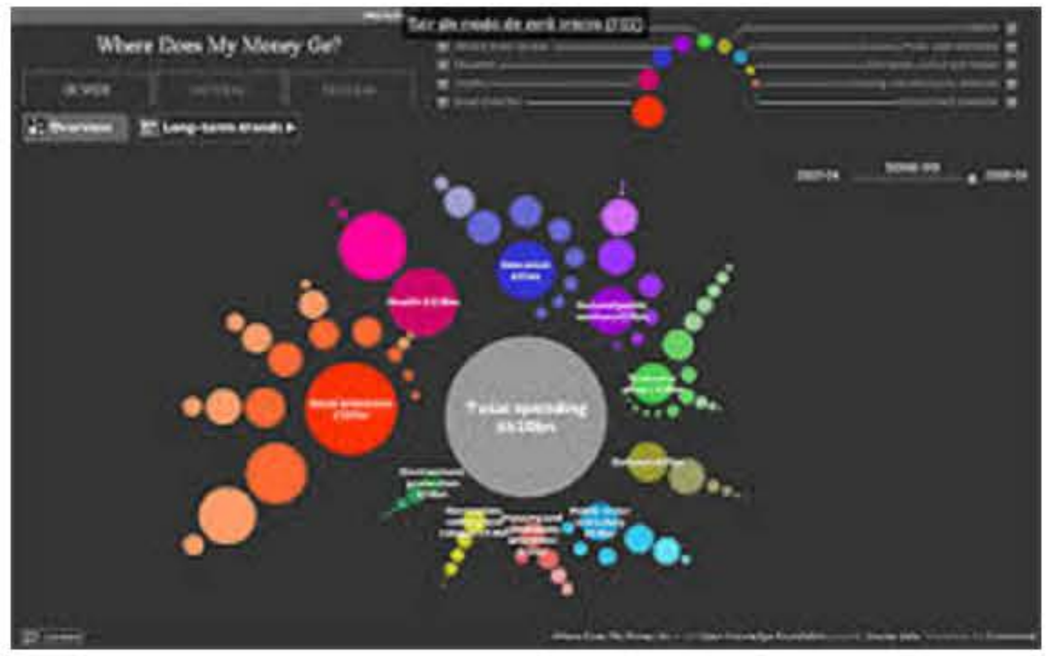


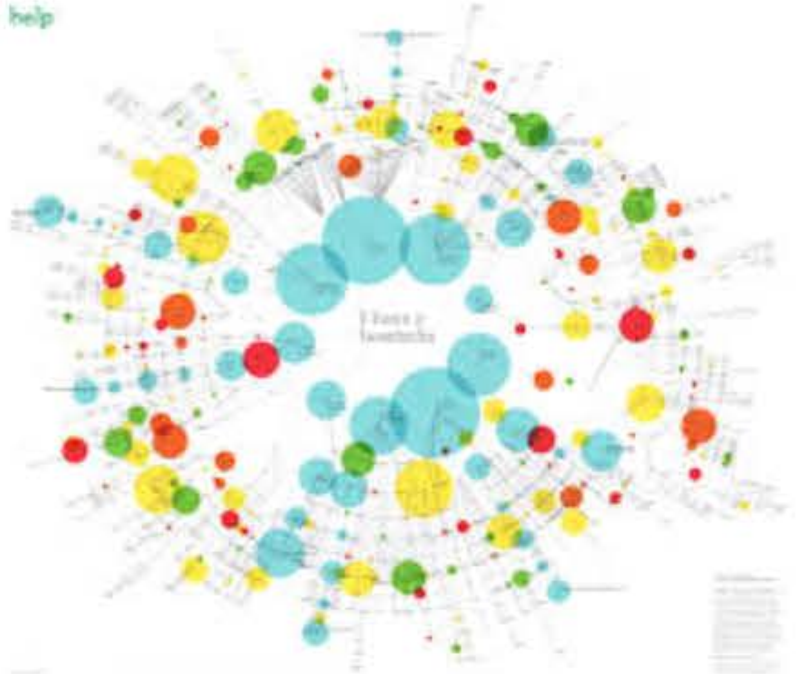
InfoVis

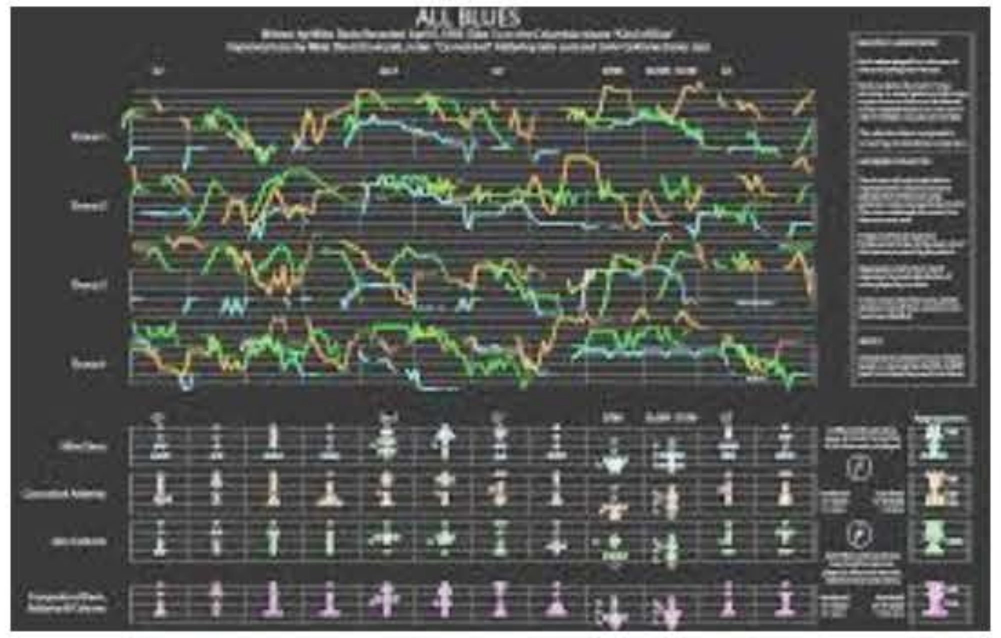

Gapminder World Map 2010
China
India
3626 × 2564 - pages.vassar.edu



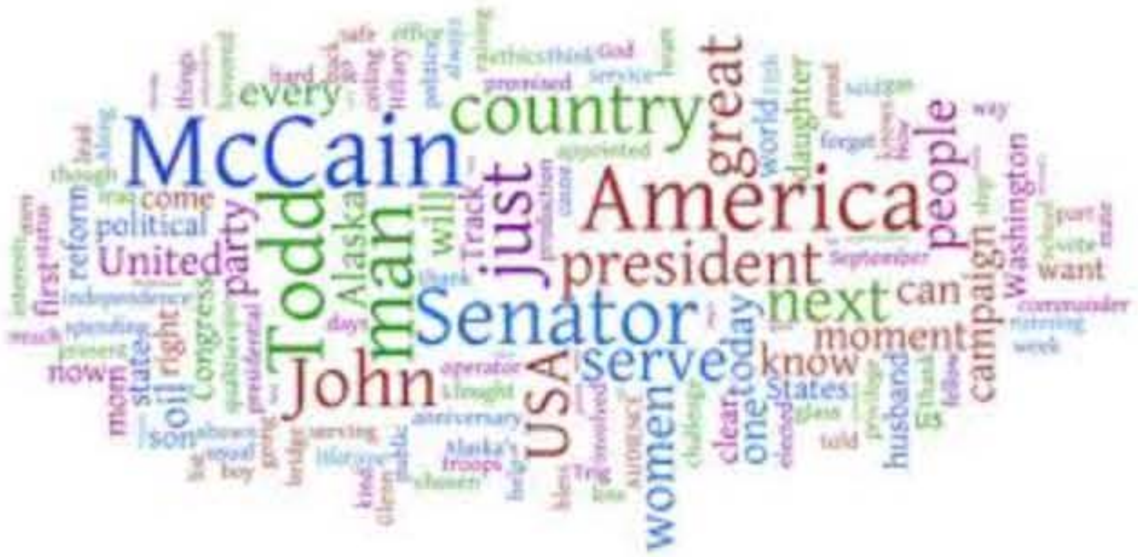

61
43

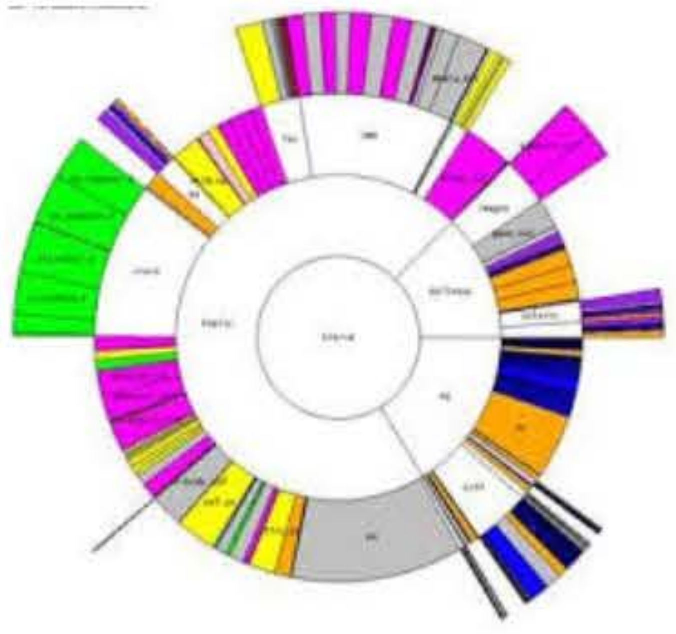

Where Does My Money Go?
Total spending

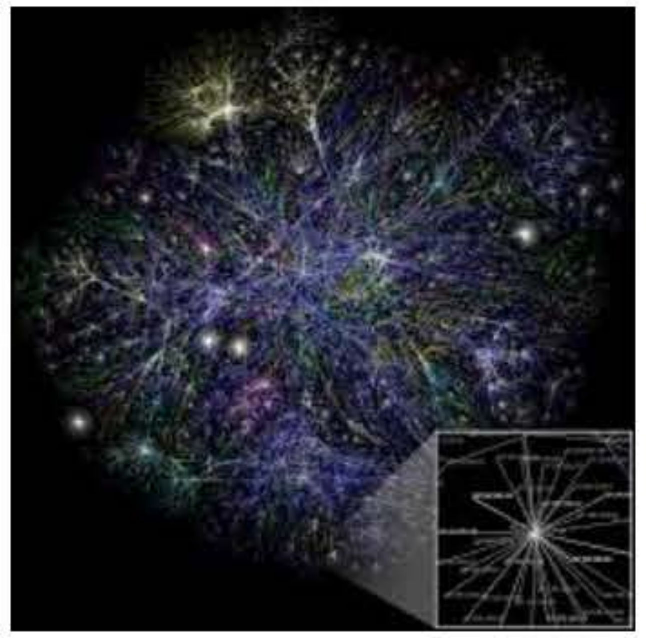


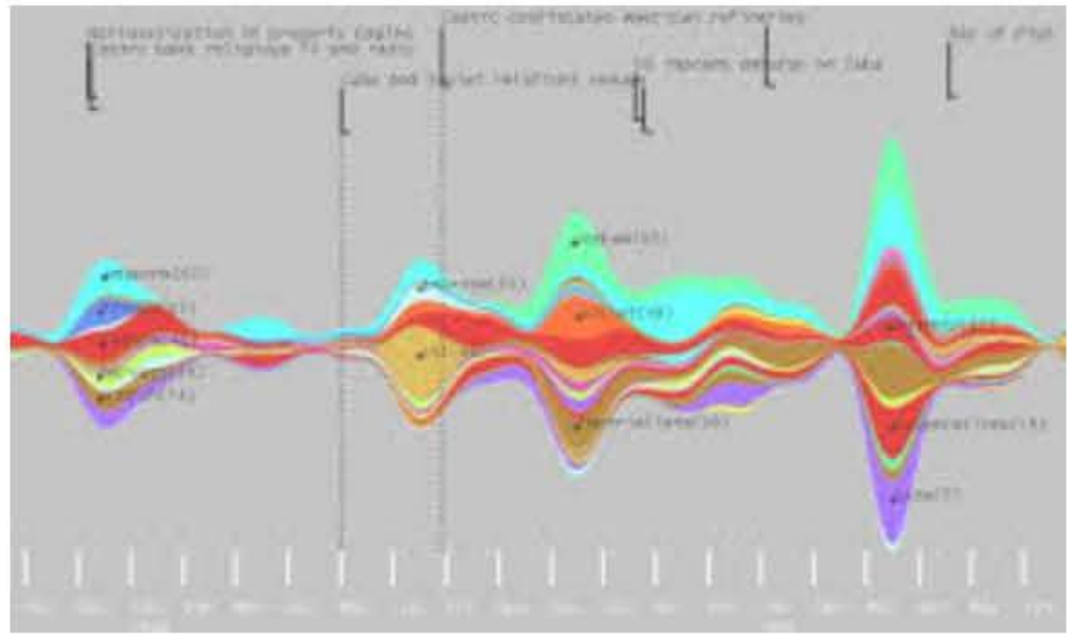

ALL BLUES

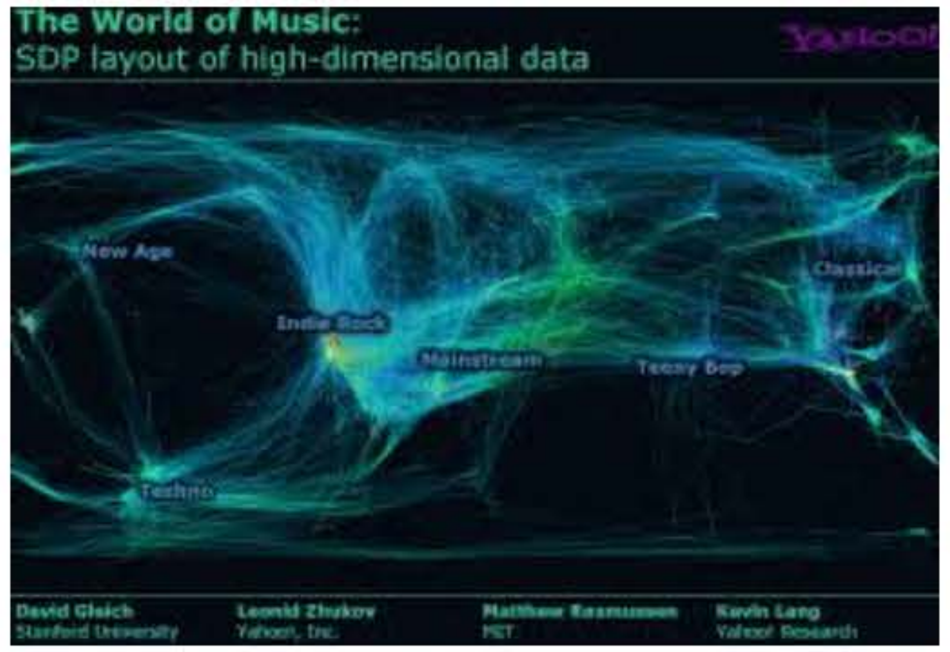

data
Information
visualization
graphics
science
interaction
Creativity
edit
research
human
design
analysis


McCain
country
America
president
Senator
John
Todd
USA
people
great
next
serve

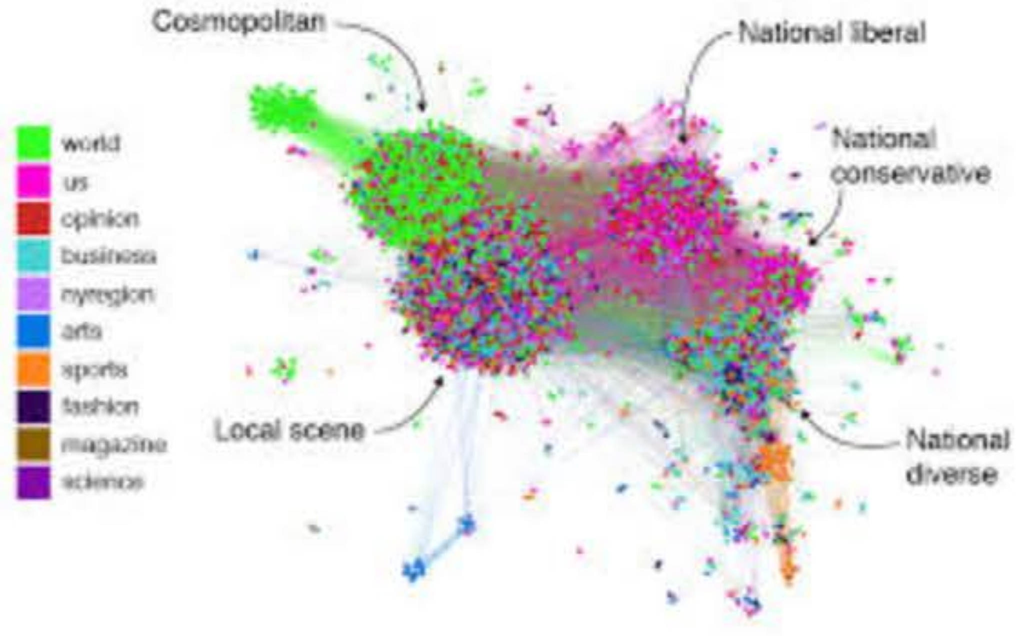







The World of Music:
SDP layout of high-dimensional data
New Age
Indie Rock
Mainstream
Classical
Teeny Bop
Techno
David Gleich
Leonid Zhukov
Matthew Rasmussen
Kevin Lang


China
Japan
United States
Congo, Dem. Rep.
South Africa
2008


Cosmopolitan
National liberal
National conservative
Local scene
National diverse
world
us
opinion
business
nyregion
arts
sports
fashion
magazine
science

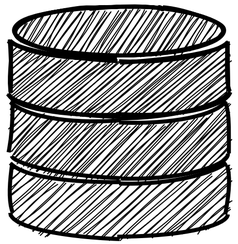

INFORMATION
VISUALIZATION AND
COMPUTATIONAL
DESIGN

"The purpose of visualization is **insight**, not pictures"

– B. Schneiderman

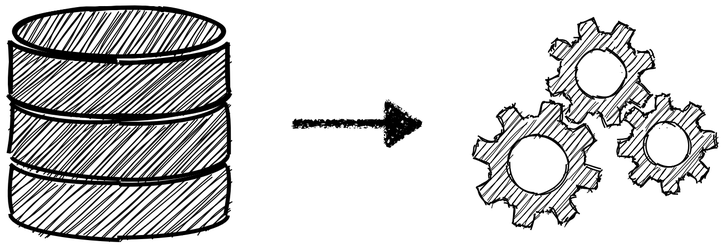
Data Analysis

Data

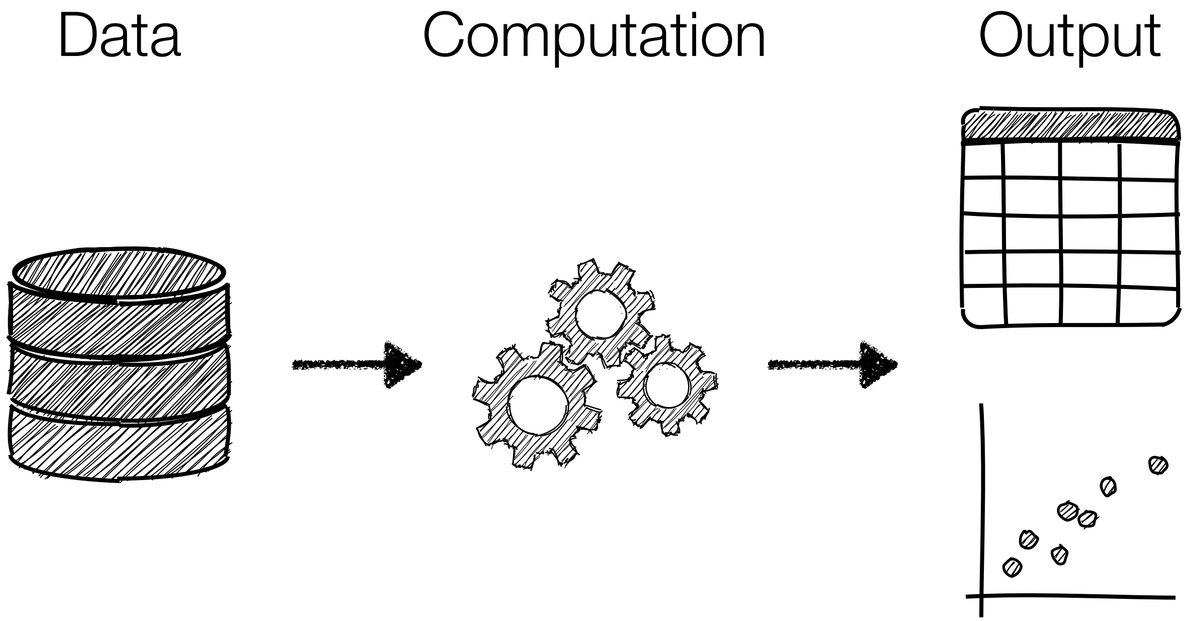


Data Analysis

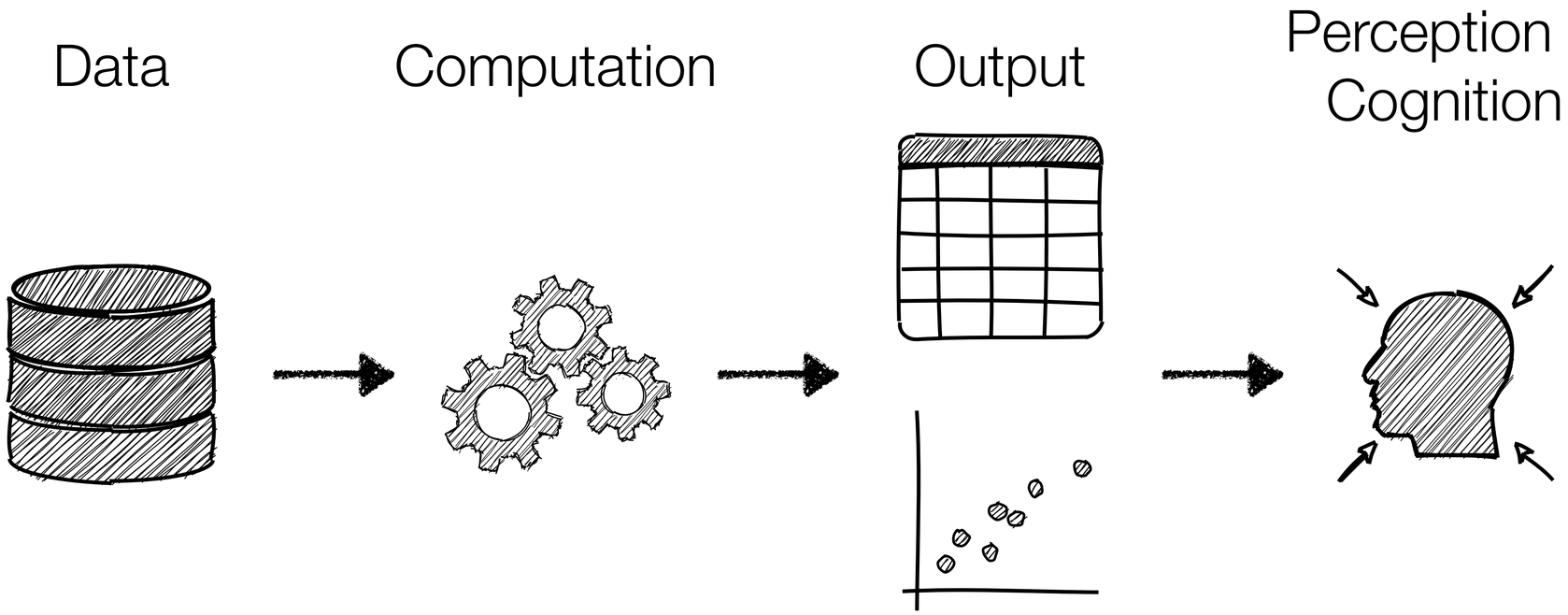
Data Computation



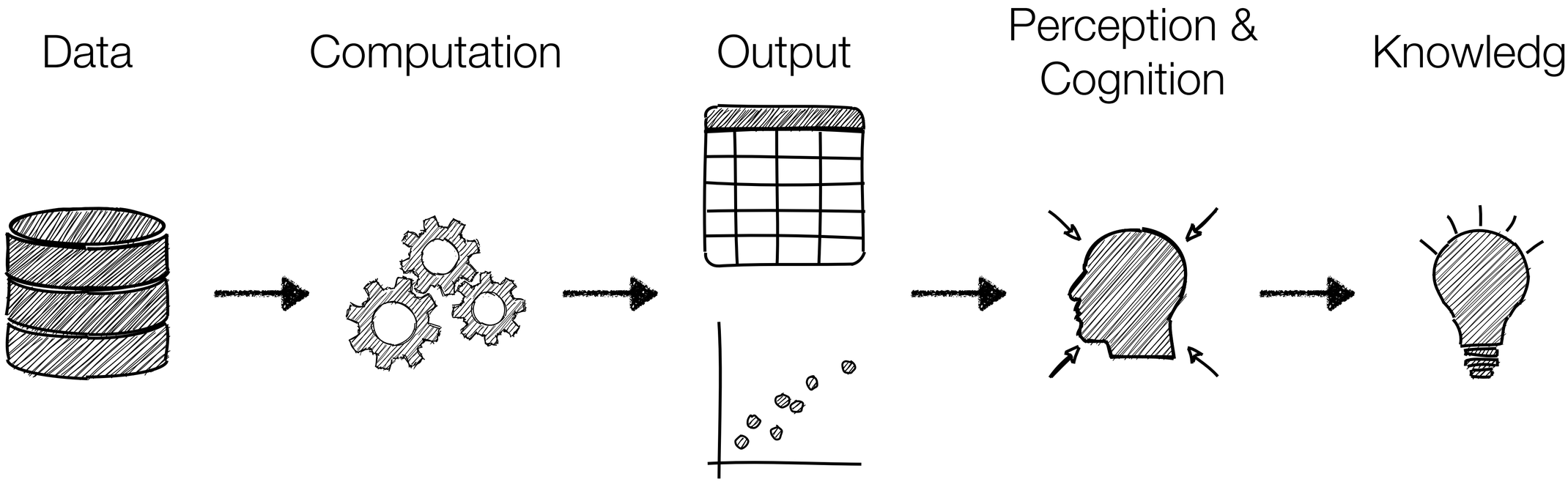
Data Analysis



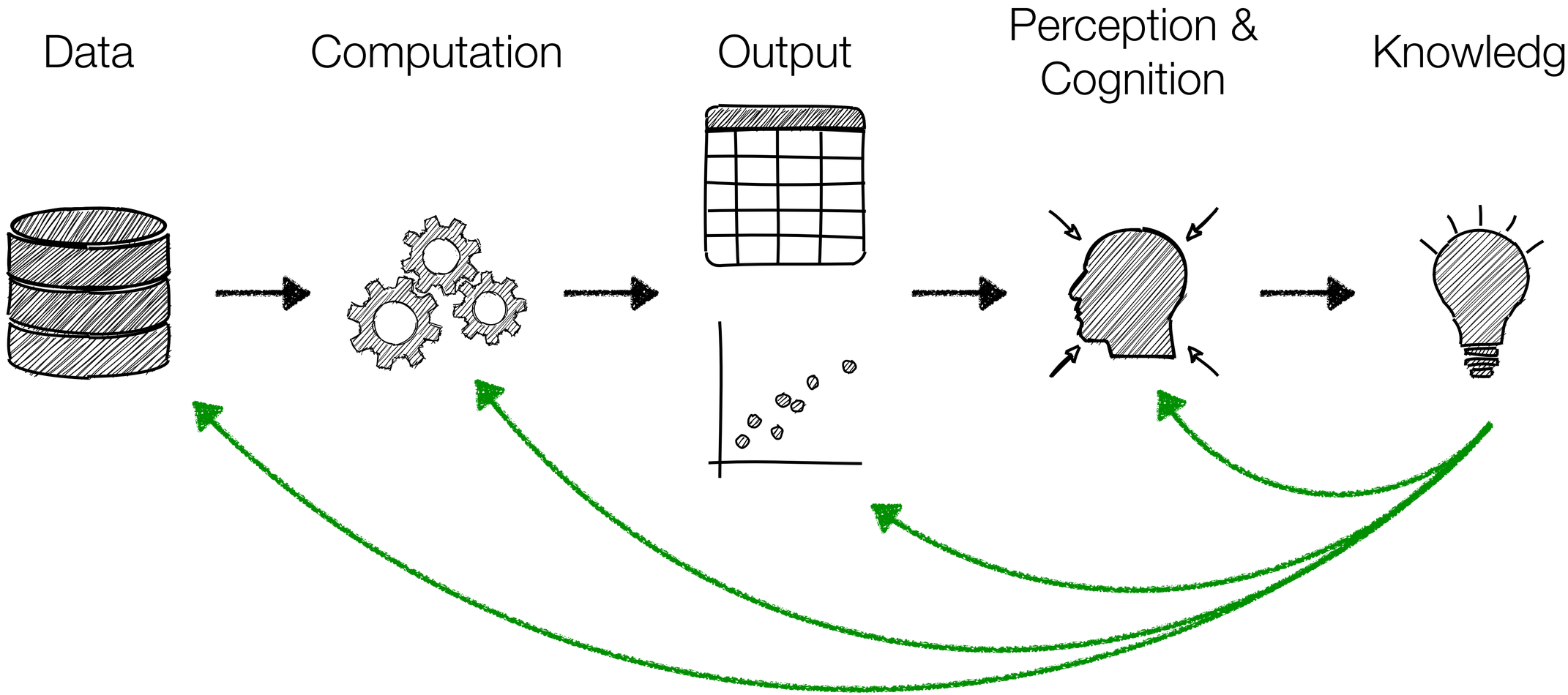
Data Analysis



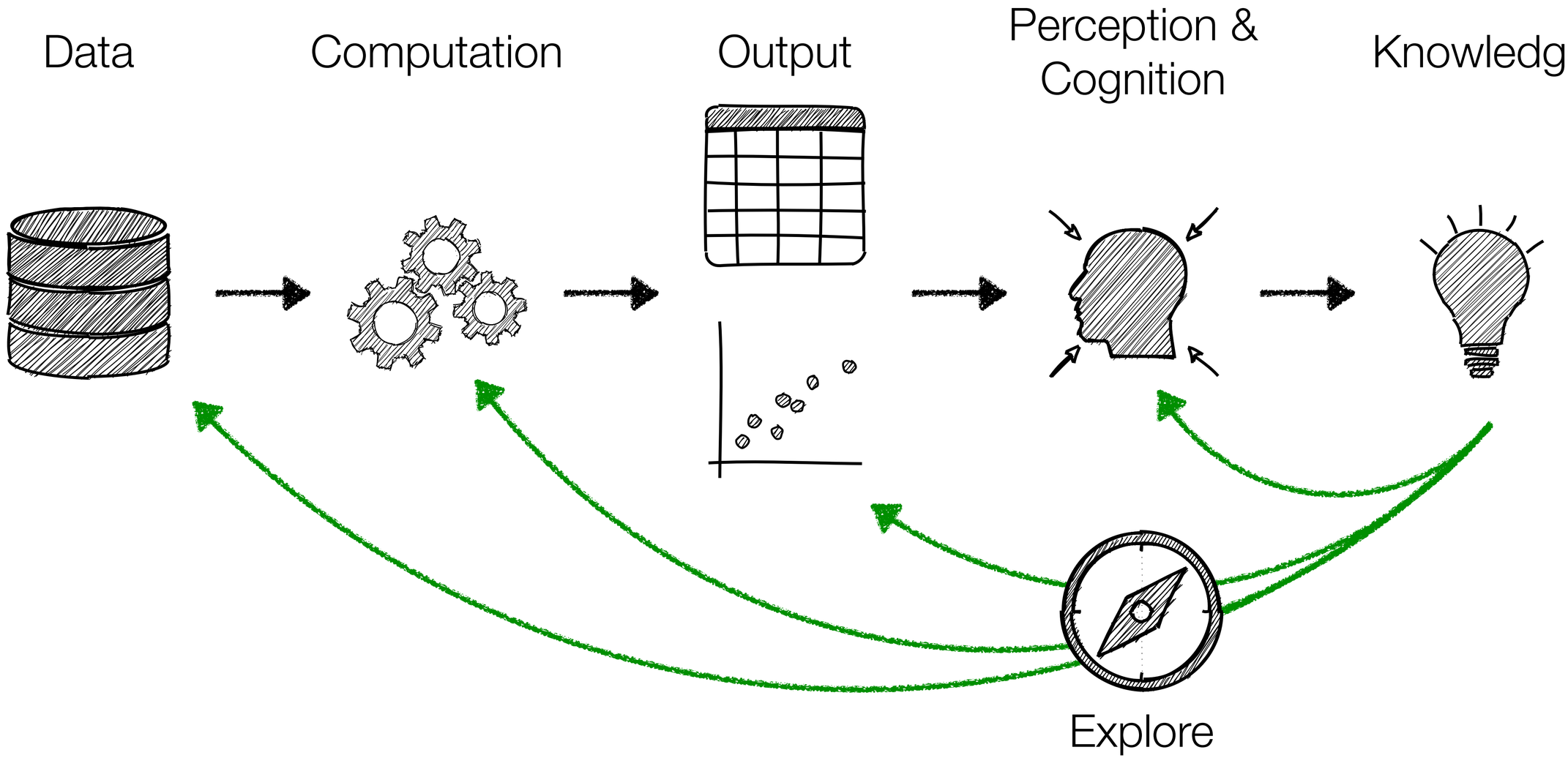
Data Analysis



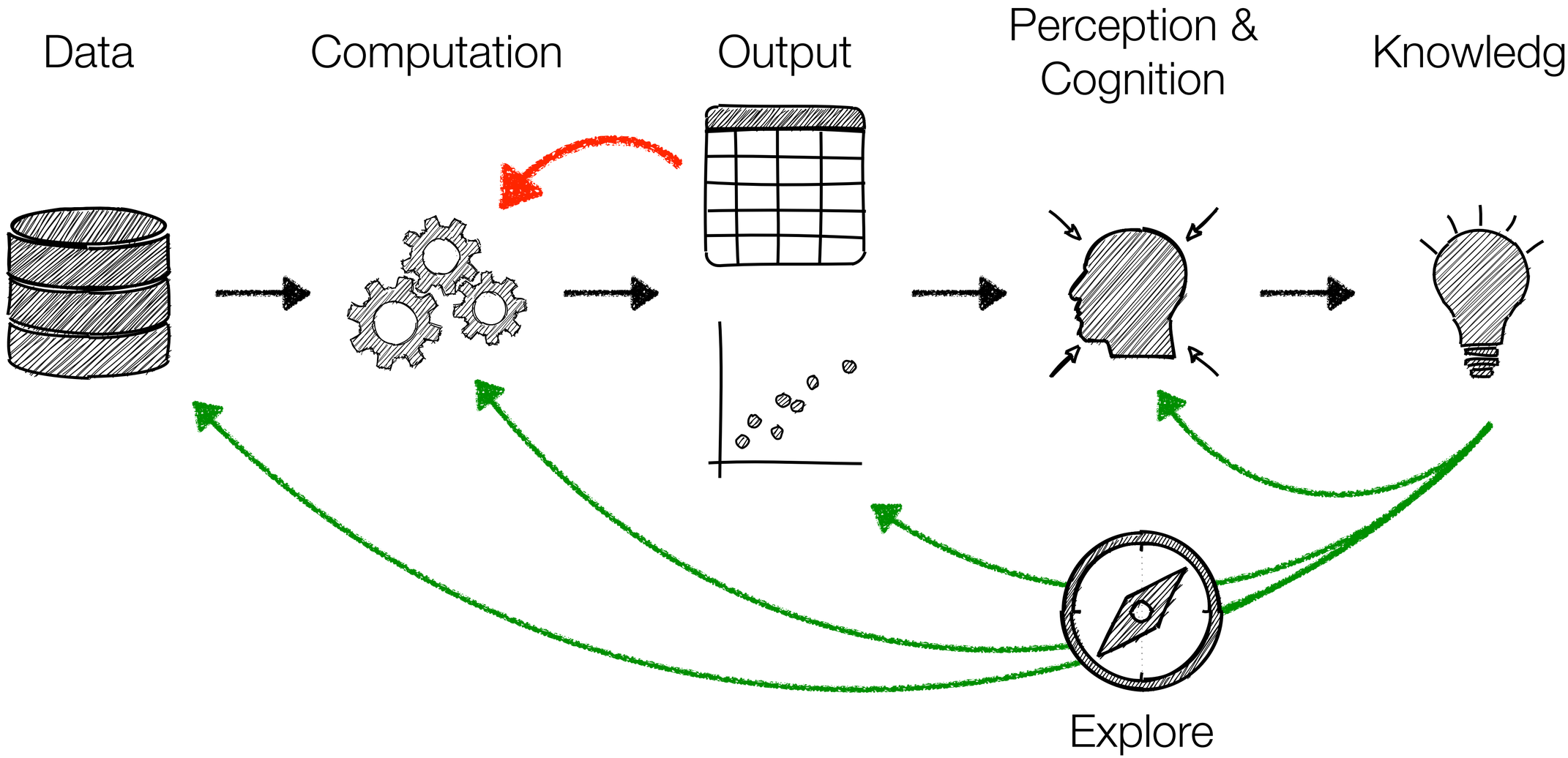
Data Analysis



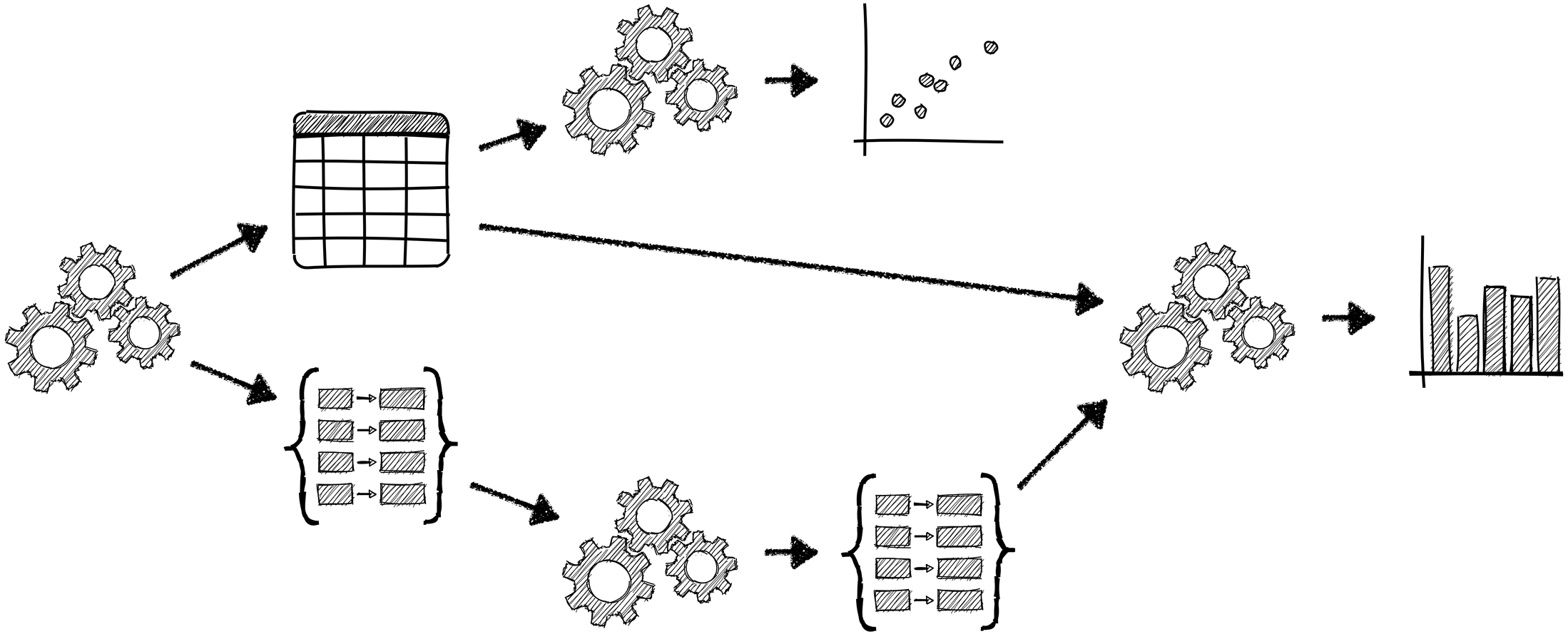
Data Analysis



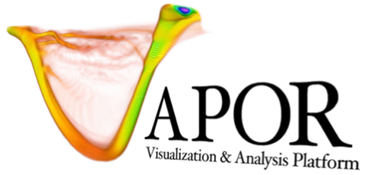
Data Analysis



Outputs Often Become Inputs



Visualization Landscape

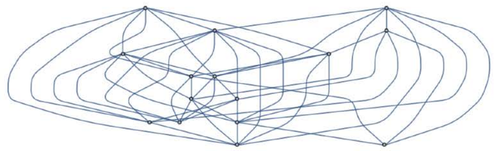
- Apps: ParaView VisIt
- Domain-Specific Apps: VMD 

- APIs: VTK, ITK
- Also… **Data Analysis Tools/Libraries**
  - JavaScript: D3, Observable Plot
  - R: ggplot
  - Python: matplotlib, altair, bokeh, …
  - Matlab
  - GNUPlot

Different Types of Notebooks, Many Similarities

```
In[1]:= RandomGraph[{15, 50}, GraphLayout → "LayeredDigraphEmbedding"]
```

Out[1]=



```
In[2]:= EigenVectorCentrality[%]

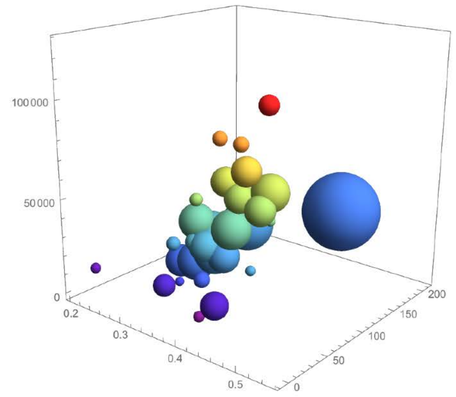
Out[2]= {0.0733294, 0.0670173, 0.0911388, 0.084084, 0.0408522, 0.058568, 0.0694066, 0.0697708,
  0.0586817, 0.0732617, 0.0785323, 0.060912, 0.0370771, 0.0646014, 0.0727667}

In[3]:= cities = GeoNearest["City", San Jose CITY, 30]

Out[3]= {Cupertino, Saratoga, Los Gatos, Milpitas, Sunol-Midtown, East Foothills,
  Campbell, Cambrian Park, Fremont, Morgan Hill, Seven Trees, Buena Vista,
  Santa Clara, Sunnyvale, Alum Rock, Burbank, Fruitdale, San Jose,
  Newark, Monte Sereno, Mountain View, Palo Alto, Los Altos, Menlo Park,
  Loyola, San Martin, East Palo Alto, Lexington Hills, Los Altos Hills, Sunol}

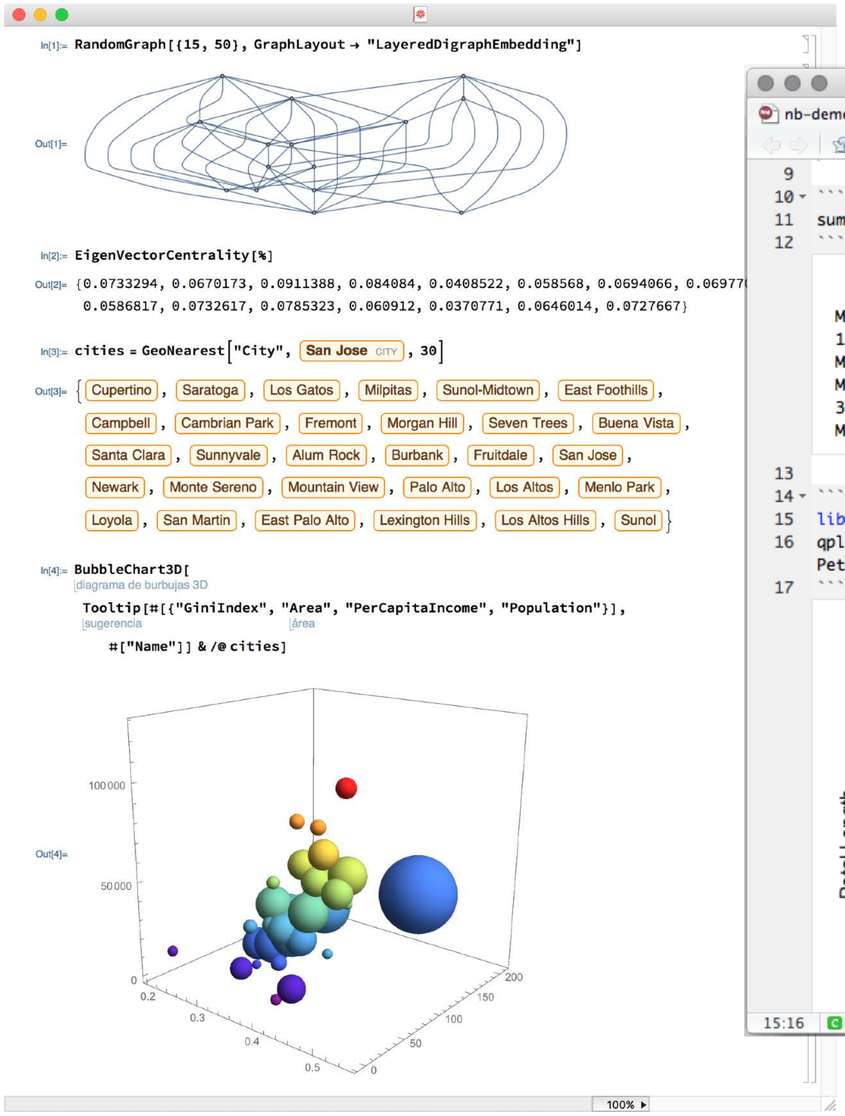
In[4]:= BubbleChart3D[
        diagrama de burbujas 3D
  Tooltip[#[{"GiniIndex", "Area", "PerCapitaIncome", "Population"}],
        sugerencia          área
    #["Name"]] & /@ cities]
```

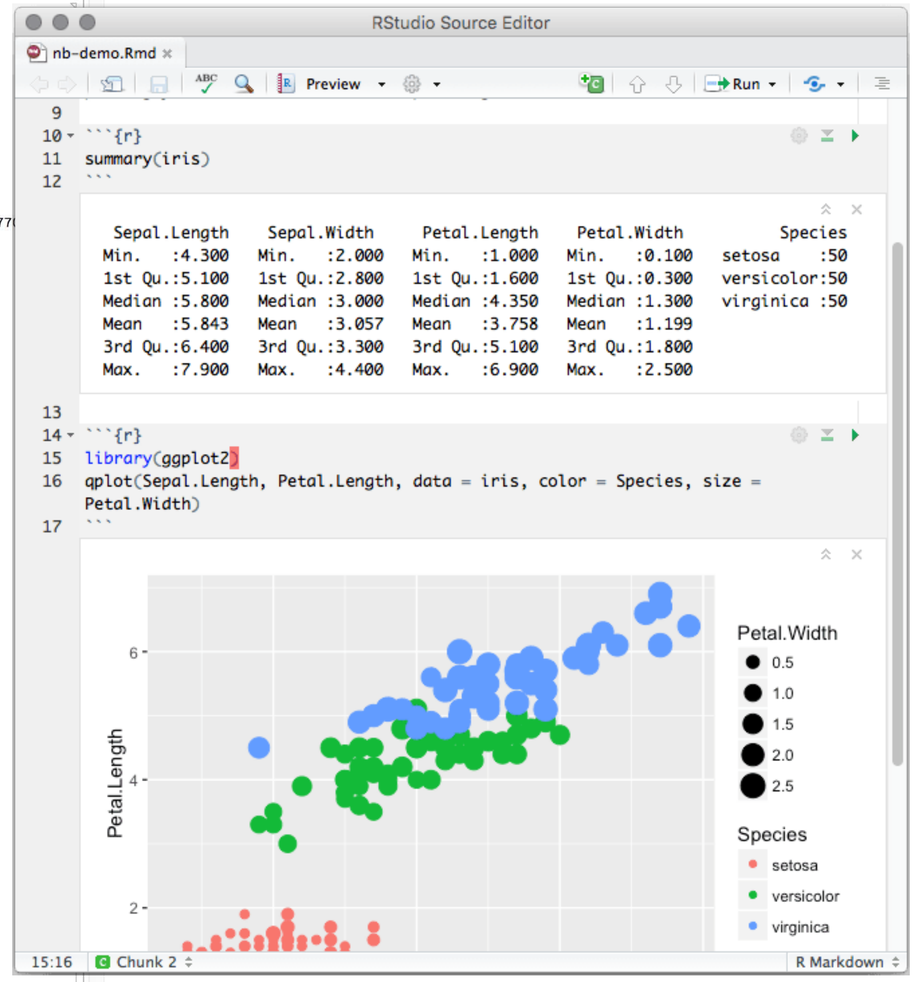
Out[4]=



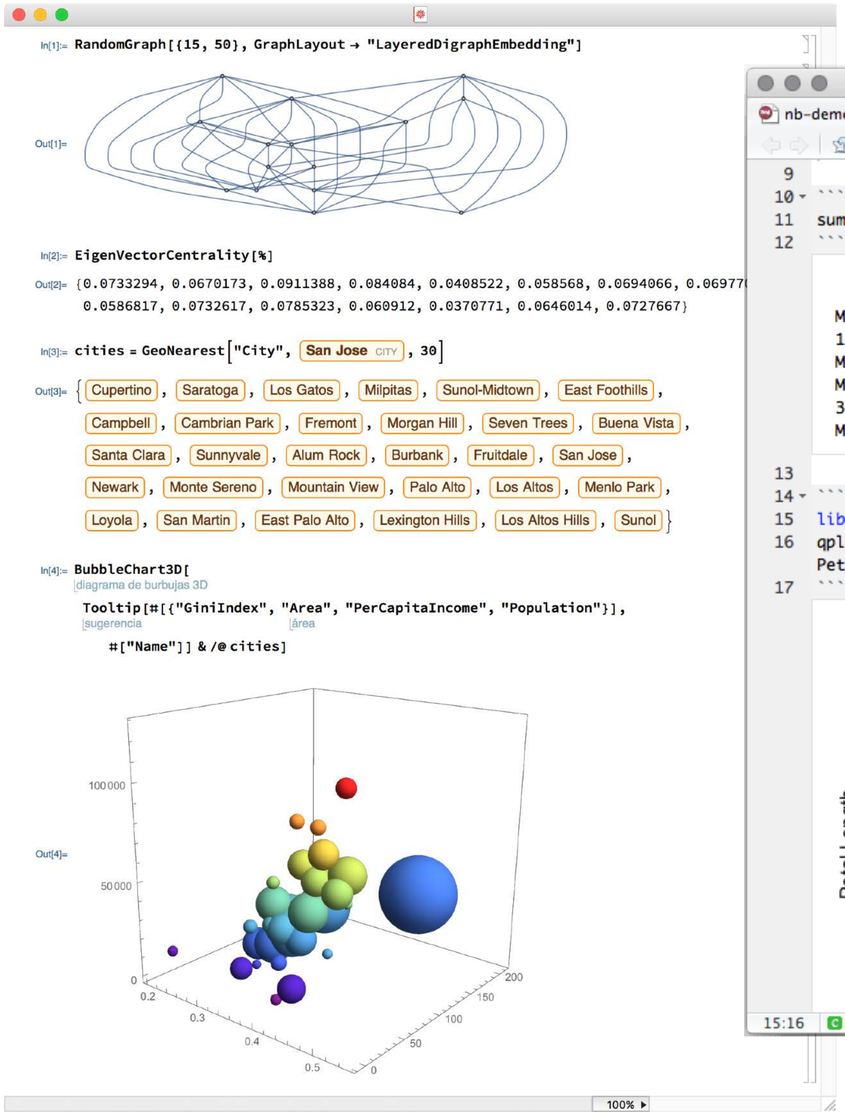
100% ▸

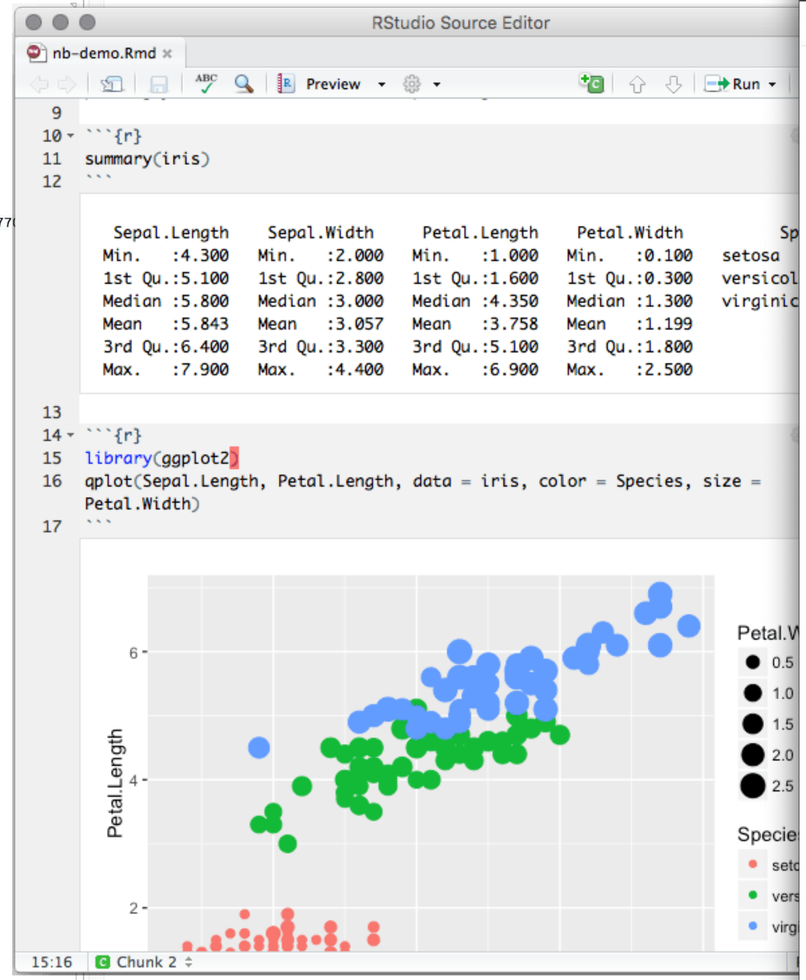
Different Types of Notebooks, Many Similarities

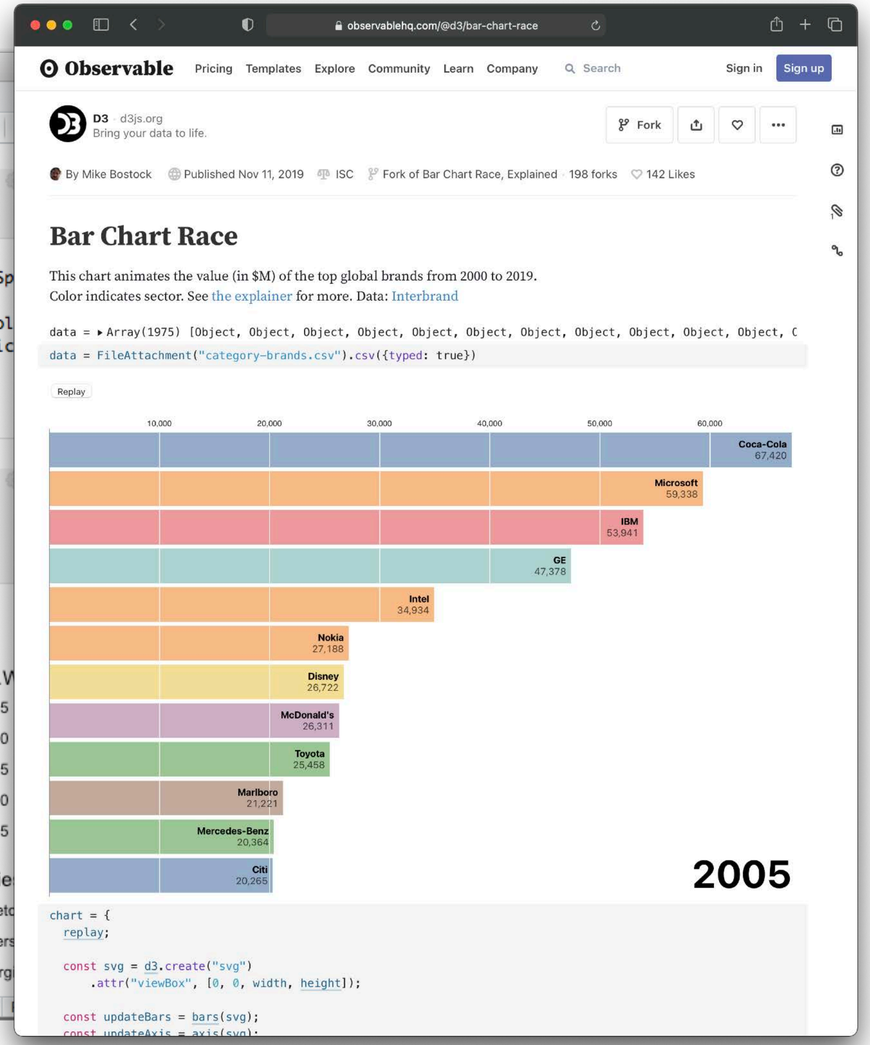




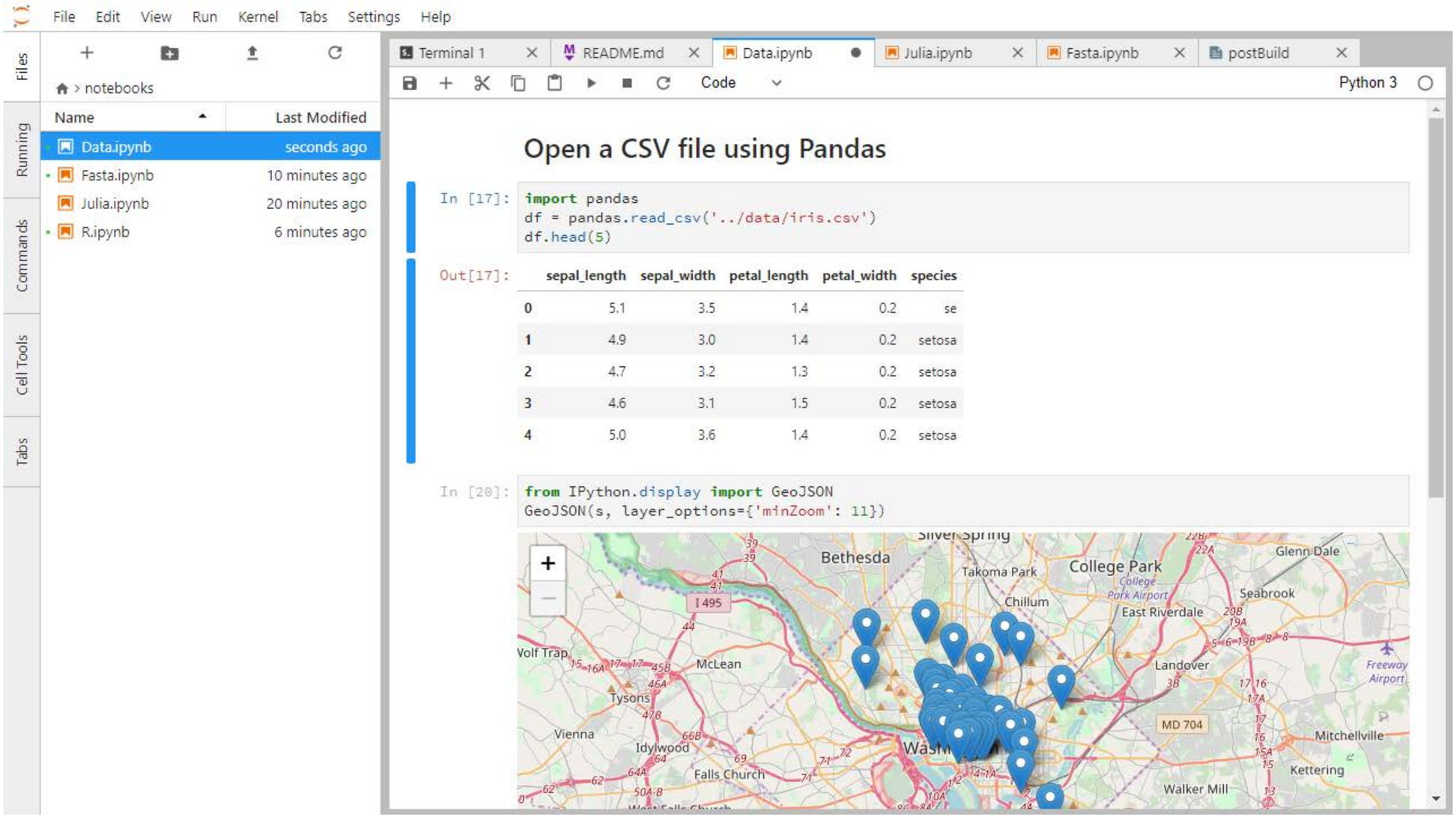
Different Types of Notebooks, Many Similarities







Focus on Jupyter Notebooks



File Edit View Run Kernel Tabs Settings Help

Lorenz.ipynb

Code

Python 3

The Lorenz Differential Equations

Before we start, we import some preliminary libraries. We will also import (below) the accompanying `lorenz.py` file, which contains the actual solver and plotting routine.

[1]:
```
%matplotlib inline
from ipywidgets import interactive, fixed
```

We explore the Lorenz system of differential equations:

$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = \rho x - y - xz$$
$$\dot{z} = -\beta z + xy$$

Let's change (σ, β, ρ) with ipywidgets and examine the trajectories.

[2]:
```
from lorenz import solve_lorenz
w=interactive(solve_lorenz,sigma=(0.0,50.0),rho=(0.0,50.0))
w
```

sigma 10.00

beta 2.67

0 $_ 1 Python 3 | Idle Saving completed Mode: Command Ln 1, Col 1 Lorenz.ipynb

File Edit View Run Kernel Tabs Settings Help

Lorenz.ipynb

Code

Python 3

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w
```

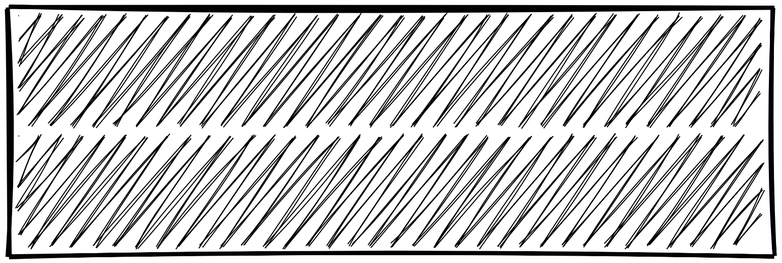
sigma 10.00

beta 2.67

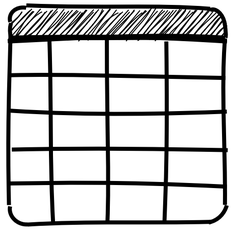
0 $_ 1 Python 3 | Idle Saving completed Mode: Command Ln 1, Col 1 Lorenz.ipynb

Notebooks Are Great for Exploration

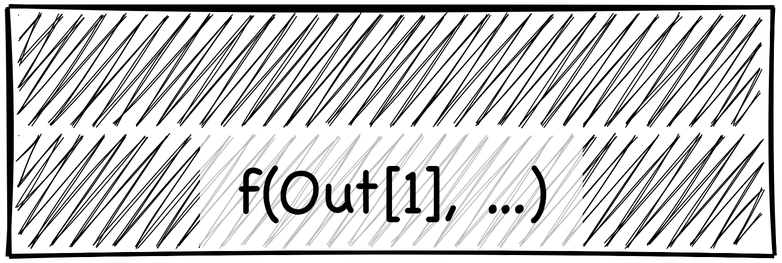
In[1]:



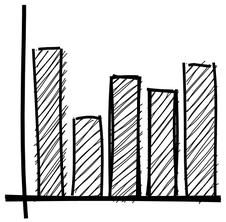
Out[1]:



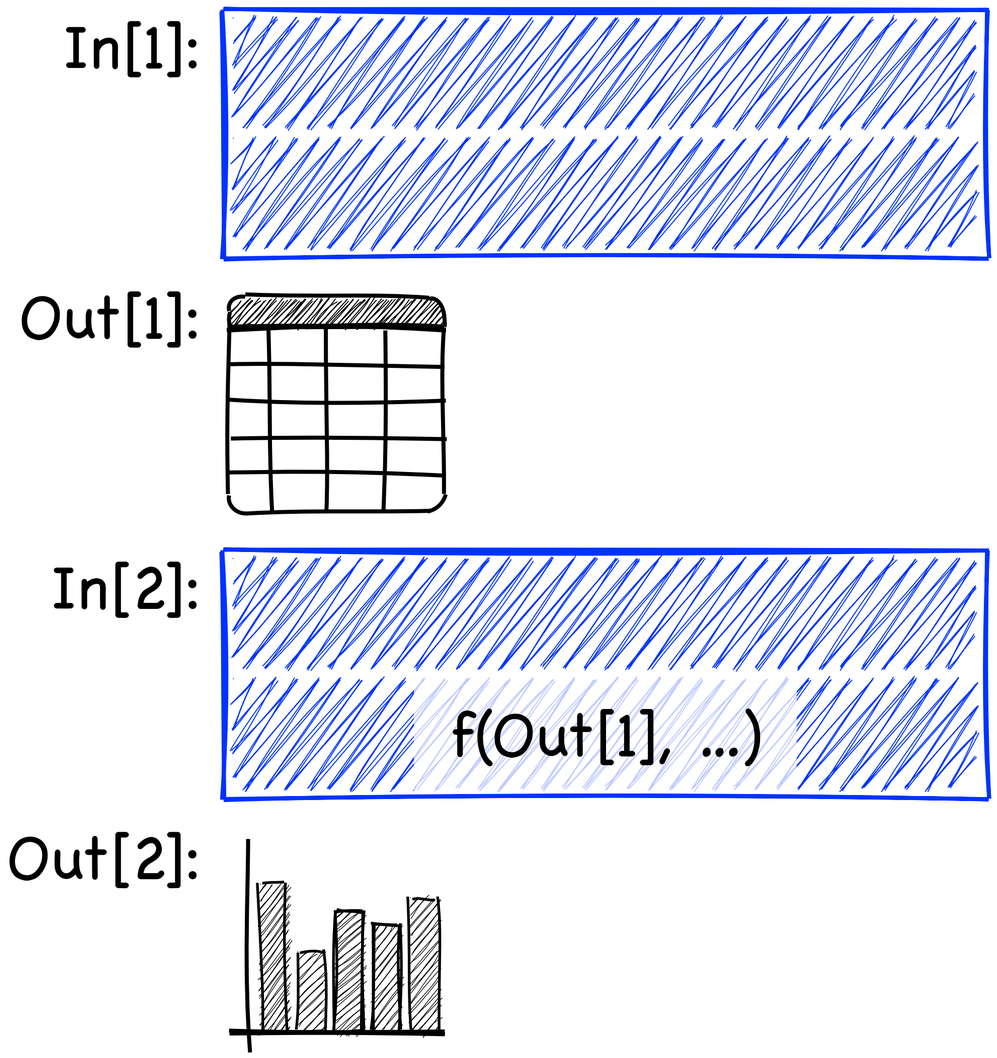
In[2]:



Out[2]:

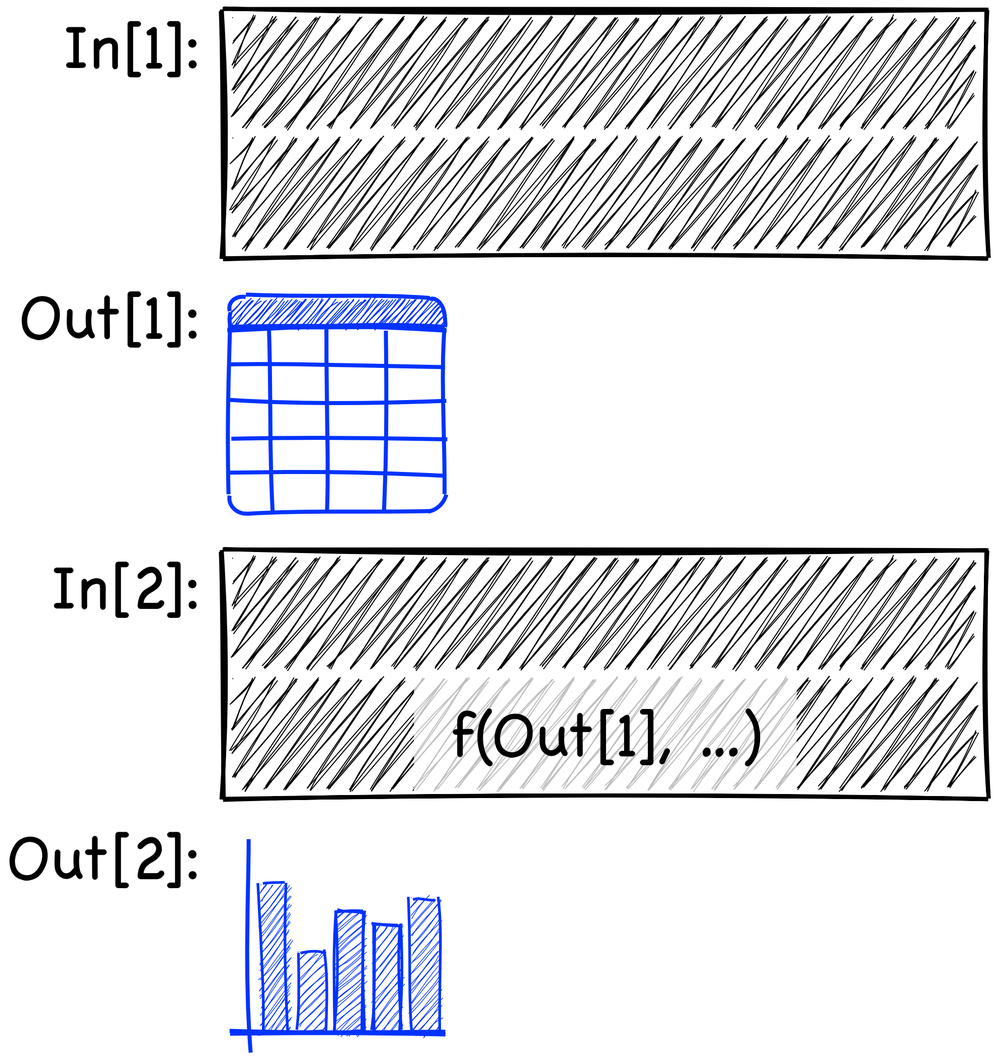


Notebooks Are Great for Exploration



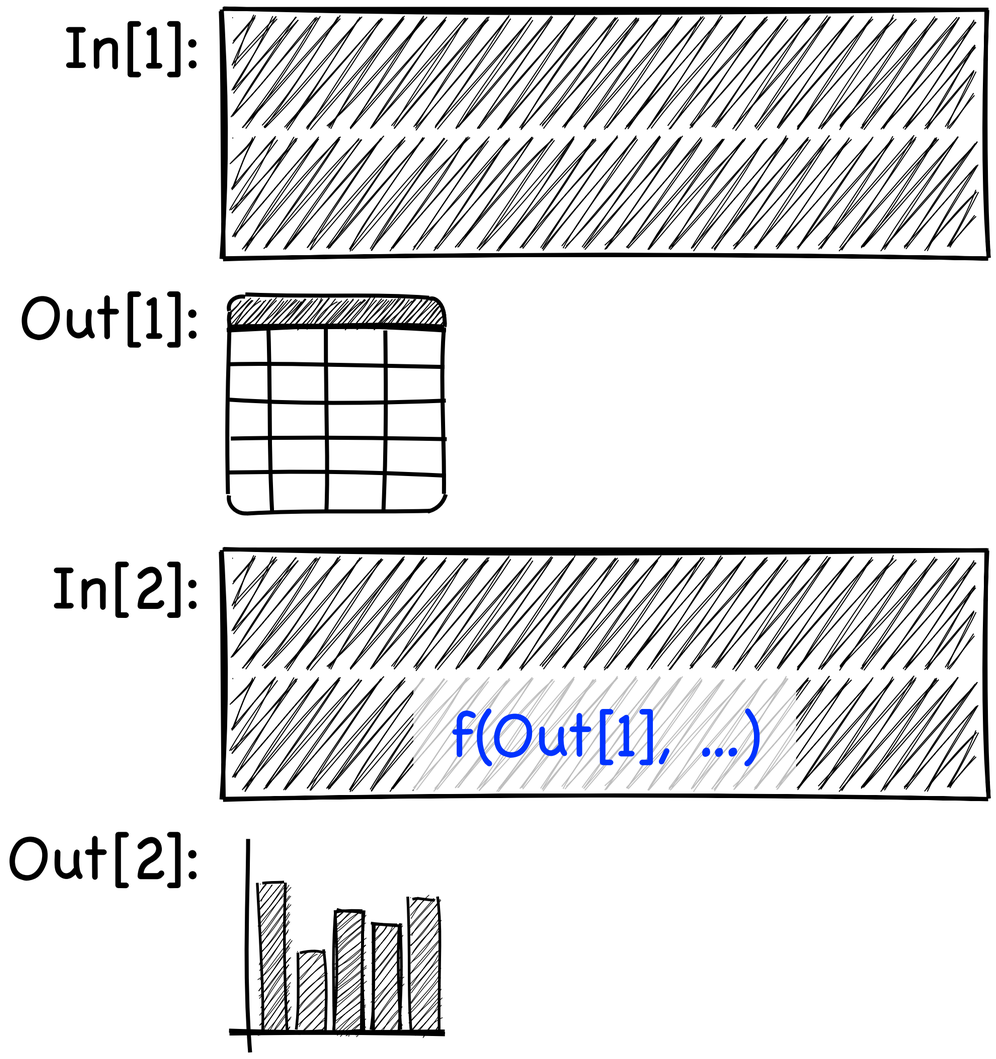
- Digestible Blocks of Code

Notebooks Are Great for Exploration



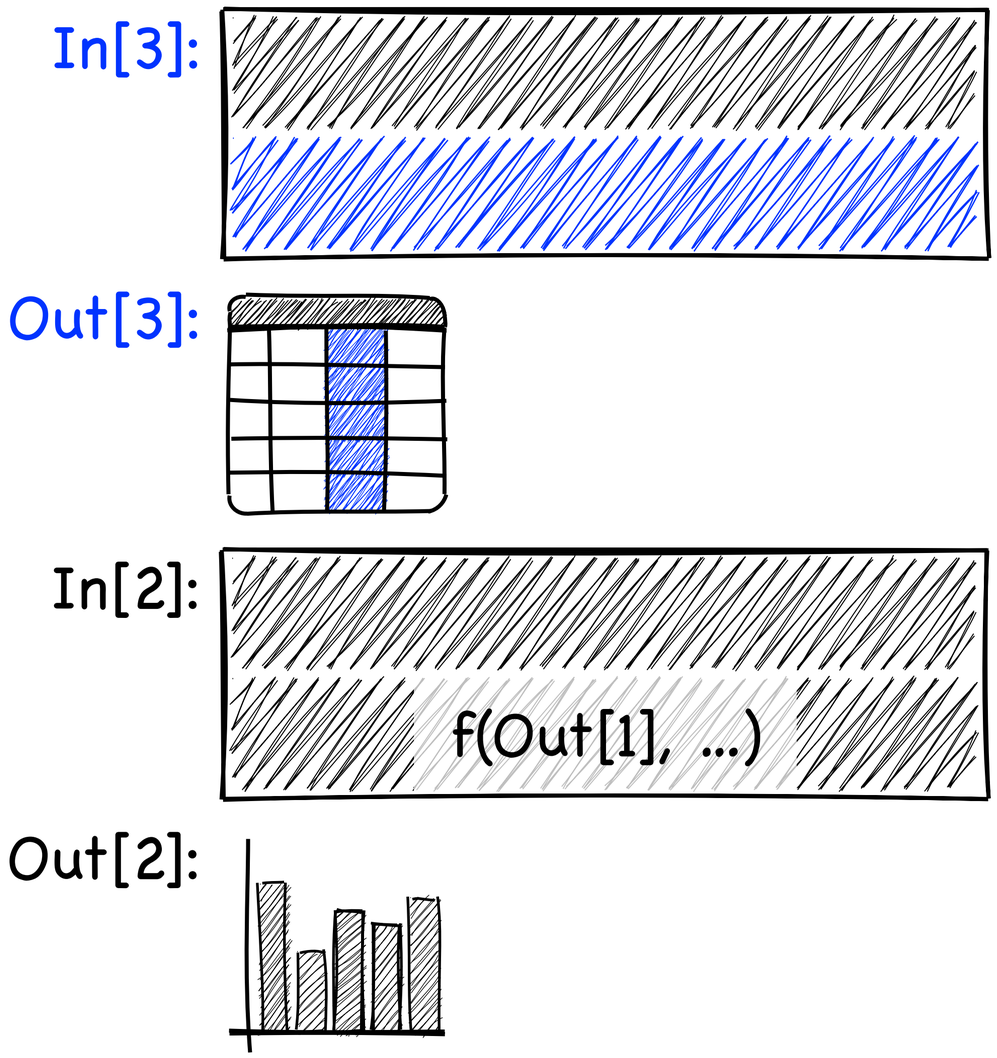
- Digestible Blocks of Code
- Rich, Inline Outputs (inc. widgets)

Notebooks Are Great for Exploration



- Digestible Blocks of Code
- Rich, Inline Outputs (inc. widgets)
- Reuse Existing Outputs

Notebooks Are Great for Exploration



- Digestible Blocks of Code
- Rich, Inline Outputs (inc. widgets)
- Reuse Existing Outputs
- Non-linear editing

Support for Rapid Exploration

- Flexible environment
  - Edit any cell whenever you want
  - Execute whichever cells you want
- Inline views of outputs
  - No context switch
  - Easily compare and trace outputs
- Explore data in situ
  - Notebooks run in browser
  - Kernels can run remotely

Notebooks Are Great for Explanation

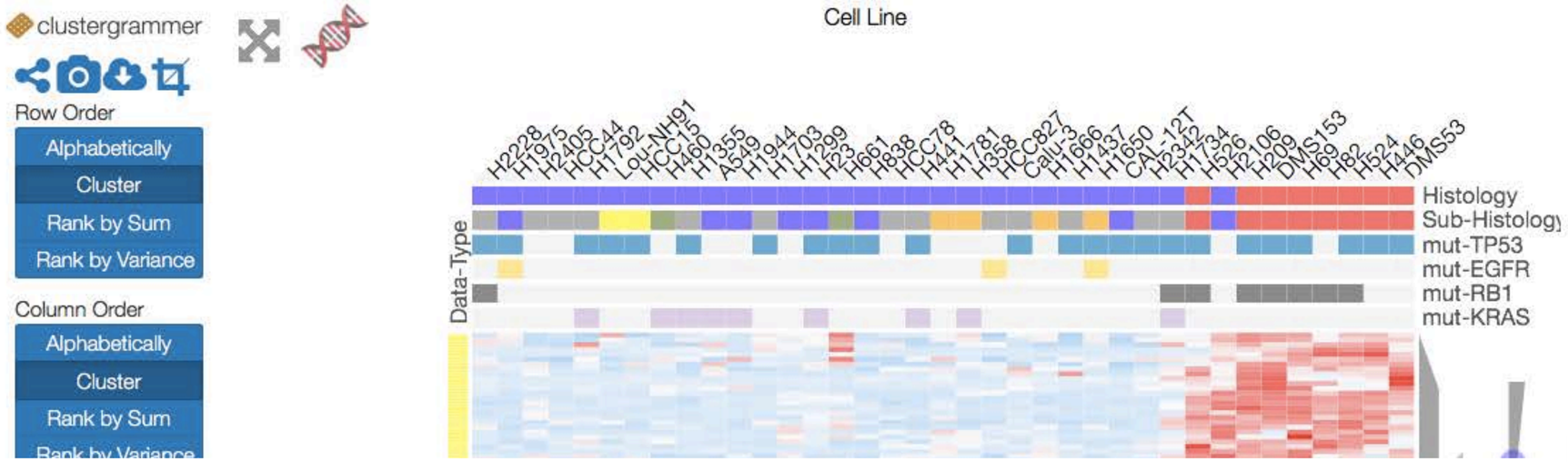
Gene Expression Data

We obtained gene expression data from the Cancer Cell Line Encyclopedia (CCLE) for 37 lung cancer cell lines assayed by our collaborators at CST. This independent dataset can be used to find novel correlations between differentially expressed genes and PTMs as well as determine whether lung cancer cell lines behave similarly in gene-expression-space and PTM-space. The gene expression data was processed in the CST_Data_Processing.ipynb notebook that: kept the top 1000 genes with the greatest variance across the cell lines, and Z-score normalized the genes across the cell lines to highlight differential expression across the lung cancer cell lines.

In [4]:
```
net.load_file('../lung_cellline_3_1_16/lung_cl_all_ptm/precalc_processed/CST_CCLE_exp.txt')
print('Expression data shape: ' + str(net.dat['mat'].shape))
```

```
Expression data shape: (1000, 37)
```

In [5]:
```
net.set_cat_color('row', 1, 'Data-Type: Exp', 'yellow')
net.cluster(views=[])
net.widget()
```



[N. Fernandez et al.]

Support for Clear Explanation

- Textual explanation: markdown cells
- Graphical explanation: inline figures
- Interactive explanation: widgets
- Publishing: Web pages, LaTeX, etc.
- Structure: clear, linear cell layout
- Reproducible

Exemplar Notebook

[1]:
```
import pandas as pd
```

[2]:
```
df.read_csv('penguins_size.csv')
```

[2]:

	species	island	culmen_length_mm	...	body_mass_g	sex
0	Chinstrap	Dream	50.9	...	3550.0	MALE
1	Gentoo	Biscoe	47.3	...	4725.0	NaN
...	...	...	...	...	...	...
342	Adelie	Torgersen	NaN	...	NaN	NaN
343	Chinstrap	Dream	47.0	...	3700.0	FEMALE

[3]:
```
df = df.dropna(subset=['culmen_length_mm', 'culmen_depth_mm',
                       'flipper_length_mm', 'body_mass_g'])
```

[3]:

	species	island	culmen_length_mm	...	body_mass_g	sex
0	Chinstrap	Dream	50.9	...	3550.0	MALE
1	Gentoo	Biscoe	47.3	...	4725.0	NaN
...	...	...	...	...	...	...
341	Gentoo	Biscoe	49.9	...	5400.0	MALE
343	Chinstrap	Dream	47.0	...	3700.0	FEMALE

[4]:
```
df.columns
```

[4]:
```
Index(['species', 'island', 'culmen_length_mm', 'culmen_depth_mm',
       'flipper_length_mm', 'body_mass_g', 'sex'],
      dtype='object')
```

[5]:
```
df = df.rename(columns={'culmen_length_mm': 'culmen length (mm)',
                        'body_mass_g': 'body mass (g)'})
```

[5]:

	species	island	culmen length (mm)	...	body mass (g)	sex
0	Chinstrap	Dream	50.9	...	3550.0	MALE
1	Gentoo	Biscoe	47.3	...	4725.0	NaN
...	...	...	...	...	...	...
341	Gentoo	Biscoe	49.9	...	5400.0	MALE
343	Chinstrap	Dream	47.0	...	3700.0	FEMALE

[6]:
```
df['body mass (g)'].max()
```

[6]:
```
6300.0
```

[7]:
```
df.groupby('island')['body mass (g)'].median()
```

[7]:
```
island
Biscoe       4775.0
Dream        3687.5
Torgersen    3700.0
Name: body mass (g), dtype: float64
```

Exemplar Notebook

```
[1]: import pandas as pd
```

```
[2]: df.read_csv('penguins_size.csv')
```

[2]:

	species	island	culmen_length_mm	...	body_mass_g	sex
0	Chinstrap	Dream	50.9	...	3550.0	MALE
1	Ge				0	NaN
...	...	...	...	...	...	...
342	Adelie	Torgersen	NaN	...	NaN	NaN
343	Chinstrap	Dream	47.0	...	3700.0	FEMALE

Linear Cell Numbering

```
[3]: df = df.dropna(subset=['culmen_length_mm', 'culmen_depth_mm',
                            'flipper_length_mm', 'body_mass_g'])
```

[3]:

	species	island	culmen_length_mm	...	body_mass_g	sex
0	Chinstrap	Dream	50.9	...	3550.0	MALE
1	Gentoo	Biscoe	47.3	...	4725.0	NaN
...	...	...	...	...	...	...
341	Gentoo	Biscoe	49.9	...	5400.0	MALE
343	Chinstrap	Dream	47.0	...	3700.0	FEMALE

```
[4]: df.columns
```

```
[4]: Index(['species', 'island', 'culmen_length_mm', 'culmen_depth_mm',
       'flipper_length_mm', 'body_mass_g', 'sex'],
      dtype='object')
```

```
[5]: df = df.rename(columns={'culmen_length_mm': 'culmen length (mm)',
                            'body_mass_g': 'body mass (g)'})
```

[5]:

	species	island	culmen length (mm)	...	body mass (g)	sex
0	Chinstrap	Dream	50.9	...	3550.0	MALE
1	Gentoo	Biscoe	47.3	...	4725.0	NaN
...	...	...	...	...	...	...
341	Gentoo	Biscoe	49.9	...	5400.0	MALE
343	Chinstrap	Dream	47.0	...	3700.0	FEMALE

```
[6]: df['body mass (g)'].max()
```

```
[6]: 6300.0
```

```
[7]: df.groupby('island')['body mass (g)'].median()
```

```
[7]: island
Biscoe       4775.0
Dream        3687.5
Torgersen    3700.0
Name: body mass (g), dtype: float64
```

Exemplar Notebook

[1]:
```
import pandas as pd
```

[2]:
```
df.read_csv('penguins_size.csv')
```

[2]:

	species	island	culmen_length_mm	...	body_mass_g	sex
0	Chinstrap	Dream	50.9	...	3550.0	MALE
1	Ge				0	NaN
...	...	...	...	...	...	...
342	Adelie	Torgersen	NaN	...	NaN	NaN
343	Chinstrap	Dream	47.0	...	3700.0	FEMALE

Linear Cell Numbering

[3]:
```
df = df.dropna(subset=['culmen_length_mm', 'culmen_depth_mm',
                       'flipper_length_mm', 'body_mass_g'])
```

[3]:

	species	island	culmen_length_mm	...	body_mass_g	sex
0	Chinstrap	Dream	50.9	...	3550.0	MALE
1	Gentoo	Biscoe	47.3	...	4725.0	NaN
...	...	...	...	...	...	...
341	Gentoo	Biscoe	49.9	...	5400.0	MALE
343	Chinstrap	Dream	47.0	...	3700.0	FEMALE

[4]:
```
df.columns
```

[4]:
```
Index(['species', 'island', 'culmen_length_mm', 'culmen_depth_mm',
       'flipper_length_mm', 'body_mass_g', 'sex'],
      dtype='object')
```

[5]:
```
df = df.rename(columns={'culmen_length_mm': 'culmen length (mm)',
                        'body_mass_g': 'body mass (g)'})
```

Code Runs Correctly
in Top-to-Bottom Order

[5]:

						sex
0	C				0	MALE
1	Gentoo	Biscoe	47.3	...	4725.0	NaN
...	...	...	...	...	...	...
341	Gentoo	Biscoe	49.9	...	5400.0	MALE
343	Chinstrap	Dream	47.0	...	3700.0	FEMALE

[6]:
```
df['body mass (g)'].max()
```

[6]:
```
6300.0
```

[7]:
```
df.groupby('island')['body mass (g)'].median()
```

[7]:
```
island
Biscoe       4775.0
Dream        3687.5
Torgersen    3700.0
Name: body mass (g), dtype: float64
```

Confusing Notebook

[1]:
```
import pandas as pd
```

[5]:
```
df = pd.read_csv('penguins_lter.csv')
```

[5]:

	study name	sample number	species	...	culmen length (mm)	body mass (g)
0	PAL0708	1	Adelie	...	39.1	3750.0
1	PAL0708	1	Gentoo	...	46.1	4500.0
...	...	...	...	...	...	...
342	PAL0910	151	Adelie	...	36.0	3700.0
343	PAL0910	152	Adelie	...	41.5	4000.0

[6]:
```
df = df.dropna(subset=['culmen_length_mm', 'culmen_depth_mm',
                       'flipper_length_mm', 'body_mass_g'])
```

```
---------------------------------------------------------------------------
KeyError                                  Traceback (most recent call last)
Input In [6], in <cell line: 1>()
----> 1 df = df.dropna(subset=['culmen_length_mm', 'culmen_depth_mm',
      2                       'flipper_length_mm', 'body_mass_g'])

KeyError: ['culmen_length_mm', 'culmen_depth_mm', 'flipper_length_mm',
           'body_mass_g']
```

[7]:
```
df.columns
```

[7]:
```
Index(['study name', 'sample number', 'species', 'region', ...,
       'flipper length (mm)', 'culmen length (mm)', 'body mass (g)'],
      dtype='object')
```

[5]:
```
df = df.rename(columns={'culmen_length_mm': 'culmen length (mm)',
                        'body_mass_g': 'body mass (g)'})
```

[5]:

	species	island	culmen length (mm)	...	body mass (g)	sex
0	Chinstrap	Dream	50.9	...	3550.0	MALE
1	Gentoo	Biscoe	47.3	...	4725.0	NaN
...	...	...	...	...	...	...
341	Gentoo	Biscoe	49.9	...	5400.0	MALE
343	Chinstrap	Dream	47.0	...	3700.0	FEMALE

[8]:
```
df['body mass (g)'].max()
```

[8]:
```
6300.0
```

[10]:
```
df.groupby('study name')['body mass (g)'].median()
```

[10]:
```
study name
PAL0708    3900.0
PAL0809    4200.0
PAL0910    4000.0
Name: body mass (g), dtype: float64
```

Confusing Notebook

[1]:
```
impor
```

Missing Cell Numbers [2,3,4]

[5]:
```
df = pd.read_csv('penguins_lter.csv')
```

[5]:

	study name	sample number	species	...	culmen length (mm)	body mass (g)
0	PAL0708	1	Adelie	...	39.1	3750.0
1	PAL0708	1	Gentoo	...	46.1	4500.0
...	...	...	...	...	...	...
342	PAL0910	151	Adelie	...	36.0	3700.0
343	PAL0910	152	Adelie	...	41.5	4000.0

[6]:
```
df = df.dropna(subset=['culmen_length_mm', 'culmen_depth_mm',
                       'flipper_length_mm', 'body_mass_g'])
```

```
---------------------------------------------------------------------------
KeyError                                  Traceback (most recent call last)
Input In [6], in <cell line: 1>()
----> 1 df = df.dropna(subset=['culmen_length_mm', 'culmen_depth_mm',
      2                       'flipper_length_mm', 'body_mass_g'])

KeyError: ['culmen_length_mm', 'culmen_depth_mm', 'flipper_length_mm',
           'body_mass_g']
```

[7]:
```
df.columns
```

[7]:
```
Index(['study name', 'sample number', 'species', 'region', ...,
       'flipper length (mm)', 'culmen length (mm)', 'body mass (g)'],
      dtype='object')
```

[5]:
```
df = df.rename(columns={'culmen_length_mm': 'culmen length (mm)',
                        'body_mass_g': 'body mass (g)'})
```

[5]:

	species	island	culmen length (mm)	...	body mass (g)	sex
0	Chinstrap	Dream	50.9	...	3550.0	MALE
1	Gentoo	Biscoe	47.3	...	4725.0	NaN
...	...	...	...	...	...	...
341	Gentoo	Biscoe	49.9	...	5400.0	MALE
343	Chinstrap	Dream	47.0	...	3700.0	FEMALE

[8]:
```
df['body mass (g)'].max()
```

[8]:
```
6300.0
```

[10]:
```
df.groupby('study name')['body mass (g)'].median()
```

[10]:
```
study name
PAL0708    3900.0
PAL0809    4200.0
PAL0910    4000.0
Name: body mass (g), dtype: float64
```

Confusing Notebook

```
[1]: import pandas as pd
```

```
[5]: df = pd.read_csv('penguins_lter.csv')
```

Same Cell Number

[5]:

	study name	sample number	species	...	(mm)	(g)
0	PAL0708	1	Adelie	...	39.1	3750.0
1	PAL0708	1	Gentoo	...	46.1	4500.0
...	...	...	...	...	...	...
342	PAL0910	151	Adelie	...	36.0	3700.0
343	PAL0910	152	Adelie	...	41.5	4000.0

```
[6]: df = df.dropna(subset=['culmen_length_mm', 'culmen_depth_mm',
                            'flipper_length_mm', 'body_mass_g'])
```

```
---------------------------------------------------------------------------
KeyError                                  Traceback (most recent call last)
Input In [6], in <cell line: 1>()
----> 1 df = df.dropna(subset=['culmen_length_mm', 'culmen_depth_mm',
      2                        'flipper_length_mm', 'body_mass_g'])

KeyError: ['culmen_length_mm', 'culmen_depth_mm', 'flipper_length_mm',
           'body_mass_g']
```

```
[7]: df.columns
```

```
[7]: Index(['study name', 'sample number', 'species', 'region', ...,
            'flipper length (mm)', 'culmen length (mm)', 'body mass (g)'],
           dtype='object')
```

```
[5]: df = df.rename(columns={'culmen_length_mm': 'culmen length (mm)',
                            'body_mass_g': 'body mass (g)'})
```

[5]:

	species	island	culmen length (mm)	...	body mass (g)	sex
0	Chinstrap	Dream	50.9	...	3550.0	MALE
1	Gentoo	Biscoe	47.3	...	4725.0	NaN
...	...	...	...	...	...	...
341	Gentoo	Biscoe	49.9	...	5400.0	MALE
343	Chinstrap	Dream	47.0	...	3700.0	FEMALE

```
[8]: df['body mass (g)'].max()
```

```
[8]: 6300.0
```

```
[10]: df.groupby('study name')['body mass (g)'].median()
```

```
[10]: study name
      PAL0708    3900.0
      PAL0809    4200.0
      PAL0910    4000.0
      Name: body mass (g), dtype: float64
```

Confusing Notebook

```
[1]: import pandas as pd
```

```
[5]: df = pd.read_csv('penguins_lter.csv')
```

[5]:

	study name	sample number	species	...	culmen length (mm)	body mass (g)
0	PAL0708	1	Adelie	...	39.1	3750.0
1	PAL0708	1	Gentoo	...	46.1	4500.0
...	...	...	...	...	...	...
342	PAL0910	151	Adelie	...	36.0	3700.0
343	PAL0910	152	Adelie	...	41.5	4000.0

```
[6]: df = df.dropna(subset=['culmen_length_mm', 'culmen_depth_mm',
                            'flipper_length_mm', 'body_mass_g'])
```

```
---------------------------------------------------------------------------
KeyError                                  Traceback (most recent call last)
Input In [6], in <cell line: 1>()
----> 1 df = df.dropna(subset=['culmen_length_mm', 'culmen_depth_mm',
      2                       'flipper_length_mm', 'body_mass_g'])

KeyError: ['culmen_length_mm', 'culmen_depth_mm', 'flipper_length_mm',
           'body_mass_g']
```

```
[7]: df.columns
```

```
[7]: Index(['study name', 'sample number', 'species', 'region', ...,
                                                    'body mass (g)'],
```

Out of Order Cell Numbers

```
[5]: df = df.rename(columns={'culmen_length_mm': 'culmen length (mm)',
                            'body_mass_g': 'body mass (g)'})
```

[5]

	species	island	culmen length (mm)	...	body mass (g)	sex
0	Chinstrap	Dream	50.9	...	3550.0	MALE
1	Gentoo	Biscoe	47.3	...	4725.0	NaN
...	...	...	...	...	...	...
341	Gentoo	Biscoe	49.9	...	5400.0	MALE
343	Chinstrap	Dream	47.0	...	3700.0	FEMALE

```
[8]: df['body mass (g)'].max()
```

```
[8]: 6300.0
```

```
[10]: df.groupby('study name')['body mass (g)'].median()
```

```
[10]: study name
      PAL0708    3900.0
      PAL0809    4200.0
      PAL0910    4000.0
      Name: body mass (g), dtype: float64
```

Confusing Notebook

```
[1]: import pandas as pd
```

```
[5]: df = pd.read_csv('penguins_lter.csv')
```

[5]:

	study name	sample number	species	...	culmen length (mm)	body mass (g)
0	PAL0708	1	Adelie	...	39.1	3750.0
1	PAL0708	1	Gentoo	...	46.1	4500.0
...	...	...	...	...	...	...
342	PAL0910	151	Adelie	...	36.0	3700.0
343	PAL0910	152	Adelie	...	41.5	4000.0

```
[6]: df = df.dropna(subset=['culmen_length_mm', 'culmen_depth_mm',
                            'flipper_length_mm', 'body_mass_g'])
```

```
---------------------------------------------------------------------------
KeyError                                  Traceback (most recent call last)
Input In [6], in <cell line: 1>()
----> 1 df = df.dropna(subset=['culmen_length_mm', 'culmen_depth_mm',
      2                       'flipper_length_mm', 'body_mass_g'])

KeyError: ['culmen_length_mm', 'culmen_depth_mm', 'flipper_length_mm',
           'body_mass_g']
```

Why is this an error?

```
[7]: df.columns
```

```
[7]: Index(['study name', 'sample number', 'species', 'region', ...,
            'flipper length (mm)', 'culmen length (mm)', 'body mass (g)'],
           dtype='object')
```

```
[5]: df = df.rename(columns={'culmen_length_mm': 'culmen length (mm)',
                            'body_mass_g': 'body mass (g)'})
```

[5]:

	species	island	culmen length (mm)	...	body mass (g)	sex
0	Chinstrap	Dream	50.9	...	3550.0	MALE
1	Gentoo	Biscoe	47.3	...	4725.0	NaN
...	...	...	...	...	...	...
341	Gentoo	Biscoe	49.9	...	5400.0	MALE
343	Chinstrap	Dream	47.0	...	3700.0	FEMALE

```
[8]: df['body mass (g)'].max()
```

```
[8]: 6300.0
```

```
[10]: df.groupby('study name')['body mass (g)'].median()
```

```
[10]: study name
      PAL0708    3900.0
      PAL0809    4200.0
      PAL0910    4000.0
      Name: body mass (g), dtype: float64
```

Confusing Notebook

```
[1]: import pandas as pd
```

```
[5]: df = pd.read_csv('penguins_lter.csv')
```

[5]:

	study name	sample number	species	...	culmen length (mm)	body mass (g)
0	PAL0708	1	Adelie	...	39.1	3750.0
1	PAL0708	1	Gentoo	...	46.1	4500.0
...	...	...	...	...	...	...
342	PAL0910	151	Adelie	...	36.0	3700.0
343	PAL0910	152	Adelie	...	41.5	4000.0

```
[6]: df = df.dropna(subset=['culmen_length_mm', 'culmen_depth_mm',
                            'flipper_length_mm', 'body_mass_g'])
```

```
---------------------------------------------------------------------------
KeyError                                  Traceback (most recent call last)
Input In [6], in <cell line: 1>()
----> 1 df = df.dropna(subset=['culmen_length_mm', 'culmen_depth_mm',
      2                       'flipper_length_mm', 'body_mass_g'])

KeyError: ['culmen_length_mm', 'culmen_depth_mm', 'flipper_length_mm',
           'body_mass_g']
```

```
[7]: df.columns
```

```
[7]: Index(['study name', 'sample number', 'species', 'region', ...,
            'flipper length (mm)', 'culmen length (mm)', 'body mass (g)'],
           dtype='object')
```

```
[5]: df = df.rename(columns={'culmen_length_mm': 'culmen length (mm)',
                            'body_mass_g': 'body mass (g)'})
```

[5]:

	species	island	culmen length (mm)	...	body mass (g)	sex
0	Chinstrap	Dream	50.9	...	3550.0	MALE
1	Gentoo	Biscoe	47.3	...	4725.0	NaN
...	...	...	...	...	...	...
341	Gentoo	Biscoe	49.9	...	5400.0	MALE
343	Chinstrap	Dream	47.0	...	3700.0	FEMALE

```
[8]: df['body mass (g)'].max()
```

```
[8]: 6300.0
```

```
[10]: df.groupby
```

Which `df` does this refer to?

```
[10]: study name
      PAL0708    3900.0
      PAL0809    4200.0
      PAL0910    4000.0
      Name: body mass (g), dtype: float64
```

Confusing Notebook

```
[1]: import pandas as pd
```

```
[5]: df = pd.read_csv('penguins_lter.csv')
```

[5]:

	study name	sample number	species	...	culmen length (mm)	body mass (g)
0	PAL0708	1	Adelie	...	39.1	3750.0
1	PAL0708	1	Gentoo	...	46.1	4500.0
...	...	...	...	...	...	...
342	PAL0910	151	Adelie	...	36.0	3700.0
343	PAL0910	152	Adelie	...	41.5	4000.0

```
[6]: df = df.dropna(subset=['culmen_length_mm', 'culmen_depth_mm',
                            'flipper_length_mm', 'body_mass_g'])
```

```
---------------------------------------------------------------------------
KeyError                                  Traceback (most recent call last)
Input In [6], in <cell line: 1>()
----> 1 df = df.dropna(subset=['culmen_length_mm', 'culmen_depth_mm',
      2                       'flipper_length_mm', 'body_mass_g'])

KeyError: ['culmen_length_mm', 'culmen_depth_mm', 'flipper_length_mm',
           'body_mass_g']
```

```
[7]: df.columns
```

```
[7]: Index(['study name', 'sample number', 'species', 'region', ...,
            'flipper length (mm)', 'culmen length (mm)', 'body mass (g)'],
           dtype='object')
```

```
[5]: df = df.rename(columns={'culmen_length_mm': 'culmen length (mm)',
                            'body_mass_g': 'body mass (g)'})
```

[5]:

	species	island	culmen length (mm)	...	body mass (g)	sex
0	Chinstrap	Dream	50.9	...	3550.0	MALE
1	Gentoo	Biscoe	47.3	...	4725.0	NaN
...	...	...	...	...	...	...
341	Gentoo	Biscoe	49.9	...	5400.0	MALE
343	Chinstrap	Dream	47.0	...	3700.0	FEMALE

```
[8]: df['body mass (g)'].max()
```

```
[8]: 6300.0
```

```
[10]: df.groupb
```

Which `df` does this refer to?

```
[10]: study name
      PAL0708    3900.0
      PAL0809    4200.0
      PAL0910    4000.0
      Name: body mass (g), dtype: float64
```

Notebook Potholes

- If you redefine or **mutate** a variable, another cell may break
- The **order** of cell execution matters
- If you forget to run an edited cell, the result may **not match** the code

Improving Notebook Output and Links Between Cells

- Improve Reuse
  - Remove ambiguities
  - Enhance recall
- Improve Display

Remove Ambiguities and Preserve Recall

```
In [5]: import pandas as pd
        df = pd.read_csv('guardian-top100-female-2019.csv')
```

Out[5]:

	Name	Rank	Position	Age on 1 Dec 2019	Nationality
0	Sam Kerr	1	Forward	26	Australia
...	...	...	...	...	...
99	Ludmila	100	Forward	25	Brazil

100 rows × 5 columns

```
In [6]: df = df.rename(columns={'Age on 1 Dec 2019': 'Age'})
```

Out[6]:

	Name	Rank	Position	Age	Nationality
0	Sam Kerr	1	Forward	26	Australia
...	...	...	...	...	...
99	Ludmila	100	Forward	25	Brazil

100 rows × 5 columns

```
In [3]: df = df[df.Age >= 31]
```

Out[3]:

	Name	Rank	Position	Age	Nationality
2	Megan Rapinoe	3	Midfielder	34	USA
...	...	...	...	...	...
96	Cláudia Neto	97	Midfielder	31	Portugal

19 rows × 5 columns

```
In [7]: df = df[df.Age <= 24]
```

Out[7]:

	Name	Rank	Position	Age	Nationality
3	Ada Hegerberg	4	Forward	24	Norway
...	...	...	...	...	...
98	Lena Oberdorf	99	Midfielder	17	Germany

25 rows × 5 columns

Remove Ambiguities and Preserve Recall

```
In [d51f8eab]: import pandas as pd
               df = pd.read_csv('guardian-top100-female-2019.csv')
```

df:

	Name	Rank	Position	Age on 1 Dec 2019	Nationality
0	Sam Kerr	1	Forward	26	Australia
...	...	...	...	...	...
99	Ludmila	100	Forward	25	Brazil

100 rows × 5 columns

```
In [full]: df = df.rename(columns={'Age on 1 Dec 2019': 'Age'})
```

df:

	Name	Rank	Position	Age	Nationality
0	Sam Kerr	1	Forward	26	Australia
...	...	...	...	...	...
99	Ludmila	100	Forward	25	Brazil

100 rows × 5 columns

```
In [over30]: df = df$full[df$full.Age >= 31]
```

df:

	Name	Rank	Position	Age	Nationality
2	Megan Rapinoe	3	Midfielder	34	USA
...	...	...	...	...	...
96	Cláudia Neto	97	Midfielder	31	Portugal

19 rows × 5 columns

```
In [under25]: df = df$full[df$full.Age <= 24]
```

df:

	Name	Rank	Position	Age	Nationality
3	Ada Hegerberg	4	Forward	24	Norway
...	...	...	...	...	...
98	Lena Oberdorf	99	Midfielder	17	Germany

25 rows × 5 columns

[dataflownb.github.io]

Improve Output Representations

```
{'setosa': (    sepal_length  sepal_width  petal_length  petal_width
  13             4.3           3.0           1.1           0.1,
  <IPython.core.display.Image object>),
 'versicolor': (    sepal_length  sepal_width  petal_length  petal_width
  99             5.7           2.8           4.1           1.3
  67             5.8           2.7           4.1           1.0,
  <IPython.core.display.Image object>),
 'virginica': (     sepal_length  sepal_width  petal_length  petal_width
  104             6.5           3.0           5.8           2.2
  121             5.6           2.8           4.9           2.0
  116             6.5           3.0           5.5           1.8,
  <IPython.core.display.Image object>)}
```

Improve Output Representations

▼ { # len=3
'setosa': ▶ (<pandas.core.frame.DataFrame>, <IPython.core.display.Image>),
'versicolor': ▼ (# len=2
0: ▶ <pandas.core.frame.DataFrame>,
1: ▶ <IPython.core.display.Image>
),
'virginica': ▼ (# len=2
0: ▼

	sepal_length	sepal_width	petal_length	petal_width
104	6.5	3.0	5.8	2.2
121	5.6	2.8	4.9	2.0
116	6.5	3.0	5.5	1.8

1: ▼

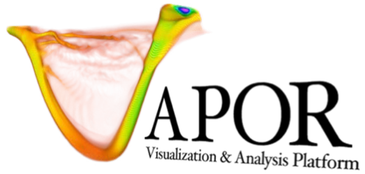
)
}

[dataflownb.github.io]

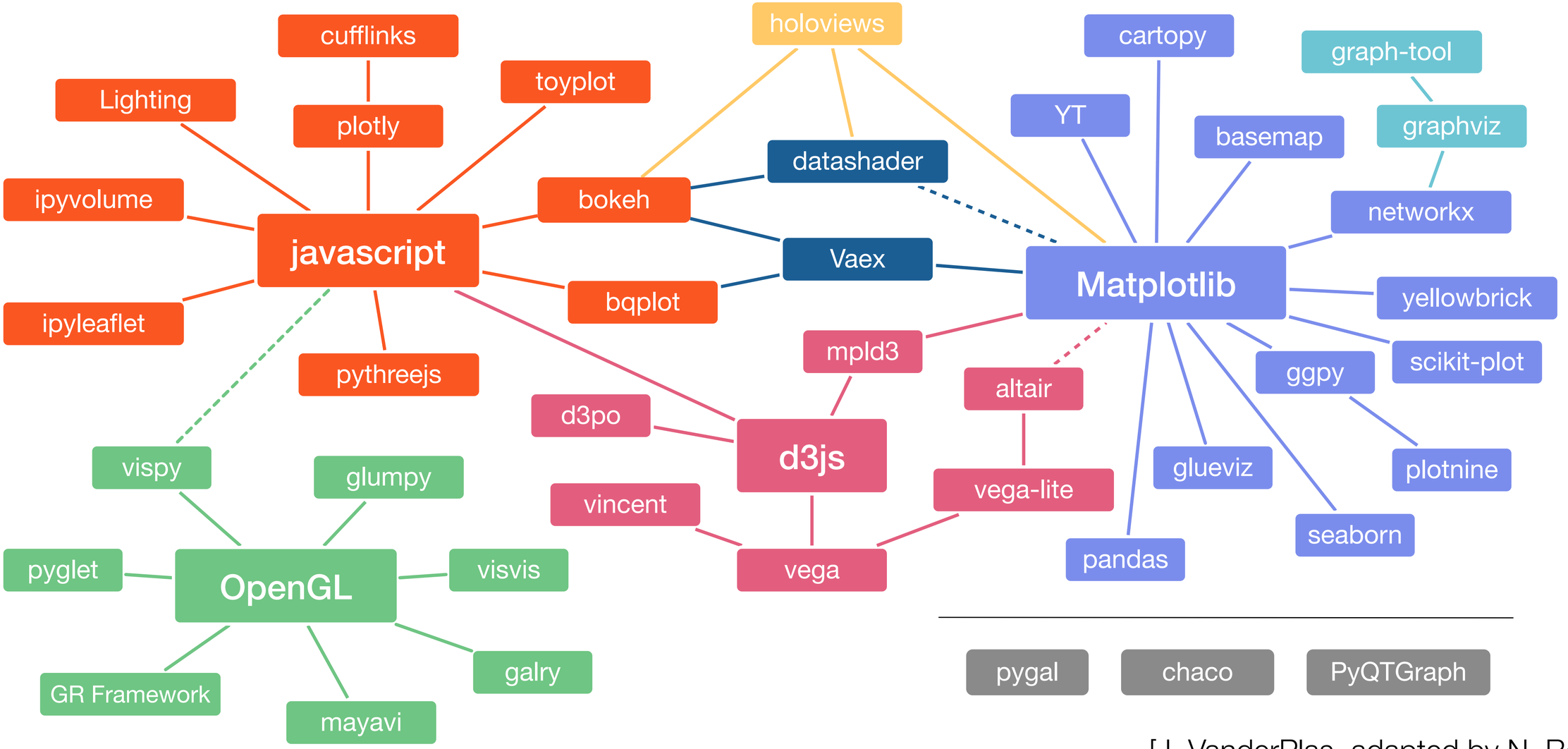
dataflownb.github.io

- Computational notebooks **facilitate efficient exploration** because users can quickly **inspect** and **reuse intermediate outputs**
- It is important to show **interactive output** that **summarizes** while providing the ability to dig into **details**
- It is important to be able to **recall and reuse** past outputs during and **after** analysis **without re-running or re-writing** code
- JupyterLab and IPython extensions to **improve notebooks**
  - Recall and reuse of past outputs (dfnotebook-extension + dfkernel)
  - Output display (ipycollections)

Visualization Landscape

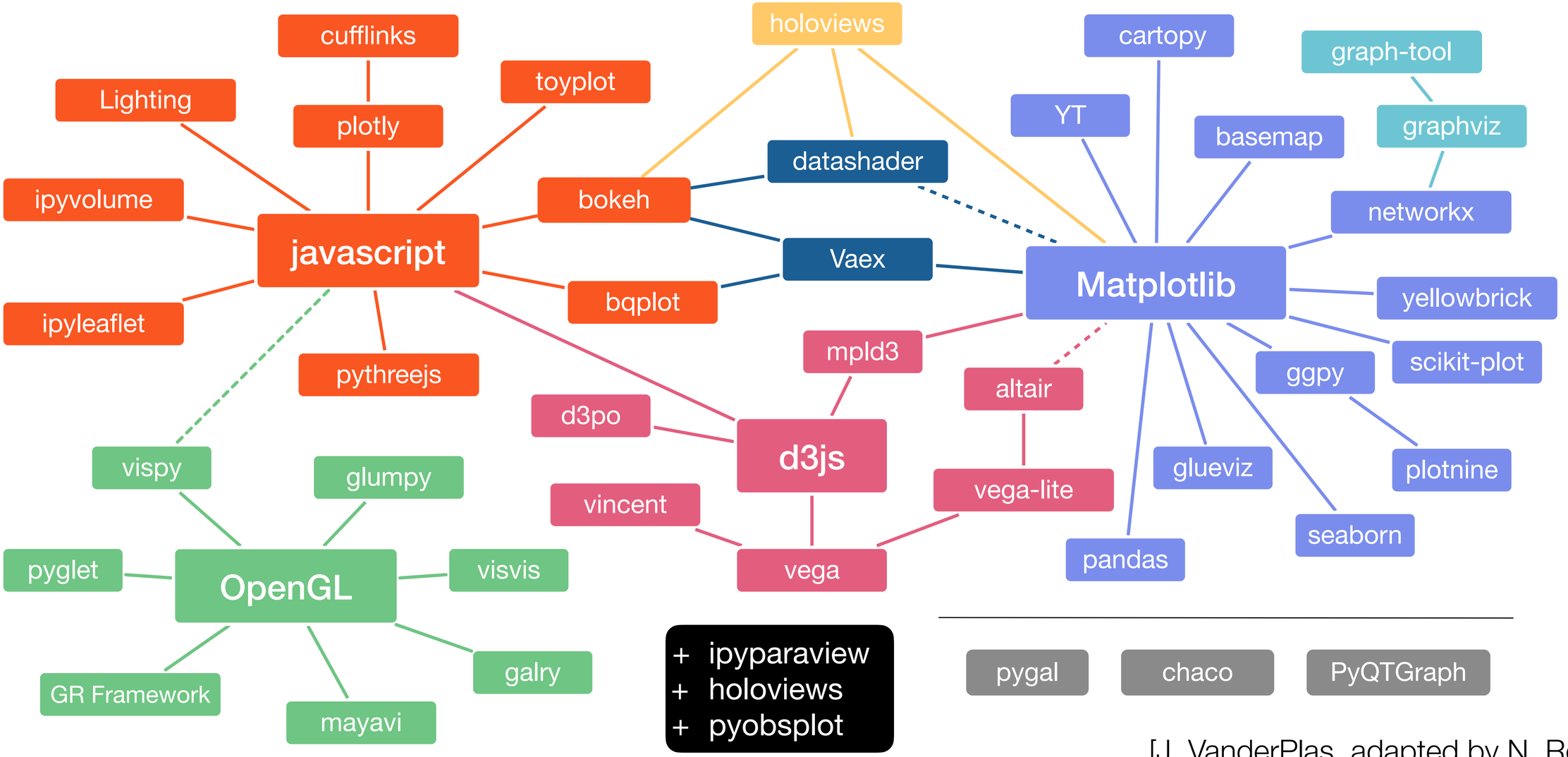
- Apps:  
- Domain-Specific Apps:  
- APIs: VTK, ITK
- Also… **Data Analysis Tools/Libraries**
  - JavaScript: D3, Observable Plot
  - R: ggplot
  - **Python**: matplotlib, altair, bokeh, …
  - Matlab
  - GNUPlot

The Python Visualization Landscape



[J. VanderPlas, adapted by N. Rougier]

The Python Visualization Landscape



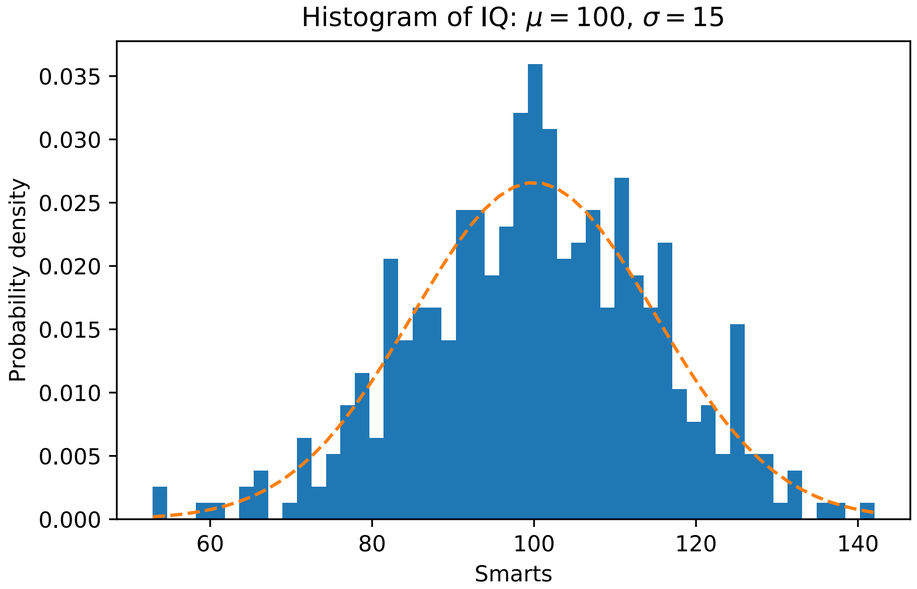
[J. VanderPlas, adapted by N. Rougier]

Examples

- Examine airfoil data on Cooley
- Login to:
  - jupyter.alcf.anl.gov
- Click on "Login Cooley"
- Copy .ipynb files from Track 4 Examples dir to your $HOME:
  /grand/projects/ATPESC2023/EXAMPLES/track-4-visualization
- …or use upload button to upload the two airfoil notebooks
  - airfoil-flow.ipynb
  - airfoil-line-plots.ipynb
- Once uploaded, click on the flow notebook to start

matplotlib

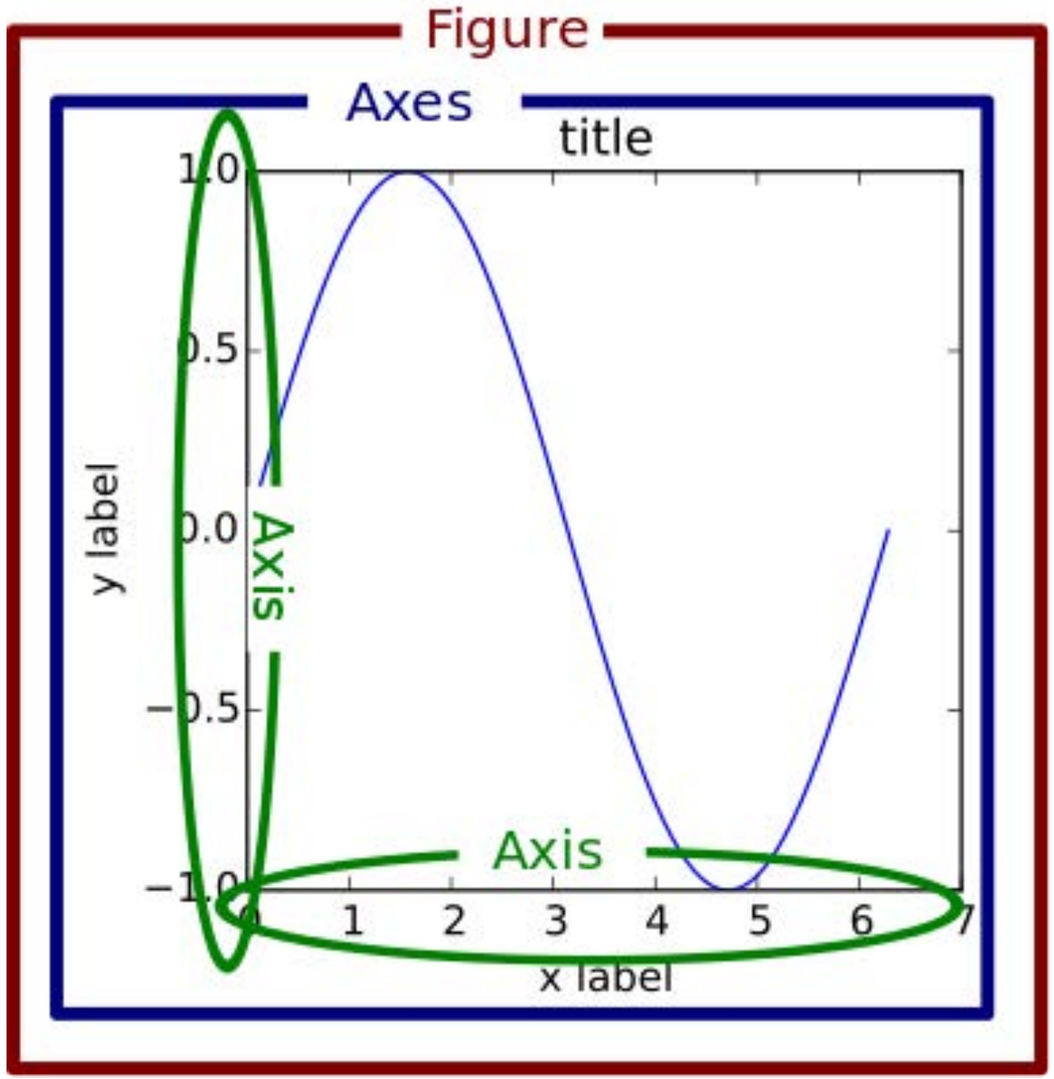
- Strengths:
  - Designed like Matlab
  - Many rendering backends
  - Can reproduce almost any plot
  - Proven, well-tested
- Weaknesses:
  - API is imperative
  - Not originally designed for the web
  - Dated styles

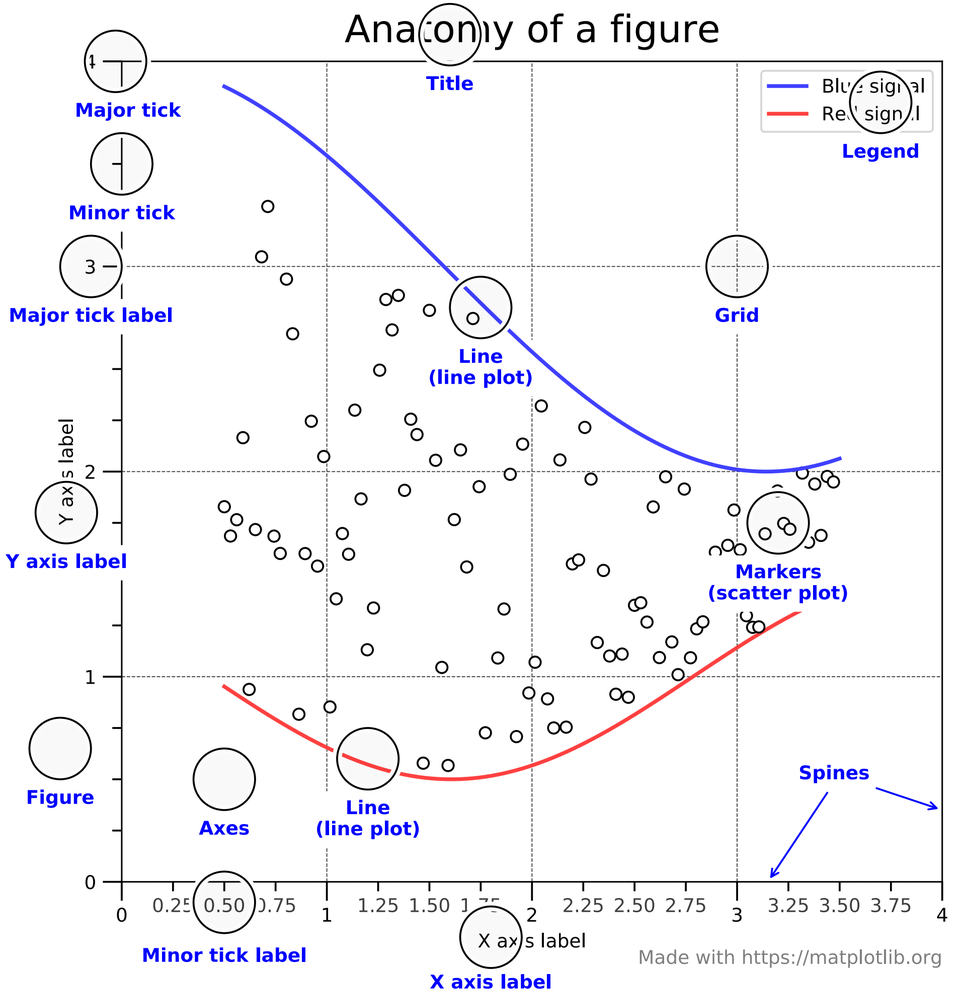


`plt.hist(…)`

[J. VanderPlas]

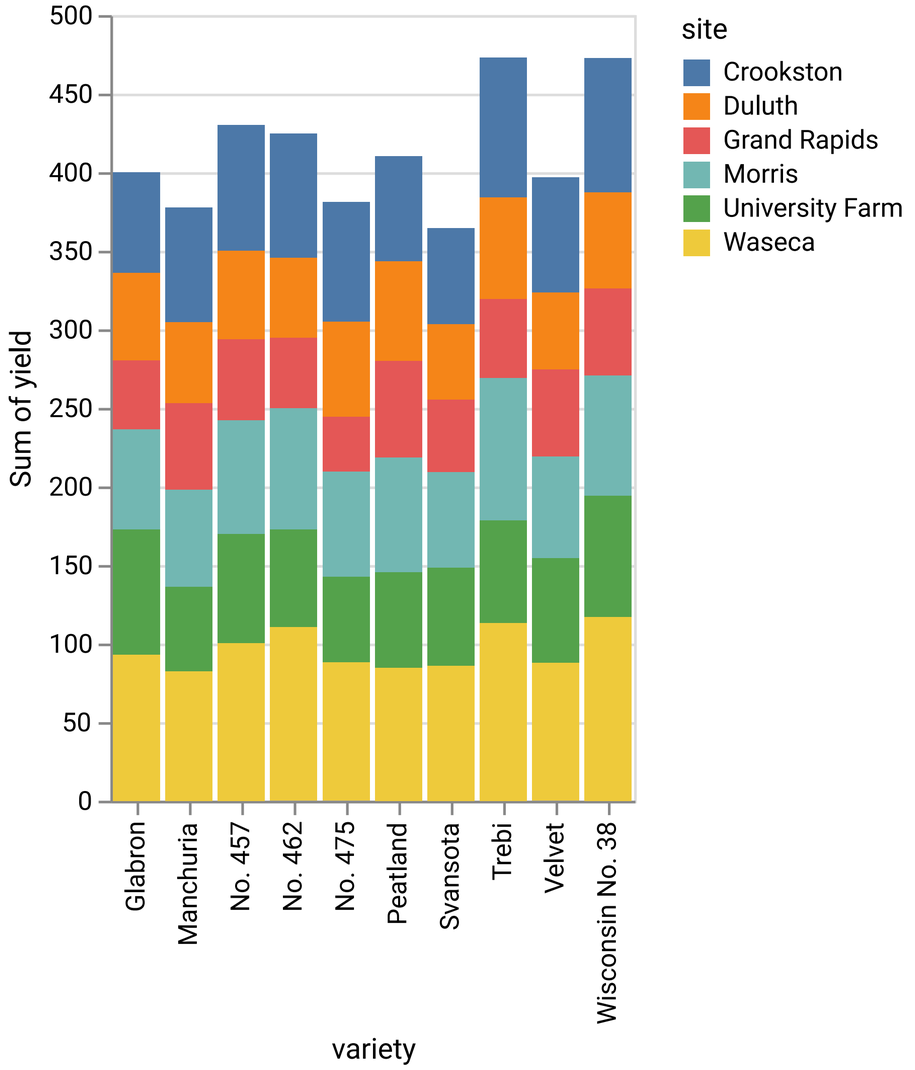
Anatomy of a Figure





Altair

- Declarative Visualization
  - Specify **what** instead of how
  - Separate specification from execution
- Based on VegaLite which is browser-based
- Strengths:
  - Declarative visualization
  - Web technologies
- Weaknesses:
  - Scaling (but see VegaFusion)
  - Specifications + translate to JavaScript



Data Items Become Visual Marks

- **Marks** are the basic graphical elements in a visualization
- Marks classified by dimensionality:

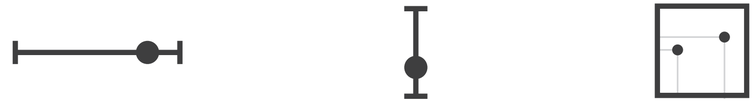
Points **Lines** **Areas**

- Also can have surfaces, volumes
- Think of marks as a mathematical definition, or if familiar with tools like Adobe Illustrator or Inkscape, the path & point definitions
- Altair: area, bar, circle, geoshape, image, line, point, rect, rule, square, text, tick
  - Also compound marks: boxplot, errorband, errorbar

[T. Munzner, E. Maguire (ill.)]

Encode Attributes via Visual Channels

- **Position**
  - Horizontal
  - Vertical
  - Both



- **Color**

- **Shape**

- **Tilt**

- **Size**
  - Length
  - Area
  - Volume

[T. Munzner, E. Maguire (ill.)]

Examples

- Examine airfoil data on Cooley
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  - jupyter.alcf.anl.gov
- Click on "Login Cooley"
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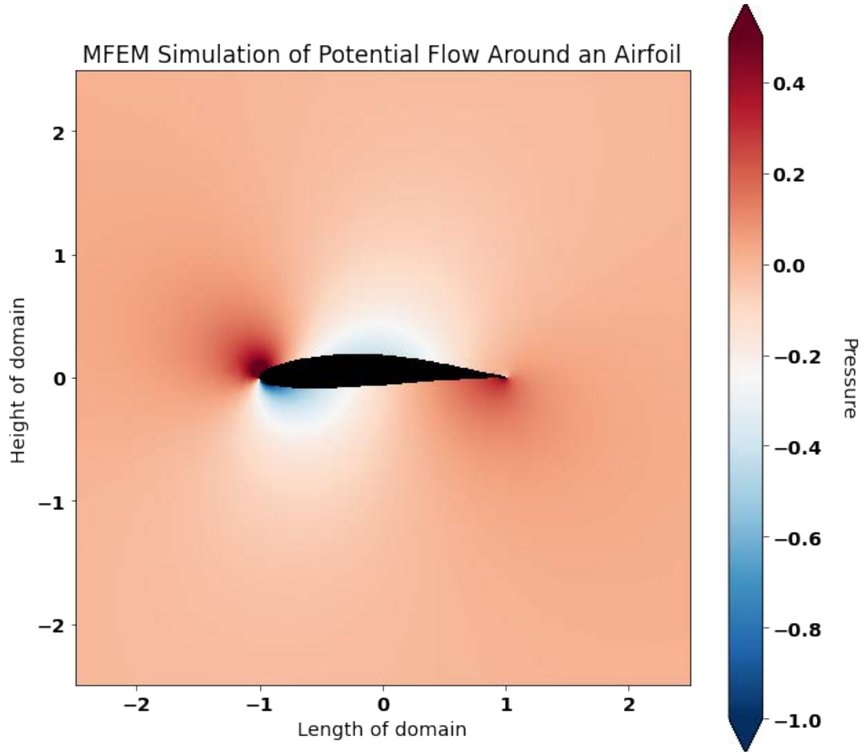
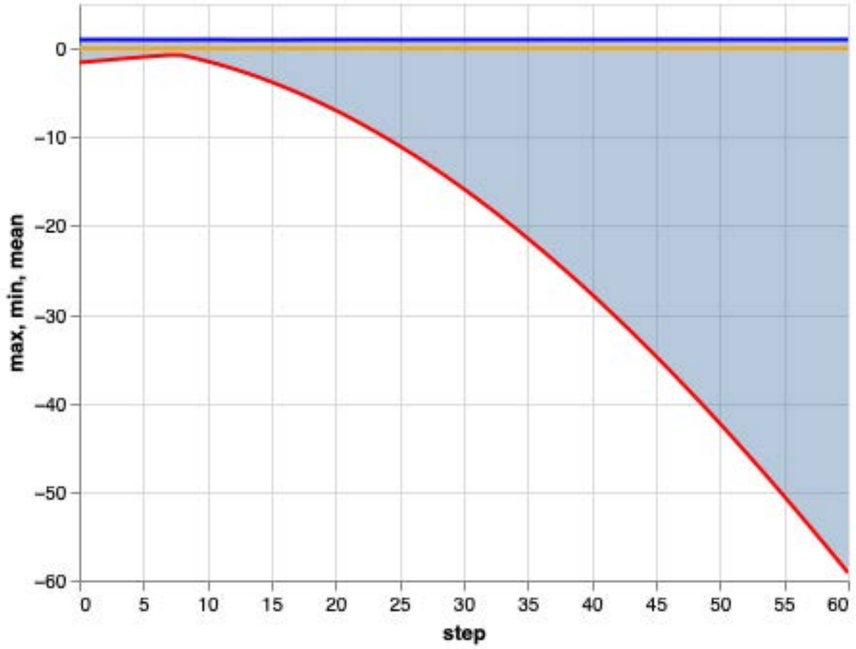
- …or use upload button to upload the two airfoil notebooks
  - airfoil-flow.ipynb
  - airfoil-line-plots.ipynb
- Once uploaded, click on the flow notebook to start

Questions?

```
plt.imshow(twod_data_array, cmap=cmap, extent=[-2.5,2.5,-2.5,2.5])
plt.clim(-1.0, 0.5); # for p
plt.title('MFEM Simulation of Potential Flow Around an Airfoil');
plt.ylabel('Height of domain');
plt.xlabel('Length of domain');
cb = plt.colorbar(extend='both');
cb.set_label('Pressure', rotation=270, labelpad=24)
```






```
chart = alt.Chart(df).encode(x='step')

area = chart.mark_area(opacity=0.4).encode(y='max', y2='min')
line = chart.mark_line(color='blue').encode(y='max')
line2 = chart.mark_line(color='orange').encode(y='mean')
line3 = chart.mark_line(color='red').encode(y='min')

area + line + line2 + line3
```