Python's Data Science Stack

Jake VanderPlas @jakevdp
JSM, July 31, 2016

Python is *not* a statistical computing language!

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Python is *not* a statistical computing language!

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

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A Quick Tour of Python's Data Science Stack

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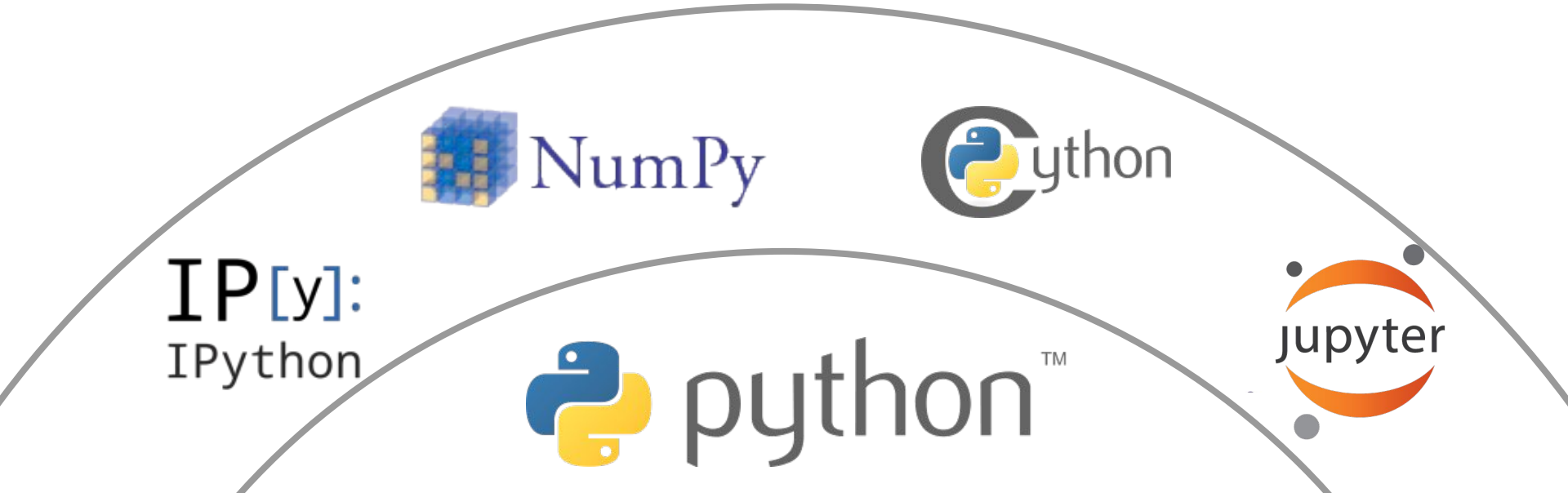
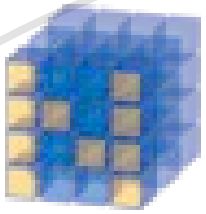
Python's Data Science Stack


NumPy
Cython
IP[y]:
IPython
python™
jupyter

NumPy = Numerical Python

Efficient array storage, manipulation, and computation



NumPy

ython

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NumPy = Numerical Python

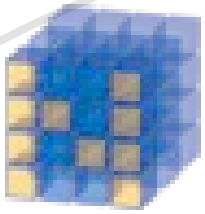
Efficient array storage, manipulation, and computation

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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NumPy

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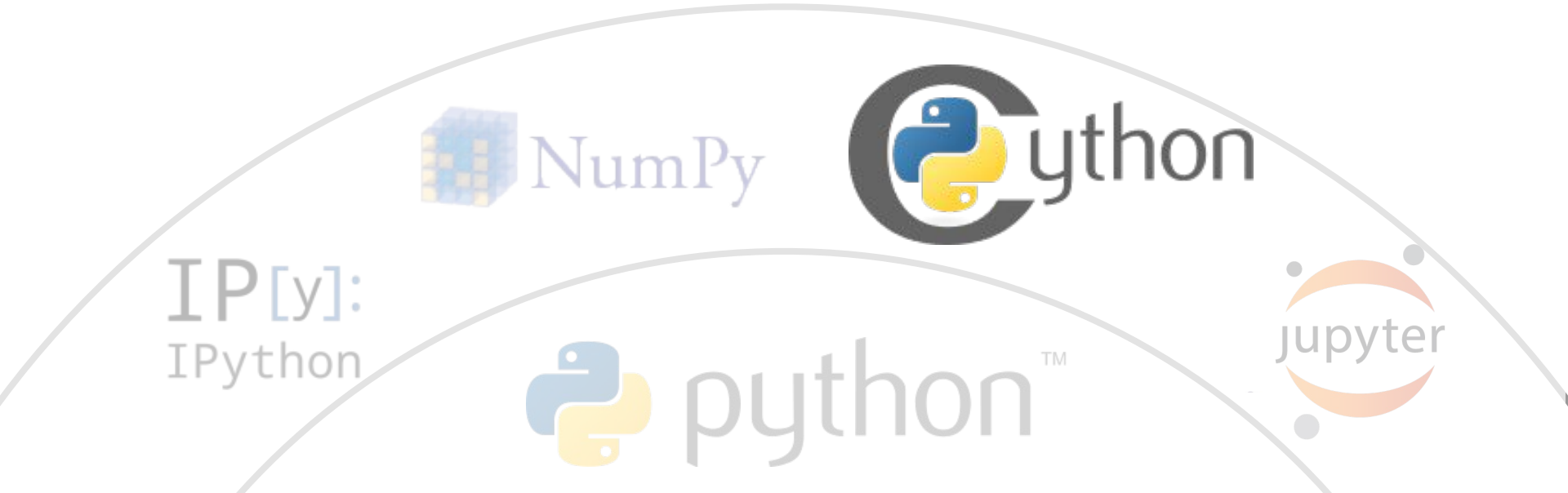
Cython = C + Python

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

ython

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IPython / Jupyter

Terminal, development environment, Notebooks, and more for efficient use of Python in day-to-day work

IPython / Jupyter

localhost:8888/notebooks/Jaynes-Cumming-model.ipynb

jupyter Jaynes-Cumming-model (unsaved changes)

File Edit View Insert Cell Kernel Help Python 3

Markdown CellToolbar

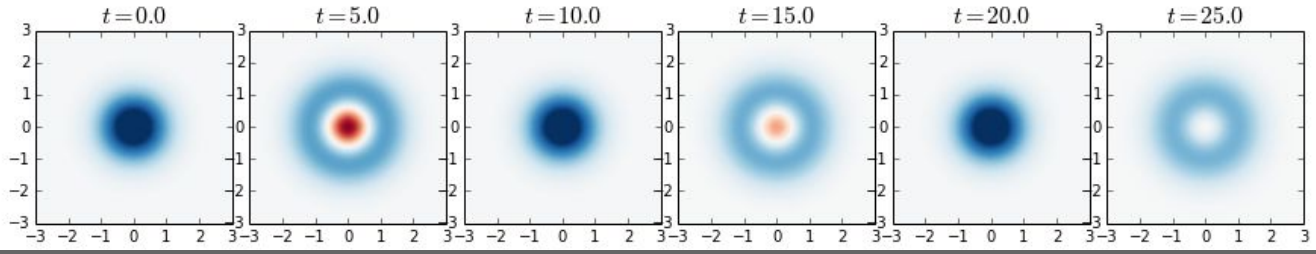
Alternative view of the model

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');
```



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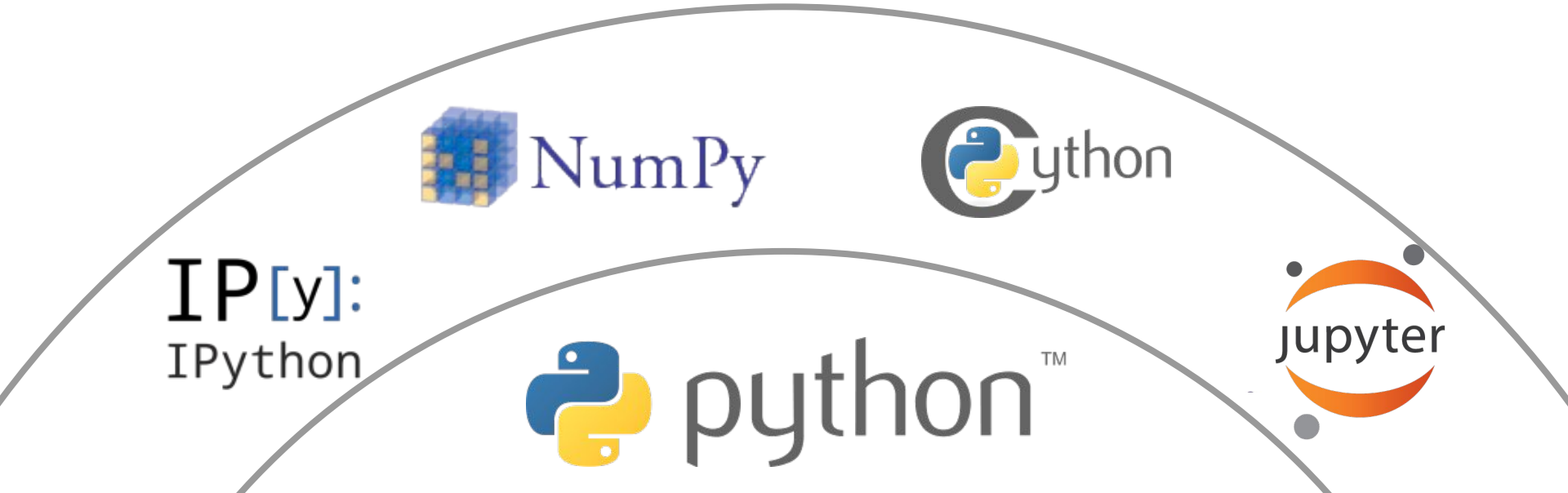
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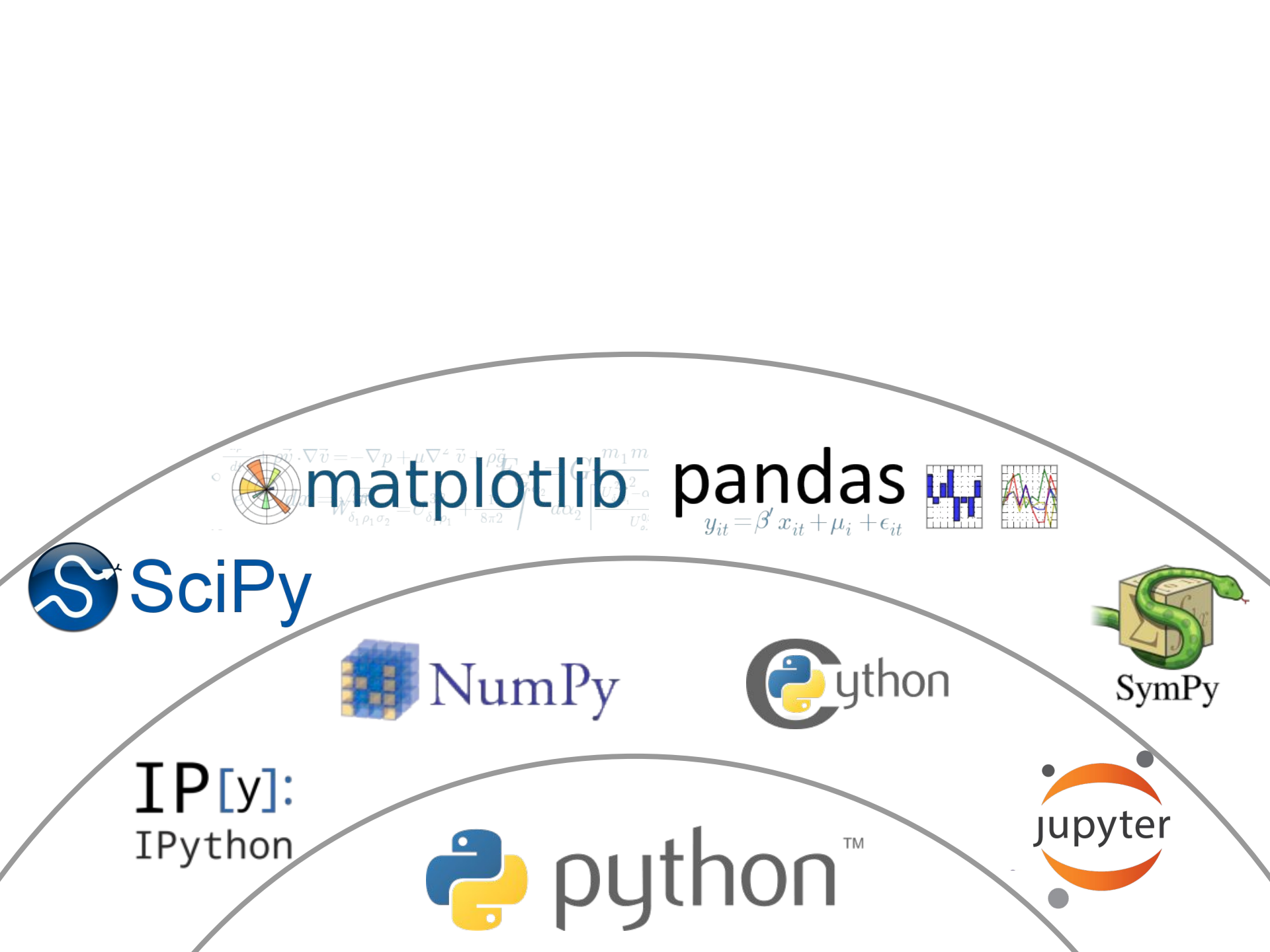
matplotlib
pandas
$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$
SciPy
NumPy
Cython
SymPy
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SciPy

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**)

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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
Cython
SymPy
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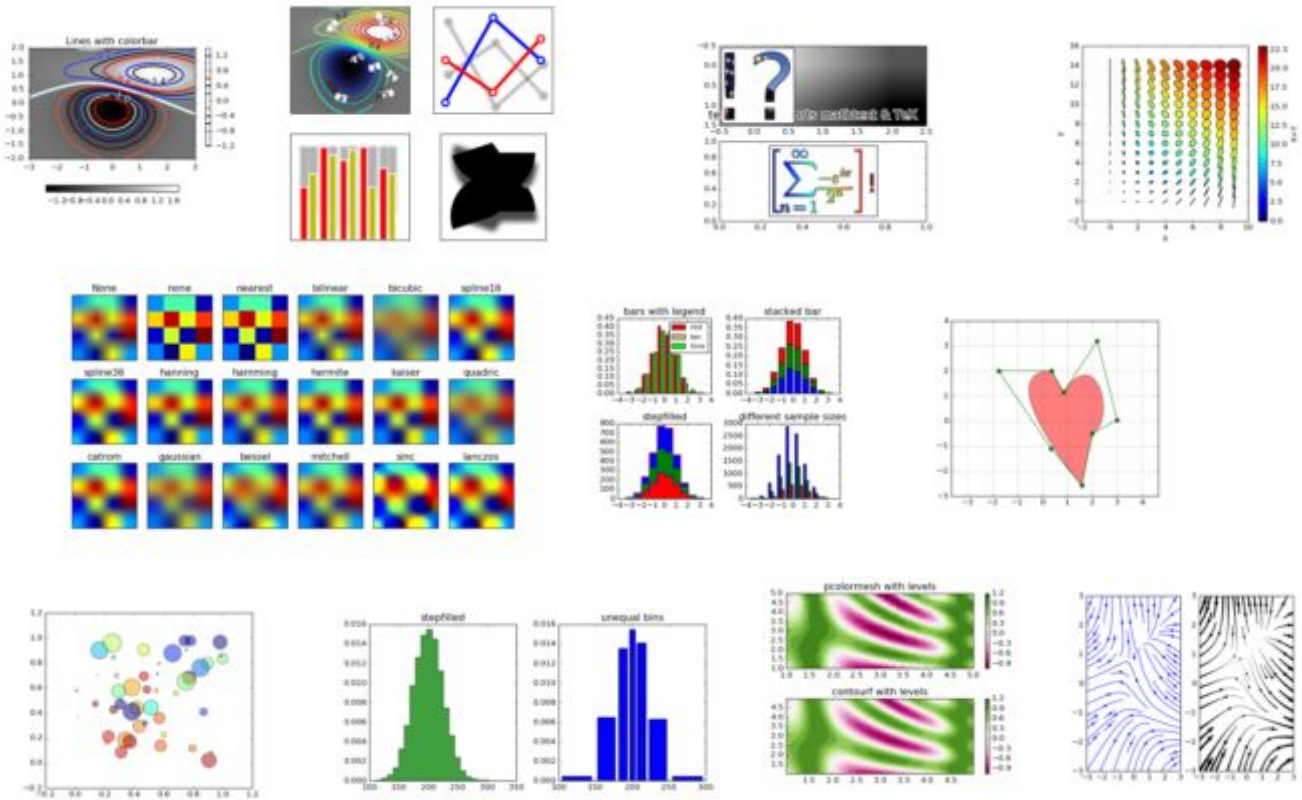
matplotlib

Matlab-inspired plotting and visualization

matplotlib

Matlab-inspired plotting and visualization

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



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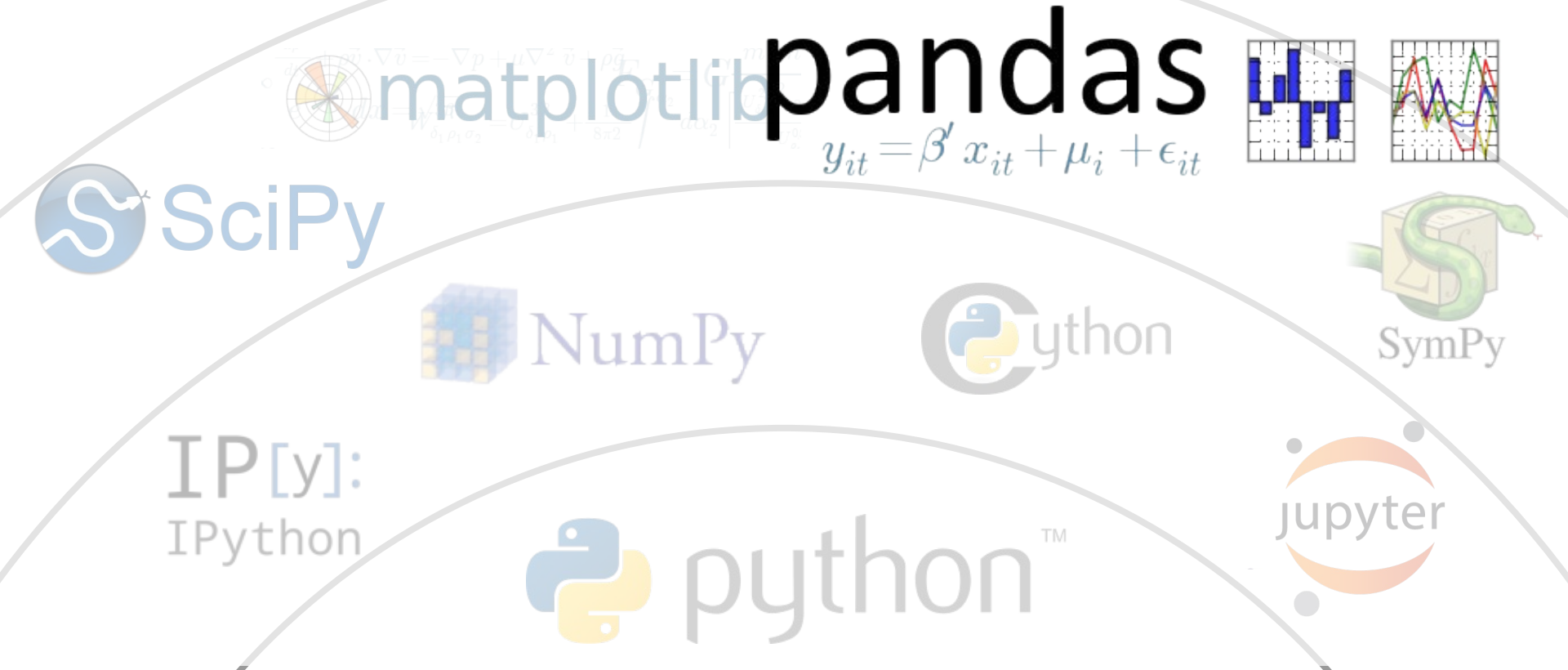
Pandas

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



Pa

```
In [1]: import pandas as pd
data = pd.read_csv('iris.csv')
data.head()
```

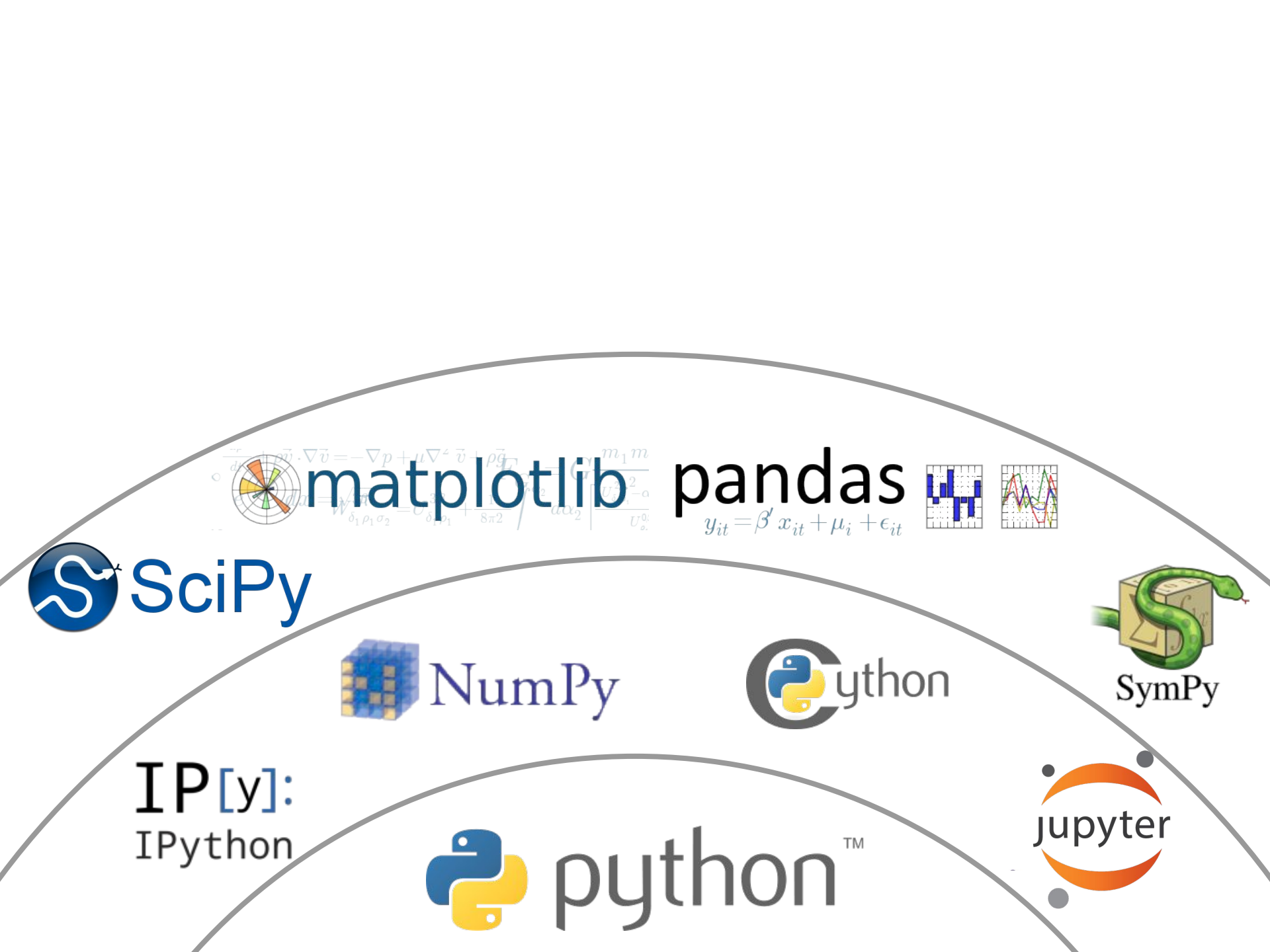
Out[1]:

	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]: 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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pandas
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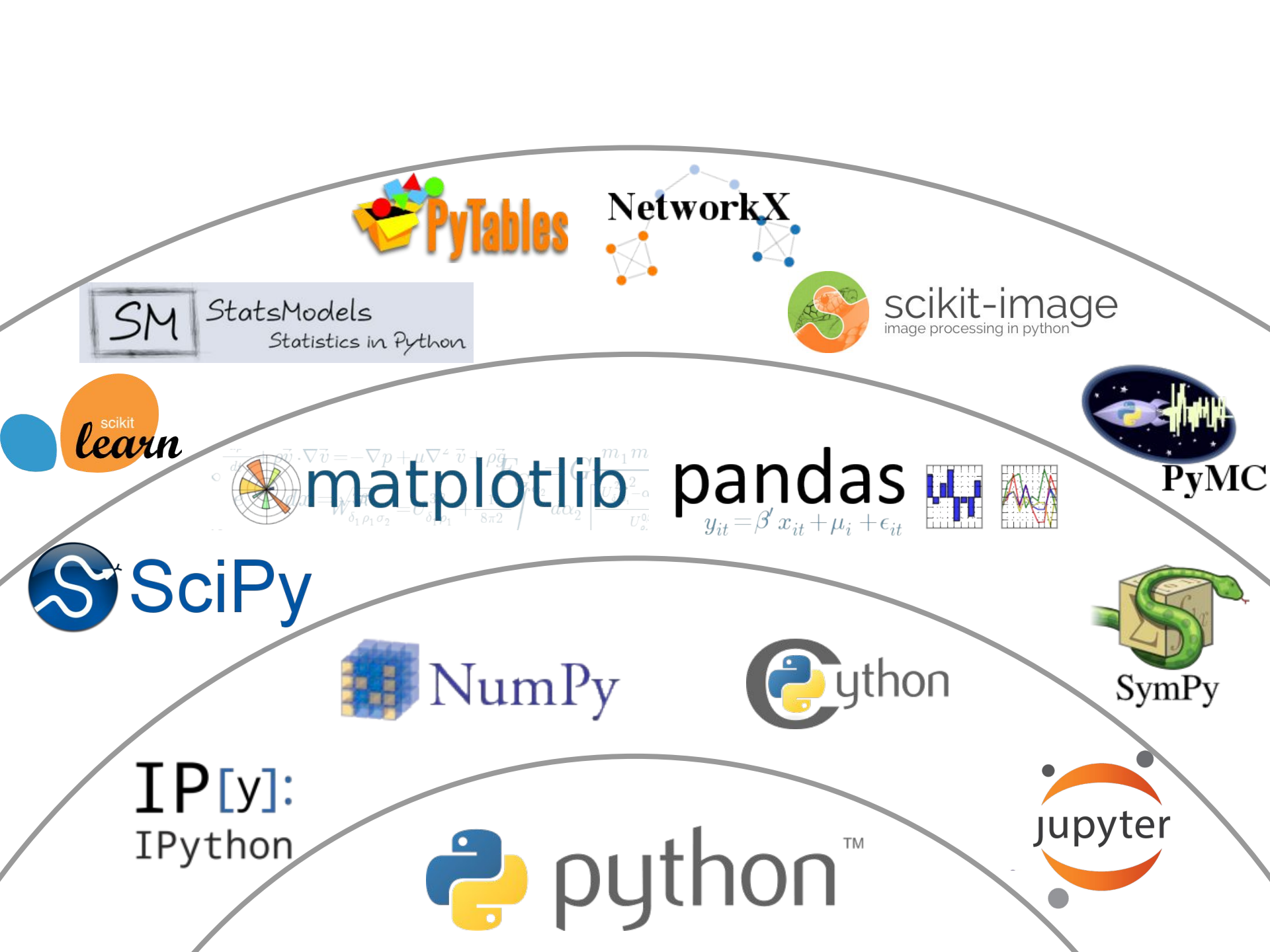
PyTables
NetworkX
SM
StatsModels
Statistics in Python
scikit-image
image processing in python
scikit
learn
matplotlib
pandas
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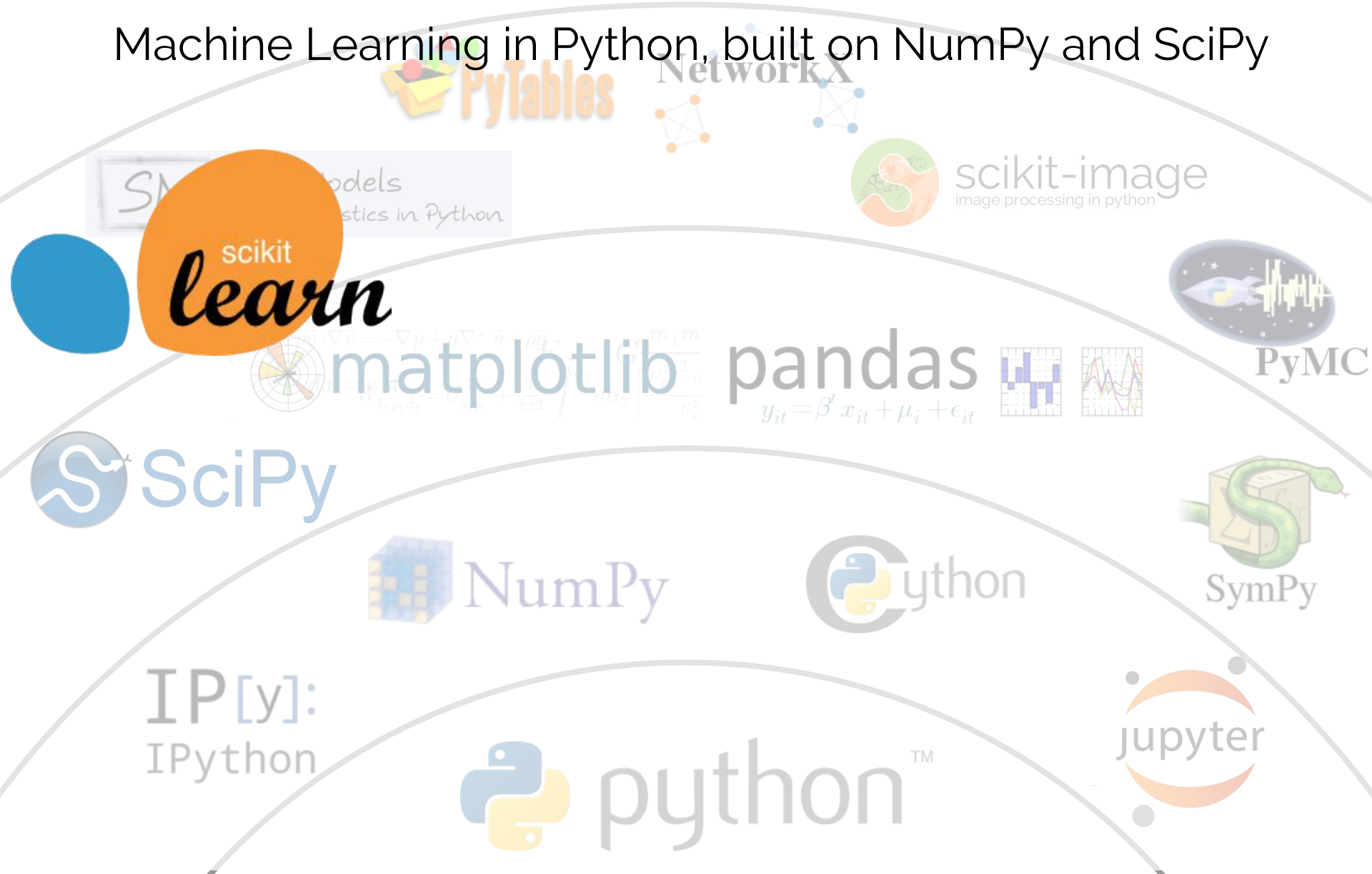
Scikit-Learn

Machine Learning in Python, built on NumPy and SciPy



Scikit-Learn

Machine Learning in Python, built on NumPy and SciPy

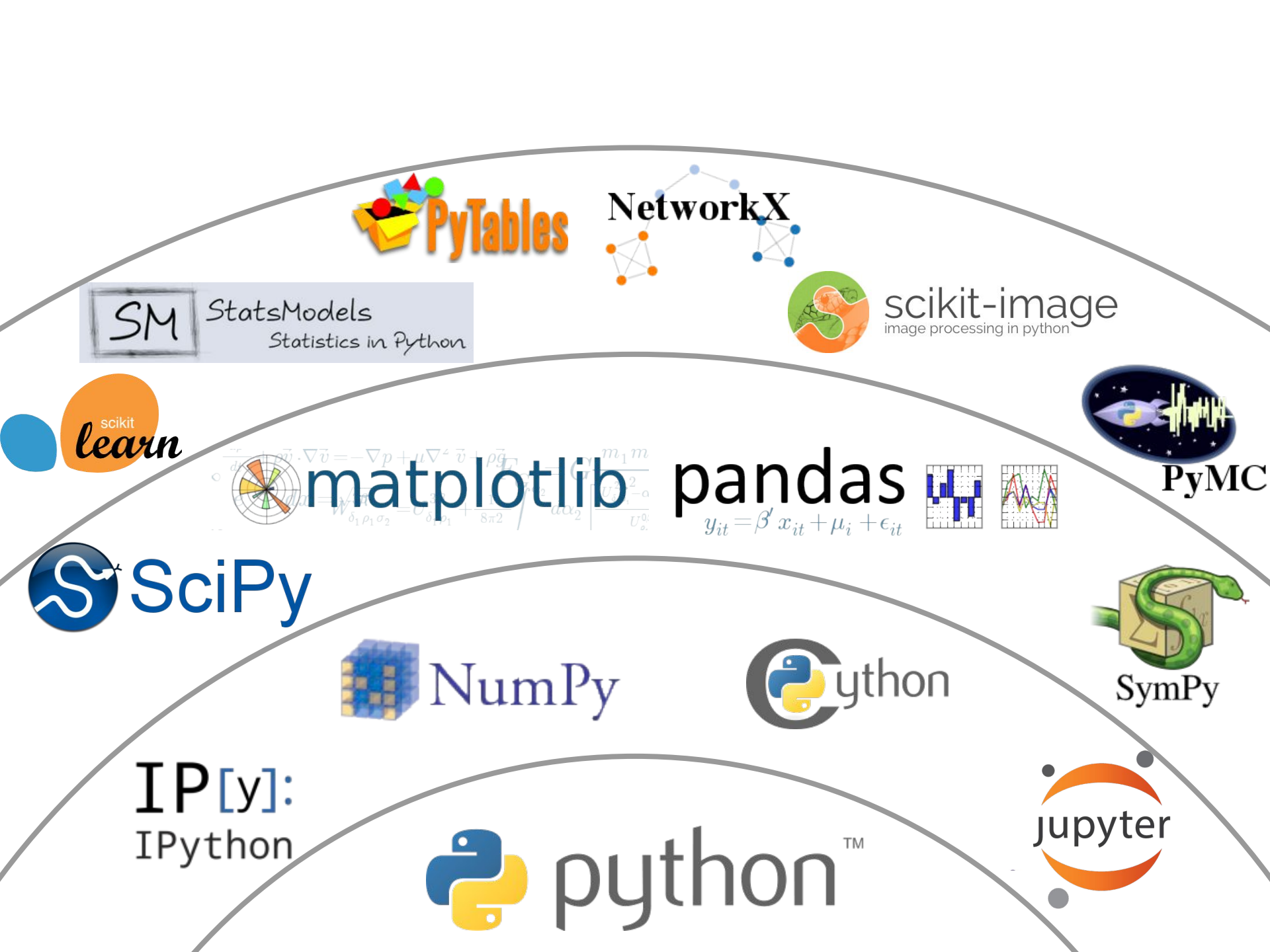
```
In [3]: from sklearn.ensemble import RandomForestClassifier

        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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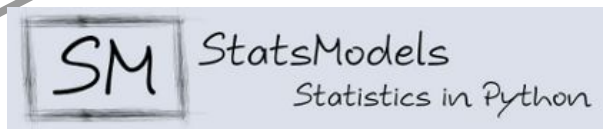
(and many, many more)



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

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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 . . .

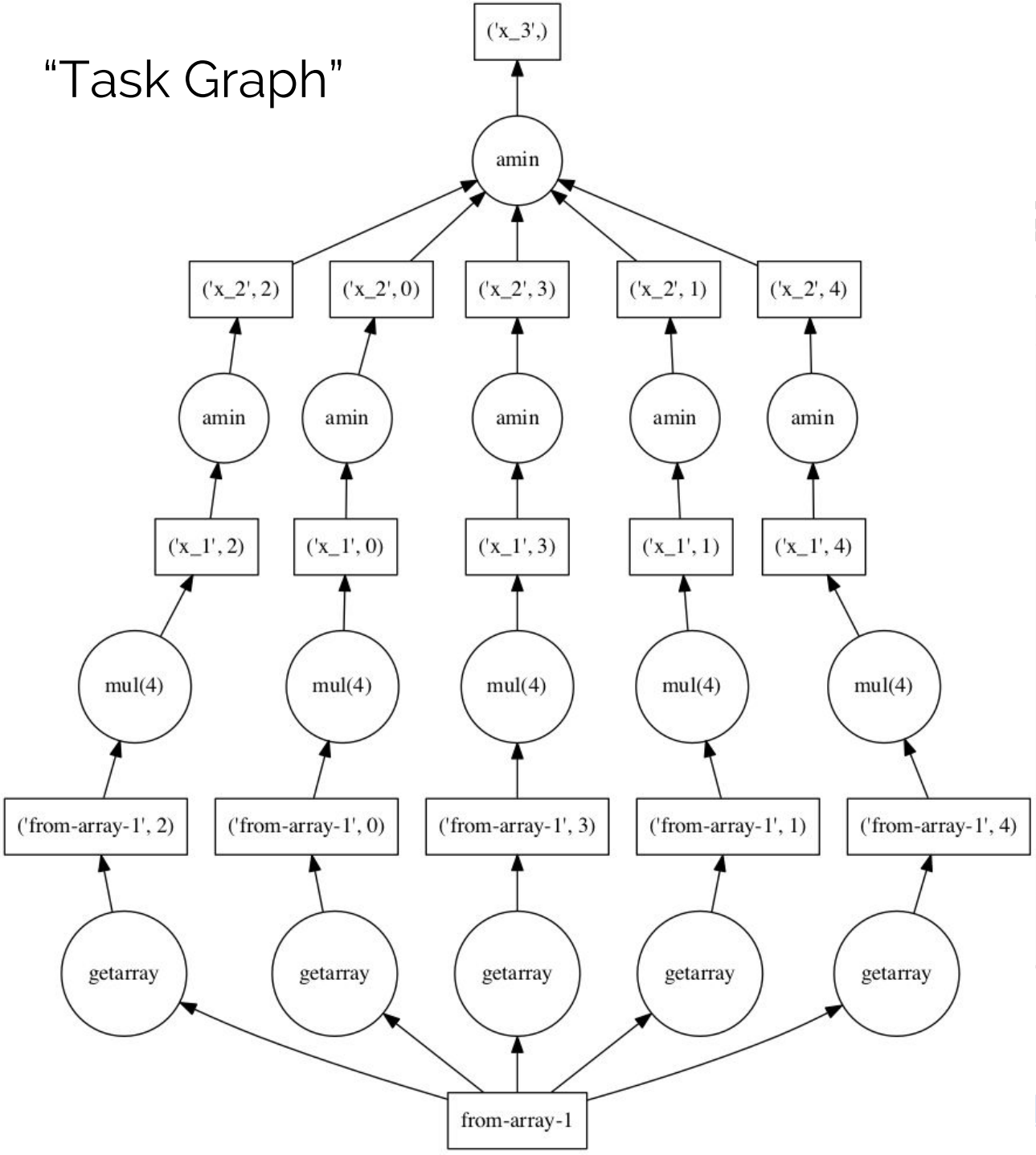
In [4]:
```
import dask.array as da

# 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

"Task Graph"



In [4

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
```

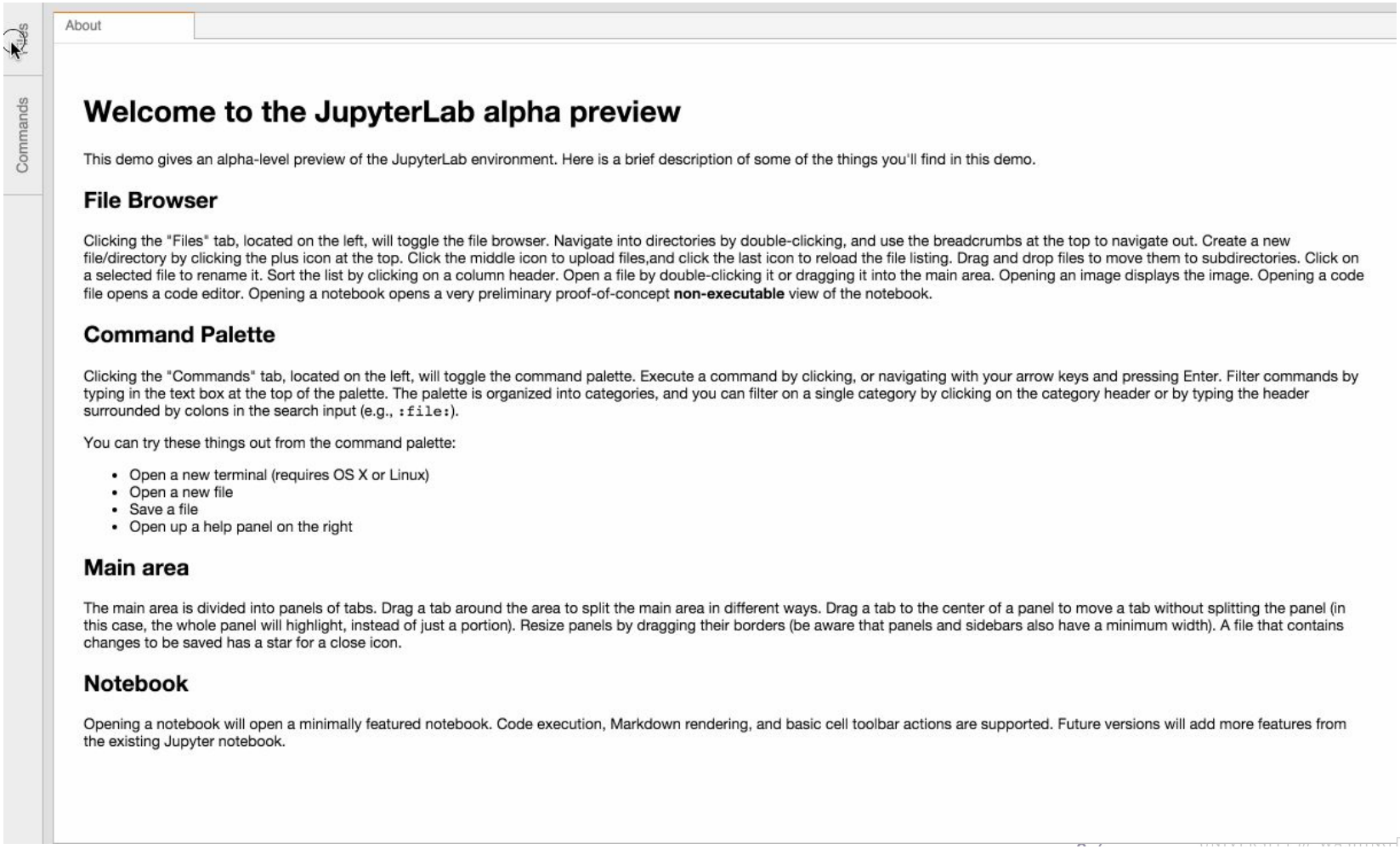
20x speedup!

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!)



Link to Animation

http://jupyter.org

Altair: Declarative Visualization based on Vega-Lite

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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.

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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.

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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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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

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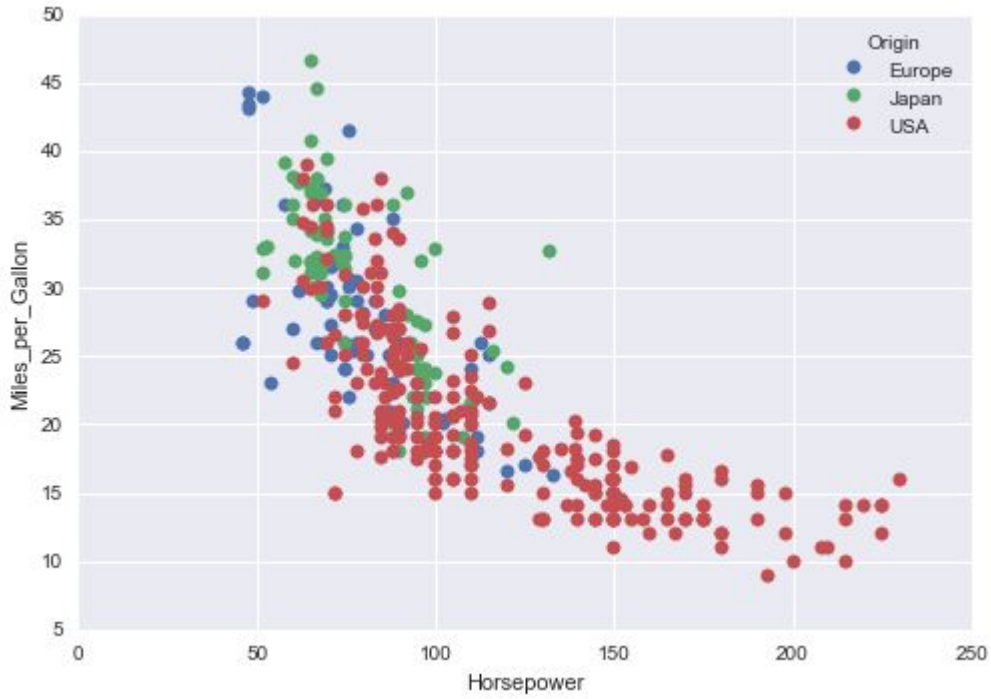
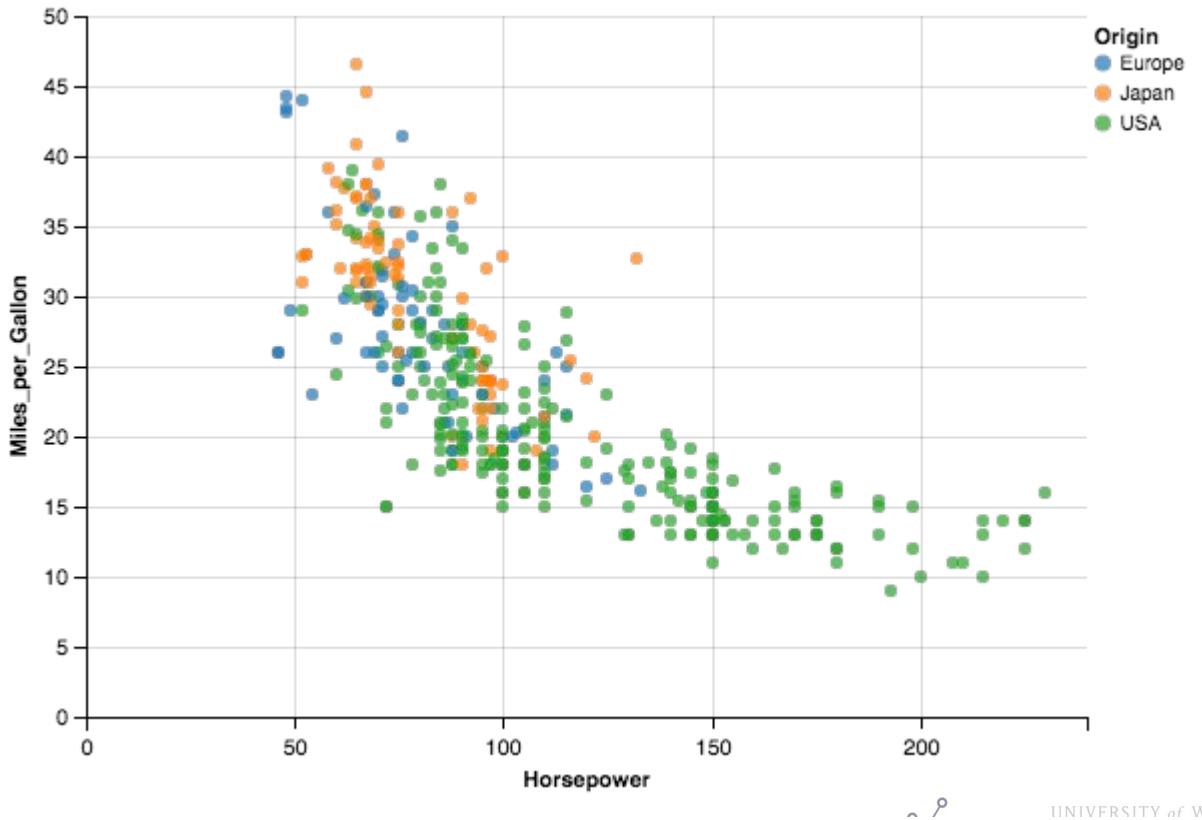
Matplotlib is an *imperative* API:

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',
)
```



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

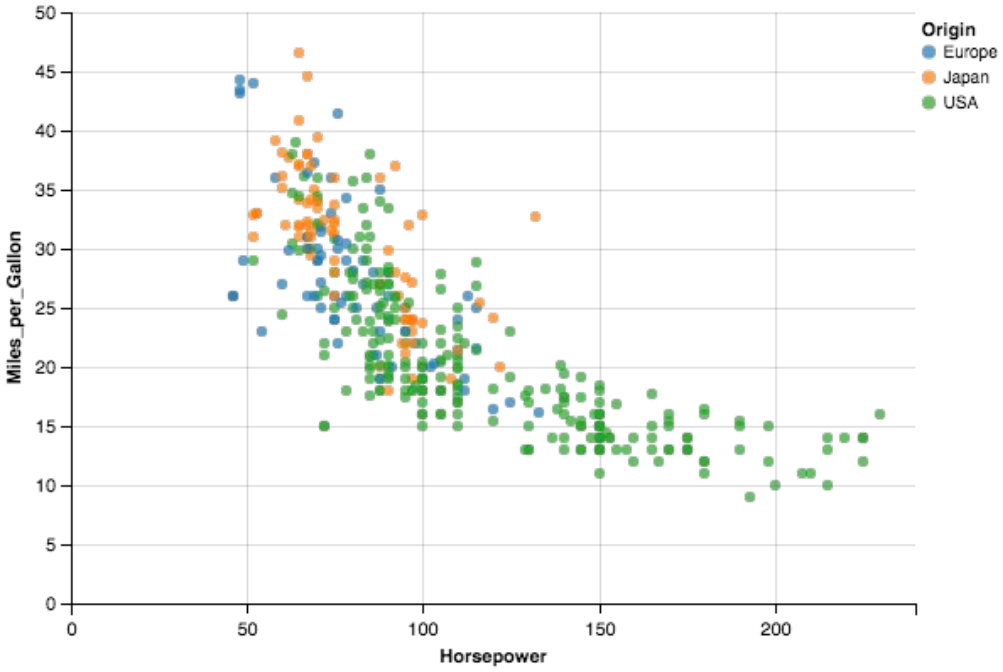
http://github.com/ellisonbg/altair

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)
```



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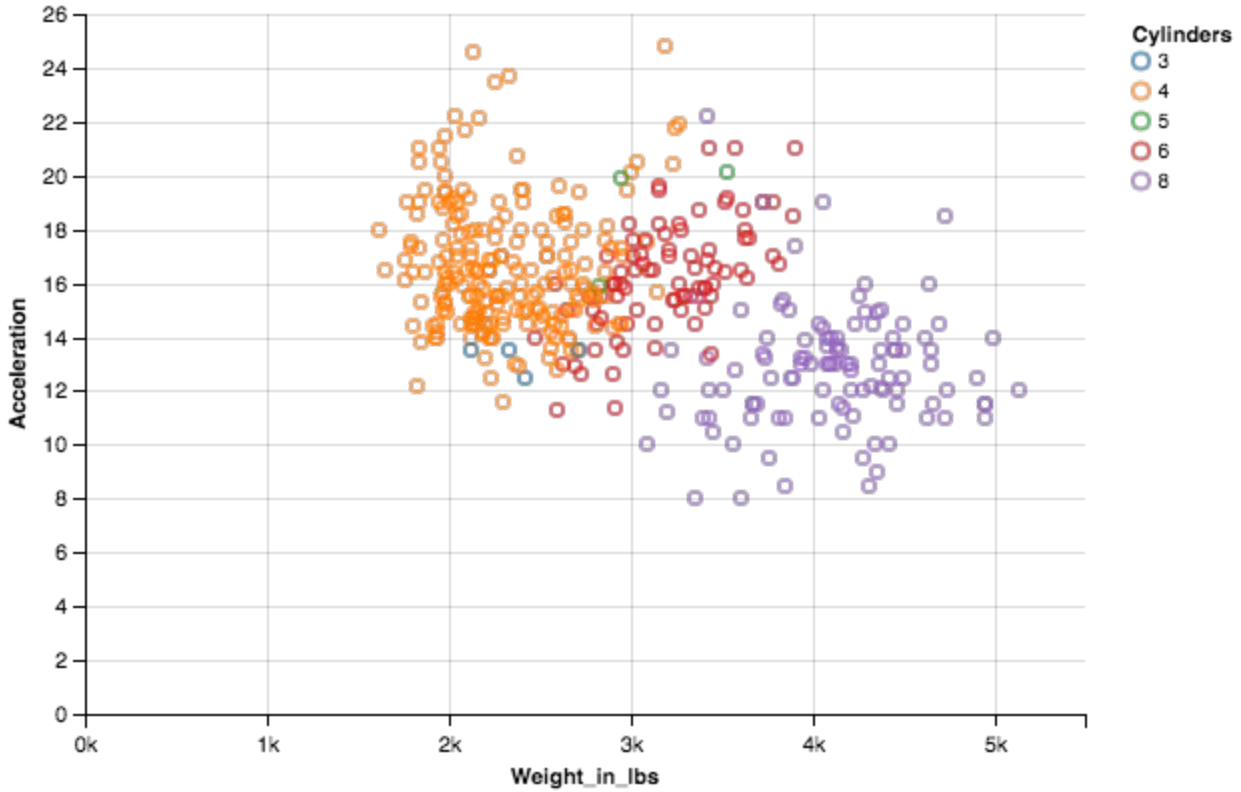
Altair/Vega-Lite supports many plot types:

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



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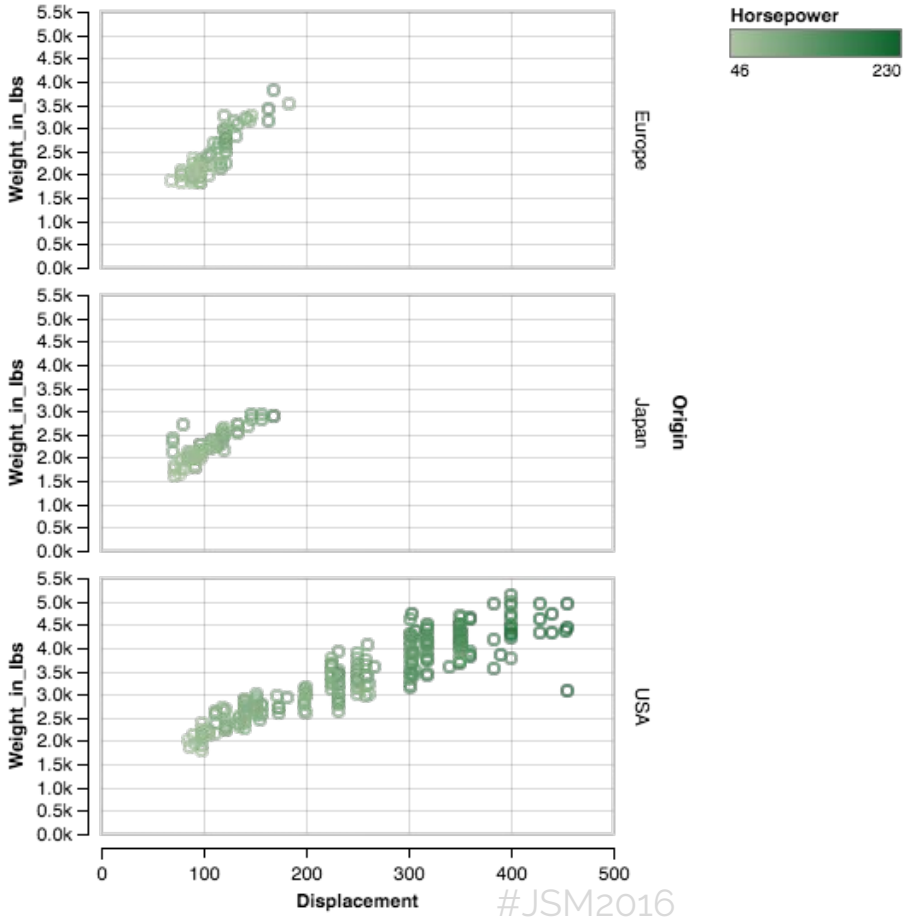
Altair/Vega-Lite supports many plot types:

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



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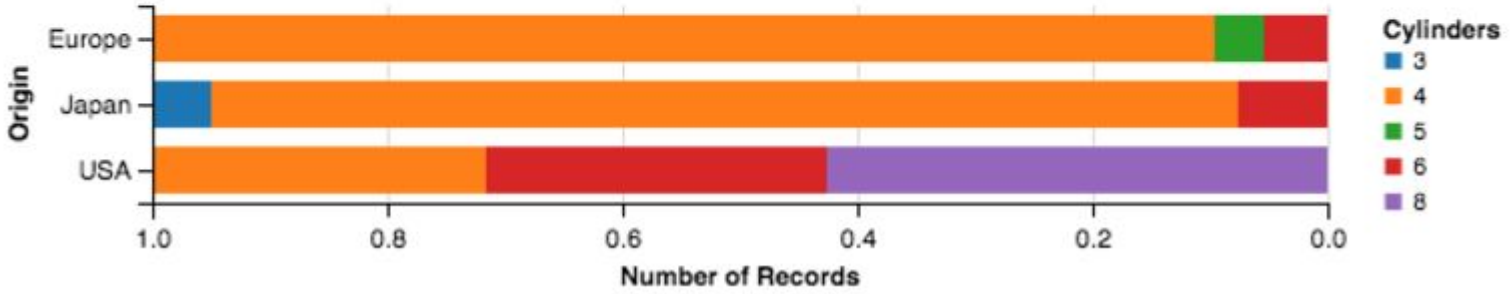
Altair/Vega-Lite supports many plot types:

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



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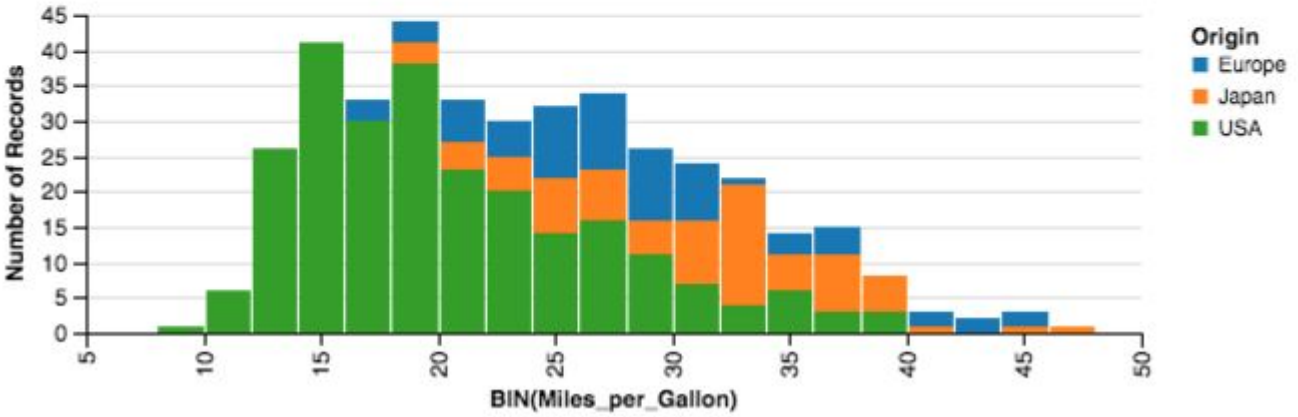
Altair/Vega-Lite supports many plot types:

```
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)
```



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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')
        )
```

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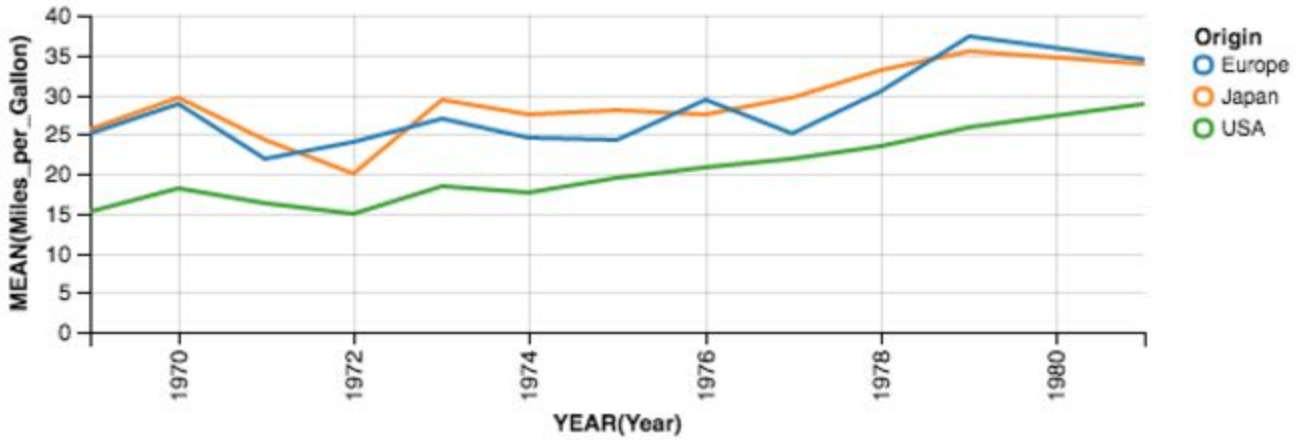
Altair/Vega-Lite supports many plot types:

```
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)
```



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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/

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Thank You!

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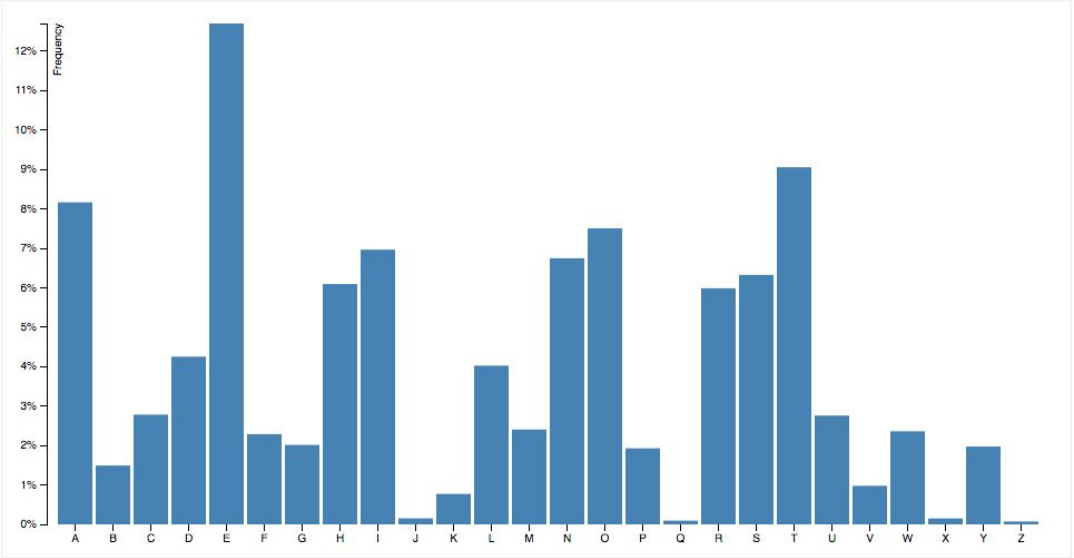
Bar Chart: d3

```
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;
}
```



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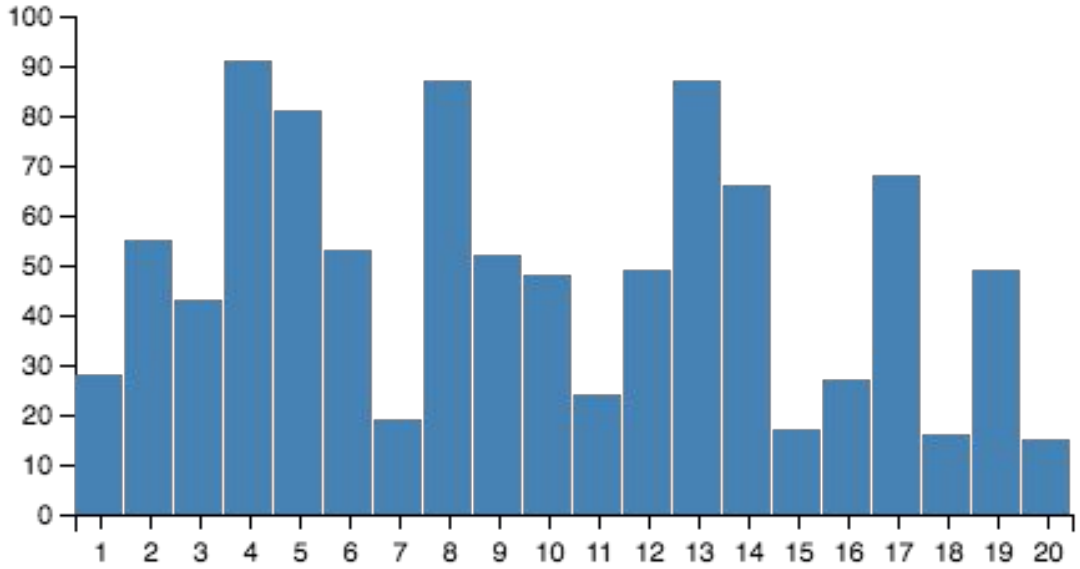
Bar Chart: Vega

```
{
  "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"}
        }
```



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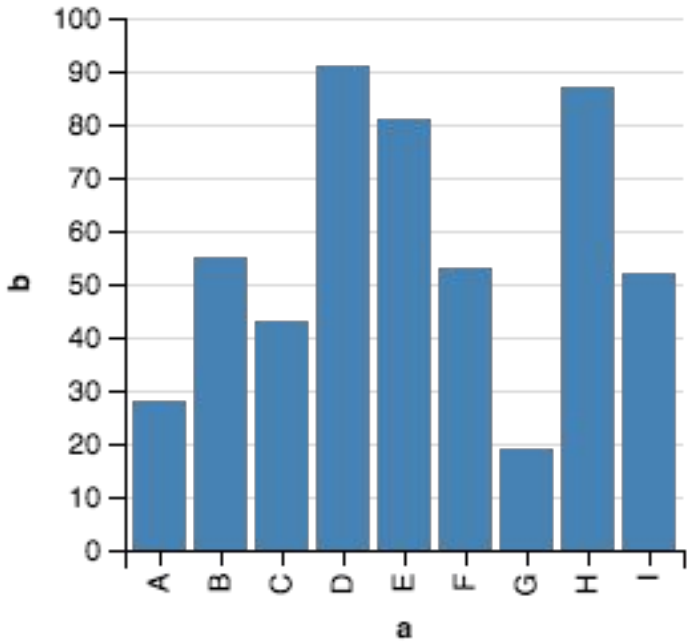
```
{
  "description": "A simple bar chart with embedded data.",
  "data": {
    "values": [
      {"a": "A","b": 28}, {"a": "B","b": 55}, {"a": "C","b": 43},
      {"a": "D","b": 91}, {"a": "E","b": 81}, {"a": "F","b": 53},
      {"a": "G","b": 19}, {"a": "H","b": 87}, {"a": "I","b": 52}
    ]
  },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

Bar Chart: Vega-Lite



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