Python for scientific computing

Python has extensive packages to help with data analysis:

- numpy: matrices, linear algebra, Fourier transform, pseudorandom number generators
- scipy: advanced linear algebra and maths, signal processing, statistics
- pandas: DataFrames, data wrangling and analysis
- matplotlib: visualizations such as line charts, histograms, scatter plots.

NumPy

NumPy is the fundamental package required for high performance scientific computing in Python. It provides:

- `ndarray`: fast and space-efficient n-dimensional numeric array with vectorized arithmetic operations
- Functions for fast operations on arrays without having to write loops
- Linear algebra, random number generation, Fourier transform
- Integrating code written in C, C++, and Fortran (for faster operations)

`pandas` provides a richer, simpler interface to many operations. We'll focus on using `ndarrays` here because they are heavily used in scikit-learn.

ndarrays

There are several ways to create numpy arrays.

In [95]:
```
# Convert normal Python array to 1-dimensional
 numpy array
np.array((1, 2, 53))
```
Out[95]:
```
array([ 1,
2, 53])
```

In [96]:
```
# Convert sequences of sequences of sequences
 ... to n-dim array
np.array([(1.5, 2, 3), (4, 5, 6)])
```
Out[96]:
```
array([[1.5,
2. , 3. ],
       [4. ,
5. , 6. ]])
```

In [97]:
```
# Define element type at creation time
np.array([[1, 2], [3, 4]], dtype=compl
ex)
```
Out[97]:
```
array([[1.+0.j, 2.+
0.j],
       [3.+0.j, 4.+
0.j]])
```

Useful properties of ndarrays:

In [98]:
```
my_array = np.array([[1, 0, 3], [0, 1, 2]])
my_array.ndim      # number of dimensions (axes), als
o called the rank
my_array.shape     # a matrix with n rows and m colum
ns has shape (n,m)
my_array.size      # the total number of elements of
 the array
my_array.dtype     # type of the elements in the arra
y
my_array.itemsize # the size in bytes of each elemen
t of the array
```

Out[98]: 2

Out[98]: (2,
3)

Out[98]: 6

Out[98]: dtype
('int
64')

Out[98]: 8

Quick array creation.
It is cheaper to create an array with placeholders than extending it later.

In [99]:

```
np.ones(3) # Default type is float64
np.zeros([2, 2])
np.empty([2, 2]) # Fills the array with wh
atever sits in memory
np.random.random((2,3))
np.random.randint(5, size=(2, 4))
```

Out[99]:

```
array([1., 1.,
1.])
```

Out[99]:

```
array([[0.,
0.],
       [0.,
0.]])
```

Out[99]:

```
array([[0.,
0.],
       [0.,
0.]])
```

Out[99]:

```
array([[0.221,
0.861, 0.549],
       [0.778,
0.125, 0.538]])
```

Out[99]:

```
array([[3, 1,
1, 1],
       [2, 0,
3, 3]])
```

Create sequences of numbers

In [100]:
```
np.linspace(0, 1, num=4)    # Linearly distributed numbers between 0 and 1
np.arange(0, 1, step=0.3)   # Fixed step size
np.arange(12).reshape(3,4) # Create and reshape
np.eye(4)                   # Identity matrix
```

Out[100]:
```
array([0.   , 0.333, 0.667, 1.   ])
```

Out[100]:
```
array([0. , 0.3, 0.6, 0.9])
```

Out[100]:
```
array([[ 0,  1,  2,  3],
       [ 4,  5,  6,  7],
       [ 8,  9, 10, 11]])
```

Out[100]:
```
array([[1., 0., 0., 0.],
       [0., 1., 0., 0.],
       [0., 0., 1., 0.],
       [0., 0., 0., 1.]])
```

Basic Operations

Arithmetic operators on arrays apply elementwise. A new array is created and filled with the result. Some operations, such as += and *=, act in place to modify an existing array rather than create a new one.

In [101]:

```
a = np.array([20, 30, 4
0, 50])
b = np.arange(4)
a, b    # Just printing
a-b
b**2
a > 32
a += 1
a
```

Out[101]:

```
(array([20, 30, 40, 50]), array
([0, 1, 2, 3]))
```

Out[101]:

```
array([20, 29, 38, 47])
```

Out[101]:

```
array([0, 1, 4, 9])
```

Out[101]:

```
array([False, False,  True,  Tru
e])
```

Out[101]:

```
array([21, 31, 41, 51])
```

The product operator * operates elementwise.
The matrix product can be performed using dot()

In [102]:

```
A, B = np.array([[1,1], [0,1]]), np.array([[2,0], [3,4
]]) # assign multiple variables in one line
A
B
A * B
np.dot(A, B)
```

Out[102]:

```
ar
ra
y
([

1]



[0

1]
```

Out[102]:

```
ar
ra
y
([

0]



[3

4]
```

Out[102]:

```
ar
ra
y
([
```

Upcasting: Operations with arrays of different types choose the more general/precise one.

In [103]:
```
a = np.ones(3, dtype=np.int) # initialize to integers
b = np.linspace(0, np.pi, 3) # default type is float
a.dtype, b.dtype, (a + b).dtype
```

Out[103]:
```
(dtype('int64'), dtype('float64'), dtype('float64'))
```

ndarrays have most unary operations (max,min,sum,...) built in

In [104]:
```
a = np.random.random((2,3))
a
a.sum(), a.min(), a.max()
```

Out[104]:
```
array([[0.057, 0.725, 0.083],
       [0.395, 0.017, 0.825]])
```

Out[104]:
```
(2.1028801738915552, 0.016881707307918936, 0.8254116092022105)
```

By specifying the axis parameter you can apply an operation along a specified axis of an array

In [105]:

```
b = np.arange(12).reshape(3,4)
b
b.sum()
b.sum(axis=0)
b.sum(axis=1)
```

Out[105]:

```
array([[ 0,  1,  2,  3],
       [ 4,  5,  6,  7],
       [ 8,  9, 10, 11]])
```

Out[105]:

```
66
```

Out[105]:

```
array([12, 15, 18, 21])
```

Out[105]:

```
array([ 6, 22, 38])
```

Universal Functions

NumPy provides familiar mathematical functions such as sin, cos, exp, sqrt, floor,... In NumPy, these are called "universal functions" (ufunc), and operate elementwise on an array, producing an array as output.

In [106]:

```
np.sin(np.arange(0, 10))
```

Out[106]:

```
array([ 0.   ,  0.841,  0.909,  0.141, -0.757, -0.959, -0.279,  0.657,
        0.989,  0.412])
```

Shape Manipulation

Transpose, flatten, reshape,...

In [107]:
```
a = np.floor(10*np.random.random((
3,4)))
a
a.transpose()
b = a.ravel() # flatten array
b
b.reshape(3, -1) # reshape in 3 ro
ws (and as many columns as needed)
```

Out[107]:
```
array([[6., 6., 8., 4.],
       [3., 5., 9., 4.],
       [2., 9., 2.,
3.]])
```

Out[107]:
```
array([[6., 3., 2.],
       [6., 5., 9.],
       [8., 9., 2.],
       [4., 4., 3.]])
```

Out[107]:
```
array([6., 6., 8., 4.,
3., 5., 9., 4., 2., 9.,
2., 3.])
```

Out[107]:
```
array([[6., 6., 8., 4.],
       [3., 5., 9., 4.],
       [2., 9., 2.,
3.]])
```

Arrays can be split and stacked together

In [108]:

```
a = np.floor(10*np.random.random((2,6
)))
a
b, c = np.hsplit(a, 2) # Idem: vsplit f
or vertical splits
b
c
np.hstack((b, c)) # Idenm: vstack for v
ertical stacks
```

Out[108]:

```
array([[7., 4.,
2., 6., 8., 5.],
       [6., 1.,
4., 3., 7., 1.]])
```

Out[108]:

```
array([[7., 4.,
2.],
       [6., 1.,
4.]])
```

Out[108]:

```
array([[6., 8.,
5.],
       [3., 7.,
1.]])
```

Out[108]:

```
array([[7., 4.,
2., 6., 8., 5.],
       [6., 1.,
4., 3., 7., 1.]])
```

Indexing and Slicing

Arrays can be indexed and sliced using [start:stop:stepsize]. Defaults are [0:ndim:1]

In [109]:
```
a = np.arange(10)
**2
a
```
Out[109]:
```
array([ 0,  1,  4,  9, 16, 25, 36, 49, 6
4, 81])
```

In [110]:
```
a[2]
```
Out[110]:

In [111]:
```
a[3:10:2]
```
Out[111]:
```
array([ 9, 25, 49, 8
1])
```

In [112]:
```
a[::-1] # Defaults are used if
 indices not stated
```
Out[112]:
```
array([81, 64, 49, 36, 25,
16,  9,  4,  1,  0])
```

In [113]:
```
a[::2]
```
Out[113]:
```
array([ 0,  4, 16, 36, 6
4])
```

For multi-dimensional arrays, axes are comma-separated: [x,y,z].

In [114]:
```
b = np.arange(16).reshape(4,4)
b
b[2,3] # row 2, column 3
```

Out[114]:
```
array([[ 0,  1,  2,
3],
       [ 4,  5,  6,
7],
       [ 8,  9, 10, 1
1],
       [12, 13, 14, 1
5]])
```

Out[114]:
```
11
```

In [115]:
```
b[0:3,1] # Values 0 to 3 in column 1
b[ : ,1] # The whole column 1
```

Out[115]:
```
array([1, 5, 9])
```

Out[115]:
```
array([ 1,  5,  9, 1
3])
```

In [116]:
```
b[1:3, : ] # Rows 1:3, all columns
```

Out[116]:
```
array([[ 4,  5,  6,
7],
       [ 8,  9, 10, 1
1]])
```

In [117]:
```
# Return the last row
b[-1]
```

Out[117]:
```
array([12, 13, 14, 1
5])
```

Note: dots (...) represent as many colons (:) as needed

- x[1,2,...] = x[1,2,:,:,:]
- x[...,3] = x[:,:,:,:,3]
- x[4,...,5,:] = x[4,:,:,5,:]

Arrays can also be indexed by arrays of integers and booleans.

In [118]:
```
a = np.arange(12)
**2
i = np.array([ 1,
1,3,8,5 ])
a
a[i]
```

Out[118]:
```
array([  0,   1,   4,   9,  16,  25,  36,
        49,  64,  81, 100, 121])
```

Out[118]:
```
array([ 1,  1,  9, 64, 25])
```

A matrix of indices returns a matrix with the corresponding values.

In [119]:
```
j = np.array([[ 3, 4], [9, 7]])
a[j]
```

Out[119]:
```
array([[ 9, 1
6],
       [81, 4
9]])
```

With boolean indices we explicitly choose which items in the array we want and which ones we don't.

In [120]:
```
a = np.arange(12).reshape(3,
4)
a
a[np.array([False,True,True
]), :]
b = a > 4
b
a[b]
```

Out[120]:
```
array([[ 0,  1,  2,  3],
       [ 4,  5,  6,  7],
       [ 8,  9, 10, 11]])
```

Out[120]:
```
array([[ 4,  5,  6,  7],
       [ 8,  9, 10, 11]])
```

Out[120]:
```
array([[False, False, False,
False],
       [False,  True,  True,
True],
       [ True,  True,  True,
True]])
```

Out[120]:
```
array([ 5,  6,  7,  8,  9, 1
0, 11])
```

Iterating

Iterating is done with respect to the first axis:

In [121]:
```
for row in b:
    print(row)
```

```
[False False False Fa
lse]
[False  True  True  T
rue]
[ True  True  True  T
rue]
```

Operations on each element can be done by flattening the array (or nested loops)

In [122]:

```python
for element in b.flat: # flat returns an iterator
    print(element)
```

```
F
a
l
s
e
F
a
l
s
e
F
a
l
s
e
F
a
l
s
e
F
a
l
s
e
T
r
u
e
T
r
u
e
```

Copies and Views (or: how to shoot yourself in a foot)

Assigning an array to another variable does NOT create a copy

In [123]:
```
a = np.arange(12)
b = a
a
```
Out[123]:
```
array([ 0,  1,  2,  3,  4,  5,  6,  7,  8,  9, 10, 11])
```

In [124]:
```
b[0] = -100
b
```
Out[124]:
```
array([-100,    1,    2,    3,    4,    5,    6,    7,    8,    9,   10,
         11])
```

In [125]:
```
a
```
Out[125]:
```
array([-100,    1,    2,    3,    4,    5,    6,    7,    8,    9,   10,
         11])
```

The view() method creates a NEW array object that looks at the same data.

In [126]:
```
a = np.arange
(12)
a
c = a.view()
c.resize((2,
6))
c
```

Out[126]:
```
array([ 0,  1,  2,  3,  4,  5,  6,  7,  8,
9, 10, 11])
```

Out[126]:
```
array([[ 0,  1,  2,  3,  4,  5],
       [ 6,  7,  8,  9, 10, 11]])
```

In [127]:
```
a[0] = 123
c # c is also changed n
ow
```

Out[127]:
```
array([[123,   1,   2,   3,   4,
5],
       [  6,   7,   8,   9,  10,
11]])
```

Slicing an array returns a view of it.

In [128]:
```
c
s = c[ : , 1:3]
s[:] = 10
s
c
```

Out[128]:
```
array([[123,   1,   2,   3,   4,
5],
       [  6,   7,   8,   9,  10,  1
1]])
```

Out[128]:
```
array([[10, 10],
       [10, 10]])
```

Out[128]:
```
array([[123,  10,  10,   3,   4,
5],
       [  6,  10,  10,   9,  10,  1
1]])
```

The copy() method makes a deep copy of the array and its data.

In [129]:
```
d = a.copy
()
d[0] = -42
d
```

Out[129]:
```
array([-42,  10,  10,   3,   4,   5,   6,  10,
10,   9,  10,  11])
```

In [130]:
```
a
```

Out[130]:
```
array([123,  10,  10,   3,   4,   5,   6,  10,  10,   9,
10,  11])
```

Numpy: further reading

- Numpy Tutorial: http://wiki.scipy.org/Tentative_NumPy_Tutorial (http://wiki.scipy.org/Tentative_NumPy_Tutorial)
- "Python for Data Analysis" by Wes McKinney (O'Reilly)

SciPy

SciPy is a collection of packages for scientific computing, among others:

- scipy.integrate: numerical integration and differential equation solvers
- scipy.linalg: linear algebra routines and matrix decompositions
- scipy.optimize: function optimizers (minimizers) and root finding algorithms
- scipy.signal: signal processing tools
- scipy.sparse: sparse matrices and sparse linear system solvers
- scipy.stats: probability distributions, statistical tests, descriptive statistics

Sparse matrices

Sparse matrices are used in scikit-learn for (large) arrays that contain mostly zeros. You can convert a dense (numpy) matrix to a sparse matrix.

In [131]:

```
from scipy import sparse
eye = np.eye(4)
eye
sparse_matrix = sparse.csr_matri
x(eye) # Compressed Sparse Row m
atrix
sparse_matrix
print("{}".format(sparse_matrix
))
```

Out[131]:

```
array([[1., 0., 0., 0.],
       [0., 1., 0., 0.],
       [0., 0., 1., 0.],
       [0., 0., 0., 1.]])
```

Out[131]:

```
<4x4 sparse matrix of type
'<class 'numpy.float64'>'
        with 4 stored elem
ents in Compressed Sparse
Row format>
```

```
  (0, 0)        1.0
  (1, 1)        1.0
  (2, 2)        1.0
  (3, 3)        1.0
```

When the data is too large, you can create a sparse matrix by passing the values and coordinates (COO format).

In [132]:
```
data = np.ones(4)                               # [1,
1,1,1]
row_indices = col_indices = np.arange(4)  # [0,
1,2,3]
col_indices = np.arange(4) * 2
eye_coo = sparse.coo_matrix((data, (row_indices,
 col_indices)))
print("{}".format(eye_coo))
```

```
  (0, 0)

1.0
  (1, 2)

1.0
  (2, 4)

1.0
  (3, 6)

1.0
```

Further reading

Check the SciPy reference guide (https://docs.scipy.org/doc/scipy/reference/) for tutorials and examples of all SciPy capabilities.

pandas

pandas is a Python library for data wrangling and analysis. It provides:

- `DataFrame`: a table, similar to an R DataFrame that holds any structured data
  - Every column can have its own data type (strings, dates, floats,...)
- A great range of methods to apply to this table (sorting, querying, joining,...)
- Imports data from a wide range of data formats (CVS, Excel) and databases (e.g. SQL)

Series

A one-dimensional array of data (of any numpy type), with indexed values. It can be created by passing a Python list or dict, a numpy array, a csv file,...

In [133]:

```python
import pandas as pd
pd.Series([1,3,np.nan]) # Default integers are integers
pd.Series([1,3,5], index=['a','b','c'])
pd.Series({'a' : 1, 'b': 2, 'c': 3 }) # when given a dic
t, the keys will be used for the index
pd.Series({'a' : 1, 'b': 2, 'c': 3 }, index = ['b', 'c',
'd']) # this will try to match labels with keys
```

Out[133]:

```
0




0

1




0

2




a
N

d
t
y
p
e

l
o
a
t
```

Functions like a numpy array, however with index labels as indices

In [134]:

```
a = pd.Series({'a' : 1, 'b': 2, 'c': 3 })
a
a['b']        # Retrieves a value
a[['a','b']] # and can also be sliced
```

Out[134]:

```
a    1
b    2
c    3
dtype: in
t64
```

Out[134]:

```
2
```

Out[134]:

```
a    1
b    2
dtype: in
t64
```

numpy array operations on Series preserve the index value

In [135]:
```
a
a[a > 1]
a * 2
np.sqrt(a)
```

Out[135]:
```
a    1
b    2
c    3
dtype: int6
4
```

Out[135]:
```
b    2
c    3
dtype: int6
4
```

Out[135]:
```
a    2
b    4
c    6
dtype: int6
4
```

Out[135]:
```
a    1.00
b    1.41
c    1.73
dtype: floa
t64
```

Operations over multiple Series will align the indices

In [136]:
```
a = pd.Series({'John' : 1000, 'Mary': 2000, 'Andre': 3000 })
b = pd.Series({'John' : 100, 'Andre': 200, 'Cecilia': 300 })
a + b
```

Out[136]:
```
Andre      3200.0
Cecilia       NaN
John       1100.0
Mary          NaN
dtype: float64
```

DataFrame

A DataFrame is a tabular data structure with both a row and a column index. It can be created by passing a dict of arrays, a csv file,...

In [137]:

```
data = {'state': ['Ohio', 'O
hio', 'Nevada', 'Nevada'],
'year': [2000, 2001, 2001, 2
002],
'pop': [1.5, 1.7, 2.4, 2.9]}
pd.DataFrame(data)
pd.DataFrame(data, columns=[
'year', 'state', 'pop', 'col
or']) # Will match indices
```

Out[137]:

	pop	state	year
0	1.5	Ohio	2000
1	1.7	Ohio	2001
2	2.4	Nevada	2001
3	2.9	Nevada	2002

Out[137]:

	year	state	pop	colo
0	2000	Ohio	1.5	NaN
1	2001	Ohio	1.7	NaN
2	2001	Nevada	2.4	NaN
3	2002	Nevada	2.9	NaN

It can be composed with a numpy array and row and column indices, and decomposed

In [138]:

```
dates = pd.date_range('20130101',periods=4)
df = pd.DataFrame(np.random.randn(4,4),index=dates,columns=list('ABCD'))
df
```

Out[138]:

	A	B	C	D
2013-01-01	1.53	0.74	-0.03	-1.84
2013-01-02	-0.62	-1.15	0.34	0.60
2013-01-03	-0.98	-0.66	-1.93	0.87
2013-01-04	-2.14	-0.31	-1.48	1.40

In [139]:

```
df.index
df.columns
df.values
```

Out[139]:

```
DatetimeIndex(['2013-01-01', '2013-01-02', '2013-01-03', '2013-01-04'], dtype='datetime64[ns]', freq='D')
```

Out[139]:

```
Index(['A', 'B', 'C', 'D'], dtype='object')
```

Out[139]:

```
array([[ 1.528,  0.744, -0.035, -1.843],
       [-0.623, -1.15 ,  0.345,  0.599],
       [-0.984, -0.661, -1.932,  0.87 ],
       [-2.142, -0.306, -1.477,  1.399]])
```

DataFrames can easily read/write data from/to files

- `read_csv(source)`: load CSV data from file or url
- `read_table(source, sep=',')`: load delimited data with separator
- `df.to_csv(target)`: writes the DataFrame to a file

In [140]:

```
df.to_csv('data.csv', index=False) # Don't export the row index
dfs = pd.read_csv('data.csv')
dfs
dfs.set_value(0, 'A', 10) # Set value in row 0, column 'A' to '10'
dfs.to_csv('data.csv', index=False)
```

Out[140]:

	A	B	C	D
0	1.53	0.74	-0.03	-1.84
1	-0.62	-1.15	0.34	0.60
2	-0.98	-0.66	-1.93	0.87
3	-2.14	-0.31	-1.48	1.40

Out[140]:

	A	B	C	D
0	10.00	0.74	-0.03	-1.84
1	-0.62	-1.15	0.34	0.60
2	-0.98	-0.66	-1.93	0.87
3	-2.14	-0.31	-1.48	1.40

Simple operations

In [141]:

```
df.head() # First 5 row
s
df.tail() # Last 5 rows
```

Out[141]:

	A	B	C	D
2013-01-01	1.53	0.74	-0.03	-1.84
2013-01-02	-0.62	-1.15	0.34	0.60
2013-01-03	-0.98	-0.66	-1.93	0.87
2013-01-04	-2.14	-0.31	-1.48	1.40

Out[141]:

	A	B	C	D
2013-01-01	1.53	0.74	-0.03	-1.84
2013-01-02	-0.62	-1.15	0.34	0.60
2013-01-03	-0.98	-0.66	-1.93	0.87
2013-01-04	-2.14	-0.31	-1.48	1.40

In [142]:

```python
# Quick stats
df.describe()
```

Out[142]:

	A	B	C	D
count	4.00	4.00	4.00	4.00
mean	-0.56	-0.34	-0.77	0.26
std	1.53	0.80	1.10	1.44
min	-2.14	-1.15	-1.93	-1.8
25%	-1.27	-0.78	-1.59	-0.0
50%	-0.80	-0.48	-0.76	0.73
75%	-0.08	-0.04	0.06	1.00
max	1.53	0.74	0.34	1.40

In [143]:

```
# Transpose
df.T
```

Out[143]:

	2013-01-01 00:00:00	2013-01-02 00:00:00	2013-01-03 00:00:00	2013-01-04 00:00:00
A	1.53	-0.62	-0.98	-2.14
B	0.74	-1.15	-0.66	-0.31
C	-0.03	0.34	-1.93	-1.48
D	-1.84	0.60	0.87	1.40

In [144]:

```
df.sort_index(axis=1, ascending=False) # Sort by index labels
df.sort(columns='B') # Sort by values
```

Out[144]:

	D	C	B	A
2013-01-01	-1.84	-0.03	0.74	1.53
2013-01-02	0.60	0.34	-1.15	-0.62
2013-01-03	0.87	-1.93	-0.66	-0.98
2013-01-04	1.40	-1.48	-0.31	-2.14

Out[144]:

	A	B	C	D
2013-01-02	-0.62	-1.15	0.34	0.60
2013-01-03	-0.98	-0.66	-1.93	0.87
2013-01-04	-2.14	-0.31	-1.48	1.40
2013-01-01	1.53	0.74	-0.03	-1.84

Selecting and slicing

In [145]:

```
df['A'] # Get single column by l
abel
df.A    # Shorthand
```

Out[145]:

```
2013-01-01    1.53
2013-01-02   -0.62
2013-01-03   -0.98
2013-01-04   -2.14
Freq: D, Name: A, dtype: f
loat64
```

Out[145]:

```
2013-01-01    1.53
2013-01-02   -0.62
2013-01-03   -0.98
2013-01-04   -2.14
Freq: D, Name: A, dtype: f
loat64
```

In [146]:

```
df[0:2]             # Get rows
 by index number
df.iloc[0:2,0:2] # Get rows
 and columns by index numbe
r
df['20130102':'20130103']
              # or row labe
l
df.loc['20130102':'2013010
3', ['A','B']] # or row and
 column label
df.ix[0:2, ['A','B']]   # a
llows mixing integers and l
abels
```

Out[146]:

	A	B	C	D
2013-01-01	1.53	0.74	-0.03	-1.84
2013-01-02	-0.62	-1.15	0.34	0.60

Out[146]:

	A	B
2013-01-01	1.53	0.74
2013-01-02	-0.62	-1.15

Out[146]:

	A	B	C	D
2013-01-02	-0.62	-1.15	0.34	0.60
2013-01-03	-0.98	-0.66	-1.93	0.87

Out[146]:

	A	B
2013-01-02	-0.62	-1.15
2013-01-03	-0.98	-0.66

Out[146]:

	A	**B**
2013-01-01	1.53	0.74
2013-01-02	-0.62	-1.15

query() retrieves data matching a boolean expression

In [147]:

```
df
df.query('A > -0.4') # Iden
tical to df[df.A > 0.4]
df.query('A > B')   # Ident
ical to df[df.A > df.B]
```

Out[147]:

	A	B	C	D
2013-01-01	1.53	0.74	-0.03	-1.84
2013-01-02	-0.62	-1.15	0.34	0.60
2013-01-03	-0.98	-0.66	-1.93	0.87
2013-01-04	-2.14	-0.31	-1.48	1.40

Out[147]:

	A	B	C	D
2013-01-01	1.53	0.74	-0.03	-1.84

Out[147]:

	A	B	C	D
2013-01-01	1.53	0.74	-0.03	-1.84
2013-01-02	-0.62	-1.15	0.34	0.60

Note: similar to NumPy, indexing and slicing returns a *view* on the data. Use copy() to make a deep copy.

Operations

DataFrames offer a wide range of operations (http://pandas.pydata.org/pandas-docs/stable/generated/pandas.DataFrame.html): max, mean, min, sum, std,...

In [148]:

```
df.mean()       # Mean of all values per
 column
df.mean(axis=1) # Other axis: means per r
ow
```

Out[148]:

```
A   -0.56
B   -0.34
C   -0.77
D    0.26
dtype: float64
```

Out[148]:

```
2013-01-01    0.
10
2013-01-02   -0.
21
2013-01-03   -0.
68
2013-01-04   -0.
63
Freq: D, dtype:
float64
```

All of numpy's universal functions also work with dataframes

In [149]:
```
np.abs(df)
```
Out[149]:

	A	B	C	D
2013-01-01	1.53	0.74	0.03	1.84
2013-01-02	0.62	1.15	0.34	0.60
2013-01-03	0.98	0.66	1.93	0.87
2013-01-04	2.14	0.31	1.48	1.40

Other (custom) functions can be applied with apply(funct)

In [150]:
```
df
df.apply(np.max)
df.apply(lambda x: x.max()
- x.min())
```

Out[150]:

	A	B	C	D
2013-01-01	1.53	0.74	-0.03	-1.84
2013-01-02	-0.62	-1.15	0.34	0.60
2013-01-03	-0.98	-0.66	-1.93	0.87
2013-01-04	-2.14	-0.31	-1.48	1.40

Out[150]:
```
A    1.53
B    0.74
C    0.34
D    1.40
dtype: float64
```

Out[150]:
```
A    3.67
B    1.89
C    2.28
D    3.24
dtype: float64
```

Data can be aggregated with groupby()

In [151]:

```
df = pd.DataFrame({'A' : ['foo', 'bar', 'foo', 'bar'], 'B' : ['one', 'one', 'two', 'three'],
                    'C' : np.random.randn(4), 'D' : np.random.randn(4)})
df
df.groupby('A').sum()
df.groupby(['A','B']).sum()
```

Out[151]:

	A	B	C	D
0	foo	one	0.74	-0.2
1	bar	one	0.73	-0.1
2	foo	two	-1.12	1.04
3	bar	three	-1.66	-0.1

Out[151]:

	C	D
A		
bar	-0.93	-0.36
foo	-0.38	0.74

Out[151]:

		C	D
A	**B**		
bar	**one**	0.73	-0.17
	three	-1.66	-0.19
foo	**one**	0.74	-0.29
	two	-1.12	1.04

Data wrangling (some examples)

Merge: combine two dataframes based on common keys

In [152]:

```
df1 = pd.DataFrame({'key': ['b', 'b',
 'a'], 'data1': range(3)})
df2 = pd.DataFrame({'key': ['a', 'b'
], 'data2': range(2)})
df1
df2
pd.merge(df1, df2)
```

Out[152]:

	data1	key
0	0	b
1	1	b
2	2	a

Out[152]:

	data2	key
0	0	a
1	1	b

Out[152]:

	data1	key	data2
0	0	b	1
1	1	b	1
2	2	a	0

Append: append one dataframe to another

In [153]:
```
df = pd.DataFrame(np.random.randn(2, 4))
df
s = pd.DataFrame(np.random.randn(1,4))
s
df.append(s, ignore_index=True)
```

Out[153]:

	0	1	2	3
0	-0.01	1.95	0.17	1.27
1	-0.38	-0.12	-0.45	-1.2[illegible]

Out[153]:

	0	1	2	3
0	0.05	-0.34	-0.73	0.38

Out[153]:

	0	1	2	3
0	-0.01	1.95	0.17	1.27
1	-0.38	-0.12	-0.45	-1.2[illegible]
2	0.05	-0.34	-0.73	0.38

Remove duplicates

In [154]:

```
df = pd.DataFrame({'k1': ['one'] * 3, 'k2': [1,
 1, 2]})
df
df.drop_duplicates()
```

Out[154]:

	k1	k2
0	one	1
1	one	1
2	one	2

Out[154]:

	k1	k2
0	one	1
2	one	2

Replace values

In [155]:
```
df = pd.DataFrame({'k1': [1, -1], 'k2': [-1, 2]}) # Say that -1 is a sentinel for missing data
df
df.replace(-1, np.nan)
```

Out[155]:

	k1	k2
0	1	-1
1	-1	2

Out[155]:

	k1	k2
0	1.0	NaN
1	NaN	2.0

Discretization and binning

In [156]:

```
ages = [20, 22, 25, 27, 21, 23
, 37, 31, 61, 45, 41, 32]
bins = [18, 25, 35, 60, 100]
cats = pd.cut(ages, bins)
cats.labels
pd.value_counts(cats)
```

Out[156]:

```
array([0, 0, 0, 1, 0, 0, 2,
1, 3, 2, 2, 1], dtype=int8)
```

Out[156]:

```
(18, 25]     5
(35, 60]     3
(25, 35]     3
(60, 100]    1
dtype: int64
```

Further reading

- Pandas docs: http://pandas.pydata.org/pandas-docs/stable/ (http://pandas.pydata.org/pandas-docs/stable/)
- https://bitbucket.org/hrojas/learn-pandas (https://bitbucket.org/hrojas/learn-pandas)
- Python for Data Analysis (O'Reilly) by Wes McKinney (the author of pandas)

matplotlib

matplotlib (http://matplotlib.sourceforge.net) is the primary scientific plotting library in Python. It provides:

- Publication-quality visualizations (http://matplotlib.org/gallery.html) such as line charts, histograms, and scatter plots.
- Integration in pandas to make plotting much easier.
- Interactive plotting in Jupyter notebooks for quick visualizations.
    - Requires some setup. See preamble and %matplotlib (http://ipython.readthedocs.io/en/stable/interactive/plotting.html?highlight=matplotlib).
- Many GUI backends, export to PDF, SVG, JPG, PNG, BMP, GIF, etc.
- Ecosystem of libraries for more advanced plotting, e.g. Seaborn (http://seaborn.pydata.org/)

Low-level usage

`plot()` is the main function (http://matplotlib.org/api/pyplot_api.html#matplotlib.pyplot.plot) to generate a plot (but many more exist):

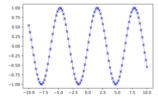
```
plot(x, y)         Plot x vs y, default settings
plot(x, y, 'bo')  Plot x vs y, blue circle markers
plot(y, 'r+')     Plot y (x = array 0..N-1), red plusses
```

Every plotting function is completely customizable through a large set of options.

In [157]:

```python
x = np.linspace(-10, 10, 100) # Sequence for X-axis

y = np.sin(x) # sine values
p = plt.plot(x, y, marker="x") # Line plot with marker x
```



pandas + matplotlib

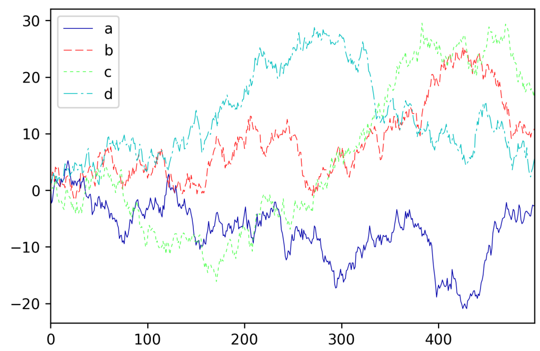
pandas DataFrames offer an easier, higher-level interface for matplotlib functions

In [158]:

```
df = pd.DataFrame(np.random.randn(500, 4),
                  columns=['a', 'b', 'c', 'd']) # random 4D data
p = df.cumsum() # Plot cumulative sum of all series
p.plot()
```

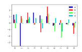
Out[158]:

```
<matplotlib.axes._subplots.AxesSubplot at 0x11dcd7b00>
```



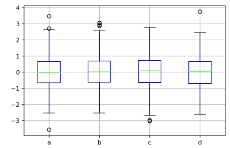
In [159]:

```
p = df[:10].plot(kind='bar') # First 10 arrays as bar p
lots
```



In [160]:

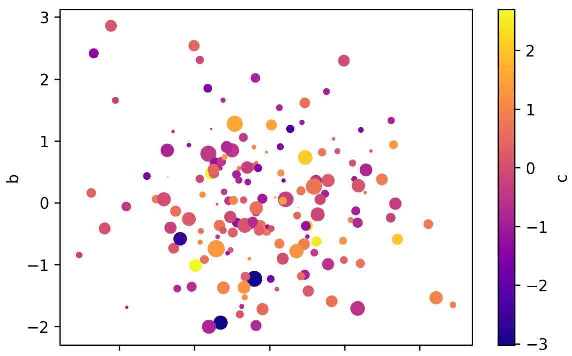
```
p = df.boxplot() # Boxplot for each of the 4 series
```



In [161]:

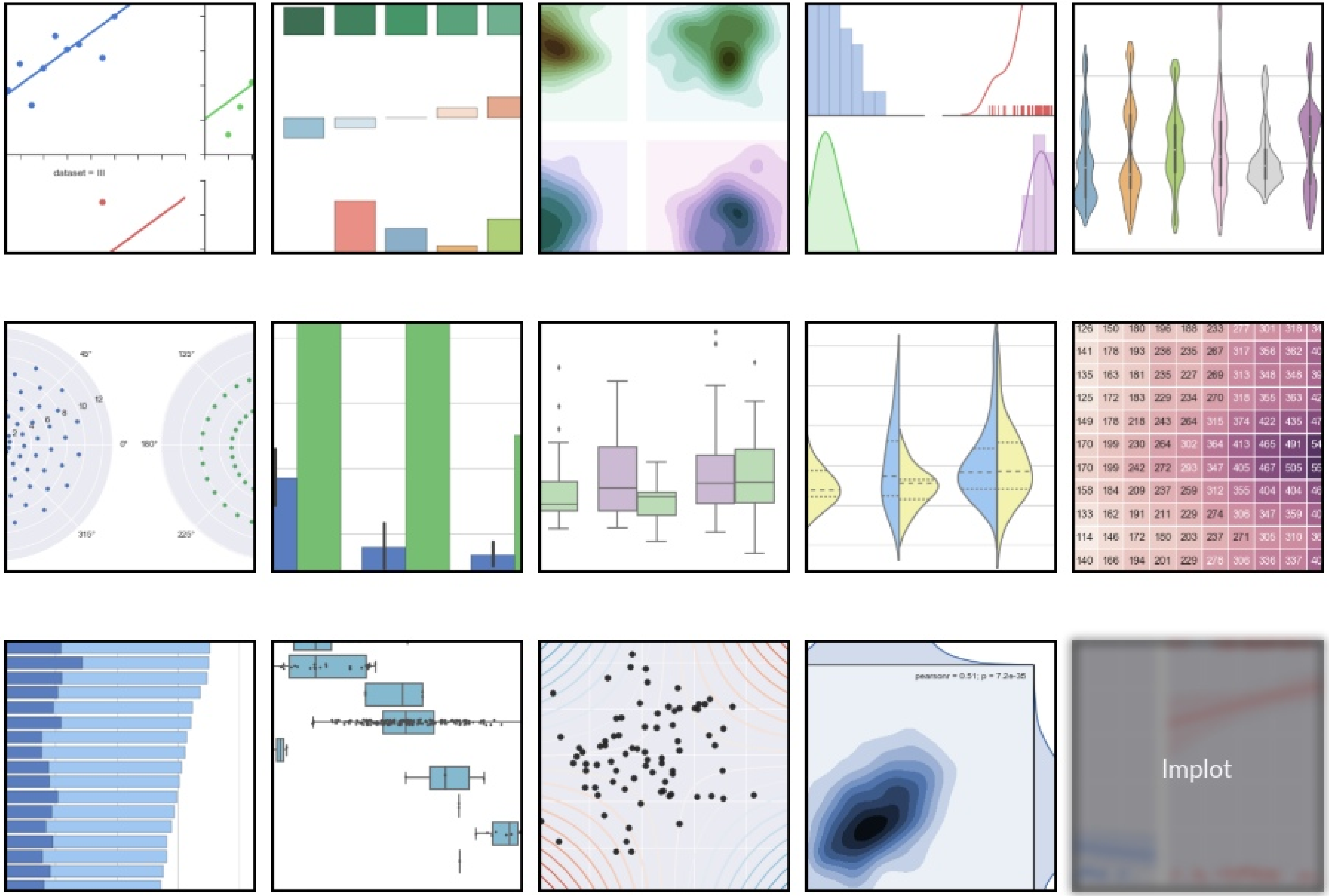
```
# Scatter plot using the 4 series for x, y, color, scale
df[:300].plot(kind='scatter', x='a', y='b', c='c',
              s=df['d']*50, linewidth='0', cmap='plasma')
```

Out[161]: <matplotlib.axes._subplots.AxesSubplot at 0x105f86a20>



Advanced plotting libraries

Several libraries, such as Seaborn (http://seaborn.pydata.org/examples/index.html) offer more advanced plots and easier interfaces.


dataset = III
pearsonr = 0.51; p = 7.2e-35
lmplot

Further reading links

- Matplotlib examples (http://matplotlib.org/gallery.html)
- Plotting with pandas (http://pandas.pydata.org/pandas-docs/version/0.18.1/visualization.html)
- Seaborn examples (http://seaborn.pydata.org/examples/index.html)