Python's Data Science Stack

Jake VanderPlas @jakevdp

JSM, July 31, 2016

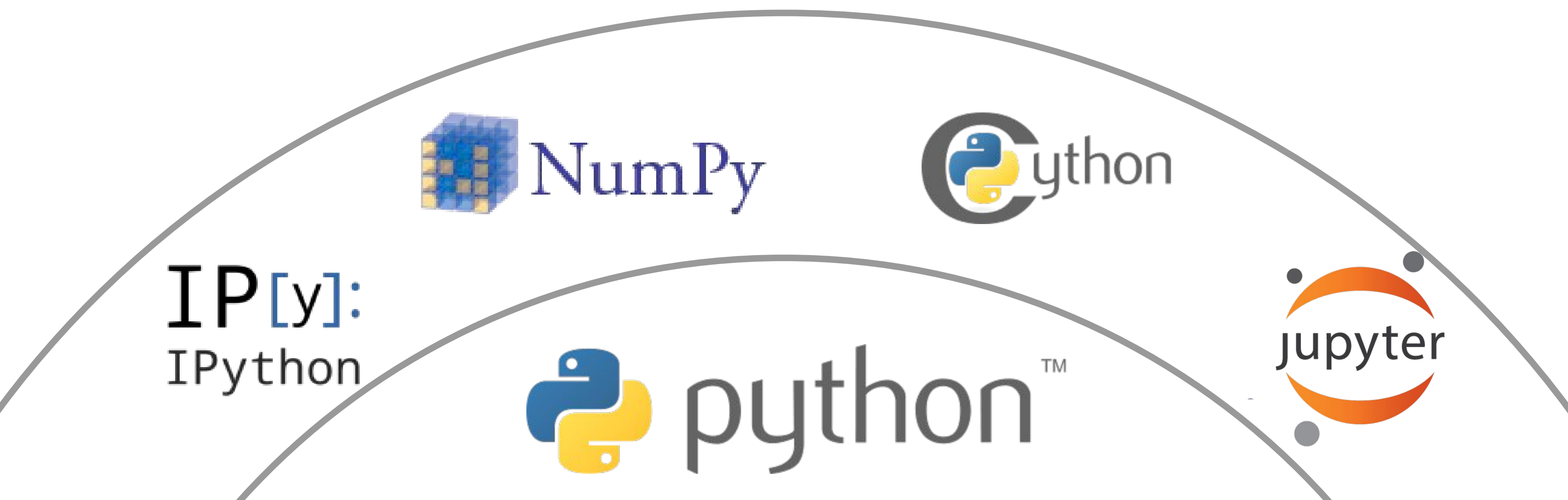
Python is *not* a statistical computing language!

Python is *not* a statistical computing language!

. . . and this may be its greatest strength as a language for statistical computing.

A Quick Tour of Python's Data Science Stack

Python's Data Science Stack


NumPy
Cython
IP[y]:
IPython
python
jupyter

NumPy = Numerical Python

Efficient array storage, manipulation, and computation

NumPy = Numerical Python

Efficient array storage, manipulation, and computation

```
In [1]: import numpy as np

        # Create a 5x5 uniform random matrix
        M = np.random.rand(5, 5)

        # Compute the SVD
        U, S, VT = np.linalg.svd(M)
        print(S)

[ 2.46102945  0.94542853  0.53550015  0.20705388  0.13071452]
```

NumPy

Cython

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Cython = C + Python

Super-set of the Python language that allows easy interfacing with C & Fortran libraries (e.g. BLAS, LAPACK, etc.) and also fast Python code.

Drives many of the packages in the data science stack.

NumPy

Cython

IPython

jupyter

python

IPython / Jupyter

Terminal, development environment, Notebooks, and more for efficient use of Python in day-to-day work localhost:8888/notebooks/Jaynes-Cumming-model.ipynb

jupyter Jaynes-Cumming-model (unsaved changes)

File Edit View Insert Cell Kernel Help | Python 3

Alternative view of the model

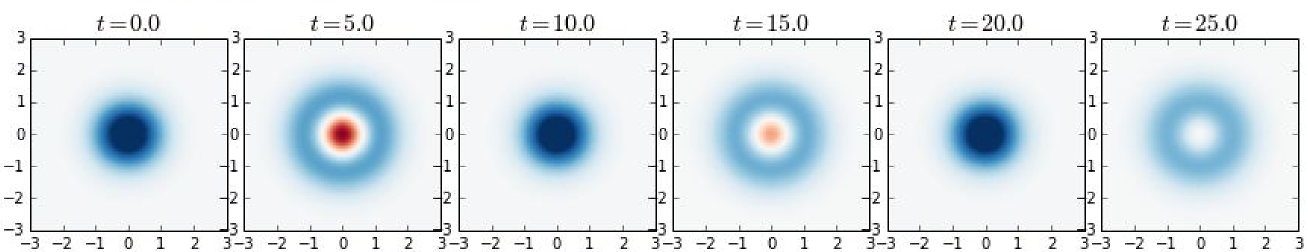
In [22]:

```
t_idx = where([tlist == t for t in [0.0, 5.0, 10, 15, 20, 25]])[1]
rho_list = array(output.states)[t_idx]

fig_grid = (2, len(rho_list)*2)
fig = plt.figure(figsize=(2.5*len(rho_list),5))

for idx, rho in enumerate(rho_list):
    rho_cavity = ptrace(rho, 0)
    W = wigner(rho_cavity, xvec, xvec)
    ax = plt.subplot2grid(fig_grid, (0, 2*idx), colspan=2)
    ax.contourf(xvec, xvec, W, 100, norm=mpl.colors.Normalize(-.25,.25), cmap=plt.get_cmap('RdBu'))
    ax.set_title(r"$t = %.1f$" % tlist[t_idx][idx], fontsize=16)

# plot the cavity occupation probability in the ground state
ax = plt.subplot2grid(fig_grid, (1, 1), colspan=(fig_grid[1]-2))
ax.plot(tlist, n_c, label="Cavity")
ax.plot(tlist, n_a, label="Atom excited state")
ax.legend()
ax.set_xlabel('Time')
ax.set_ylabel('Occupation probability');
```



NumPy

Cython

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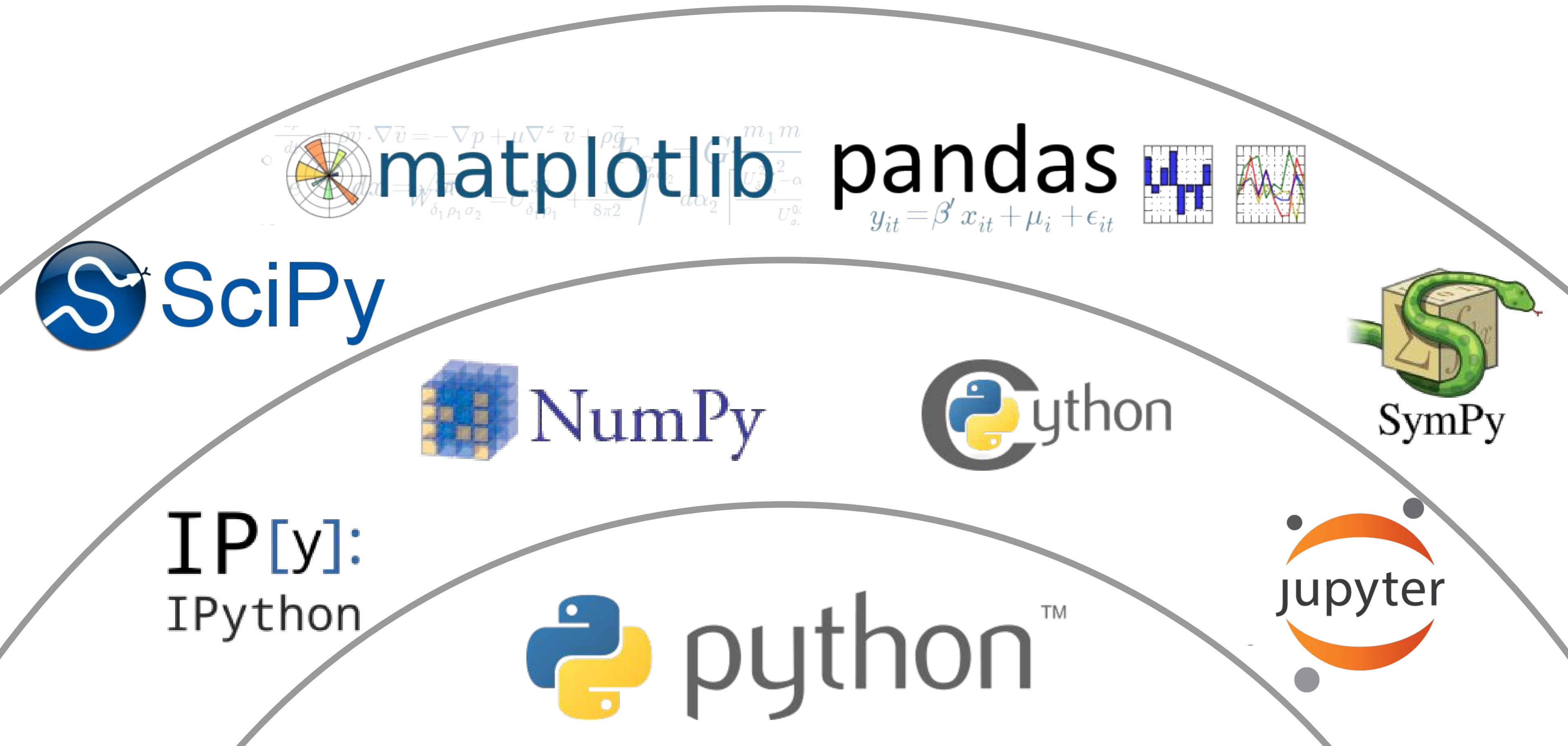
matplotlib
pandas
$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$
SciPy
NumPy
Cython
SymPy
IP[y]:
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jupyter
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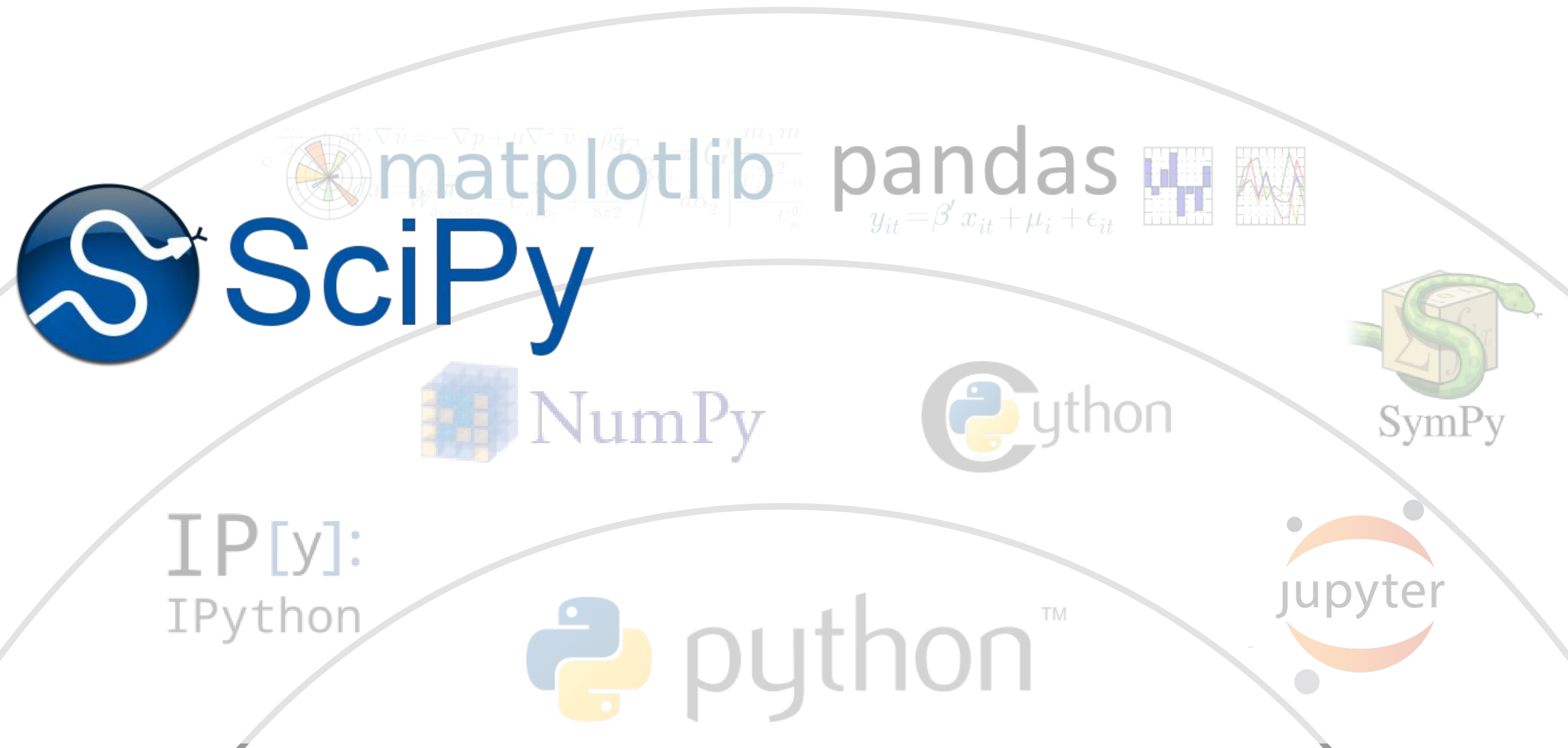
SciPy

Provides an interface to common scientific computing Tasks, including wrappers of many NetLib packages.



SciPy

Provi
Tasks

List from http://docs.scipy.org/doc/scipy/reference/

- Special functions (**scipy.special**)
- Integration (**scipy.integrate**)
- Optimization (**scipy.optimize**)
- Interpolation (**scipy.interpolate**)
- Fourier Transforms (**scipy.fftpack**)
- Signal Processing (**scipy.signal**)
- Linear Algebra (**scipy.linalg**)
- Sparse Eigenvalue Problems with ARPACK
- Compressed Sparse Graph Routines (**scipy.sparse.csgraph**)
- Spatial data structures and algorithms (**scipy.spatial**)
- Statistics (**scipy.stats**)
- Multidimensional image processing (**scipy.ndimage**)
- File IO (**scipy.io**)


matplotlib
pandas
$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$
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Sympy

Library for symbolic computation: algebraic operations, differentiation & integration, optimization, etc.

Sympy

Library for symbolic computation: algebraic operations, differentiation & integration, optimization, etc.

Polynomials and rational functions

`SymPy` does not expand brackets automatically. The function `expand` is used for this.

In [6]:
```
a=(x+y-z)**6
a
```

Out[6]: $(x+y-z)^6$

In [7]:
```
a=expand(a)
a
```

Out[7]:
$$x^6 + 6x^5y - 6x^5z + 15x^4y^2 - 30x^4yz + 15x^4z^2 + 20x^3y^3 - 60x^3y^2z + 60x^3yz^2 - 20x^3z^3 + 15x^2y^4 - 60x^2y^3z + 90x^2y^2z^2 - 60x^2yz^3 + 15x^2z^4 + 6xy^5 - 30xy^4z + 60xy^3z^2 - 60xy^2z^3 + 30xyz^4 - 6xz^5 + y^6 - 6y^5z + 15y^4z^2 - 20y^3z^3 + 15y^2z^4 - 6yz^5 + z^6$$


matplotlib
pandas
SciPy
NumPy
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SymPy
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jupyter
python

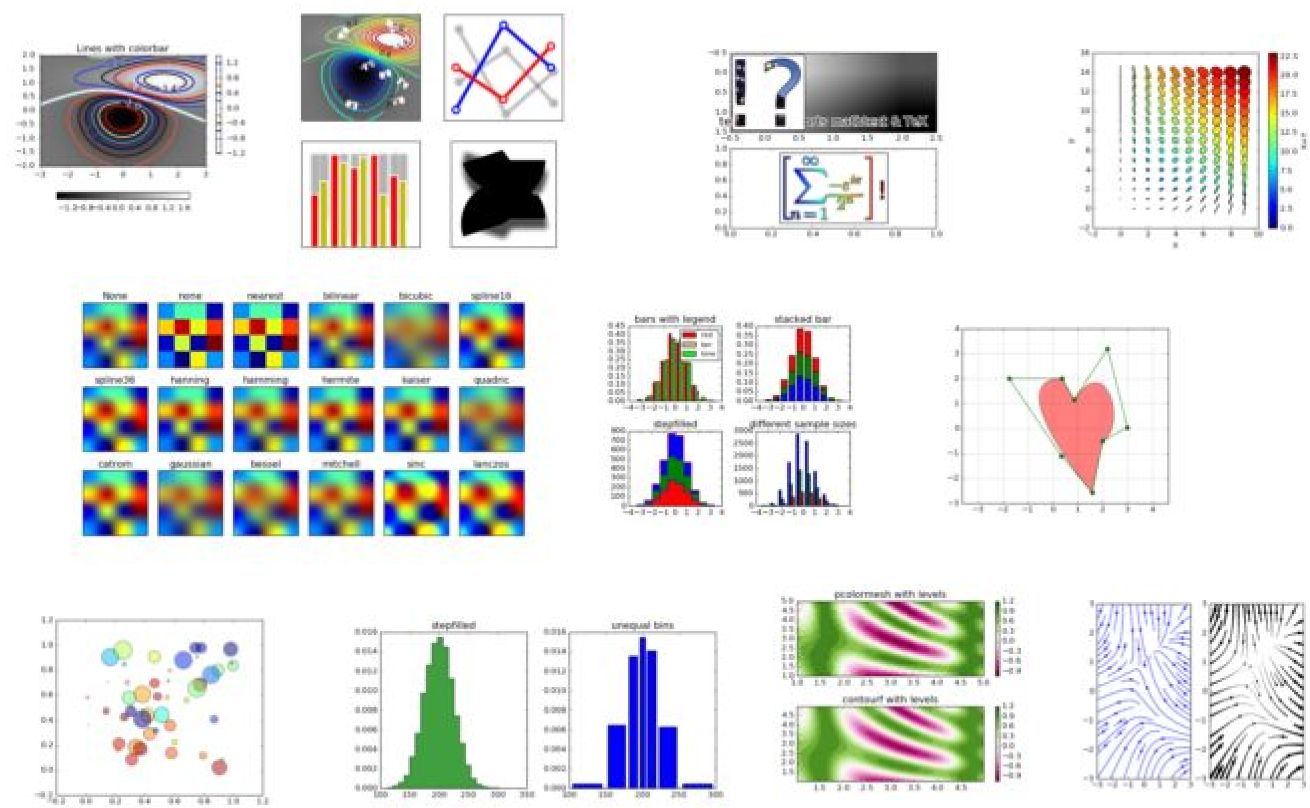
matplotlib

Matlab-inspired plotting and visualization

matplotlib

Matlab-inspired plotting and visualization

From http://matplotlib.org/gallery.html




matplotlib
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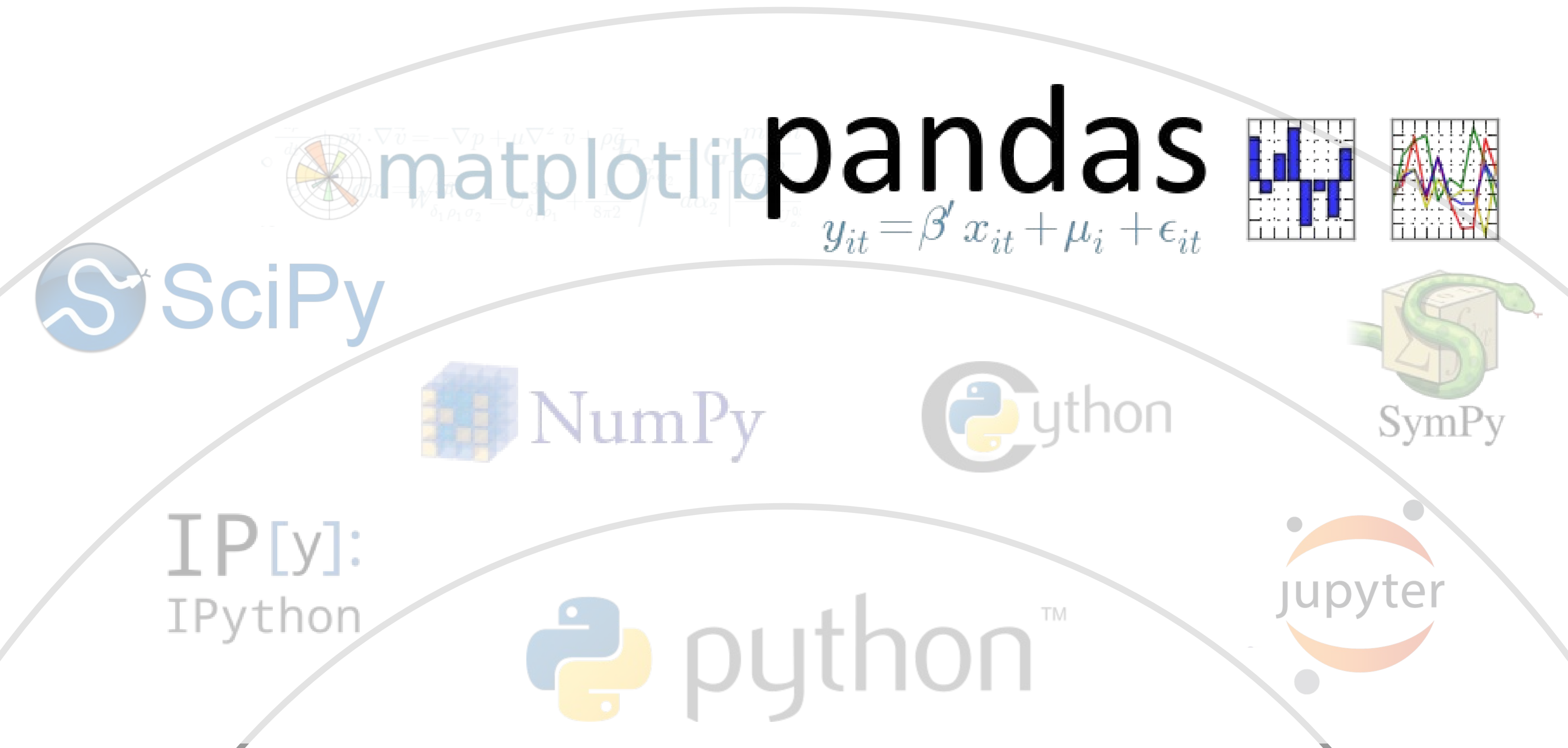
Pandas

R-inspired DataFrames & associated functionality (data munging & cleaning, group-by & transformations, and much more)



Pa

In [1]:

```python
import pandas as pd
data = pd.read_csv('iris.csv')
data.head()
```

Out[1]:

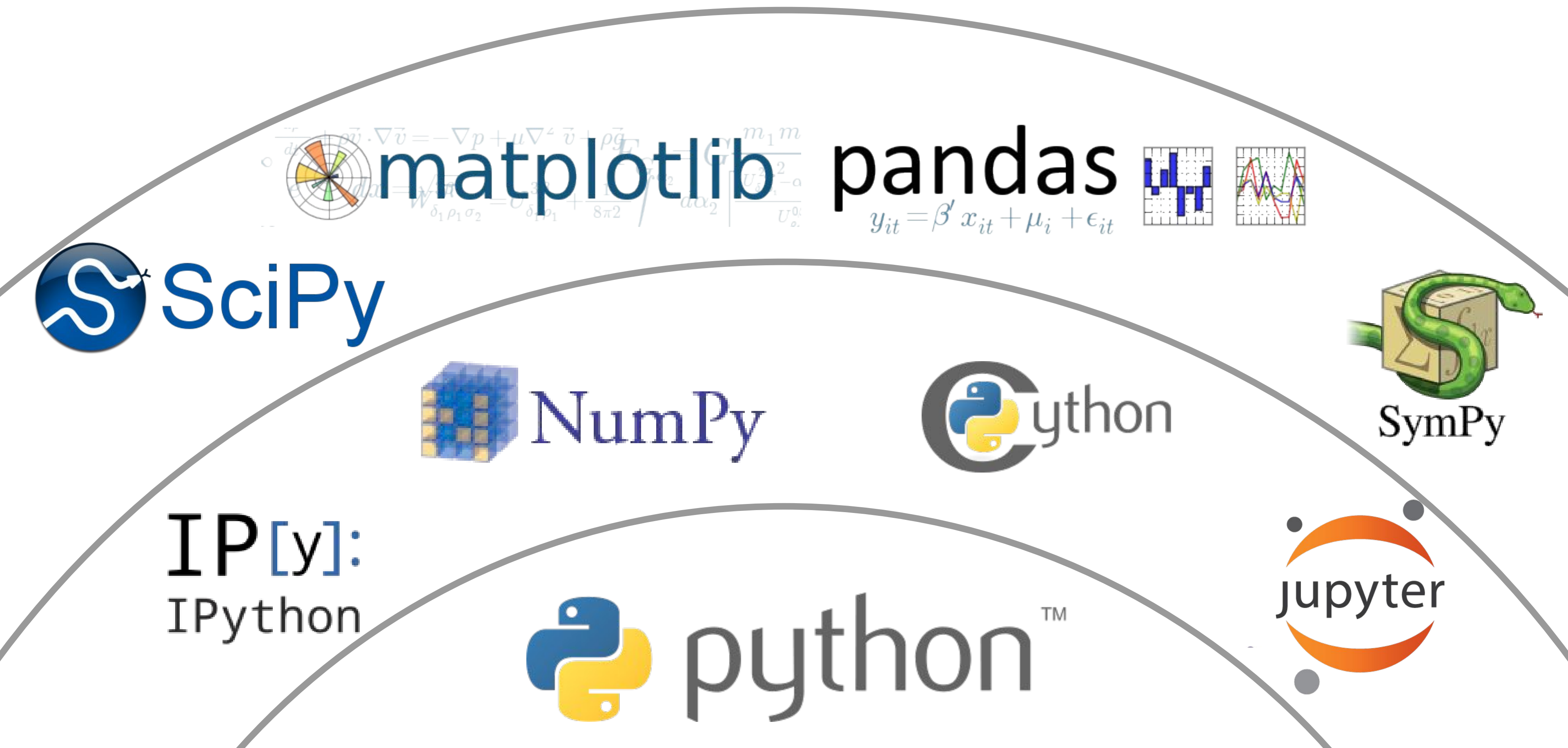
	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
0	5.1	3.5	1.4	0.2	setosa
1	4.9	3.0	1.4	0.2	setosa
2	4.7	3.2	1.3	0.2	setosa
3	4.6	3.1	1.5	0.2	setosa
4	5.0	3.6	1.4	0.2	setosa

In [2]:

```python
data.groupby('Species').mean()
```

Out[2]:

	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width
Species				
setosa	5.006	3.428	1.462	0.246
versicolor	5.936	2.770	4.260	1.326
virginica	6.588	2.974	5.552	2.026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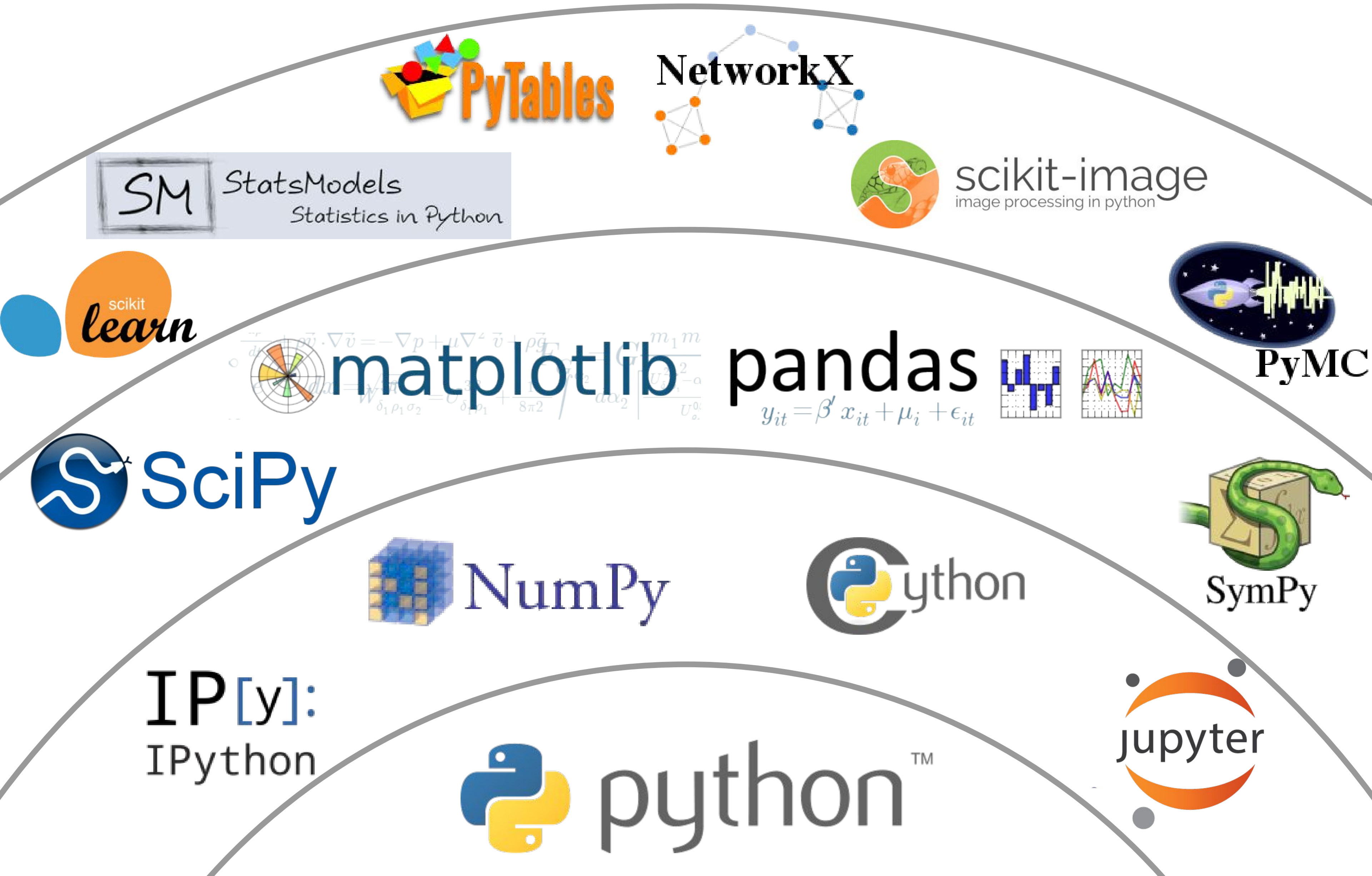
PyTables
NetworkX
SM
StatsModels
Statistics in Python
scikit-image
image processing in python
scikit
learn
PyMC
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pandas
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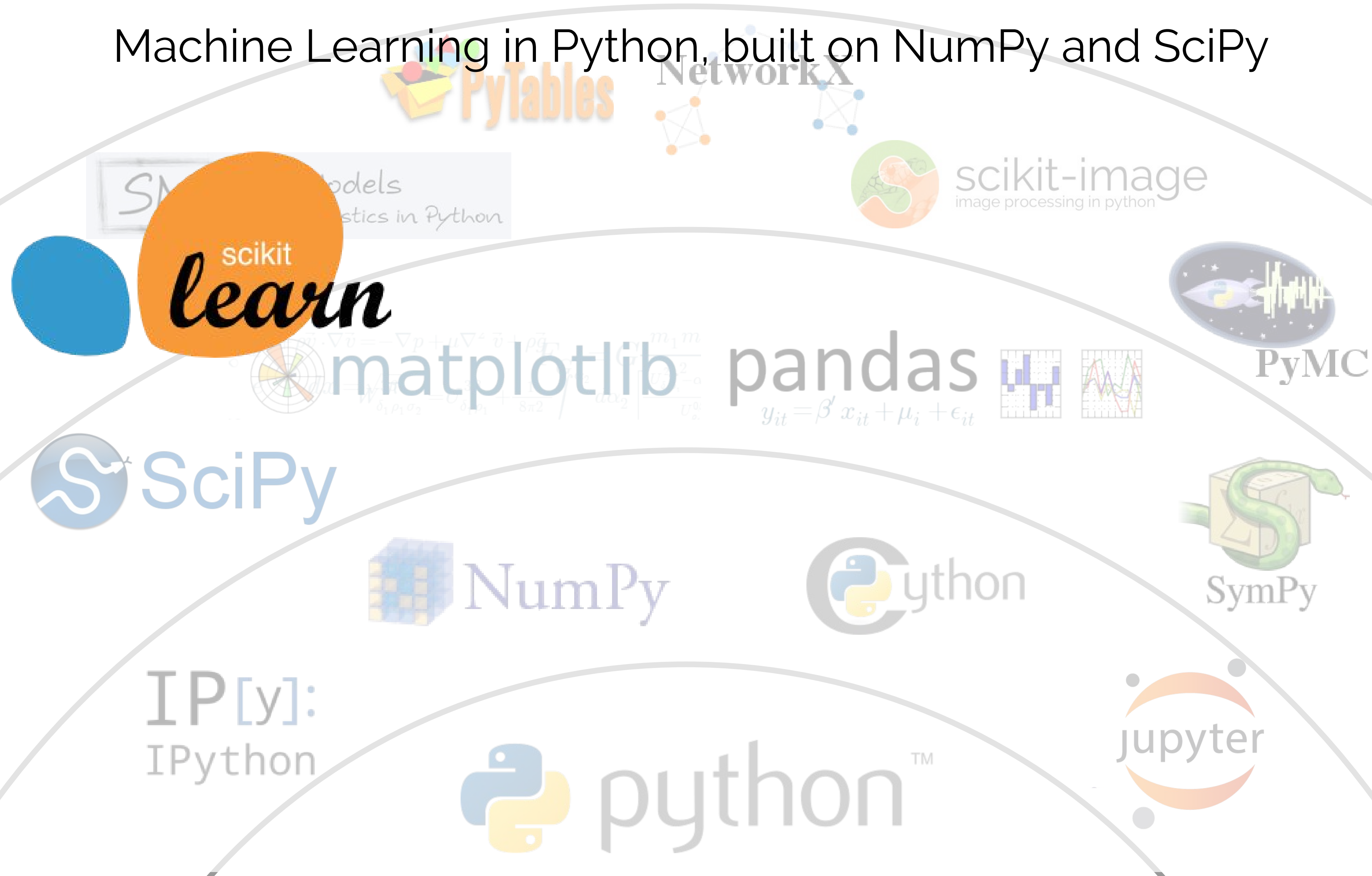
python ™

Scikit-Learn

Machine Learning in Python, built on NumPy and SciPy



Scikit-Learn

Machine Learning in Python, built on NumPy and SciPy

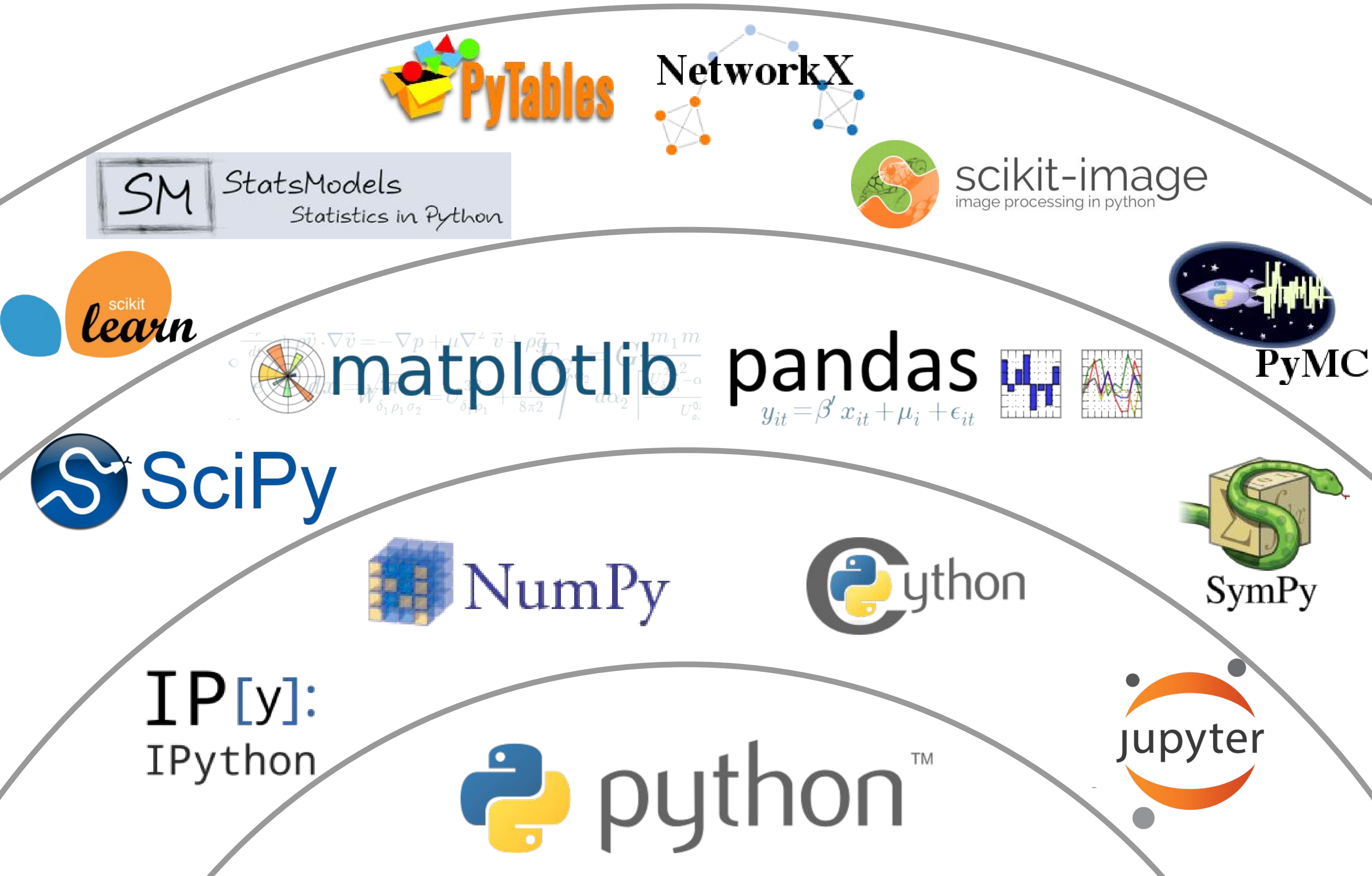
```
In [3]: from sklearn.ensemble import RandomForestClassifier

        features = data.drop('Species', axis=1)
        labels = data['Species']

        model = RandomForestClassifier()
        model.fit(features, labels)

        predicted = model.predict(features.iloc[:5])
        print(predicted)

        ['setosa' 'setosa' 'setosa' 'setosa' 'setosa']
```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PyMC
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astropy
BIOPYTHON
DIPY
NIPY
SunPy
(and many, many more)

PyTables
NetworkX

StatsModels
Statistics in Python
scikit-image
image processing in python

scikit learn
matplotlib
pandas
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PyMC

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Recent-ish Developments

- **Dask**: Parallelization of Data & Computation
- **Numba**: LLVM compilation of Python code
- **Jupyter Lab**: interactive & extensible polyglot development environment
- **Altair**: Declarative Visualization based on Vega-Lite

Dask: Parallel Computation for Distributed Arrays & DataFrames

With minimal changes to your NumPy & Pandas expressions, parallelize your computations over distributed data!

http://dask.pydata.org/

Dask: Parallel Computation for Distributed Arrays & DataFrames

A straightforward NumPy computation:

```
In [3]: import numpy as np

        # create an array of normally-distributed random numbers
        a = np.random.randn(1000)

        # multiply this array by a factor
        b = a * 4

        # find the minimum value
        b_min = b.min()
        print(b_min)

        -11.4051061336
```

http://dask.pydata.org/

Dask: Parallel Computation for Distributed Arrays & DataFrames

Dask uses the same expressions . . .

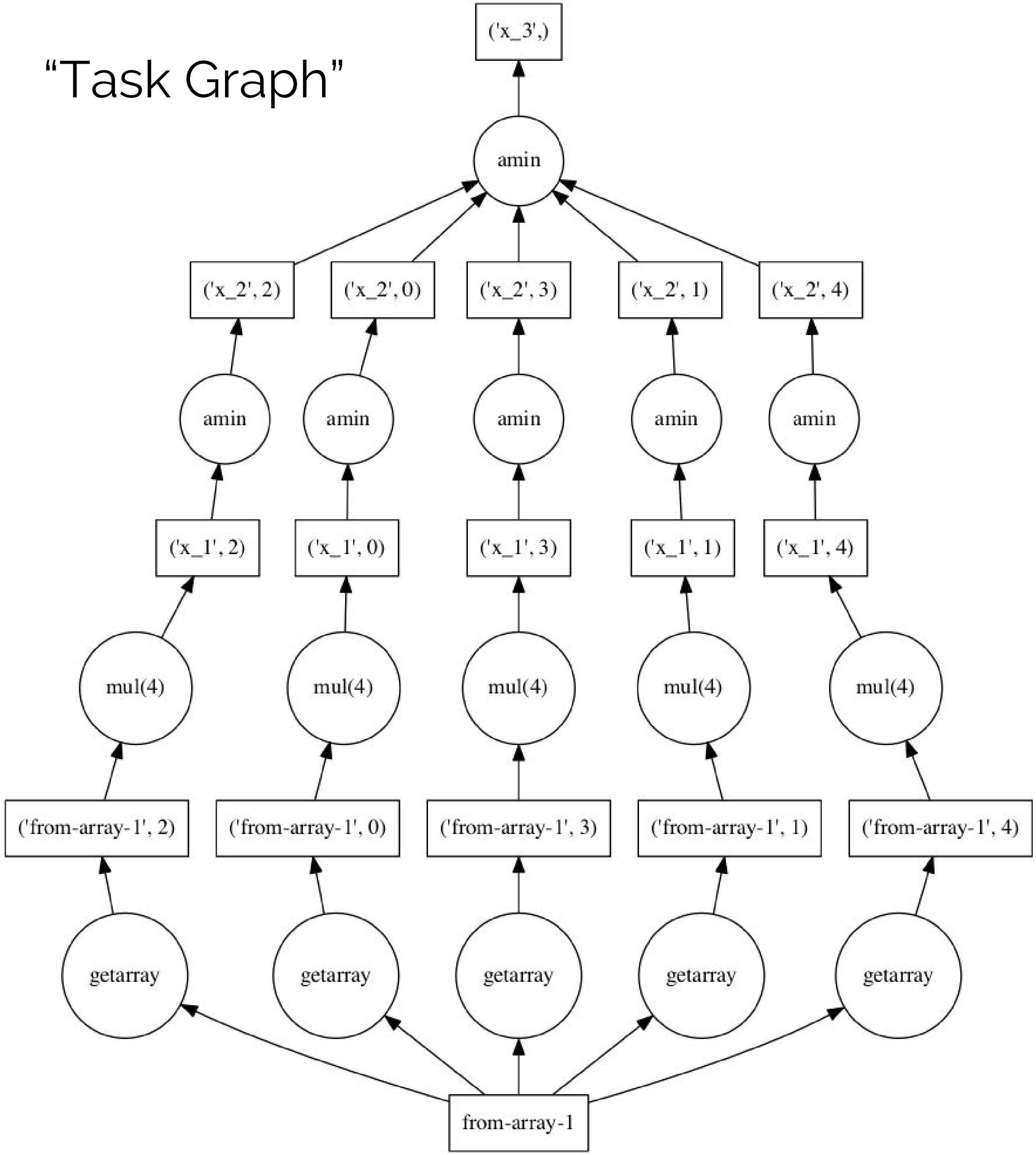
```
In [4]: import dask.array as da

        # create a dask array from the above array
        a2 = da.from_array(a, chunks=200)

        # multiply this array by a factor
        b2 = a2 * 4

        # find the minimum value
        b2_min = b2.min()
        print(b2_min)

        dask.array<x_3, shape=(), chunks=(), dtype=float64>
```

http://dask.pydata.org/

Dask
Distr

In [4

“Task Graph”



k.pydata.org/

Dask: Parallel Computation for Distributed Arrays & DataFrames

```
In [6]: b2_min.compute()

Out[6]: -11.405106133564583
```

http://dask.pydata.org/

Numba: JIT-compilation of Python code

With a simple decorator, Python is compiled to LLVM and executes at near C/Fortran speed!

```
def fib(n):
    a, b = 0, 1
    for i in range(n):
        a, b = b, a + b
    return a

%timeit fib(50)
```

```
100000 loops, best of 3: 3.83 µs per loop
```

Still some features missing, but very promising (see my blog posts for some examples).

http://numba.pydata.org/

Numba: JIT-compilation of Python code

With a simple decorator, Python is compiled to LLVM and executes at near C/Fortran speed!

```
@numba.jit
def fib(n):
    a, b = 0, 1
    for i in range(n):
        a, b = b, a + b
    return a

%timeit(fib(50))
```

```
1 loops, best of 3: 468 ns per loop
```

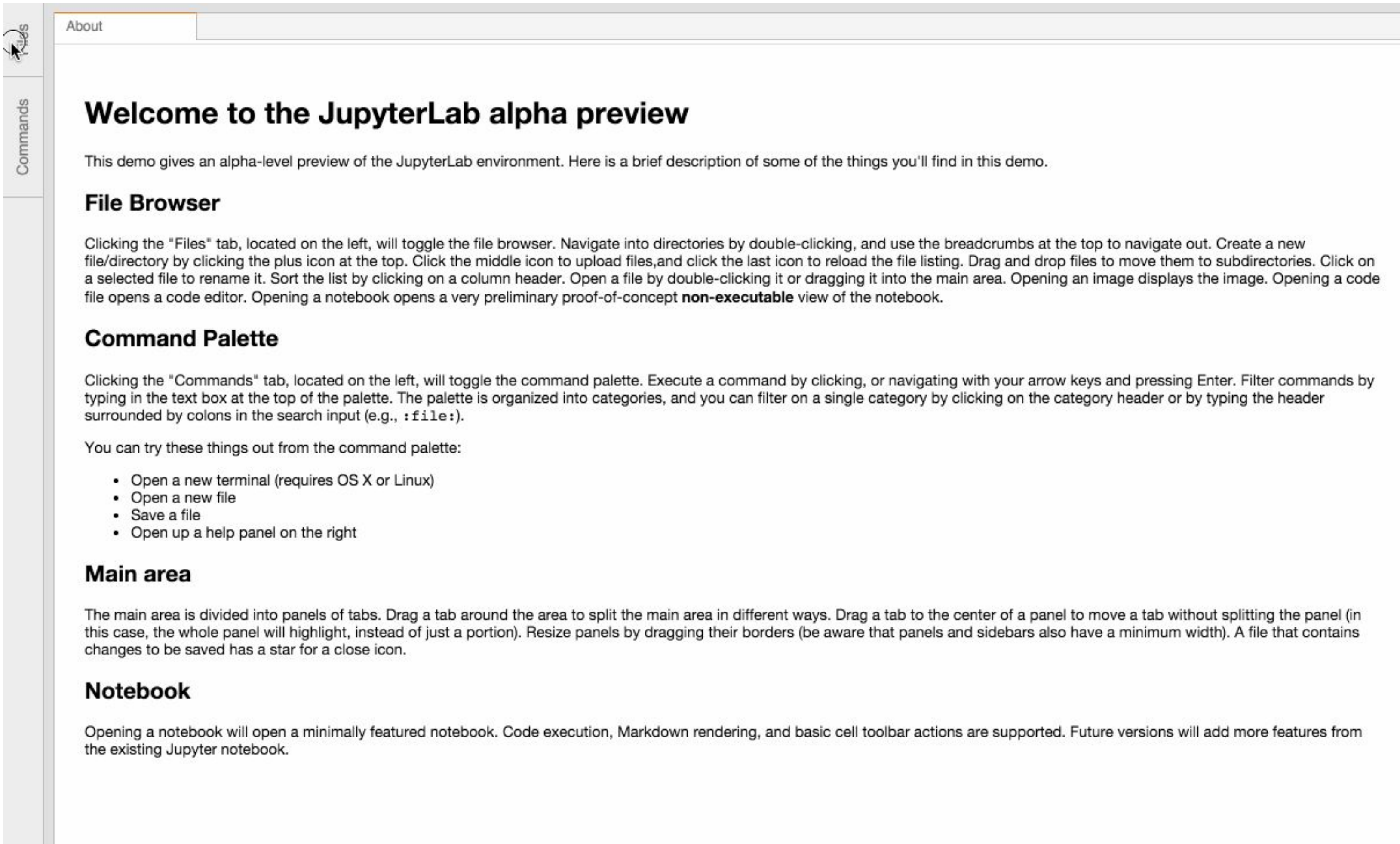
20x speedup!

Still some features missing, but very promising (see my blog posts for some examples).

http://numba.pydata.org/

Jupyter Lab

Jupyter beyond notebooks: extensible cross-platform interactive computing environment (release soon!)



Welcome to the JupyterLab alpha preview

This demo gives an alpha-level preview of the JupyterLab environment. Here is a brief description of some of the things you'll find in this demo.

File Browser

Clicking the "Files" tab, located on the left, will toggle the file browser. Navigate into directories by double-clicking, and use the breadcrumbs at the top to navigate out. Create a new file/directory by clicking the plus icon at the top. Click the middle icon to upload files,and click the last icon to reload the file listing. Drag and drop files to move them to subdirectories. Click on a selected file to rename it. Sort the list by clicking on a column header. Open a file by double-clicking it or dragging it into the main area. Opening an image displays the image. Opening a code file opens a code editor. Opening a notebook opens a very preliminary proof-of-concept **non-executable** view of the notebook.

Command Palette

Clicking the "Commands" tab, located on the left, will toggle the command palette. Execute a command by clicking, or navigating with your arrow keys and pressing Enter. Filter commands by typing in the text box at the top of the palette. The palette is organized into categories, and you can filter on a single category by clicking on the category header or by typing the header surrounded by colons in the search input (e.g., `:file:`).

You can try these things out from the command palette:

- Open a new terminal (requires OS X or Linux)
- Open a new file
- Save a file
- Open up a help panel on the right

Main area

The main area is divided into panels of tabs. Drag a tab around the area to split the main area in different ways. Drag a tab to the center of a panel to move a tab without splitting the panel (in this case, the whole panel will highlight, instead of just a portion). Resize panels by dragging their borders (be aware that panels and sidebars also have a minimum width). A file that contains changes to be saved has a star for a close icon.

Notebook

Opening a notebook will open a minimally featured notebook. Code execution, Markdown rendering, and basic cell toolbar actions are supported. Future versions will add more features from the existing Jupyter notebook.

Altair: Declarative Visualization based on Vega-Lite

The Visualization story in Python is somewhat confusing . . .

- Matplotlib
- Bokeh
- Plotly
- Seaborn
- Holoviews
- VisPy
- ggplot
- pandas plot
- Lightning

Each library has strengths, but arguably none is yet the “killer viz app” for Data Science.

Most Useful for Data Science is *Declarative Visualization*

Imperative

- Specify *How* something should be done.
- Must manually specify plotting steps
- Specification & Execution intertwined.

Declarative

- Specify *What* should be done
- Details determined automatically
- Separates Specification from Execution

Declarative visualization lets you think about **data** and **relationships**, rather than incidental details.

Enter Altair.

Declarative statistical visualization library for Python, driven by Vega-Lite

http://github.com/ellisonbg/altair

Collaboration with Brian Granger (Jupyter team), myself, and University of Washington's Interactive Data Lab

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jupyter

Example: Cars Dataset

In [1]:
```
from altair import Chart, load_dataset
data = load_dataset('cars')
```

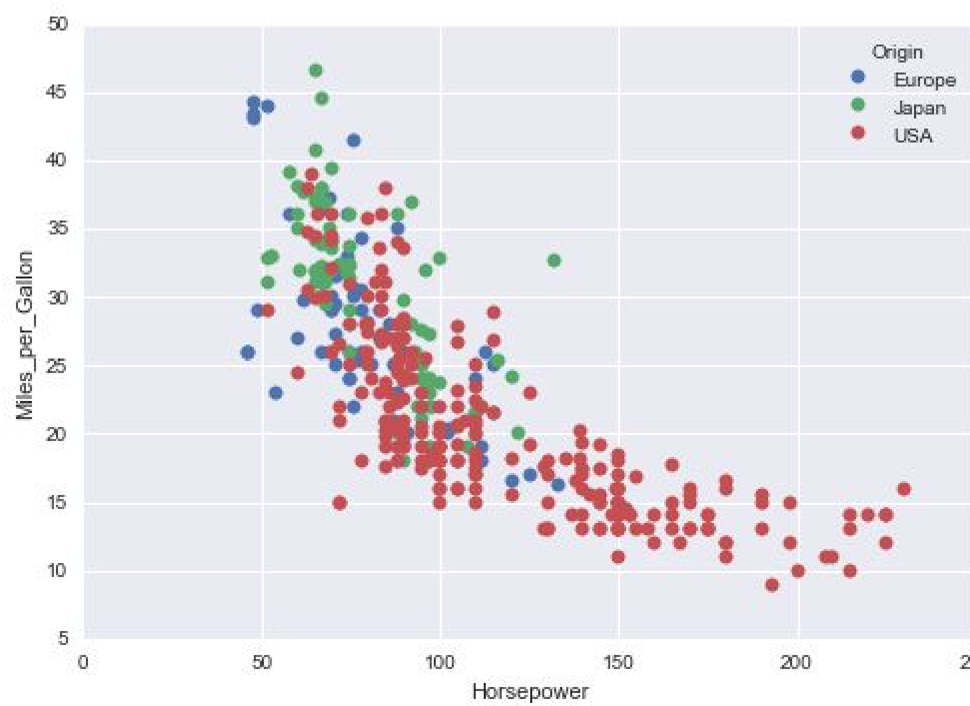
In [2]:
```
data.head()
```

Out[2]:

	Acceleration	Cylinders	Displacement	Horsepower	Miles_per_Gallon	Name	Origin
0	12.0	8	307.0	130.0	18.0	chevrolet chevelle malibu	USA
1	11.5	8	350.0	165.0	15.0	buick skylark 320	USA
2	11.0	8	318.0	150.0	18.0	plymouth satellite	USA
3	12.0	8	304.0	150.0	16.0	amc rebel sst	USA
4	10.5	8	302.0	140.0	17.0	ford torino	USA

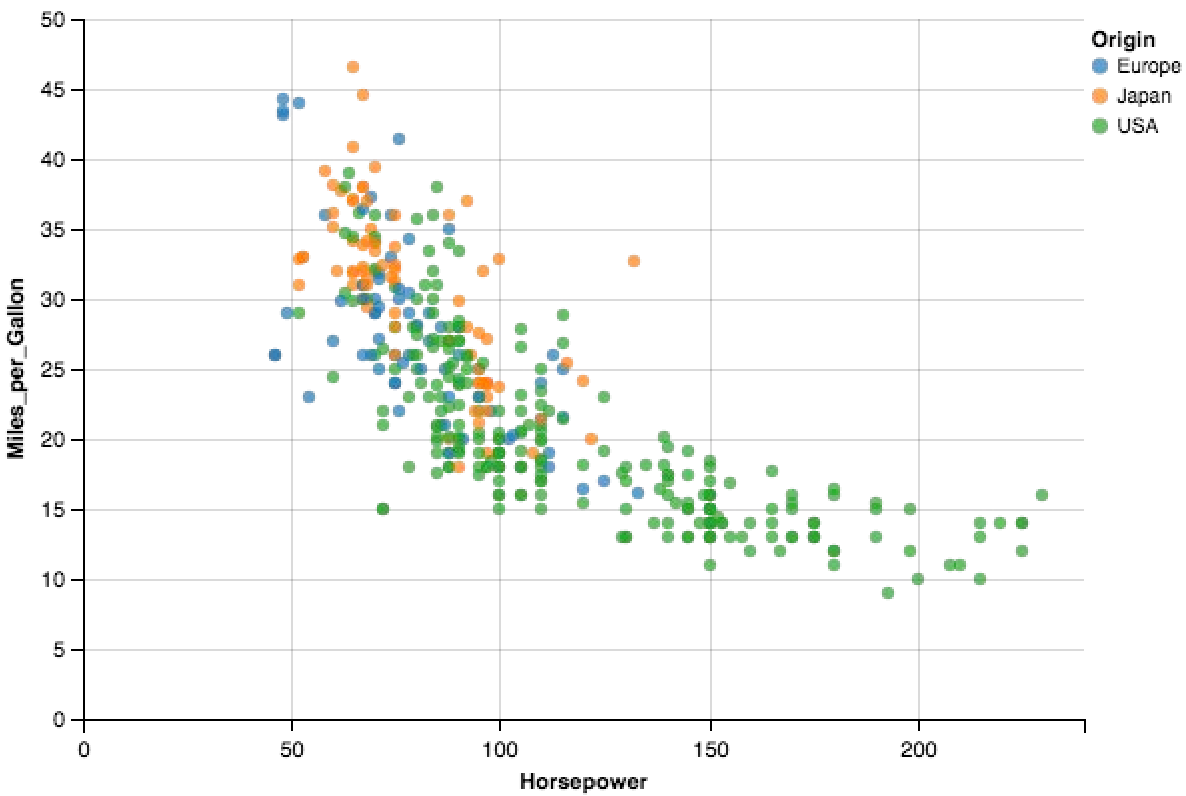
Matplotlib is an *imperative* API:

In [4]:
```
import matplotlib.pyplot as plt

def scatter(group):
    plt.plot(group['Horsepower'],
             group['Miles_per_Gallon'],
             'o', label=group.name)

data.groupby('Origin').apply(scatter)
plt.legend(title='Origin')
plt.xlabel('Horsepower')
plt.ylabel('Miles_per_Gallon');
```



Altair is a *declarative* API:

In [5]:
```
from altair import datasets, Chart

Chart(data).mark_circle().encode(
    x='Horsepower',
    y='Miles_per_Gallon',
    color='Origin',
)
```



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http://github.com/ellisonbg/altair

Altair is a *declarative* API:

Altair itself contains no renderers, but simply outputs a Vega-Lite visualization specification:

```
In [11]: chart.to_dict(data=False)

Out[11]: {'encoding': {'color': {'field': 'Origin', 'type': 'nominal'},
           'x': {'field': 'Horsepower', 'type': 'quantitative'},
           'y': {'field': 'Miles_per_Gallon', 'type': 'quantitative'}},
          'mark': 'circle'}
```

- Portable JSON serialization (Vega-Lite spec)
- Interest from other viz libraries (matplotlib, Bokeh, Plotly) in supporting this serialization.
- Potential for cross-language compatibility

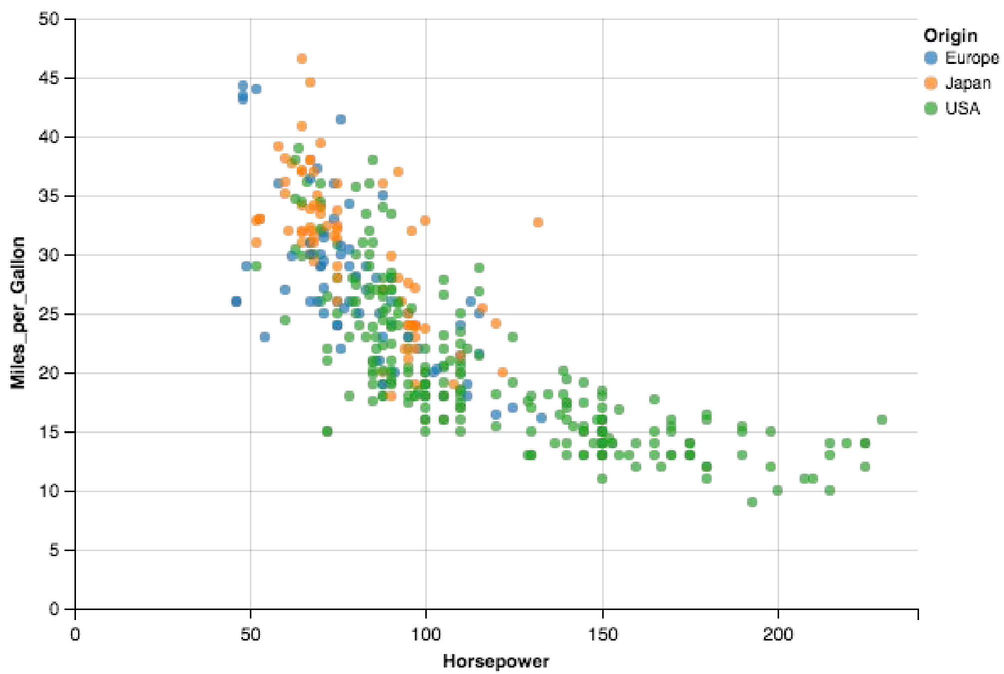
http://github.com/ellisonbg/altair

Vega-Lite schema is well-defined; allows round-trip between spec and code:

In [15]:
```
code = Chart.from_dict(spec).to_altair(data='data')
print(code)
```

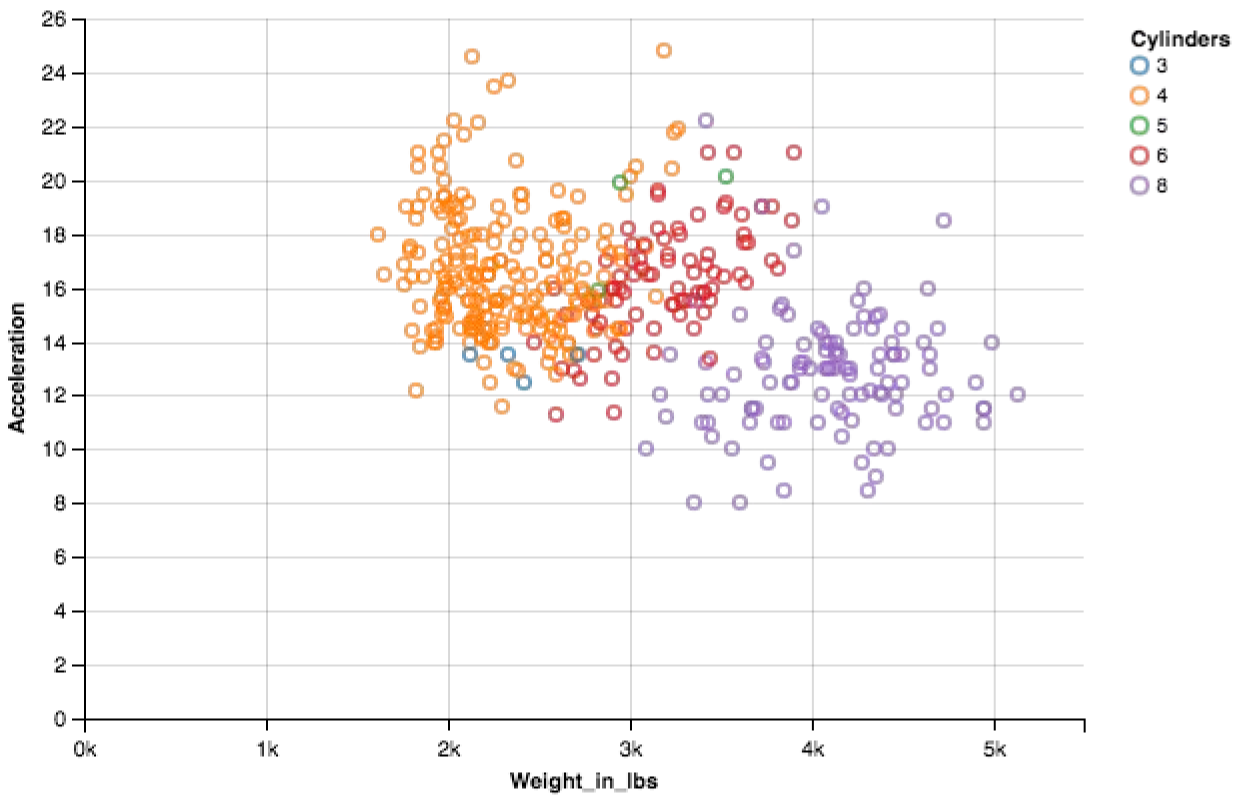
```
Chart(data).mark_circle().encode(
    color='Origin:N',
    x='Horsepower:Q',
    y='Miles_per_Gallon:Q',
)
```

In [16]:
```
eval(code)
```



Altair/Vega-Lite supports many plot types:

In [4]:
```
Chart(cars).mark_point().encode(
    x='Weight_in_lbs',
    y='Acceleration',
    color='Cylinders:N'
)
```



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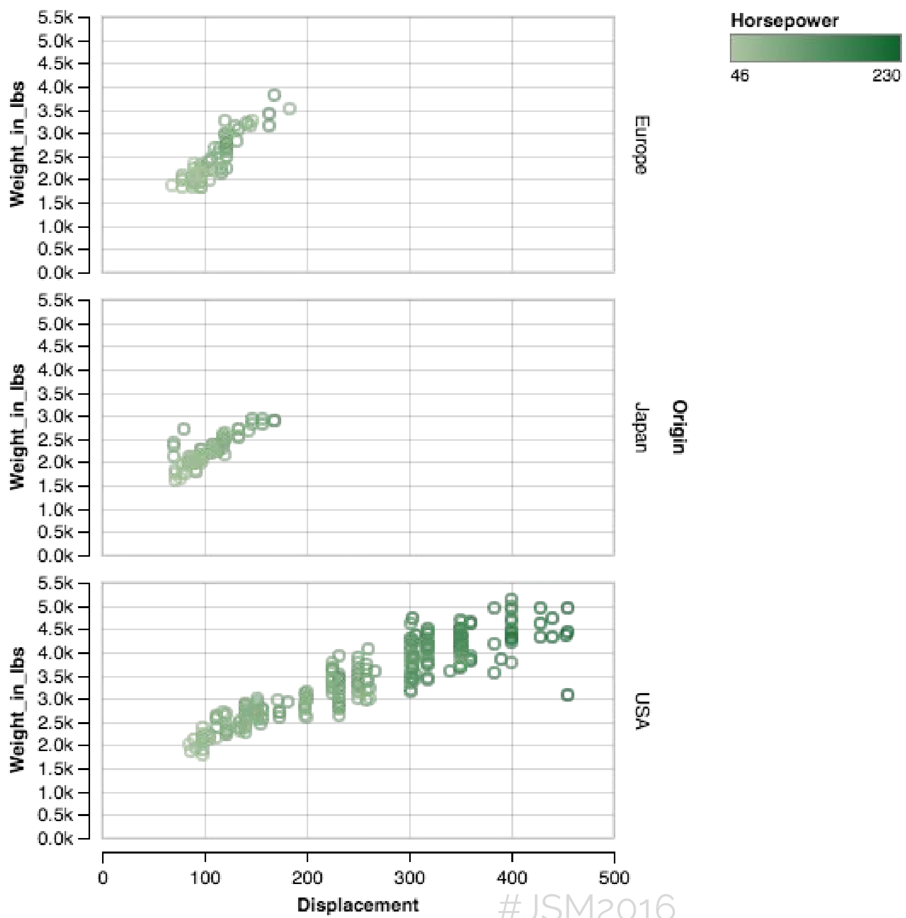
ADVANCING DATA-INTENSIVE DISCOVERY IN ALL FIELDS

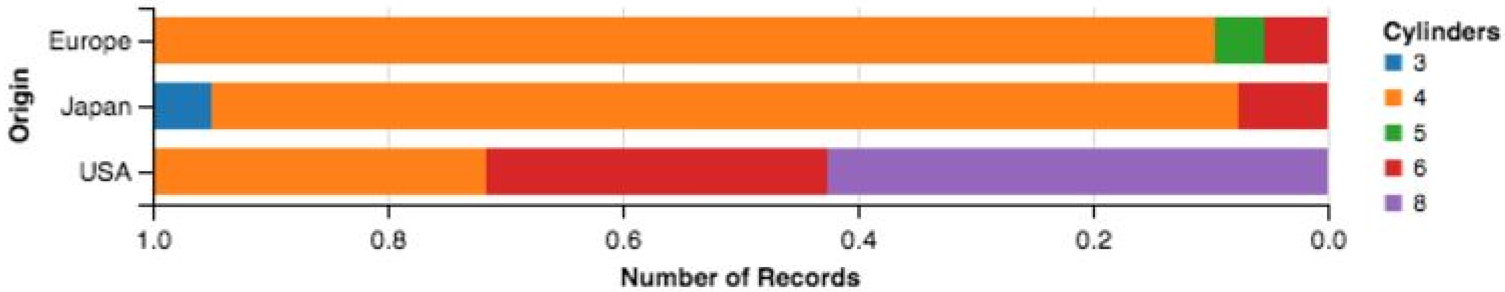
Altair/Vega-Lite supports many plot types:

In [6]:
```
Chart(cars).mark_point().encode(
    x='Displacement',
    y='Weight_in_lbs',
    color='Horsepower',
    row='Origin'
).configure_cell(width=300, height=150)
```



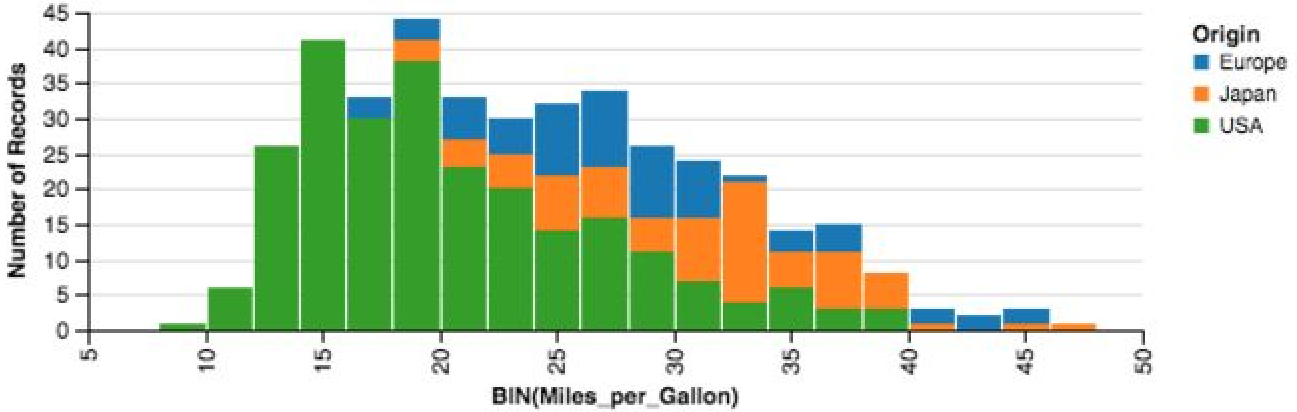
Altair/Vega-Lite supports many plot types:

```
In [7]: Chart(cars).mark_bar(stacked='normalize').encode(
            Y('Origin'),
            X('*:Q', aggregate='count', sort='descending'),
            Color('Cylinders:N')
        )
```



Altair/Vega-Lite supports many plot types:

In [8]:
```
Chart(cars).mark_bar().encode(
    X('Miles_per_Gallon', bin=Bin(maxbins=20)),
    Y('*:Q', aggregate='count'),
    Color('Origin')
).configure_cell(height=150)
```

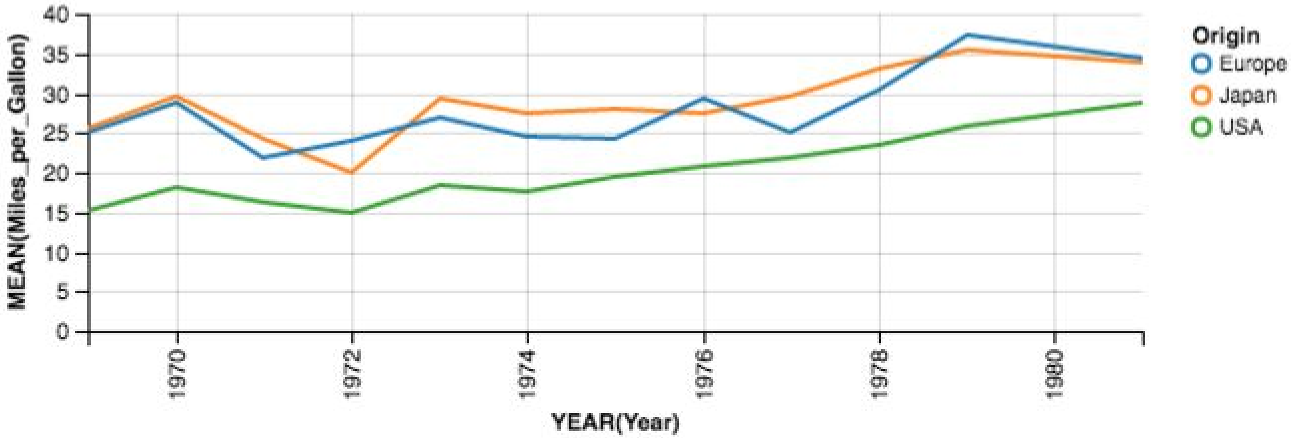


Altair/Vega-Lite supports many plot types:

In [9]:
```
Chart(cars).mark_text(applyColorToBackground=True).encode(
    Row('Origin:O'),
    Column('Cylinders:O'),
    Color('mean(Miles_per_Gallon):Q', sort='descending'),
    Text('mean(Miles_per_Gallon):Q')
)
```

Altair/Vega-Lite supports many plot types:

In [10]:
```
Chart(cars).mark_line().encode(
    X('Year:T', timeUnit='year'),
    Y('Miles_per_Gallon:Q', aggregate='mean'),
    Color('Origin:N')
).configure_cell(height=150)
```



Try Altair:

```
$ conda install altair --channel conda-forge
```

or

```
$ pip install altair
$ jupyter nbextension install --sys-prefix --py vega
```

For a Jupyter notebook tutorial, type

```
import altair
altair.tutorial()
```

http://github.com/ellisonbg/altair/

Thank You!

Email: jakevdp@uw.edu

Twitter: @jakevdp

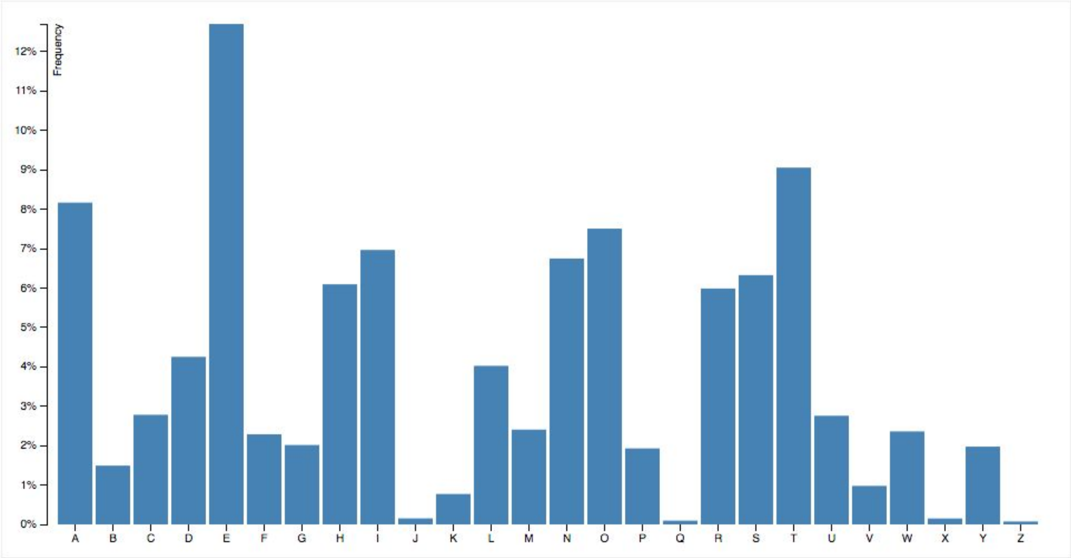
Github: jakevdp

Web: http://vanderplas.com

Blog: http://jakevdp.github.io

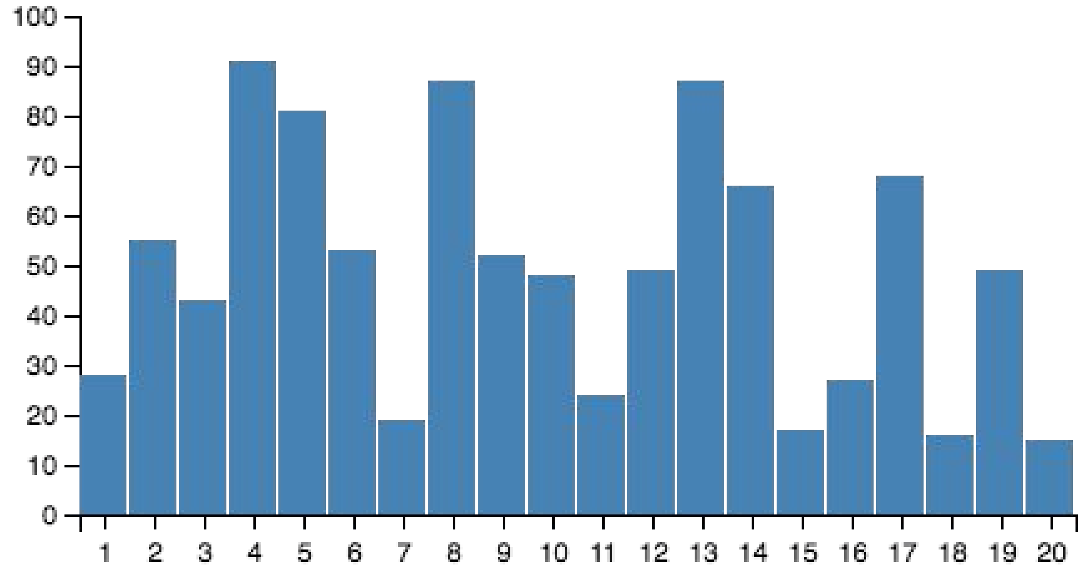
Bar Chart: d3

```
var margin = {top: 20, right: 20, bottom: 30, left: 40},
    width = 960 - margin.left - margin.right,
    height = 500 - margin.top - margin.bottom;

var x = d3.scale.ordinal()
    .rangeRoundBands([0, width], .1);

var y = d3.scale.linear()
    .range([height, 0]);

var xAxis = d3.svg.axis()
    .scale(x)
    .orient("bottom");

var yAxis = d3.svg.axis()
    .scale(y)
    .orient("left")
    .ticks(10, "%");

var svg = d3.select("body").append("svg")
    .attr("width", width + margin.left + margin.right)
    .attr("height", height + margin.top + margin.bottom)
  .append("g")
    .attr("transform", "translate(" + margin.left + "," + margin.top +
")");

d3.tsv("data.tsv", type, function(error, data) {
  if (error) throw error;

  x.domain(data.map(function(d) { return d.letter; }));
  y.domain([0, d3.max(data, function(d) { return d.frequency; })]);

  svg.append("g")
      .attr("class", "x axis")
      .attr("transform", "translate(0," + height + ")")
      .call(xAxis);

  svg.append("g")
      .attr("class", "y axis")
      .call(yAxis)
    .append("text")
      .attr("transform", "rotate(-90)")
      .attr("y", 6)
      .attr("dy", ".71em")
      .style("text-anchor", "end")
      .text("Frequency");

  svg.selectAll(".bar")
      .data(data)
    .enter().append("rect")
      .attr("class", "bar")
      .attr("x", function(d) { return x(d.letter); })
      .attr("width", x.rangeBand())
      .attr("y", function(d) { return y(d.frequency); })
      .attr("height", function(d) { return height - y(d.frequency);
});
});

function type(d) {
  d.frequency = +d.frequency;
  return d;
}
```



Bar Chart: Vega

```
{
  "width": 400,
  "height": 200,
  "padding": {"top": 10, "left": 30, "bottom": 30, "right": 10},
  "data": [
    {
      "name": "table",
      "values": [
        {"x": 1,  "y": 28}, {"x": 2,  "y": 55},
        {"x": 3,  "y": 43}, {"x": 4,  "y": 91},
        {"x": 5,  "y": 81}, {"x": 6,  "y": 53},
        {"x": 7,  "y": 19}, {"x": 8,  "y": 87},
        {"x": 9,  "y": 52}, {"x": 10, "y": 48},
        {"x": 11, "y": 24}, {"x": 12, "y": 49},
        {"x": 13, "y": 87}, {"x": 14, "y": 66},
        {"x": 15, "y": 17}, {"x": 16, "y": 27},
        {"x": 17, "y": 68}, {"x": 18, "y": 16},
        {"x": 19, "y": 49}, {"x": 20, "y": 15}
      ]
    }
  ],
  "scales": [
    {
      "name": "x",
      "type": "ordinal",
      "range": "width",
      "domain": {"data": "table", "field": "x"}
    },
    {
      "name": "y",
      "type": "linear",
      "range": "height",
      "domain": {"data": "table", "field": "y"},
      "nice": true
    }
  ],
  "axes": [
    {"type": "x", "scale": "x"},
    {"type": "y", "scale": "y"}
  ],
  "marks": [
    {
      "type": "rect",
      "from": {"data": "table"},
      "properties": {
        "enter": {
          "x": {"scale": "x", "field": "x"},
          "width": {"scale": "x", "band": true, "offset": -1},
          "y": {"scale": "y", "field": "y"},
          "y2": {"scale": "y", "value": 0}
        },
        "update": {
          "fill": {"value": "steelblue"}
        }
```



```
{
  "description": "A simple bar chart with embedded data.",
  "data": {
    "values": [
      {"a": "A","b": 28}, {"a": "B","b": 55}, {"a": "C","b": 43},
      {"a": "D","b": 91}, {"a": "E","b": 81}, {"a": "F","b": 53},
      {"a": "G","b": 19}, {"a": "H","b": 87}, {"a": "I","b": 52}
    ]
  },
  "mark": "bar",
  "encoding": {
    "x": {"field": "a", "type": "ordinal"},
    "y": {"field": "b", "type": "quantitative"}
  }
}
```

Bar Chart: Vega-Lite