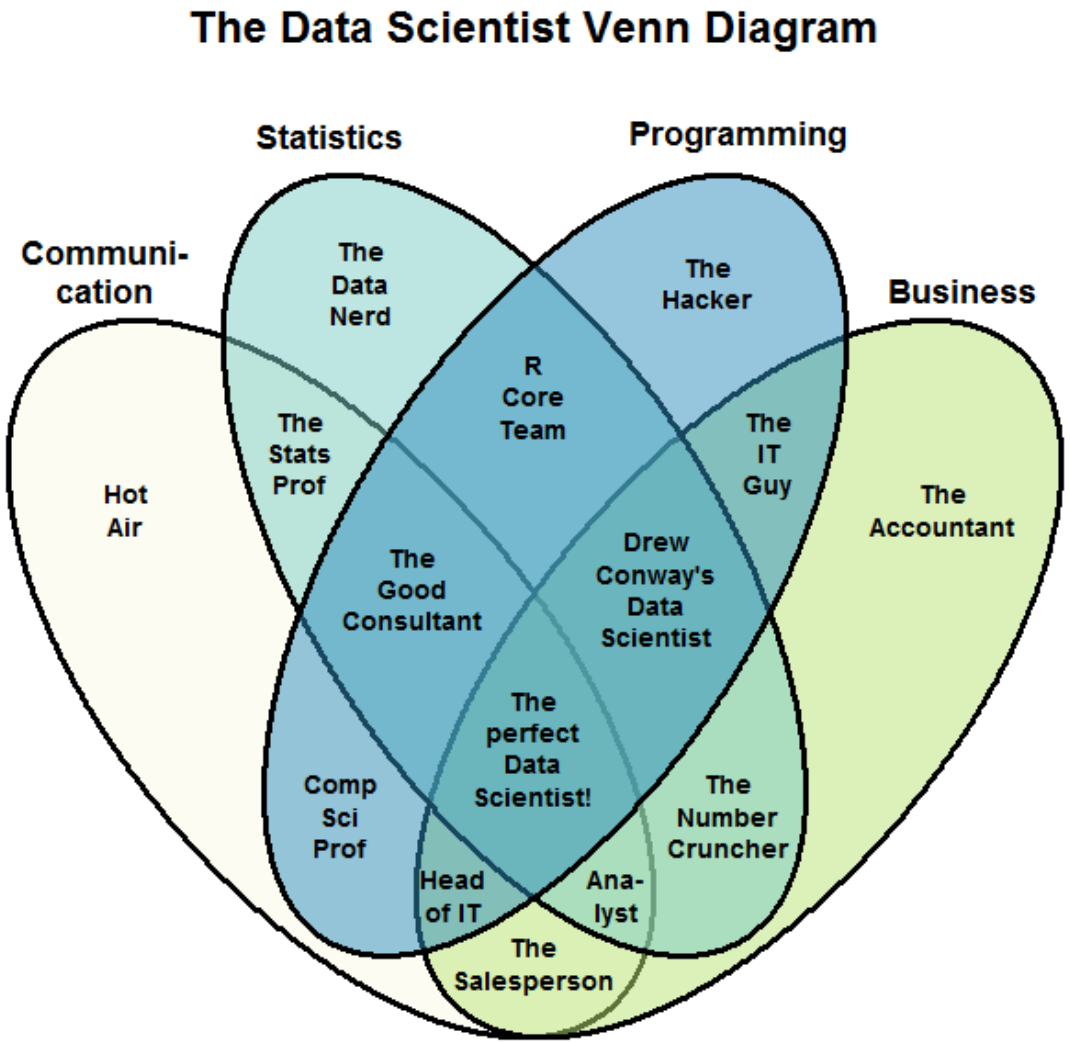
The Python Ecosystem for Data Science: A Guided Tour

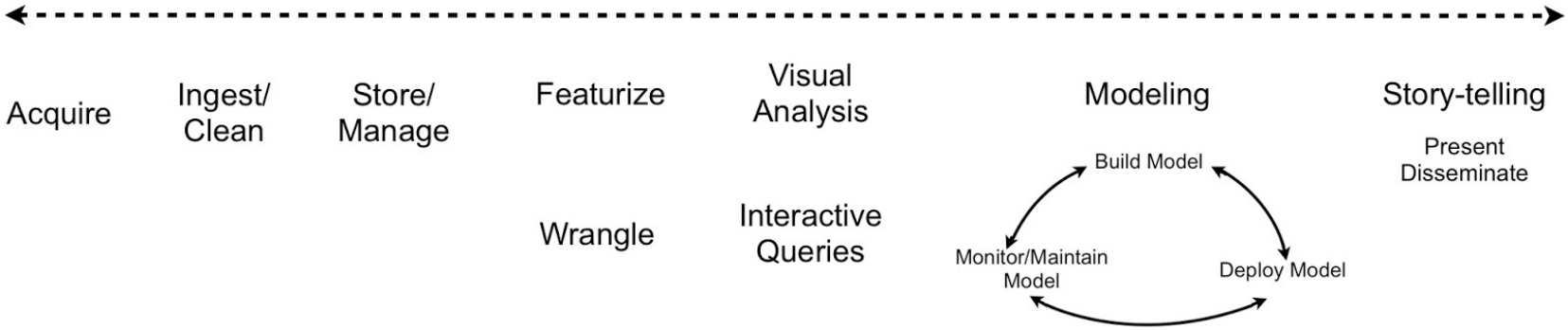
PyData Warsaw 2017 | at the Copernicus Science Centre | 19-20 October 2017

Christian Staudt | Independent Data Scientist



Source: Stephan Kolassa @ Stackexchange (https://datascience.stackexchange.com/questions/2403/data-science-without-knowledge-of-a-specific-topic-is-it-worth-pursuing-as-a-ca)

The (?) Data Science Workflow



Source: Ben Lorica @ O'Reilly (https://www.oreilly.com/ideas/data-analysis-just-one-component-of-the-data-science-workflow)

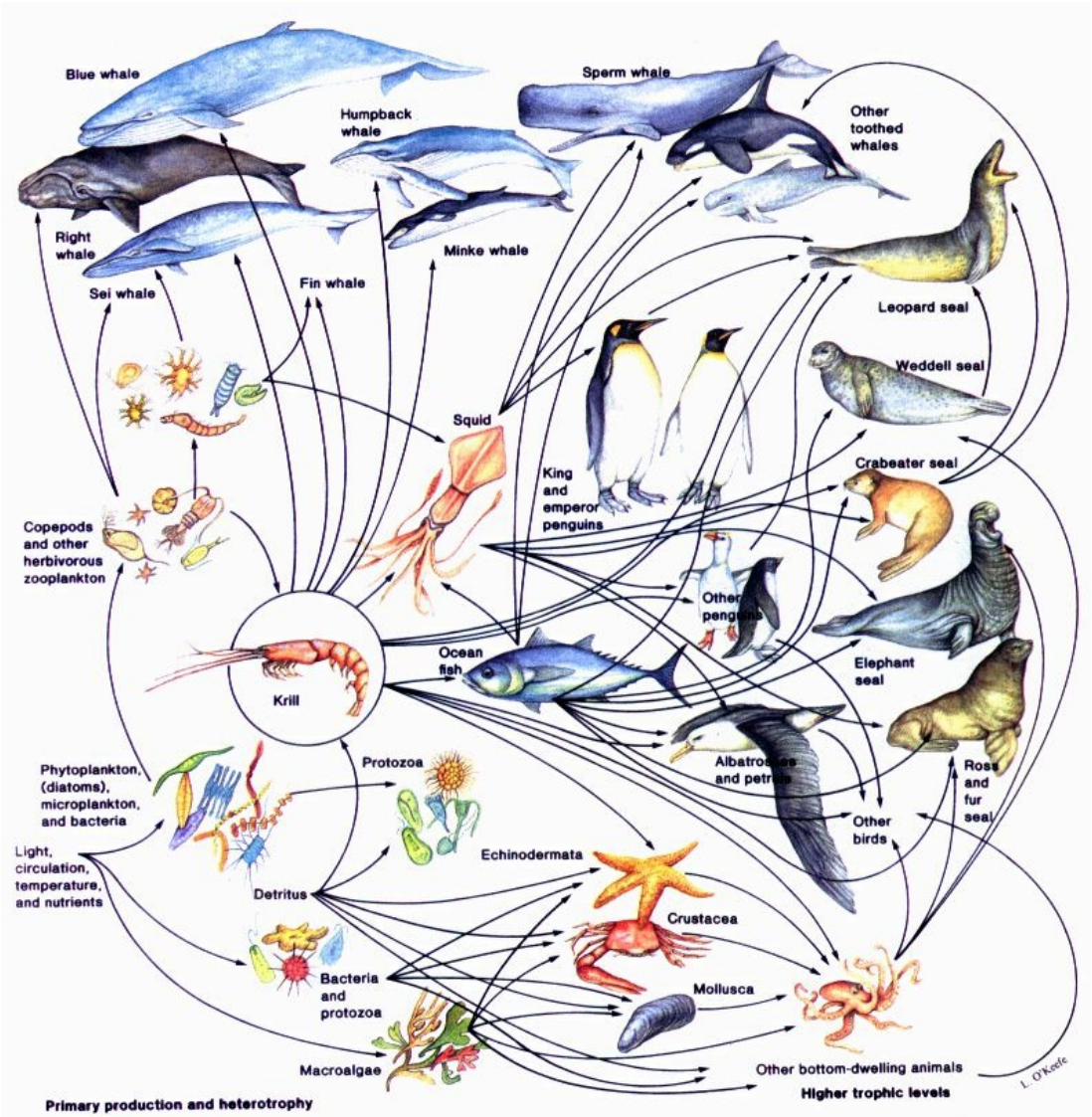
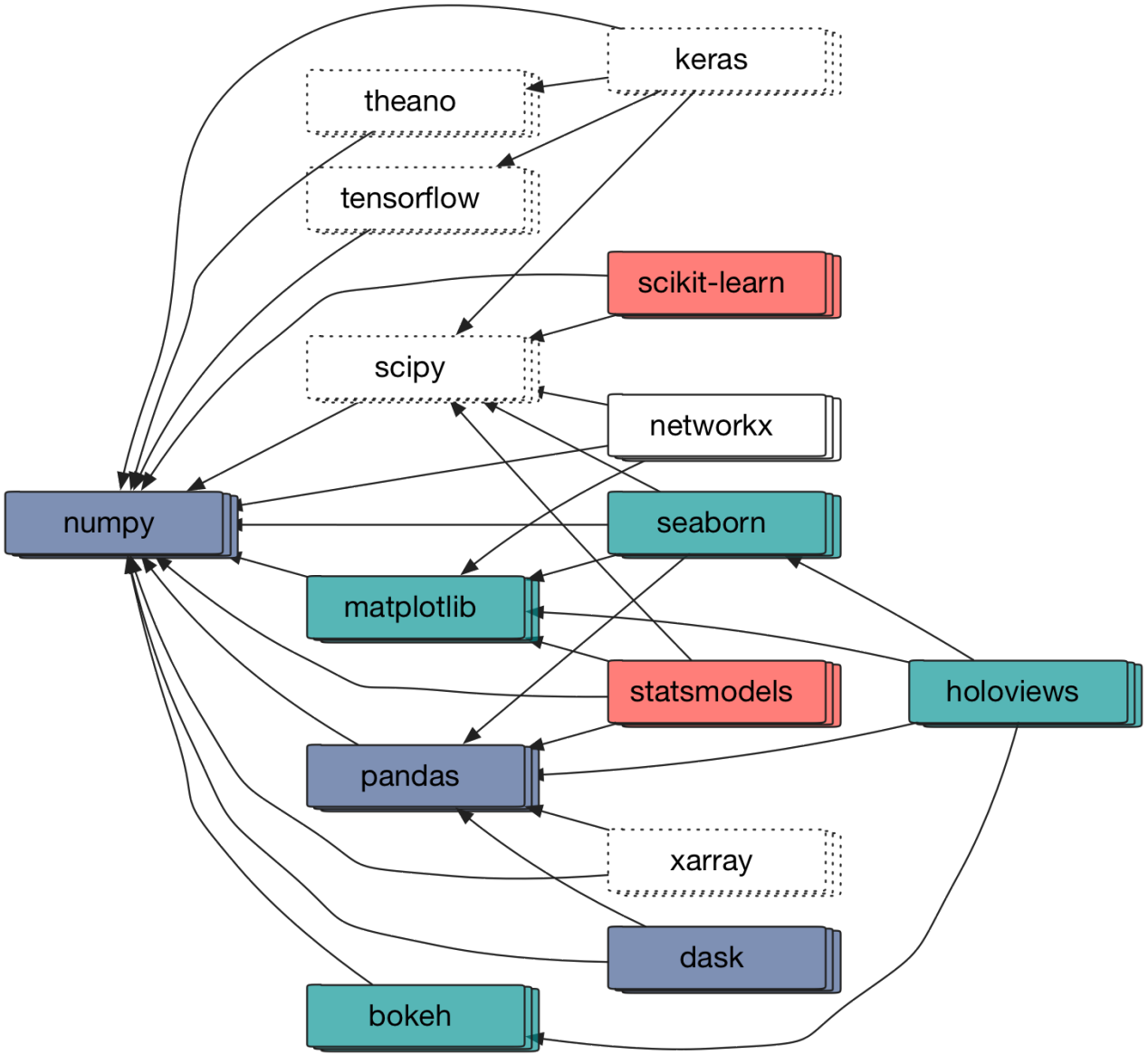
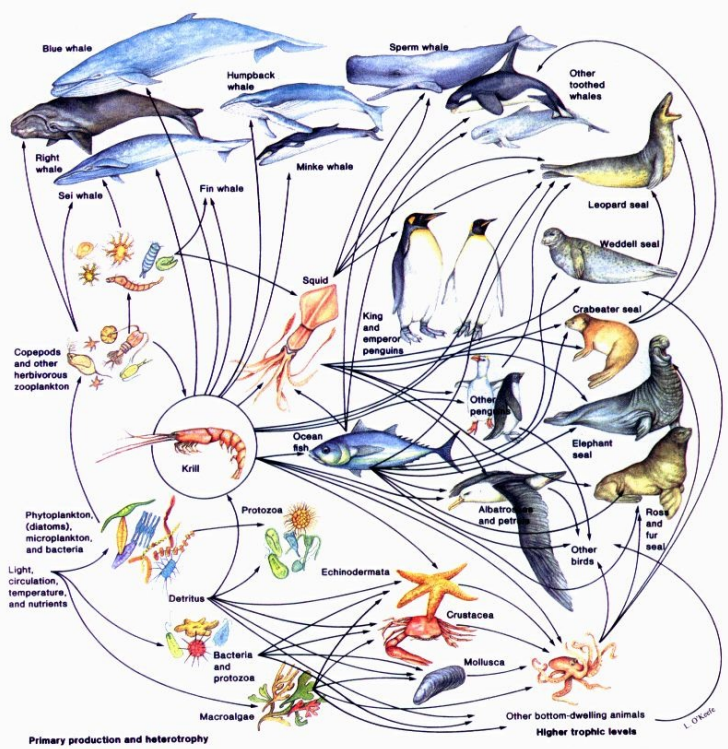


FIGURE 15.3 Food Webs. An Antarctic food web. Small crustaceans called krill support nearly all life in Antarctica. Krill are eaten by 6 species of baleen whales, 20 species of squid, over 100 species of fish, 35 species of birds, and 7 species of seals. Krill feed on algae, protozoa, other small crustaceans, and various larvae.


keras
theano
tensorflow
scikit-learn
scipy
networkx
numpy
seaborn
matplotlib
statsmodels
holoviews
pandas
xarray
dask
bokeh



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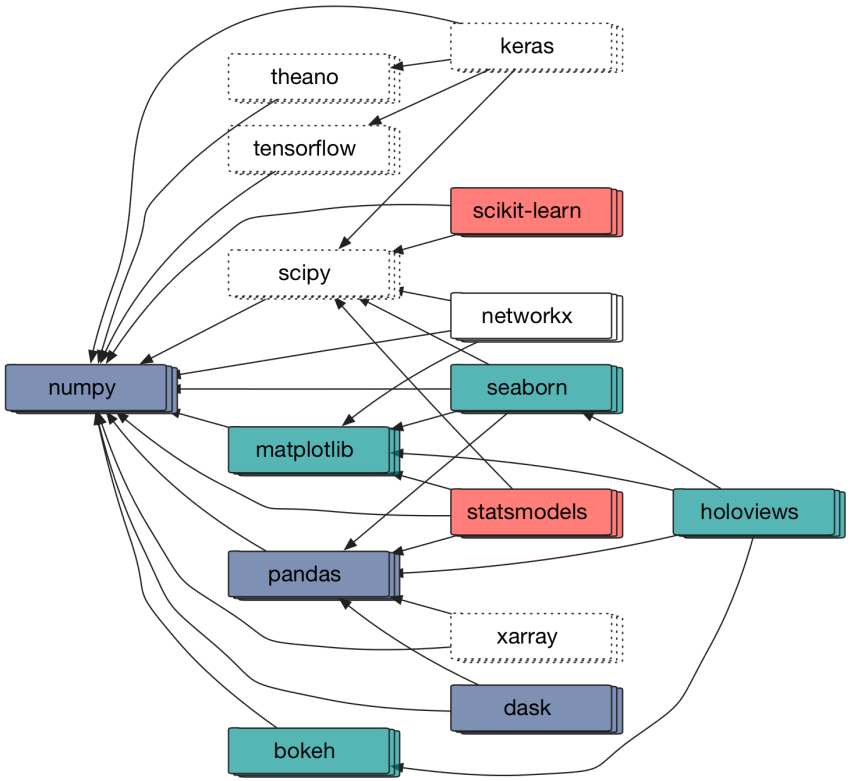
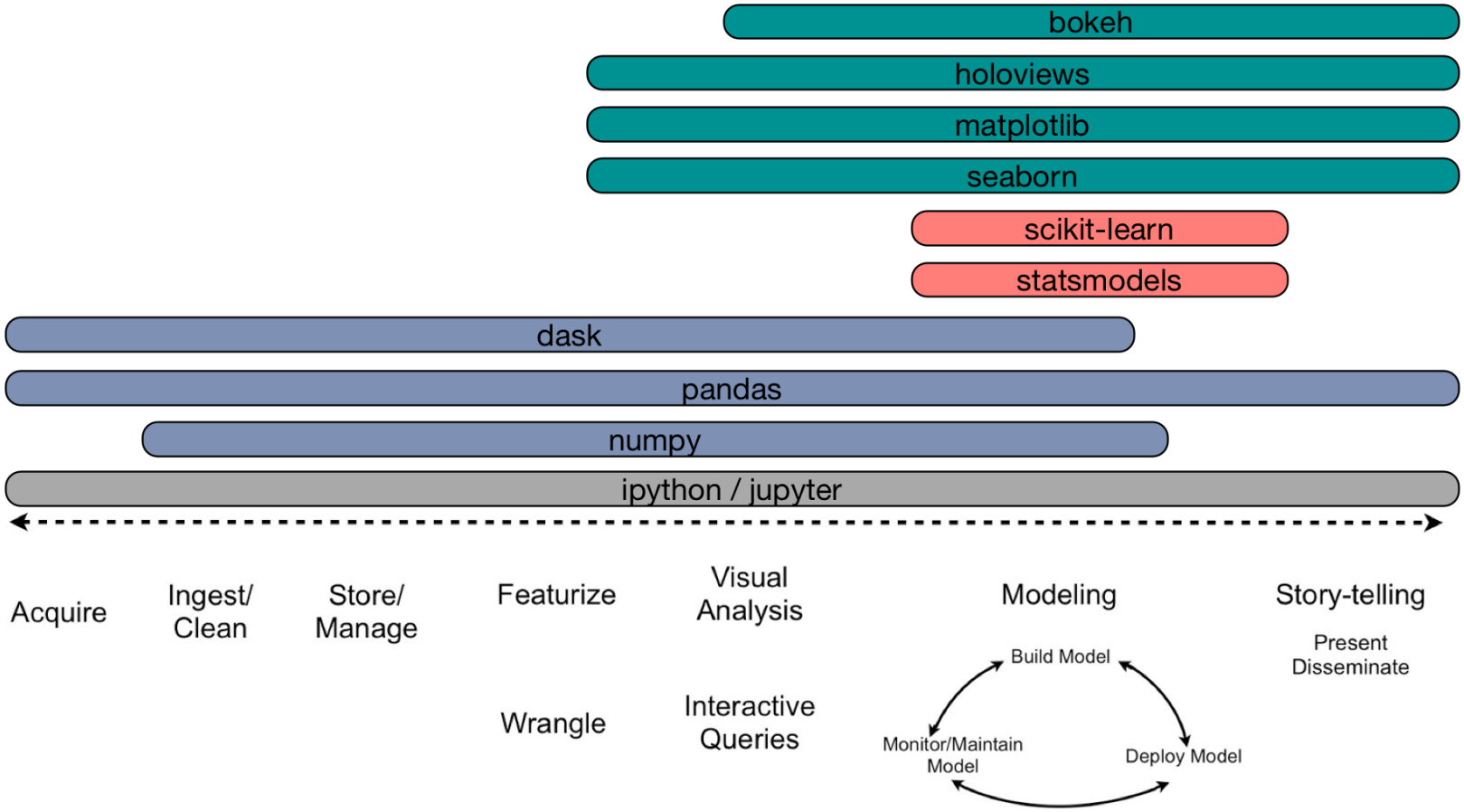


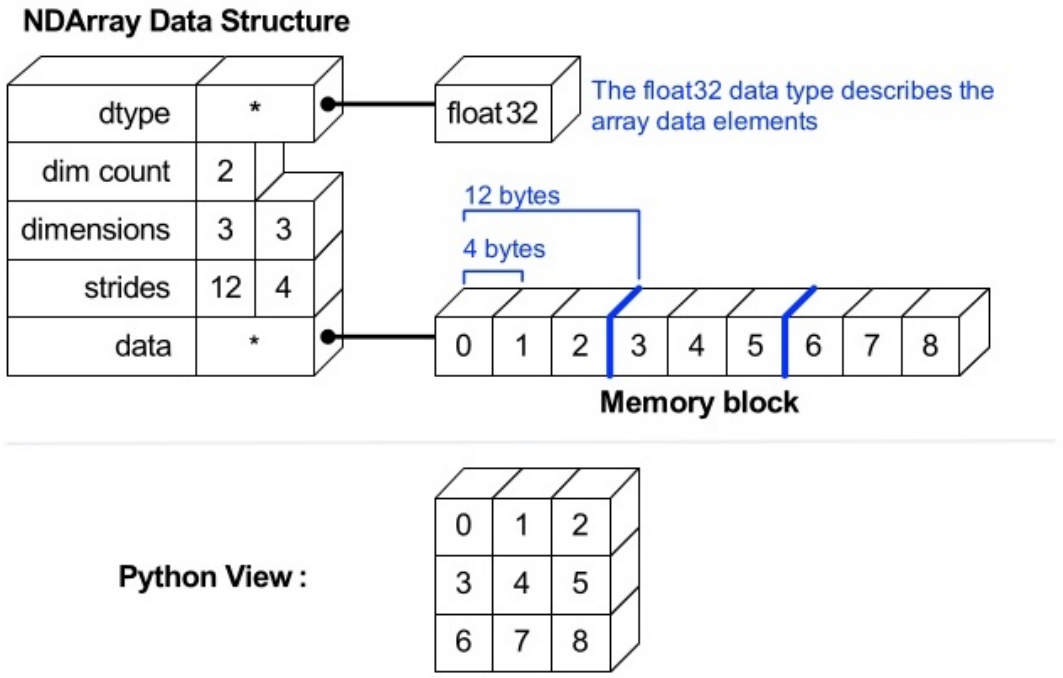
Wrangling


bokeh
holoviews
matplotlib
seaborn
scikit-learn
statsmodels
dask
pandas
numpy
ipython / jupyter
Acquire
Ingest/ Clean
Store/ Manage
Featurize
Wrangle
Visual Analysis
Interactive Queries
Modeling
Build Model
Deploy Model
Monitor/Maintain Model
Story-telling
Present
Disseminate

numpy

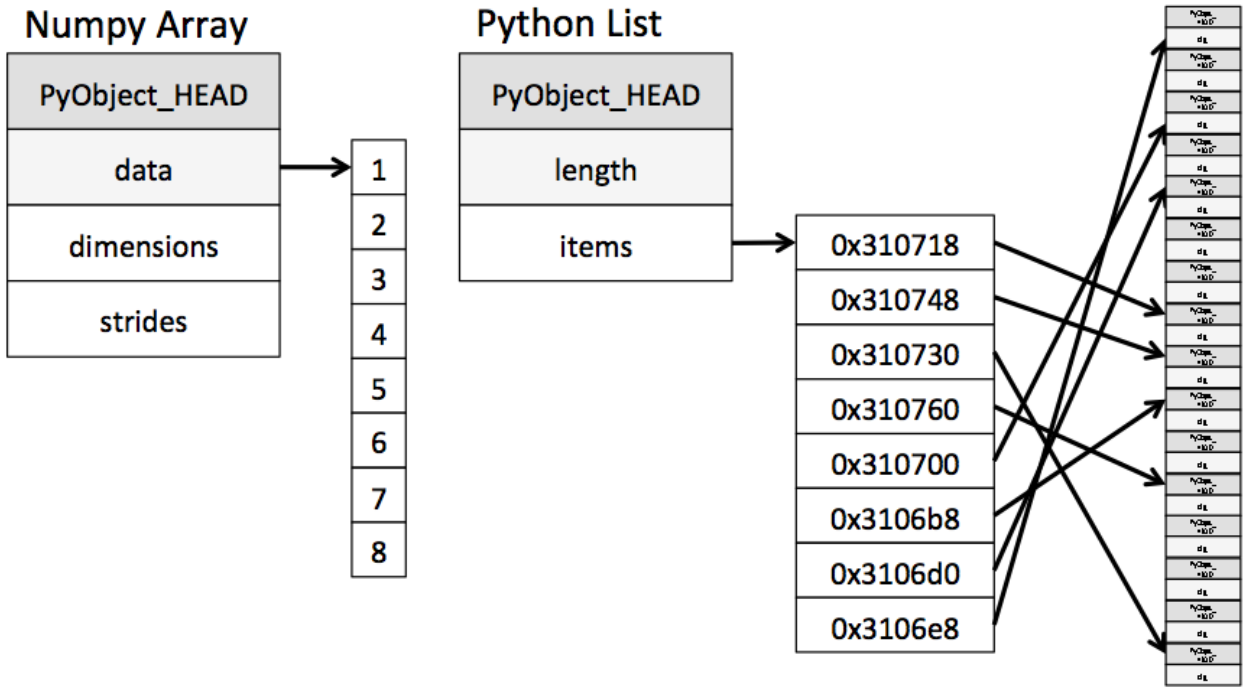
- the fundamental package for numeric computing in Python
- provides
  - n-dimensional array object
  - powerful array functions
  - math: linear algebra, random numbers, ...

numpy ndarray



Source: Travis Oliphant @ SIAM 2011 (https://www.slideshare.net/enthought/numpy-talk-at-siam)

numpy array vs python list



Source: Python Data Science Handbook by Jake VanderPlas (https://jakevdp.github.io/PythonDataScienceHandbook/02.01-understanding-data-types.html)

understand numpy - lose your loops

In [5]:
```
n = int(1e6)
```

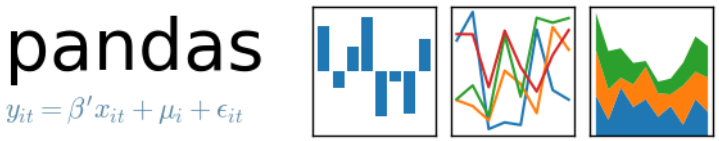
In [6]:
```
%%timeit
a = [random.random() for i in range(n)]
b = [math.log(x) for x in a]
```

```
440 ms ± 66.3 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

In [7]:
```
%%timeit
a = numpy.random.rand(n)
b = numpy.log(a)
```

```
22.2 ms ± 904 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

pandas



- labeled, indexed array data structures (e.g. Series, DataFrame)
- operations (e.g. `join`, `groupby`, ...)
- time series support (e.g. selection by date range)
- input/output tools (e.g. CSV, Excel, ...)
- some statistics

pandas example

task: find the correlation between inhabitants and number of museums of the departements of France

In [8]:
```
ls heresthedata/
```

```
Departements.csv            Liste_musees_de_France.xls
```

In [9]:
```
import pandas
```

In [10]:
```
departements = pandas.read_csv("heresthedata/Departements.csv", sep=";")
departements.head()
```

Out[10]:

	Nom du département	Nombre d'arrondissements	Nombre de cantons	Nombre de communes	Population municipale	Populat to
0	Ain	4	23.0	410	626.127	643.30
1	Aisne	5	21.0	805	539.783	554.04
2	Allier	3	19.0	318	343.062	353.26
3	Alpes-de-Haute-Provence	4	15.0	199	161.588	166.29
4	Hautes-Alpes	2	15.0	168	139.883	145.21

In [11]:
```
departements = departements[["Nom du département", "Population totale"]]
```

In [12]:
```
museums = pandas.read_excel("heresthedata/Liste_musees_de_France.xls")
museums.head(2)
```

Out[12]:

	NOMREG	NOMDEP	DATEAPPELLATION	FERME	ANNREOUV	ANNEXI
0	ALSACE	BAS-RHIN	01/02/2003	NON	NaN	NaN
1	ALSACE	BAS-RHIN	01/02/2003	NON	NaN	NaN

In [13]:
```
museum_count = museums.groupby("NOMDEP").size()
museum_count.head(5)
```

Out[13]:
```
NOMDEP
AIN                          14
AISNE                        15
ALLIER                        9
ALPES DE HAUTE PROVENCE       9
ALPES-MARITIMES              33
dtype: int64
```

In [14]:
```
departements["Nom du département"] = departements["Nom du département"].apply(lamb
da s: s.upper())
departements["Nom du département"] = departements["Nom du département"].apply(lamb
da s: s.replace("-", " "))
```

In [15]:
```
departements.index = departements["Nom du département"]
departements.drop(["Nom du département"], axis=1, inplace=True)
```

In [16]:
```
joined = departements.join(pandas.DataFrame(museum_count,
index=museum_count.index, columns=["number of museums"]))
joined.head(3)
```

Out[16]:

	Population totale	number of museums
Nom du département		
AIN	643.309	14.0
AISNE	554.040	15.0
ALLIER	353.262	9.0

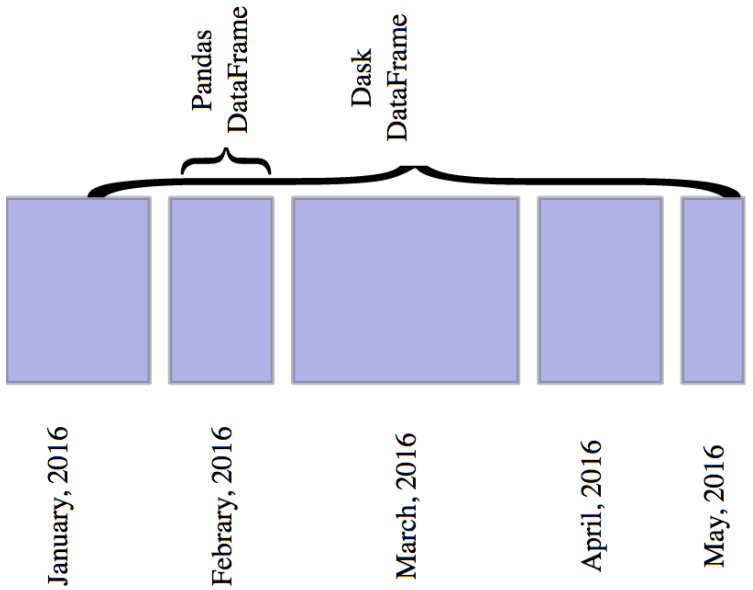
In [17]:
```
joined["Population totale"] = joined["Population totale"].apply(lambda s: pandas.to_numeric(s, errors="drop"))
joined.corr()
```

Out[17]:

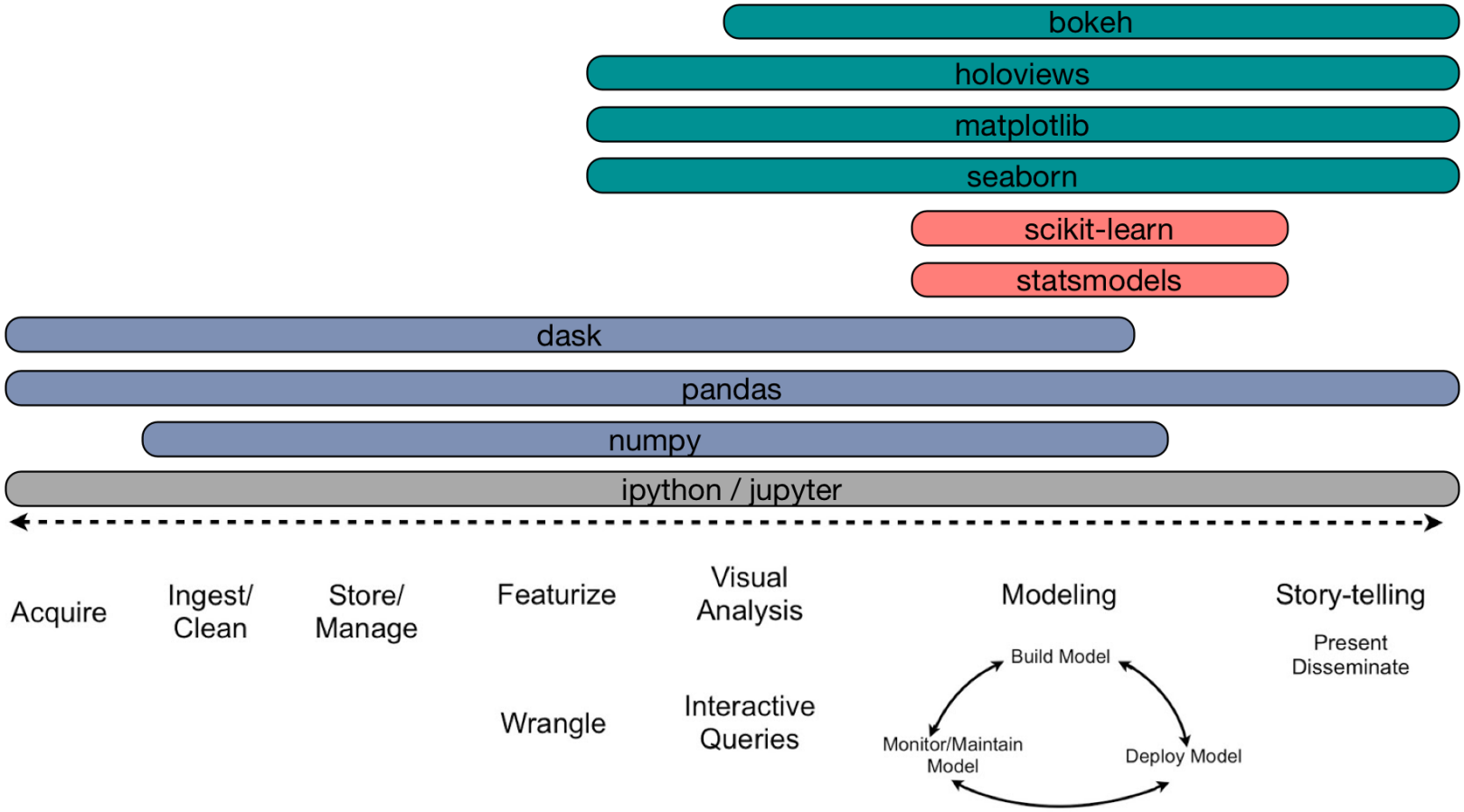
	Population totale	number of museums
Population totale	1.000000	0.601027
number of museums	0.601027	1.000000

dask

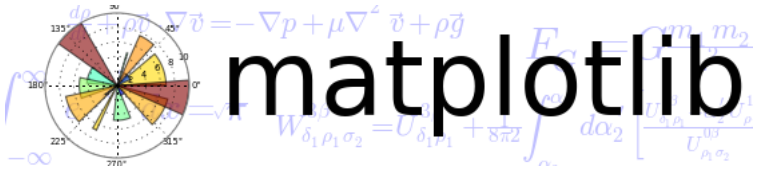
- **dask dataframe**
  - combines many pandas dataframes (split along the index), **mimic pandas API**
  - use cases
    - manipulating **datasets not fitting comfortably into memory** on a single machine
    - **parallelizing** many pandas operations across **many cores**
    - **distributed computing** of very large tables (e.g. stored in parallel file systems)



Visual Exploration & Presentation



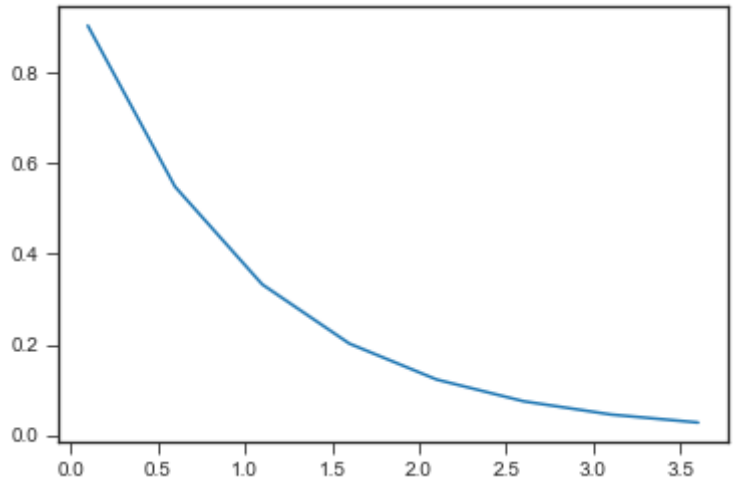
matplotlib



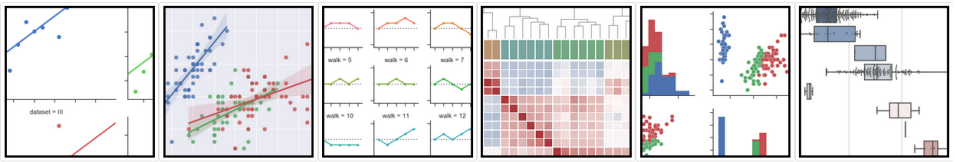
- 2D plotting library
- provides
  - MATLAB-like interface via the `pyplot` API

In [18]:
```
import matplotlib.pyplot as plt
%matplotlib inline
```

In [19]:
```
x = numpy.arange(0.1, 4, 0.5)
y = numpy.exp(-x)

fig, ax = plt.subplots()
ax.plot(x, y)
plt.show()
```



seaborn



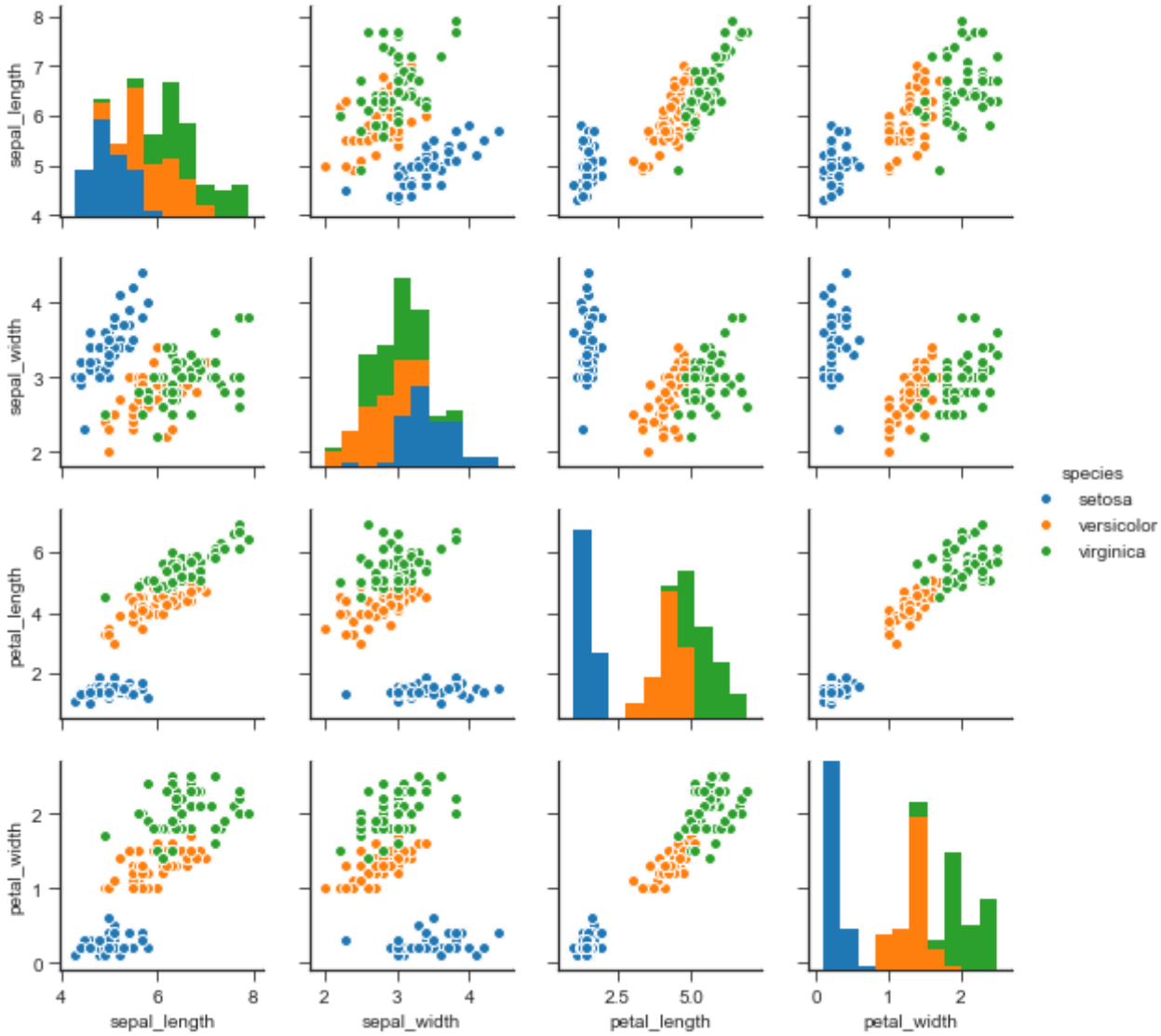
- production-ready **statistical graphics** on top of matplotlib
  - fit and visualize linear regression models
  - visualize and cluster matrix data
  - plot time series data
  - structuring grids of plots
- support for pandas and numpy data structures
- improved styling of matplotlib graphics (themes, color palettes, ...)

In [20]:
```
irisData = seaborn.load_dataset("iris")
irisData.head()
```

Out[20]:

	sepal_length	sepal_width	petal_length	petal_width	species
0	5.1	3.5	1.4	0.2	setosa
1	4.9	3.0	1.4	0.2	setosa
2	4.7	3.2	1.3	0.2	setosa
3	4.6	3.1	1.5	0.2	setosa
4	5.0	3.6	1.4	0.2	setosa

In [21]:
```
seaborn.pairplot(irisData, hue="species", size=2);
```



bokeh

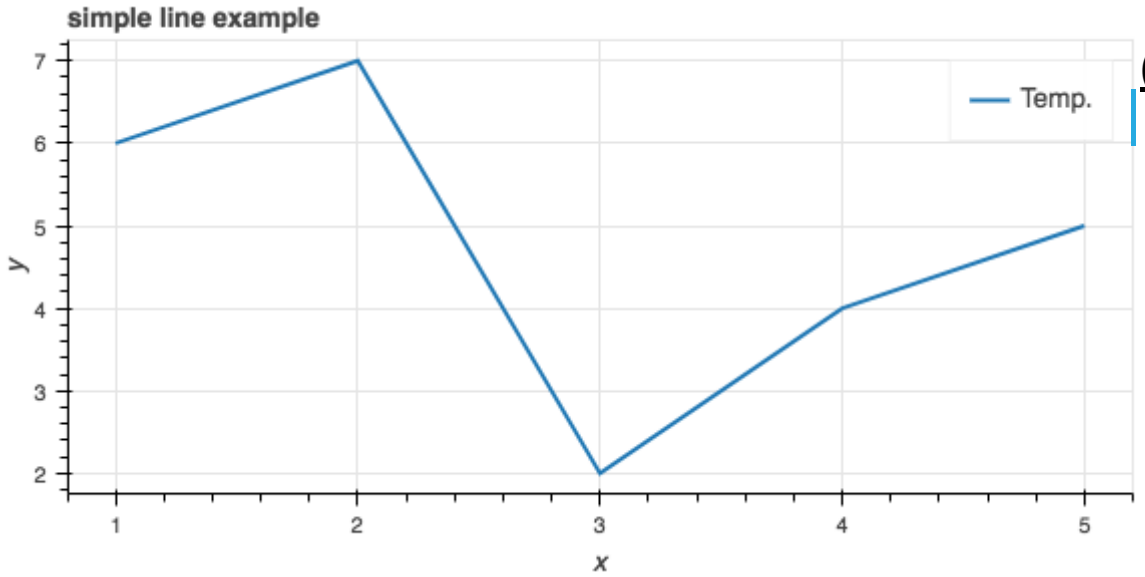
- interactive visualization library that targets modern web browsers for presentation
  - build e.g. interactive dashboards, data applications, ...
  - inspired by D3.js

In [22]:

```
from bokeh import plotting

x = [1, 2, 3, 4, 5]
y = [6, 7, 2, 4, 5]

plotting.output_notebook()
plot = plotting.figure(title="simple line example", x_axis_label='x',
y_axis_label='y', width=600, height=300)
plot.line(x, y, legend="Temp.", line_width=2)
plotting.show(plot)
```

(https://bokeh.pydata.org)

Bokeh JS 0.12.9 successfully loaded.



(https://bokeh.pydata.o

holoviews

- "focus on what you are trying to explore and convey, not on the process of plotting"
- annotate data with semantic metadata, then "let it plot itself"
- use **matplotlib** or **bokeh** as backend (and easily switch between them)

In [24]:
```
macro_df = pandas.read_csv('data/macro.csv', '\t')
macro_df.head()
```

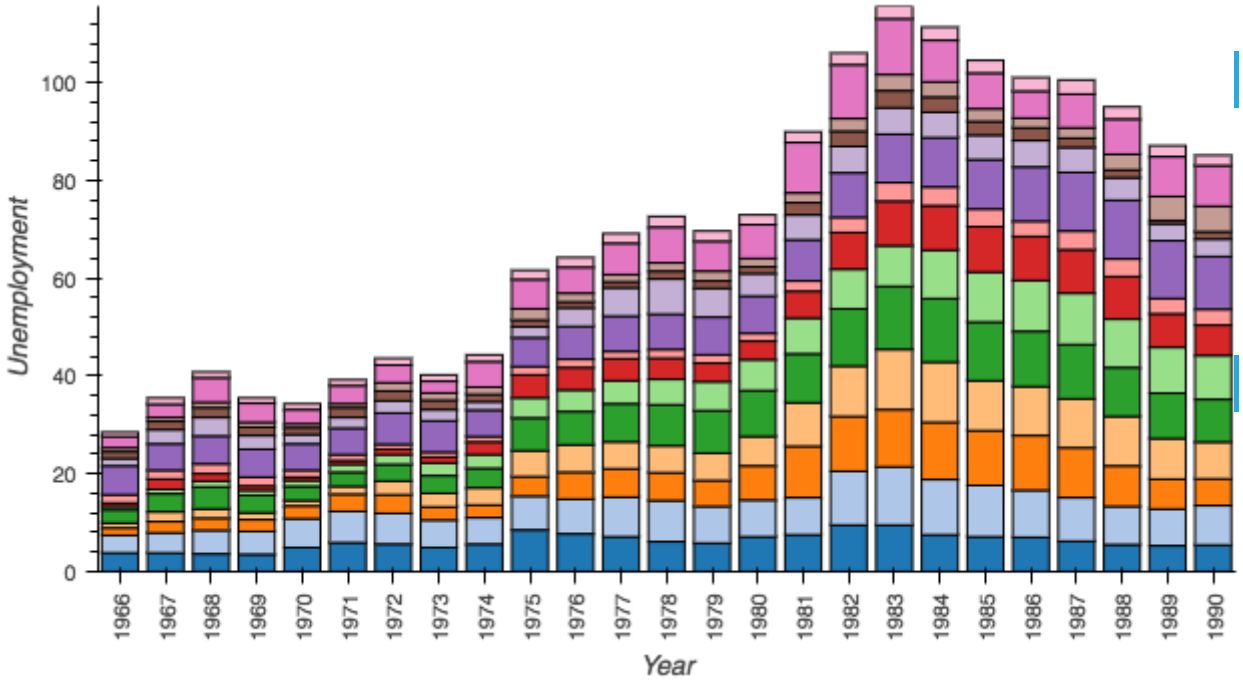
Out[24]:

	country	year	gdp	unem	capmob	trade
0	United States	1966	5.111141	3.8	0	9.622906
1	United States	1967	2.277283	3.8	0	9.983546
2	United States	1968	4.700000	3.6	0	10.089120
3	United States	1969	2.800000	3.5	0	10.435930
4	United States	1970	-0.200000	4.9	0	10.495350

In [25]:
```
import holoviews
holoviews.extension('bokeh')

key_dimensions   = [('year', 'Year'), ('country', 'Country')]
value_dimensions = [('unem', 'Unemployment'), ('capmob', 'Capital Mobility'),
                    ('gdp', 'GDP Growth'), ('trade', 'Trade')]
macro = holoviews.Table(macro_df, kdims=key_dimensions, vdims=value_dimensions)
```

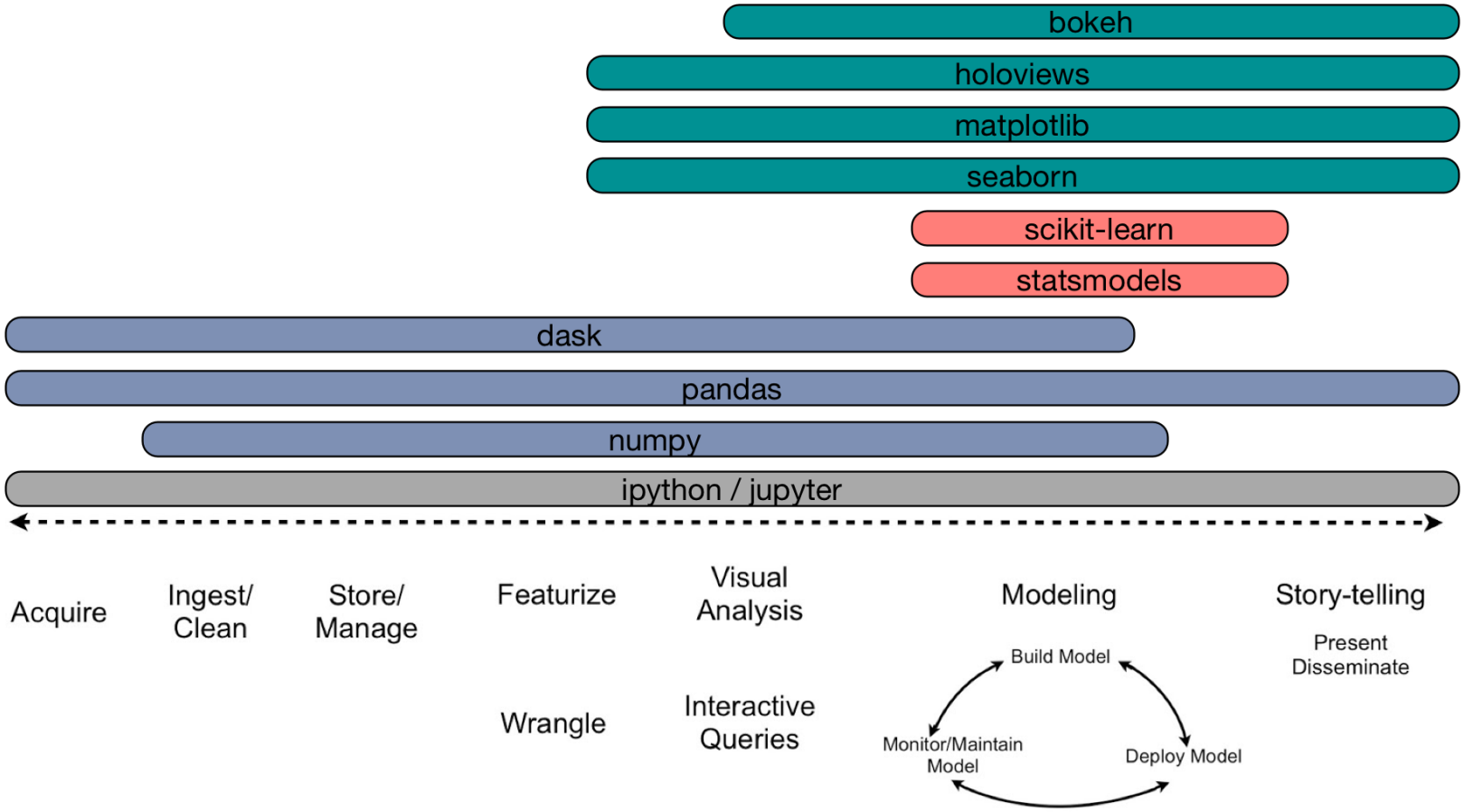
In [26]:
```
%%opts Bars [stack_index=1 xrotation=90 legend_cols=7 show_legend=False  show_fram
e=False tools=['hover']]
%%opts Bars (color=Cycle('Category20'))
%%opts Bars [width=650 height=350]

macro.to.bars([ 'Year', 'Country'], 'Unemployment', [])
```

Out[26]:



(https://bok

Modeling


bokeh
holoviews
matplotlib
seaborn
scikit-learn
statsmodels
dask
pandas
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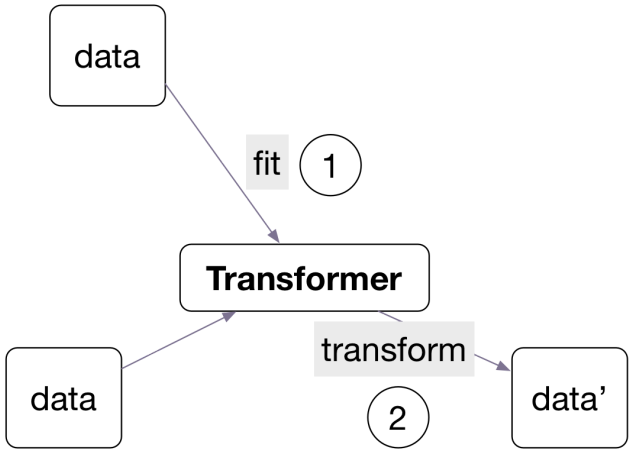
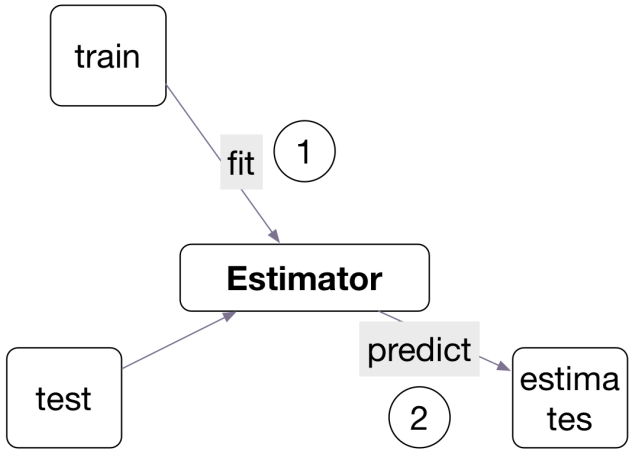
Acquire
Ingest/ Clean
Store/ Manage
Featurize
Wrangle
Visual Analysis
Interactive Queries
Modeling
Build Model
Deploy Model
Monitor/Maintain Model
Story-telling
Present
Disseminate

scikit-learn

- machine learning in Python
- provides
  - machine learning algorithms for classification, regression, clustering, dimensionality reduction, ...
  - building blocks of preprocessing and model selection workflows

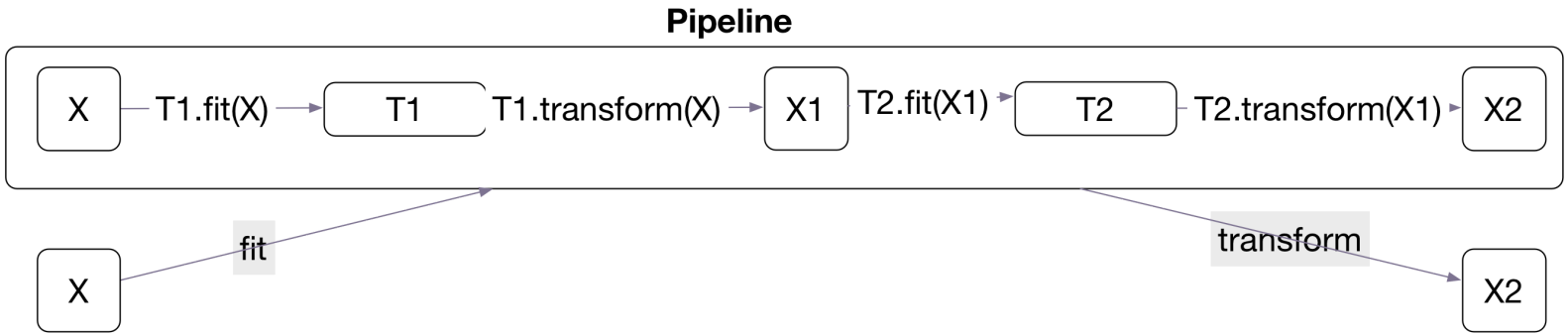
scikit-learn's modular approach: estimators, transformers, pipelines






```
transformer.fit(X)
X_t = transformer.transform(X)
```

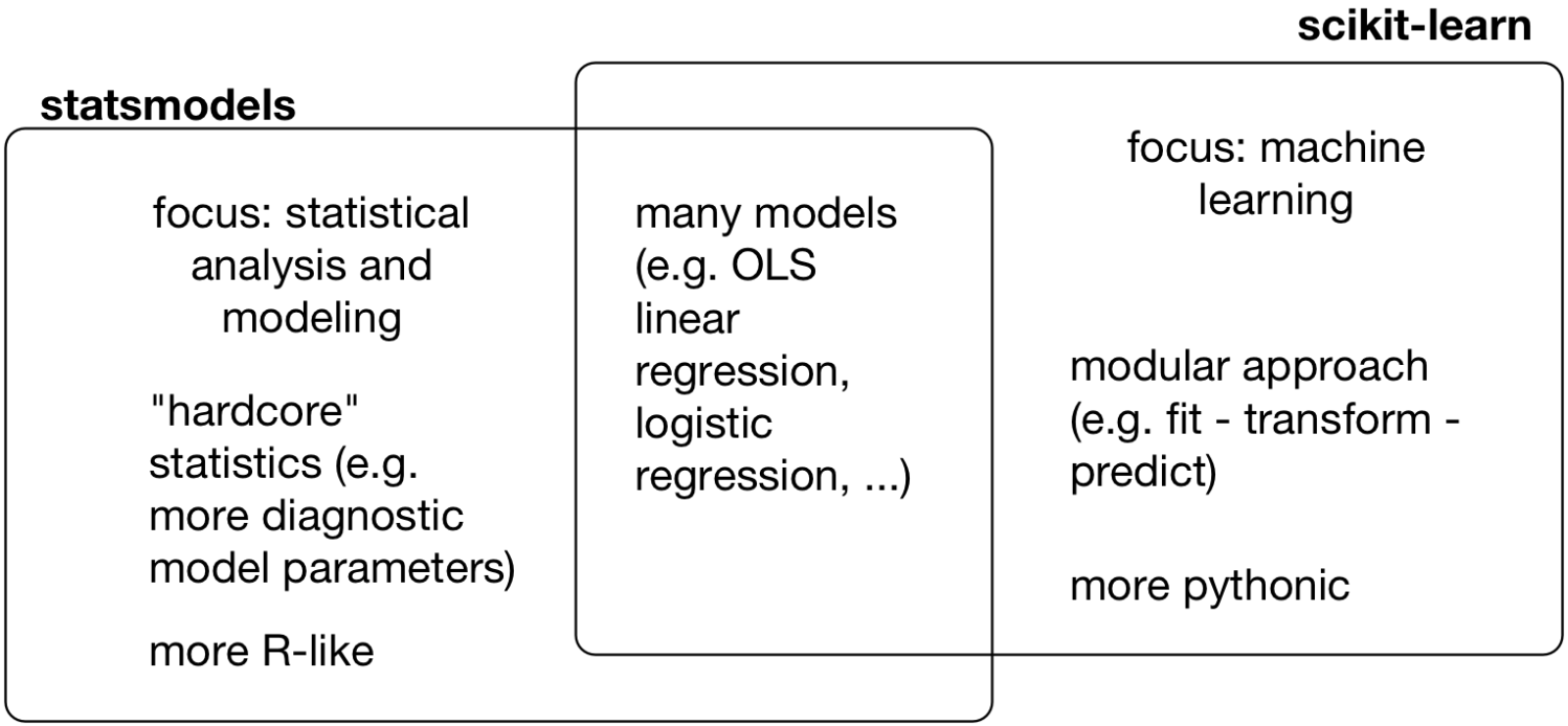
```
estimator.fit(X_train)
p = estimator.predict(X_test)
```



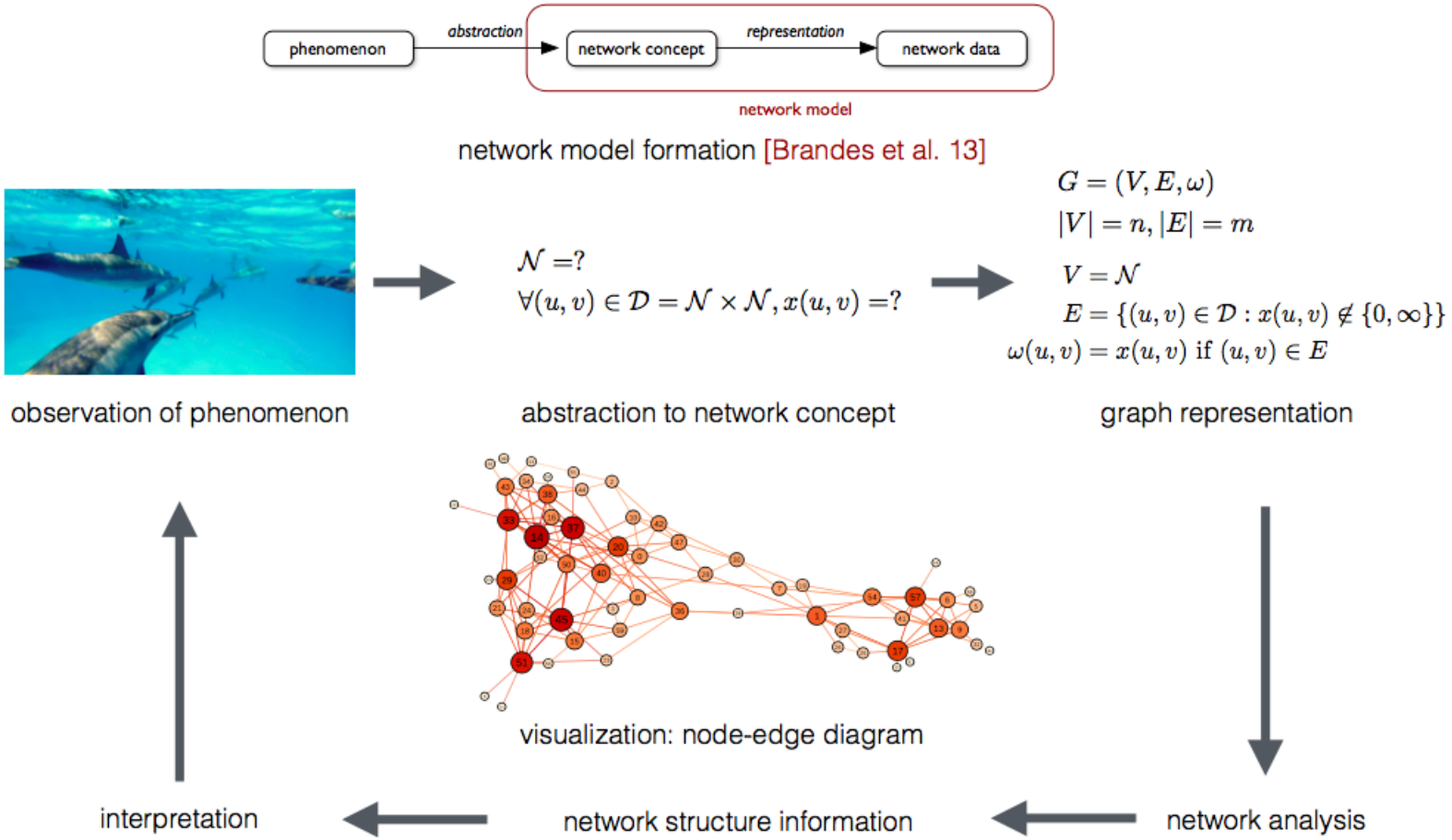
statsmodels

- statistical models, test, and exploration
  - R replacement
- contents, e.g.
  - regression models
  - time series analysis (e.g. ARIMA)
  - statistical test (e.g. t-test)

statsmodels vs scikit-learn



and now for something completely different: network analysis

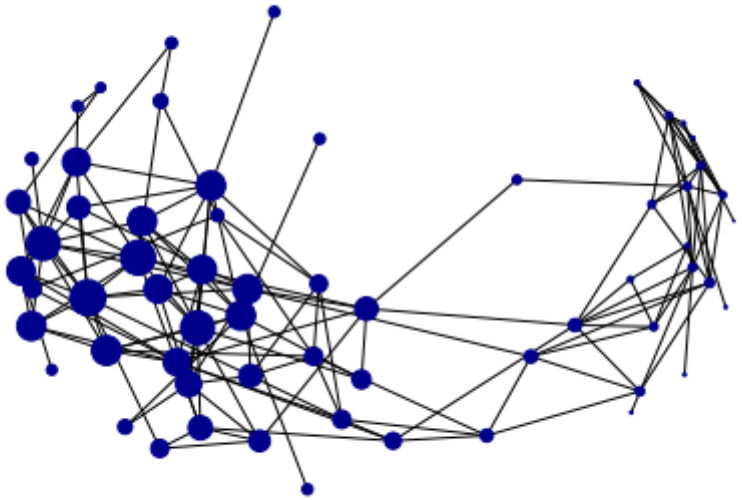


networkx

- creation, manipulation, and study of the structure of complex networks
- provides
  - algorithms for network analysis (centrality, diameter, ...)
  - algorithms for constructing graphs
  - ...
- pure Python
  - any object can be a node

In [27]:

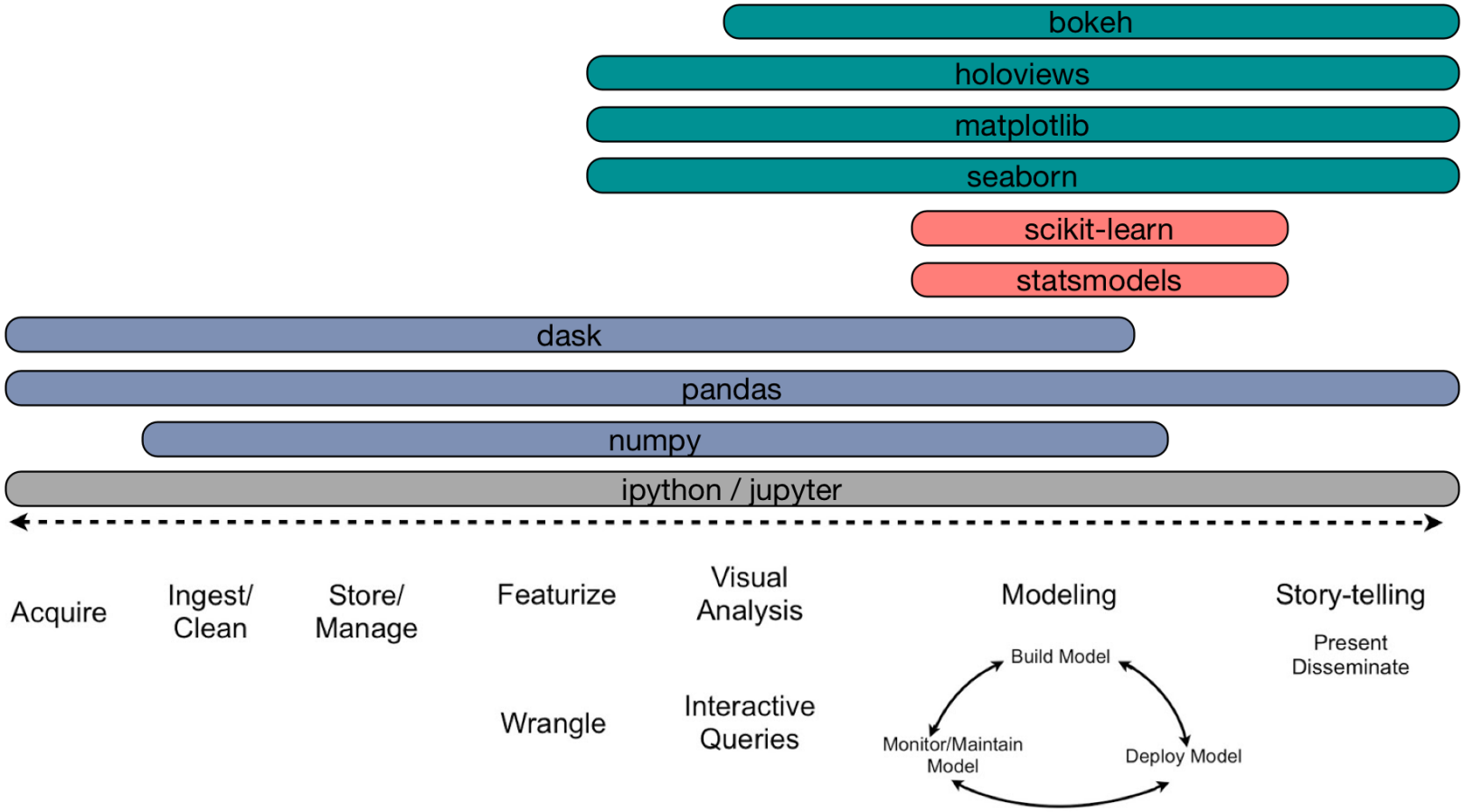
```
import networkx

G = networkx.read_edgelist("data/dolphins.edgelist")
ec = networkx.eigenvector_centrality(G)
networkx.draw(G,
              node_size=numpy.fromiter(iter(ec.values()), dtype=float) * 1000,
              node_color='darkblue',  pos=networkx.spring_layout(G))
```



need to do graph data analysis at scale?

- again, put algorithms and data structures into compiled code with
  - **igraph**
  - **graph-tool**
  - **networkit**

meta-tools


bokeh
holoviews
matplotlib
seaborn
scikit-learn
statsmodels
dask
pandas
numpy
ipython / jupyter
Acquire
Ingest/ Clean
Store/ Manage
Featurize
Wrangle
Visual Analysis
Interactive Queries
Modeling
Build Model
Deploy Model
Monitor/Maintain Model
Story-telling
Present
Disseminate

ipython

IP[y]

- powerful interactive Python shell
- tools for parallel computing (ipyparallel)

ipython extension: rpy2.ipython (formerly known as rmagic)

- seamless conversion of R and pandas dataframes between cells

In [29]:
```
%load_ext rpy2.ipython
```

In [30]:
```
df = pandas.read_csv("data/iris.csv", sep=";")
```

In [31]:
```
%%R -i df
head(df)
```

```
  Unnamed..0 sepal_length sepal_width petal_length petal_width species
0          0          5.1         3.5          1.4         0.2  setosa
1          1          4.9         3.0          1.4         0.2  setosa
2          2          4.7         3.2          1.3         0.2  setosa
3          3          4.6         3.1          1.5         0.2  setosa
4          4          5.0         3.6          1.4         0.2  setosa
5          5          5.4         3.9          1.7         0.4  setosa
```

In [32]:
```
%%R -o df2
df2 <- read.csv(file="data/iris.csv", header=TRUE, sep=";")
```

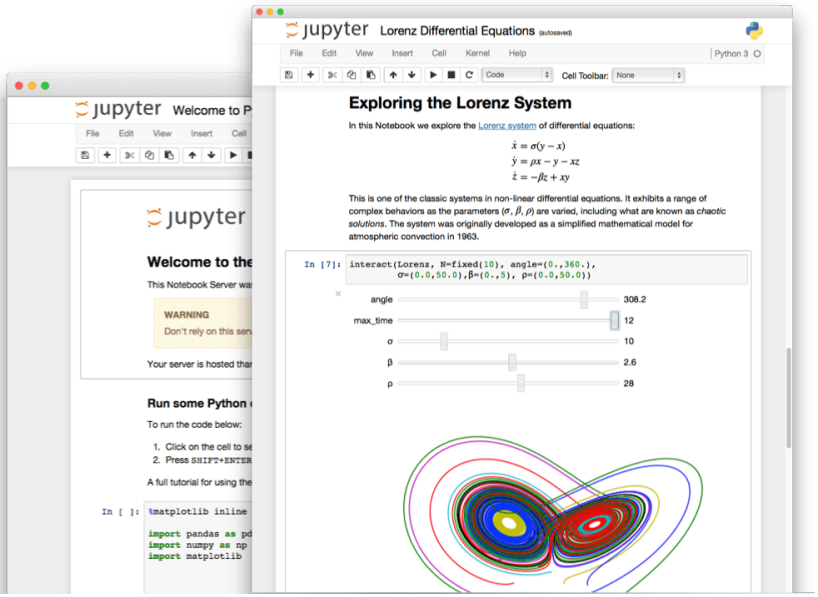
In [33]:
```
df2.describe()
```

Out[33]:

	X	sepal_length	sepal_width	petal_length	petal_width
count	150.000000	150.000000	150.000000	150.000000	150.000000
mean	74.500000	5.843333	3.057333	3.758000	1.199333
std	43.445368	0.828066	0.435866	1.765298	0.762238
min	0.000000	4.300000	2.000000	1.000000	0.100000
25%	37.250000	5.100000	2.800000	1.600000	0.300000
50%	74.500000	5.800000	3.000000	4.350000	1.300000
75%	111.750000	6.400000	3.300000	5.100000	1.800000
max	149.000000	7.900000	4.400000	6.900000	2.500000

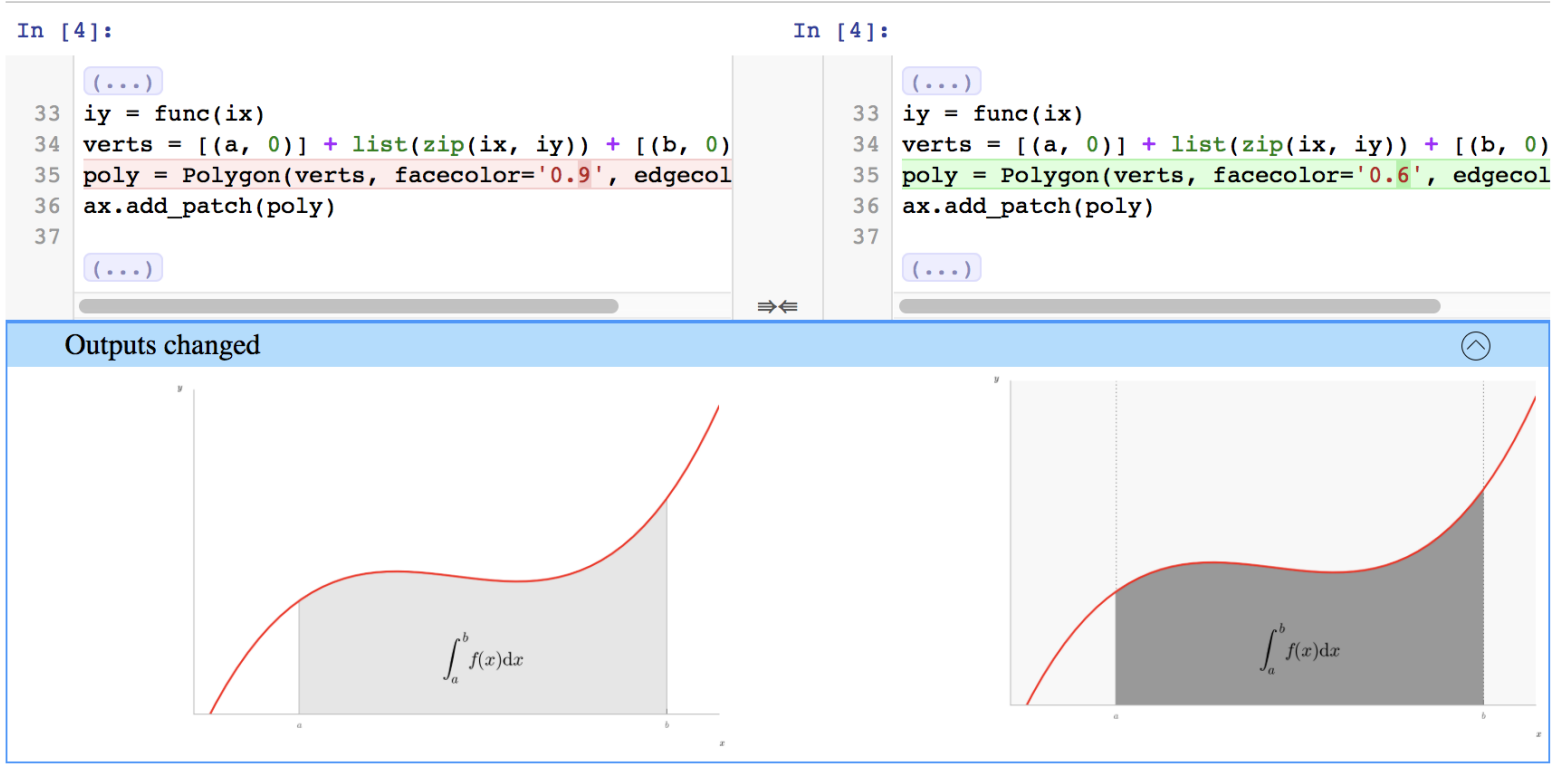
jupyter

- interactive notebooks, combining code, documentation, visualizations
  - Donald Knuth's literate programming (1992)
- language-agnostic, with support for e.g. R, Julia, Scala
- **nbconvert**: export notebooks to PDF, HTML, slides (e.g. this presentation)...



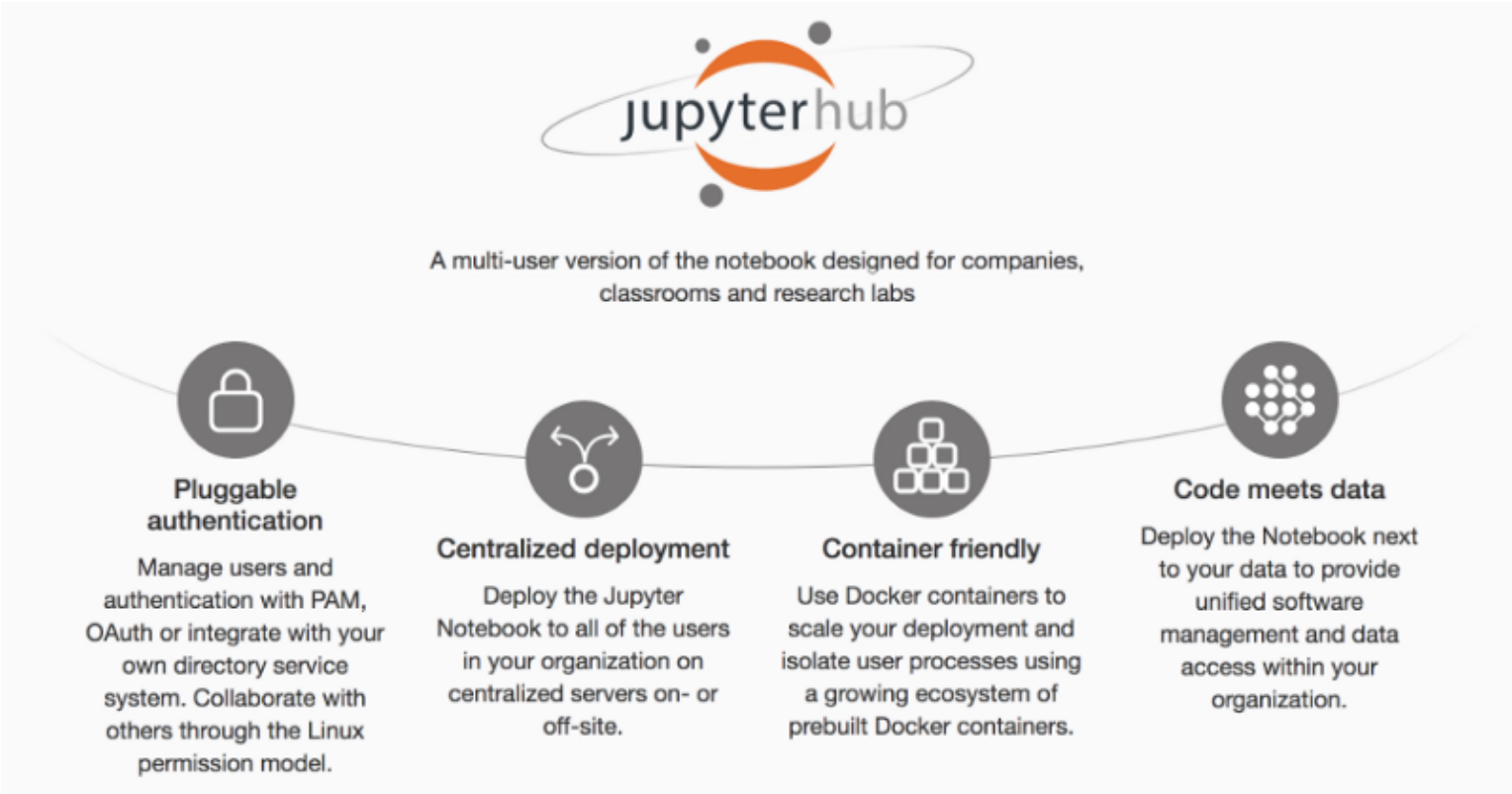
nbdime

- diff and merge tools for jupyter notebooks
- git integration!



jupyterhub

- multi-user server for jupyter notebooks



thank you for your attention!