

Scientific Programming in Python

Inteligencia Artificial en los Sistemas de Control Autónomo
Máster Universitario en Ingeniería Industrial

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Objectives

1. Introduce some Python tools for scientific programming.
2. Motivate the need of efficient matrix manipulation.
3. Handle matrices and dataframes in Python.
4. Basic data visualization with Python.

Bibliography

Jake VanderPlas. Python Data Science Handbook. Chapters 1, 2, 3 and 4. O'Reilly. (Link).

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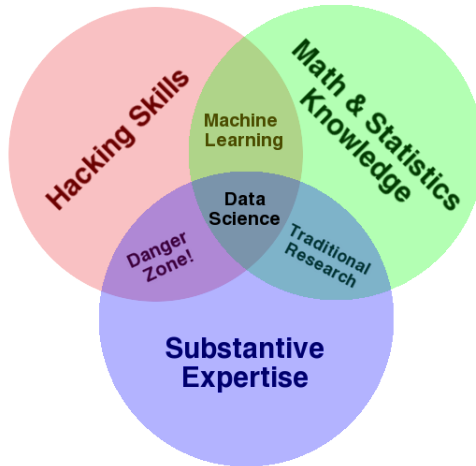
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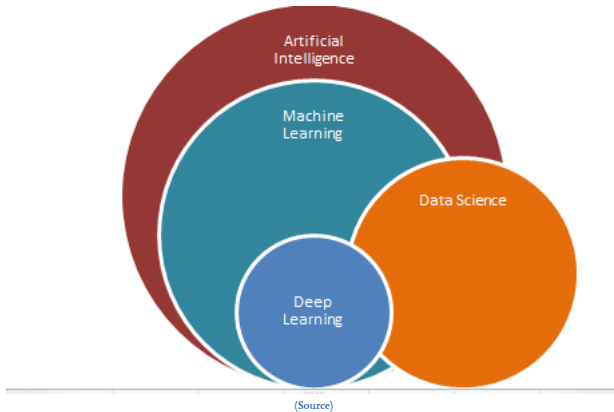
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Data Science (I)



Data Science (II)



Data Science

The data scientist toolkit (I)

Data science is about manipulating data

- Need of specialized tools
- Two main languages: R and Python

Python is a general purpose programming language

- Easy integration
- Huge ecosystem of packages and tools

Need of data-oriented tools

- Features provided by third-party tools

Data Science

The data scientist toolkit (II)

Tool	Type	Description
conda	Software	Python environments and package management
iPython	Software	Advanced Python interpreter
Jupyter	Software	Python notebooks (Python interpreter)
Numpy	Package	Efficient array operations
Pandas	Package	Dataframe support
Matplotlib	Package	Data visualization
Seaborn	Package	Data visualization with dataframes
Scikit-learn	Package	AI/ML package for Python

Conda crush introduction

Conda environment for Data Science

1. `conda create --name ml
seaborn=0.9.0`
2. `source activate ml`
3. `conda install ipython`
4. `conda install nb_conda`

List environments:

```
conda info --envs
```

Activate environment:

```
source activate <env>
```

Install package:

```
conda install <package>
```

List packages:

```
conda list
```

Exit environment (Linux):

deactivate

Python IDEs for Data Science (II)

Exercises

Write a Python script that shows the multiplication table of the number 5. Write the script using each one of the following environments:

1. iPython + text editor of your choice.
2. Jupyter.
 - Bonus track: Publish the notebook in GitHub.
3. Spyder.
4. Rodeo (optional).

Basics (I)

- most objects come with a docstring attribute
- docstring accessible through `help()`

- len?, list?, list.append?
- Try to type just '?'

- Does not work with most builtin functions!

iPython

Basics (II)

Press <tab> to complete almost everything

- Object contents

```
In [21]: a = [1,2,3]
In [22]: a.
```

a.append	a.count	a.insert	a.reverse
a.clear	a.extend	a.pop	a.sort
a.copy	a.index	a.remove	

- Packages

```
In [26]: import num
```

- Wildcards

```
In [29]: *Warning?
```

%%!	BaseException
ArithmeticError	BlockingIOError
AssertionError	BrokenPipeError
AttributeError	BufferError

iPython

Basics (III): Keyboard shortcuts

Navigation

KEYSTROKE	ACTION
Ctrl-a	Move cursor to the beginning of the line
Ctrl-e	Move cursor to the end of the line
Ctrl-b	Move cursor back one character
Ctrl-f	Move cursor forward one character

History

KEYSTROKE	ACTION
Ctrl-p (↑)	Previous command
Ctrl-n (↓)	Next command
Ctrl-r	Reverse-search

Text entry

KEYSTROKE	ACTION
Ctrl-d	Delete next character in line
Ctrl-k	Cut text from cursor to end of line
Ctrl-u	Cut text from beginning of line to cursor
Ctrl-y	Yank (paste) previously cut text

iPython magic commands

- Not valid in regular Python
- Provides handy features
- Widely used in DS and ML

- % prefix: Line magics - single line
- %% prefix: Cell magics - several lines

- %magic: Magic commands
- %lsmagic: List of magic commands

Pasting code blocks: %paste and %cpaste

- %paste: Paste one time
- %%cpaste: Paste several times

```
In [25]: %cpaste
Pasting code; enter '--' alone on the line
to stop or use Ctrl-D.
:         def donothing(x):
:             return x:
:--
```

```
In [20]: %paste
def donothing(x):
    return x

## -- End pasted text --
```


Running external code: %run and %timeit

- Executes a single line
- Automatic adjustment of runs
- Shows basic statistics

- Many optional arguments
- Checkout %run?

```
In [41]: donothing(10)
Out[41]: 10
```

```
In [34]: %timeit [n ** 2 for n in range(2000)]
753 µs ± 16.2 µs per loop
(mean ± std. dev. of 7 runs, 1000 loops each)
```

%%timeit: Several lines

iPython

Input and output history (II)

Fast access to history: Underscore ()

- Variable containing the last output
- Example: `print(_)`

Double and triple underscores

- Example: `print(__)`
- Example: `print(____)`

Trick: Shortcut to access (`_n`)

- Out[n] = _n, with n=number
- Example: `print(_2)`

Magic command to show history

- %history

Supressing command output (;)

- Example: $4 * 2$;

iPython shell commands

- Execution of shell commands from iPython
- Use prefix `!`
- Example: `!ls`, `!pwd`

- Example: `files = !ls`

- Example: `!echo {files}`

iPython
Automagic

Problems with some shell commands

```
In [23]: !pwd
/repositorios/pythonCourse
In [24]: !cd ..
In [25]: !pwd
/repositorios/pythonCourse
```

Some magic commands here to help

- %cd,%ls,%mkdir,%pwd,

Those magics are regularly used ...

- ... so common that % is no longer required (automagic)
- Working with iPython is almost like working with a Unix-like shell

Automagic commands

cat, cp, env, ls, man, mkdir, more,
mb, pwd, rm and rmdir

NumPy

Understanding Data Types in Python (I)

Static typing

```
/* C code */
int result = 0;
for(int i=0; i<100; i++){
    result += i;
}
```

- Data types must be declared
- Data types cannot change
- Error detection in compilation
- Variables names are, basically, labels

Dynamic typing

```
# Python code
result = 0
for i in range(100):
    result += i
```

- Data types are not declared
- Data types can change
- Error detection in run-time
- Variables are complex data structures (even for simple types)

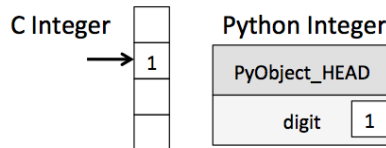
NumPy

Understanding Data Types in Python (II)

Dynamic typing must be implemented somewhere ...

Python 3.4 source code

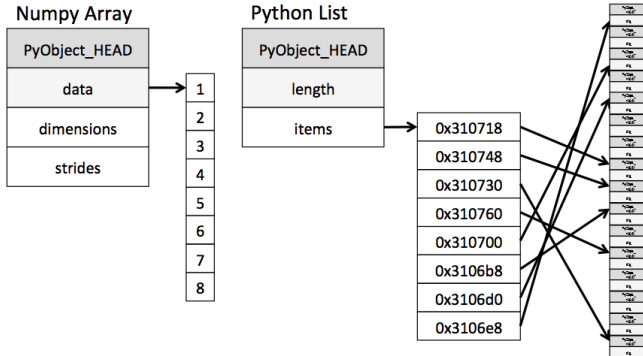
```
struct _longobject {
    long ob_refcnt;
    PyTypeObject *ob_type;
    size_t ob_size;
    long ob_digit[1];
};
```



Understanding Data Types in Python (III)

A Python list may contain different types

```
In [1]: L3 = [True, "2", 3.0, 4]
...: [type(item) for item in L3]
Out[1]: [bool, str, float, int]
```



NumPy

Understanding Data Types in Python (IV)

Standard Python data types are powerful and flexible

- Flexibility has a price: Reduced performance
- Not an big issue in generic programming
- A big issue in scientific programming
- We require efficient data manipulation mechanisms: NumPy

NumPy: Python package for numeric computation

- Efficient array implementation
- Fast mathematical functions
- Random numbers generation
- Static data types: Less flexibility

Most Python modules for AI/ML depend on NumPy, in particular

- Pandas (dataframes), Scikit-learn (ML), Seaborn (data visualization)

Introduction

NumPy must be imported in order to be available

- Remember, you can use `np?` or `np.<TAB>`

The main component of NumPy is `ndarray`

- Python object
- Efficient matrix representation
- Homogeneous elements

Convention

```
import numpy as np
```

```
In [1]: array = np.array
        ([1, 2, 3])
In [2]: array
Out[1]: array([1, 2, 3])
In [3]: array = np.array
        ([ [1, 2], [3, 4] ])
```


NumPy

NumPy data types

Python is implemented in C

- Data types in NumPy are based on those in C

Two styles to declare types

- String:
`np.zeros(10,
dtype='int16')`
- NumPy object:
`np.zeros(10,
dtype=np.int16)`

DATA TYPE	DESCRIPTION
bool_	Boolean (True or False) stored as a byte
int_	Default integer type
intc	Identical to C
intp	Integer used for indexing
int8	Byte
int16	Integer
int32	Integer
int64	Integer
uint8	Unsigned integer
uint16	Unsigned integer
uint32	Unsigned integer
uint64	Unsigned integer
float_	Shorthand for float64
float16	Half precision float
float32	Single precision float
float64	Double precision float
complex_	Shorthand for complex128
complex64	Complex number
complex128	Complex number

NumPy

Accessing single elements

Unidimensional array

- `array[index]`

Unidimensional array from the end

- `array[-index]`

Multidimensional array

- `array[row,column]`

```
x = np.array([5, 0, 3, 3, 7, 9])
x[0] # 5
x[4] # 7
x[-1] # 9
x[-2] # 7
x = np.array([[3, 5, 2, 4],
               [7, 6, 8, 8],
               [1, 6, 7, 7]])
x2[2, 0] # 1
x2[2, -1] # 7
```

Warning

Ndarray has fixed types, values can be truncated without warning. Big source of problems!

NumPy

Accessing subarrays

Slice notation can be used with ndarray

- `x[start:stop:step]`

Default values

- Start = 0
- Stop = Size of dimension
- Step = 1

Step may take a negative value

- Reverse order

These operations return a view

- Use `copy()` to get a copy

```
x[:5]      # first five elements
x[5:]      # elements after index 5
x[4:7]     # middle sub-array
x[::2]     # every other element
x[1::2]    # every other element,
           # starting at index 1
x[::-1]    # all elements, reversed
```

```
x[:2, :3] # 2 rows, 3 columns
x[:3, ::2] # all rows, every
            other column
x[:, :-1, ::-1]
```


Splitting of arrays

Three methods to split arrays

- `np.split()`
- `np.vsplit()`
- `np.hsplit()`

```
In [1]: x = [1, 2, 3, 99, 99, 3, 2, 1]
In [2]: x1, x2, x3 = np.split(x, [3, 5])
In [3]: print(x1, x2, x3)
[1 2 3] [99 99] [3 2 1]
```

```
In [1]: grid = np.arange(16).reshape((4, 4))
In [2]: print(grid)
[[ 0  1  2  3]
 [ 4  5  6  7]
 [ 8  9 10 11]
 [12 13 14 15]]
In [3]: upper, lower = np.vsplit(grid, [2])
In [4]: print(upper)
[[0  1  2  3]
 [4  5  6  7]]
```


NumPy

Universal functions (II)

Vectorized operations: Functions that are aware of NumPy's static typing

- Avoid dynamic type-checking
- Loop related code pushed into the compiled layer
- Hugely improved performance
- Perform an operation with the first element and then it to the rest

In NumPy, vectorized operations are named **universal functions**, or **ufuncs**

- Regular functions
- Arrays as arguments (one or multi-dimensional)
- Operates between arrays of different sizes (**broadcasting**)

In order to take advantage of NumPy's performance, ufuncs must be used

NumPy

Universal functions: Arithmetic functions

NumPy makes use of Python's native arithmetic operators

- Used like regular Python operators
- Operators are wrappers for NumPy's functions

Operator	Equivalent UFunc	Description
+	<code>np.add</code>	Addition (e.g., $1 + 1 = 2$)
-	<code>np.subtract</code>	Subtraction (e.g., $3 - 2 = 1$)
-	<code>np.negative</code>	Unary negation (e.g., -2)
*	<code>np.multiply</code>	Multiplication (e.g., $2 * 3 = 6$)
/	<code>np.divide</code>	Division (e.g., $3 / 2 = 1.5$)
//	<code>np.floor_divide</code>	Floor division (e.g., $3 // 2 = 1$)
**	<code>np.power</code>	Exponentiation (e.g., $2 ** 3 = 8$)
%	<code>np.mod</code>	Modulus/remainder (e.g., $9 \% 4 = 1$)

NumPy

Universal functions (III)

```
x = np.arange(4)
print("x      =", x)
print("x + 5 =", x + 5)
print("x - 5 =", x - 5)
print("x * 2 =", x * 2)
print("x / 2 =", x / 2)
print("x // 2 =", x // 2) # floor division
np.add(x, 2)             # array plus scalar
```

```
print("-x      = ", -x)
print("x ** 2  = ", x ** 2)
print("x % 2   = ", x % 2)
```

NumPy

Universal functions: Basic functions

Absolute value

- `np.absolute(x)` and `np.abs(x)`

Trigonometric functions

- `np.sin(theta)`, `np.cos(theta)`, `np.tan(theta)`
- `np.arcsin(theta)`, `np.arccos(theta)`, `np.arctan(theta)`

Exponents and logarithms

- `np.exp(x)`, `np.exp2(x)`, `np.power(base, x)`
- `np.log(x)`, `np.log2(x)`, `np.log10(x)`

Advanced mathematical functions

- Checkout module `scipy.special` for exotic mathematical functions

Output as argument

- Avoid temporal variables using `out` argument in ufuncs
- Example: `np.multiply(x, 10, out=y)`

NumPy

Universal functions: Special functions

Aggregation functions

- Applied to any ufunc
- `reduce(x)`: Repeatedly applies an ufunc to the elements of an array until only a single result remains
- `accumulate(x)`: Like `reduce()`, but it stores intermediate values
- `outer(x)`: Compute the output of all pairs of two different inputs

```
In [1]: x = np.arange(1, 6)
In [2]: np.add.reduce(x)
Out[1]: 15
```

```
In [1]: np.add.reduce(x)
Out[1]: 15
```

```
In [132]: np.multiply.outer(x, x)
array([[ 1,  2,  3,  4,  5],
       [ 2,  4,  6,  8, 10],
       [ 3,  6,  9, 12, 15],
       [ 4,  8, 12, 16, 20],
       [ 5, 10, 15, 20, 25]])
```


NumPy

Universal functions: Aggregations (I)

Many ufuncs to summarize data

- Basic step in exploratory data analysis
- Argument `axis` determines to which dimension the summary is to be applied

FUNCTION	NaN-SAFE VERSION	DESCRIPTION
<code>np.sum</code>	<code>np.nansum</code>	Compute sum of elements
<code>np.prod</code>	<code>np.nanprod</code>	Compute product of elements
<code>np.mean</code>	<code>np.nanmean</code>	Compute mean of elements
<code>np.std</code>	<code>np.nanstd</code>	Compute standard deviation
<code>np.var</code>	<code>np.nanvar</code>	Compute standard deviation
<code>np.min</code>	<code>np.nanmin</code>	Find minimum value
<code>np.max</code>	<code>np.nanmax</code>	Find maximum value
<code>np.argmin</code>	<code>np.nanargmin</code>	Find index of minimum value
<code>np.argmax</code>	<code>np.nanargmax</code>	Find index of maximum value
<code>np.median</code>	<code>np.nanmedian</code>	Compute median of elements
<code>np.percentile</code>	<code>np.nanpercentile</code>	Compute rank-based statistics of elements
<code>np.any</code>	N/A	Evaluate whether any elements are true
<code>np.all</code>	N/A	Evaluate whether all elements are true

NumPy

Universal functions: Aggregations (II)

(Download dataset)

- Use `wget` or `curl` to download the file within `iPython`

```
import pandas as pd
data = pd.read_csv('president_heights.csv')
heights = np.array(data['height(cm)'])
print(heights)

print("Mean height: ", heights.mean())
print("Standard deviation: ", heights.std())
print("Minimum height: ", heights.min())
print("Maximum height: ", heights.max())

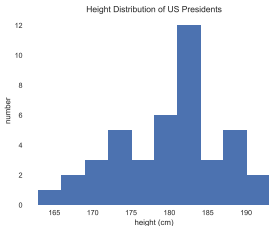
print("25th percentile: ", np.percentile(heights, 25))
print("Median: ", np.median(heights))
print("75th percentile: ", np.percentile(heights, 75))
```

NumPy

Universal functions: Aggregations (III)

```
%matplotlib inline
import matplotlib.pyplot as plt
import seaborn; seaborn.set() # set plot style

plt.hist(heights)
plt.title('Height Distribution of US Presidents')
plt.xlabel('height (cm)')
plt.ylabel('number');
```



NumPy

Universal functions: Broadcasting (I)

Broadcasting is a mechanism to operate over arrays of different sizes

- Used in ufuncs
- Implicit array expansion through three rules

Broadcasting rules

1. Rule 1: If the two arrays differ in their number of dimensions, the shape of the one with fewer dimensions is padded with ones on its leading (left) side.
2. Rule 2: If the shape of the two arrays does not match in any dimension, the array with shape equal to 1 in that dimension is stretched to match the other shape.
3. Rule 3: If in any dimension the sizes disagree and neither is equal to 1, an error is raised.

Universal functions: Broadcasting (II)

A visual representation of the addition problem using base ten blocks. The first addend is represented by three blocks labeled 0, 1, and 2. The second addend is represented by three blocks labeled 5, 5, and 5. The sum is represented by three blocks labeled 5, 6, and 7.

Diagram illustrating the addition of two 3x3 matrices:

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} + \begin{bmatrix} 0 & 1 & 2 \\ 0 & 1 & 2 \\ 0 & 1 & 2 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \\ 1 & 2 & 3 \end{bmatrix}$$

Diagram illustrating the addition of two 3x3 matrices. The first matrix has values [0, 1, 2] in the first column and [0, 1, 2] in the second column. The second matrix has values [0, 1, 2] in the first column and [0, 1, 2] in the second column. The result matrix has values [0, 1, 2] in the first column, [1, 2, 3] in the second column, and [2, 3, 4] in the third column.

Array expansion does not
consume memory!

NumPy

Comparisons, masks, and Boolean logic (I)

(Download dataset)

Example

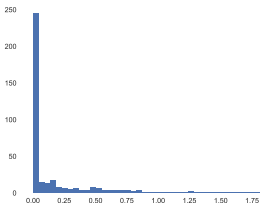
```
import numpy as np
import pandas as pd

# pandas to extract rainfall inches as a ndarray
rainfall = pd.read_csv('Seattle2014.csv')['PRCP'].values
inches = rainfall / 254.0 # 1/10mm -> inches
inches.shape
# Outputs (365,)
```

```
%matplotlib
import matplotlib.pyplot as plt
import seaborn; seaborn.set()
plt.hist(inches, 40);
```

NumPy

Comparisons, masks, and Boolean logic (II)



Data filtering is a recurrent task

- How many rainy days were there in the year?
- What is the average precipitation on those rainy days?
- How many days were there with more than half an inch of rain?

Two filtering methods in NumPy

- Boolean arrays masks
- Fancy indexing

NumPy

Comparisons, masks, and Boolean logic: Booleans arrays masks (I)

```
x [ x < 5 ]
x [ x == 3 ]
x [ ( x > 3 ) & ( x <= 5 ) ]
```

We've seen arithmetic ufuncs ...

- ... but they also support comparison and boolean operations
- Return an array of booleans

OPERATOR	UFUNC
==	np.equal
!=	np.not_equal
<	np.less
<=	np.less_equal
>	np.greater
>=	np.greater_equal

OPERATOR	UFUNC
&	np.bitwise_and
	np.bitwise_or
^	np.bitwise_xor
~	np.bitwise_not

Comparisons, masks, and Boolean logic: Booleans arrays masks (II)

```
print(x)
[[5, 0, 3, 3]
 [7, 9, 3, 5]
 [2, 4, 7, 6]]

np.count_nonzero(x < 6) # Returns 8
np.sum(x < 6) # Returns 8
np.sum(x < 6, axis=1) # By row, returns
    array([4, 2, 2])
np.any(x > 8) # Returns True
np.any(x < 0) # Returns False
np.all(x < 10) # Returns True

np.sum(~((inches <= 5) | (inches >= 1)))
```

Comparisons, masks, and Boolean logic: Fancy indexing

So far we've seen three accessing methods

- Simple indices (`x[1]`)
- Slices (`x[:5]`)
- Boolean masks (`x[x>0]`)

Fancy indexing: Pass arrays on indices instead of scalars

```
x = rand.randint(100, size=10)
[x[3], x[7], x[2]] # Simple indices
ind = [3, 7, 4] # Array of indices
x[ind] # Fancy indexing
x[[3, 5, 6]] # Also valid
```

The shape of the result reflects the shape of the index arrays rather than the shape of the array being indexed

Structured arrays (II)

```
data['name'] = name
data['age'] = age
data['weight'] = weight

# Get all names
data['name']

# Get first row of data
data[0]

# Get the name from the last row
data[-1]['name']

# Get names where age is under 30
data[data['age'] < 30]['name']
```

These kind of structures are day-to-day used

- Pandas is a much better choice

Pandas

Introduction

A data science workflow needs more features

- Label columns and rows
- Missing data
- Operations on groups
- Data input

Pandas implements all those features, and more

- Built on NumPy's ndarray

Pandas provides two main objects

- Series
- DataFrame

Convention

```
import numpy as np
import pandas as pd
```


The Pandas Series object (I)

A **Series** is a one-dimensional array of indexed data

- NumPy arrays indices are implicit (i.e. its position)
- Series indices are explicit, and can be any type

INDEX	VALUES
'a'	0.25
'b'	0.5
'c'	0.75
'd'	0.99

Two attributes

- values: ndarray
- index: pd.Index object

Two indices

- Implicit: Regular index
- Explicit: Custom index

```
data = pd.Series([0.25,
                  0.5, 0.75, 1.0])
data.values
data.index
data[1:3]
```


Pandas

The Pandas Series object (II)

```
In [1] : data = pd.Series([0.25, 0.5, 0.75, 1.0],
                           index=['a', 'b', 'c', 'd'])
```

```
In [2]: data
```

Out [1] :

a 0.25

b 0.50

c 0.75

d 1.00

```
dtype: float64
```

```
In [3]: data['a']
```

Out [2]: 0.25

```
In [4]: data[o]
```

Out [3]: 0.25

The Pandas DataFrame object (II)

```
In [1]: import seaborn as sns
```

```
In [2]: iris = sns.load_dataset('iris')
```

```
In [3]: iris.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 [246]: iris.columns
```

Out [2 4 6]:

```
Index(['sepal_length', 'sepal_width', 'petal_length',
      'petal_width', 'species'], dtype='object')
```

Pandas

Constructing DataFrame objects

Manual initialization

- From a single Series object
`pd.DataFrame(population, columns=['population'])`
- From several Series objects
`pd.DataFrame('population': population, 'area': area)`
- From a dictionary
`pd.DataFrame([{'a': 0, 'b': 0}, {'a': 1, 'b': 2}])`
- From a NumPy 2-D array
`pd.DataFrame(np.random.rand(3, 2),
columns=['foo', 'bar'], index=['a', 'b', 'c'])`

Read from a file

- CSV (very common!!!): `pd.read_csv('filename.csv')`
- Excel:
`pd.read_excel('filename.xlsx', sheetname='mysheet')`

Data indexing and selection: Series

Pandas

Data indexing and selection: DataFrame

Dictionary-like syntax

```
>>> data['area']
>>> data.area
>>> data.area is data['area']
True
>>> data['density'] = data['pop']
    / data['area']
```

Array-like syntax

```
>>> data.values # Get values
array
>>> data.T # Transpose
>>> data[0] # First row
>>> data['area'] # Area column
```

Remember indexing conventions

- Indexing refers to columns (`data['area']`)
- Slicing refers to rows (`data['Florida':'Illinois']`)
- Masking refers to rows (`data[data.density > 100]`)

Pandas

Data indexing and selection: loc, iloc and ix

Two types of indices in Pandas

- Explicit and implicit
- Indexing (`data[0]`) is explicit
- Slicing (`data[:2]`) is implicit (Python-like)
- Source of troubles!

Pandas makes explicit the used scheme

- loc: Explicit index
- iloc: Implicit index
- ix: Hybrid

Series

```
>>> serie.loc[1]
```

```
>>> serie.loc[1:3]
```

```
>>> serie.iloc[1]
```

```
>>> serie.iloc[1:3]
```

Dataframes

```
>>> df.iloc[:3, :2]
```

```
>>> df.loc[:, 'illinois', : 'pop']
```

```
>>> df.ix[:3, : 'pop']
```

```
>>> df.loc[df.data > 100, ['pop',  
                             'density']]
```

```
>>> df.iloc[0, 2] = 90
```

Pandas

Operating on data (I)

Pandas fully supports NumPy's ufuncs

- Efficient computations

Additional Pandas features

- Index and column name preservation
- Index aligning
- Easy data combination

```
>>> rng = np.random.RandomState(42)
>>> df = pd.DataFrame(rng.randint(0,
    10, (3,4)))
>>> df = pd.DataFrame(rng.randint(0,
    10, (3,4)), columns=[ 'A', 'B', 'C',
    , 'D' ])
>>> print(df)
   A  B  C  D
0  7  2  5  4
1  1  7  5  1
2  4  0  9  5
>>> np.sin(df * np.pi / 4)
      A          B          C          D
0  -7.07e-01    1.0   -0.7   1.22e-16
1   7.07e-01   -0.7   -0.7   7.07e-01
2   1.22e-16    0.0    0.7  -7.07e-01
```


Operating on data (II)

```
>>> A = pd.Series([2, 4, 6], index=[0, 1, 2])
>>> B = pd.Series([1, 3, 5], index=[1, 2, 3])
>>> A + B
0      NaN
1      5.0
2      9.0
3      NaN
dtype: float64
>>> A.add(B, fill_value=0)
0      2.0
1      5.0
2      9.0
3      5.0
dtype: float64
```

Pandas

Missing data (I)

NumPy supports missing data in floating-point data

- Specific value defined by IEEE
- Available as `np.nan`

Pandas supports missing data through two mechanisms

- `None` object, interpreted as NaN (Not a Number)
- `np.nan`: for floating-point data
- Almost automatic NaN handling (types upcast)

```
>>> pd.Series([1, np.nan, 2, None])
0    1.0
1    NaN
2    2.0
3    NaN
dtype: float64
```


Pandas

Combining datasets: `pd.concat()` (I)

Many times we need to combine two or more datasets

- Pandas provides `pd.concat()`, `append()` and `pd.merge()`

`pd.concat()` signature

```
pd.concat(objs, axis=0, join='outer',
          join_axes=None, ignore_index=False, keys
          =None, levels=None, names=None,
          verify_integrity=False, copy=True)
```

By default, `pd.concat()` joins rows preserving index

- `axis`: Join columns (`axis=1`)
- `verify_integrity`: Raise error if duplicates (`verify_integrity=True`)
- `ignore_index`: Create new index (`ignore_index=True`)
- `join`: Can be 'outer' (union) or 'inner' (intersection)

Combining datasets: `pd.concat()` (II)

```
>> df1 = pd.DataFrame([{'A': 'Ao', 'B': 'Bo'}, {'A': 'A1', 'B': 'B1'}
    ])
>> df2 = pd.DataFrame([{'A': 'A2', 'B': 'B2'}, {'A': 'A3', 'B': 'B3'}
    ])

>> print(df1), print(df2); print(pd.concat([df1, df2]))
  A  B      A  B      A  B
0  Ao Bo    0  A2 B2    0  Ao Bo
1  A1 B1    1  A3 B3    1  A1 B1
                        0  A2 B2
                        1  A3 B3

>> pd.concat([df1, df2], axis=1)
  A  B  A  B
0  Ao Bo A2 B2
1  A1 B1 A3 B3
>> df1.append(df2)
```


Pandas

Combining datasets: `pd.merge()` (II)

One-to-one

```
>> print(df1); print(df2)
  employee      group
0      Bob  Accounting
1      Jake  Engineering
2      Lisa  Engineering
3       Sue           HR
  employee  hire_date
0      Lisa      2004
1       Bob      2008
2       Jake      2012
3       Sue      2014
>> print(pd.merge(df1, df2))
  employee      group  hire_date
0       Bob  Accounting      2008
1       Jake  Engineering      2012
2       Lisa  Engineering      2004
3       Sue      HR           2014
```

Many-to-one

```
>>> print(df3); print(df4)
  employee  group  hire_date
0      Bob  Accounting  2008
1      Jake  Engineering  2012
2      Lisa  Engineering  2004
3       Sue           HR  2014

  group  supervisor
0  Accounting  Carly
1  Engineering  Guido
2           HR  Steve

>>> print(pd.merge(df3, df4))
  employee  group  hire_date  supervisor
0      Bob  Accounting  2008      Carly
1      Jake  Engineering  2012      Guido
2      Lisa  Engineering  2004      Guido
3       Sue           HR  2014      Steve
```

Pandas

Combining datasets: `pd.merge()` (III)

Many-to-many

```
>>> print(df1); print(df5)
```

	employee	group
0	Bob	Accounting
1	Jake	Engineering
2	Lisa	Engineering
3	Sue	HR

	group	skills
0	Accounting	math
1	Accounting	spreadsheets
2	Engineering	coding
3	Engineering	linux
4	HR	spreadsheets
5	HR	organization

```
>>> pd.merge(df1, df5)
```

	employee	group	skills
0	Bob	Accounting	math
1	Bob	Accounting	spreadsheets
2	Jake	Engineering	coding
3	Jake	Engineering	linux
4	Lisa	Engineering	coding
5	Lisa	Engineering	linux
6	Sue	HR	spreadsheets
7	Sue	HR	organization

Pandas

Combining datasets: `pd.merge()` (IV)

pd.merge() signature

```
pd.merge(left, right, how='inner', on=None,
         left_on=None, right_on=None, left_index=
         False, right_index=False, sort=False,
         suffixes=('_x', '_y'), copy=True,
         indicator=False, validate=None)
```

Arguments:

- `on`: Key column name
- `left_on`: Left table key column name
- `right_on`: Right table key column name
- `how`: Set arithmetic, `'inner'` (default, intersection), `'outer'` (union, fills missings with NaNs), `'left'` (left entries), `'right'` (right entries)

Pandas

Combining datasets: `pd.merge()` (V)

```
>>> A
   lkey  value
0  foo    1
1  bar    2
2  baz    3
3  foo    4

>>> B
   rkey  value
0  foo    5
1  bar    6
2  qux    7
3  bar    8

>>> A.merge(B, left_on='lkey', right_on='rkey', how='outer')
   lkey  value_x  rkey  value_y
0  foo    1      foo    5
1  foo    4      foo    5
2  bar    2      bar    6
3  bar    2      bar    8
4  baz    3      NaN    NaN
5  NaN    NaN     qux    7
```

Pandas

Aggregation in Pandas (I)

The first step in data analysis is summarization

- First contact with data
- Insight to the dataset

Aggregation methods

- Applied to columns

AGGREGATION	DESCRIPTION
<code>count()</code>	Total number of items
<code>first(), last()</code>	First and last item
<code>mean(), median()</code>	Mean and median
<code>min(), max()</code>	Minimum and maximum
<code>std(), var()</code>	Standard dev. and variance
<code>mad()</code>	Mean absolute deviation
<code>prod()</code>	Product of all items
<code>sum()</code>	Sum of all items
<code>describe()</code>	Data summary

```
>>> import seaborn as sns
>>> planets = sns.load_dataset('planets')
>>> planets.head()
```

		method	number	orbital_period	mass	distance	year
0	Radial Velocity	1	269.300	7.10	77.40	2006	
1	Radial Velocity	1	874.774	2.21	56.95	2008	
2	Radial Velocity	1	763.000	2.60	19.84	2011	
3	Radial Velocity	1	326.030	19.40	110.62	2007	
4	Radial Velocity	1	516.220	10.50	119.47	2009	

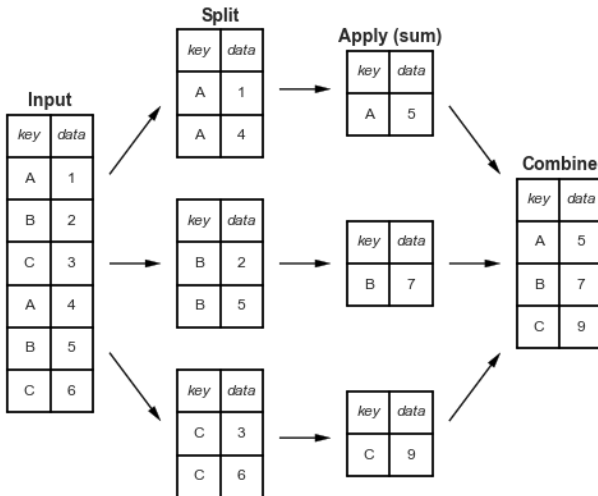
```
>>> planets.dropna().describe()
```

	number	orbital_period	mass	distance	year
count	498.00	498.000000	498.00	498.0000	498.000
mean	1.73	835.778671	2.50	52.0682	2007.377
std	1.17	1469.128259	3.63	46.5960	4.167
min	1.00	1.328300	0.00	1.3500	1989.000
25%	1.00	38.272250	0.21	24.4975	2005.000
50%	1.00	357.000000	1.24	39.9400	2009.000
75%	2.00	999.600000	2.86	59.3325	2011.000
max	6.00	17337.500000	25.00	354.0000	2014.000

```
>>> planets.mean()
```

number	1.785507
orbital_period	2002.917596
mass	2.638161
distance	264.069282
year	2009.070531
dtype:	float64

Grouping in Pandas (II)



Grouping in Pandas (III)

```
>>> df = pd.DataFrame({'key': ['A', 'B', 'C', 'A', 'B', 'C'],
                        'data': range(6)})
```

```
>>> print(df)
```

key data

O A O

I B I

$$2 \quad C \quad 2$$

3 A 3

4 B 4

5 C 5

```
>>> df.groupby('key')
```

```
<pandas.core.groupby.groupby.DataFrameGroupBy object at 0x102685438>
```

```
>>> df.groupby( 'key' ).sum()
      data
```

key

A 3

B 5

C 7

Pandas

Grouping in Pandas (III)

Several mapping methods available

- List

```
df.groupby([2,3,4,1]).sum()
```

- Dictionary

```
df.groupby('A': 'vowel', 'B': 'consonant', 'C':  
'vowel')
```

- Python function

```
df.groupby(str.lower)
```

- Multiple keys

```
planets.groupby(['method', 'year'])
```

- Mixed keys

```
df.groupby(['key1', 'key2', str.lower])
```


Pandas

Grouping in Pandas (IV)

The method `groupby()` returns an object `groupby`

- Basicly, it is a collection of dataframes

```
planets.groupby('method').get_group('Transit')
```

- Column selection as dataframe

```
planets.groupby('method')['year']
```

Interesting groupby attribute, groups

- Dictionary with groups

```
planets.groupby('method').groups
```

- Compatible with the `len()` method

```
len(planets.groupby('method'))
```

Pandas

Grouping in Pandas (V)

Usual operations with groupings

- Aggregation:
`df.groupby('key').aggregate(['min', np.median, max])`
`df.groupby('key').aggregate('data1': 'min', 'data2': 'max')`
- Filtering:
`planets.groupby('method').filter(lambda x: x['distance'].mean() > 50.)`
- Transformation:
`df.groupby('key').transform(lambda x: x - x.mean())`

Apply(): Apply arbitrary function and combine results

- Takes a function as argument that takes a DataFrame
- ```
planets.groupby("method").apply(lambda x: x / x.sum())
```

# Pandas

## Grouping in Pandas (VI)

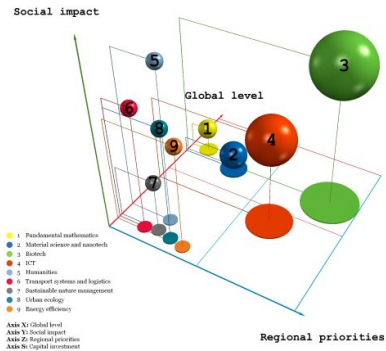
## Grouping by decade

```
decade = 10 * (planets['year'] // 10)
decade = decade.astype(str) + 's'
decade.name = 'decade'
planets.groupby(['method', decade])['number'].sum()
 .unstack().fillna(0)
```

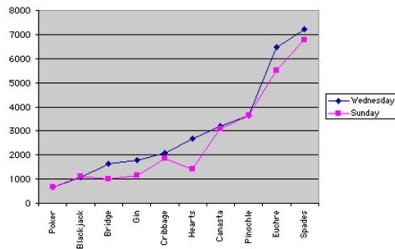


## Visualization

## Bad visualization examples (II)

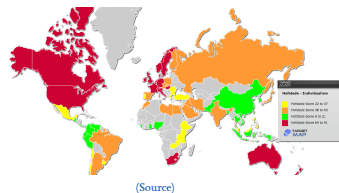
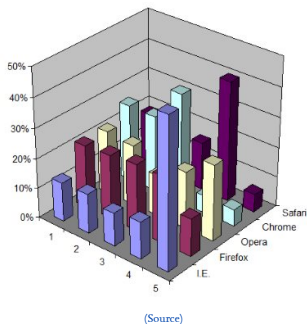


(Source)



(Source)

## Bad visualization examples (III)

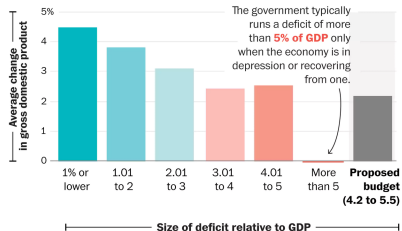


## Visualization

## Bad visualization examples (IV)

## Strange time for a stimulus

What annual **economic growth** averaged under various deficit-to-GDP ratios, since 1967



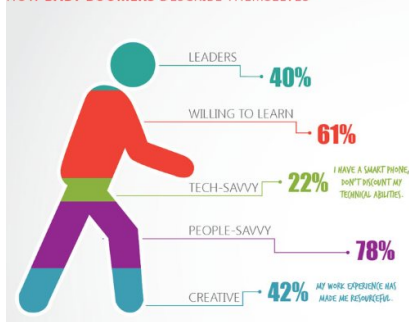
Notes: To capture the environment in which the budget was set, deficit-to-GDP ratios are compared with the economic climate of the prior fiscal year. GDP growth is adjusted for inflation and seasonality. Indicators for the current budget are based on the average of available data in fiscal 2017 and 2018 years. Fiscal years end in September.

Sources: Commerce Department (GDP); Congressional Budget Office (historical deficit); Committee for a Responsible Federal Budget (deficit forecasts, budget changes)

THE WASHINGTON POST

(Source)

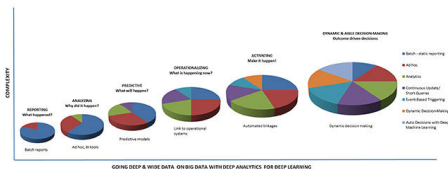
## HOW BABY BOOMERS DESCRIBE THEMSELVES



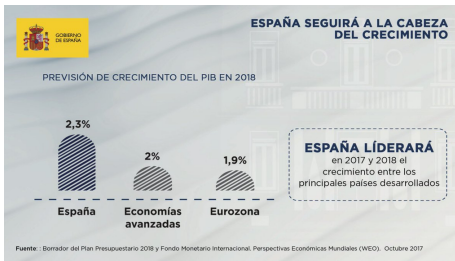
(Source)

## Visualization

## Bad visualization examples (V)



(Source)



(Source)



## Visualization

## Motivation (I)

## Efficient data visualization tips

- **Define your story**
- The chart must tell the story
- Don't distract from your story (with irrelevant data or visual elements)
- One story, one chart
- Put the story comprehension in first term
- Better several simple charts than one complex chart
- Choose colors wisely (color scale or high contrast)
- Elements order must support the story (legend, bars, etc)
- There is life beyond pies and bars
- Keep it simple, stupid!

## Visualization

## Motivation (II)

## Know your data

- Categorical or numerical
- Number of dimensions to represent (1D, 2D, 3D, more dimensions)

## Can you use other representation?

- Chart better than table? ...
- ... that depends

## What do you want to represent?

- Distribution, relationship, comparison or composition

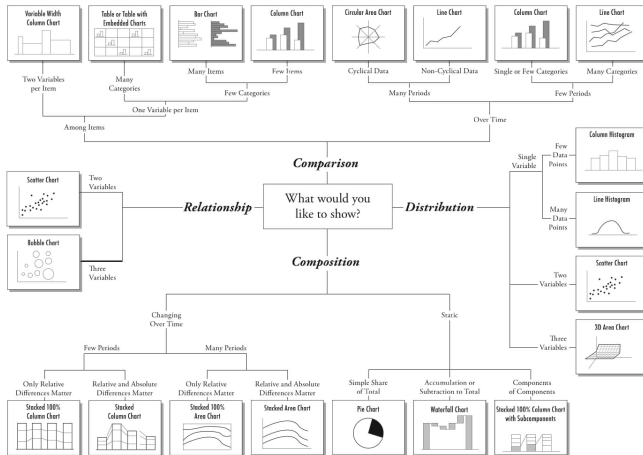
Look for templates: (<https://python-graph-gallery.com/>)

# Visualization

## Motivation (III)

### Chart Suggestions—A Thought-Starter

www.ExtremePresentation.com  
© 2009 A. Abela — a.x.abela@gmail.com



(Source)

## Visualization

## Introduction to Matplotlib (I)

## Matplotlib is a Python package

- Based on NumPy
- Imitates Matlab

### Three operation modes

- Scripts.  
Must use `plt.show()` to enter event loop. Use it once!
- IPython shell.  
Must use `%matplotlib`
- IPython notebook. Two modes
  - `%matplotlib inline`
  - `%matplotlib notebook`

## Convention

```
import matplotlib as mpl
import matplotlib.pyplot as plt
```

```
import matplotlib.pyplot as plt
import numpy as np

x = np.linspace(0, 10, 100)

plt.plot(x, np.sin(x))
plt.plot(x, np.cos(x))

plt.show()
```

## Visualization

## Introduction to Matplotlib (II)

## Matplotlib comes with two interfaces

- Matlab-like. Old-fashioned function-oriented API.
- Object-oriented. Object-oriented and more powerfull API.

## Matlab API

```
plt.figure() # create a plot

create the first of two panels
and set current axis
plt.subplot(2, 1, 1) # (rows,
columns, panel number)
plt.plot(x, np.sin(x))

create the second panel and
set current axis
plt.subplot(2, 1, 2)
plt.plot(x, np.cos(x));
```

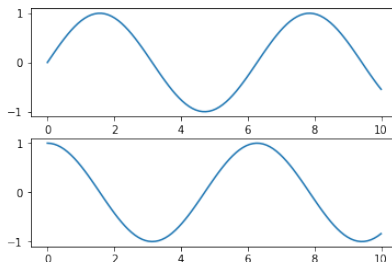
## OO API

```
plt.figure() # create a plot

create the first of two panels
and set current axis
plt.subplot(2, 1, 1) # (rows,
columns, panel number)
plt.plot(x, np.sin(x))

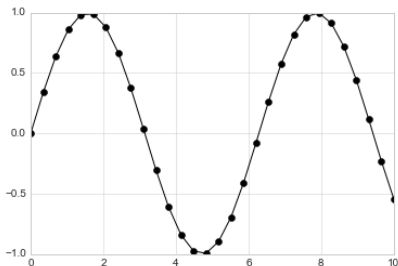
create the second panel and
set current axis
plt.subplot(2, 1, 2)
plt.plot(x, np.cos(x));
```

## Introduction to Matplotlib (III)

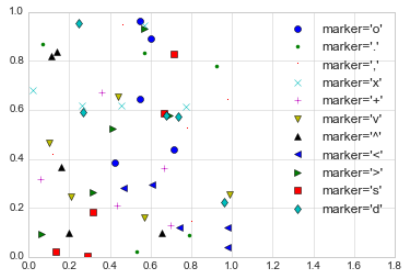


## Visualization

## Introduction to Matplotlib (IV)



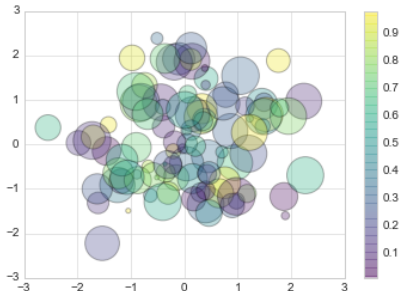
```
plt.plot(x, np.sin(x), '-ok',
 color='black')
```



```
for marker in ['o', '.', 'x', '+', 'v', '^', '<', '>', 's', 'd']:
 plt.plot(rng.rand(5), rng.rand(5), marker,
 label="marker='{0}'".format(marker))
plt.legend(numpoints=1)
plt.xlim(0, 1.8);
```

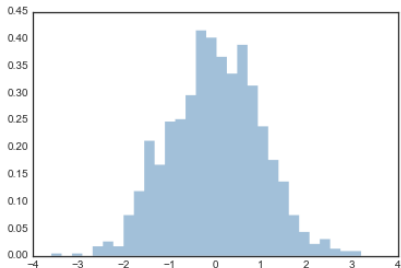
## Visualization

## Introduction to Matplotlib (V)



```
rng = np.random.RandomState(0)
x = rng.randn(1000)
y = rng.randn(1000)
colors = rng.rand(1000)
sizes = 1000 * rng.rand(1000)

plt.scatter(x, y, c=colors, s=sizes, alpha=0.3,
 cmap='viridis')
plt.colorbar(); # show color scale
```



```
data = np.random.randn(1000)

plt.hist(data, bins=30, normed=True, alpha=0.5,
 histtype='stepfilled', color='steelblue',
 edgecolor='none');
```





## Visualization

## Introduction to Seaborn (I)

## Seaborn is a modern data-visualization Python package

- Based on matplotlib
- ... it uses matplotlib indeed
- Pandas-aware
- High level
- Advanced visualizations
- Easy to use

Still under development! (v. 0.9)

## Convention

```
import seaborn as sns
```

This documentation is for Seaborn  
0.9 or newer

## Introduction to Seaborn (II)

## Display initialization

- `plt.show()`
- `%matplotlib`

## Style initialization

- Default Seaborn style `sns.set()`
- By default, same style than `matplotlib`

Several functions ...

- ... similar parameters

## Parameters

- x: Data axis x
- y: Data axis Y
- data: Dataframe name
- hue: Color
- style: Style
- sizes: Size
- kind: Alternate representation

## Visualization

## Introduction to Seaborn (III)

## Typical Seaborn usage

1. Prepare data
2. Set up aesthetics
3. Plot
4. Customize the plot

```
import matplotlib.pyplot as plt
import seaborn as sns

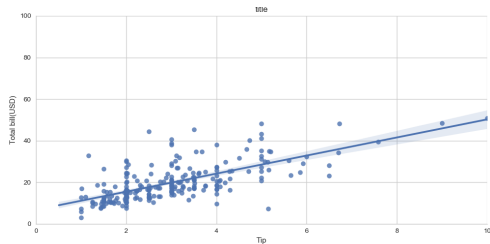
Prepare data
tips = sns.load_dataset("tips")

Set up aesthetics
sns.set_style("whitegrid")

Plot
g = sns.lmplot(x="tip", y="total_bill", data=tips, aspect=2)

Plot customization
g = (g.set_axis_labels("Tip", "Total bill (USD)").set(xlim=(0, 10), ylim=(0, 10)))

plt.title("title")
plt.show(g)
```



## Visualization

## Seaborn datasets (I)

## Seaborn comes with several dummy datasets

- `sns.load_dataset('name')`

We will use two datasets

- 'iris': The classical iris dataset, numerical
- 'tips': Numeric and categorical variables

```
>>> tips = sns.load_dataset('tips')
```

```
>>> print(tips.head())
```

|   | total_bill | tip  | sex    | smoker | day | time   | size |
|---|------------|------|--------|--------|-----|--------|------|
| 0 | 16.99      | 1.01 | Female | No     | Sun | Dinner | 2    |
| 1 | 10.34      | 1.66 | Male   | No     | Sun | Dinner | 3    |
| 2 | 21.01      | 3.50 | Male   | No     | Sun | Dinner | 3    |
| 3 | 23.68      | 3.31 | Male   | No     | Sun | Dinner | 2    |
| 4 | 24.59      | 3.61 | Female | No     | Sun | Dinner | 4    |

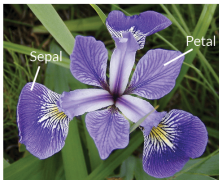
## Visualization

## Seaborn datasets (II)

```
>>> iris = sns.load_dataset('iris')
```

```
>>> print(iris.head())
```

|   | 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  |



## Iris Versicolor



## Iris Setosa

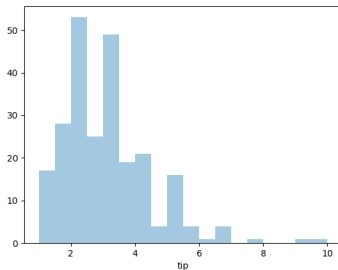


## Iris Virginica

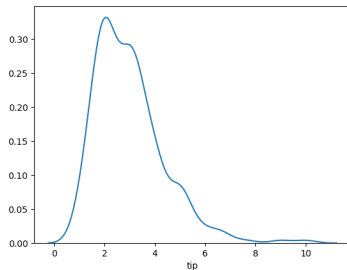
(Source)

## Visualization

## Seaborn: Distributions (I)



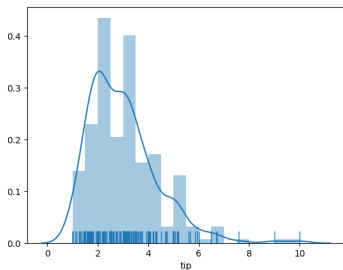
```
sns.distplot(tips['tip'],
 kde=False)
```



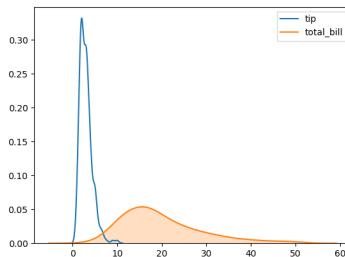
```
sns.distplot(tips['tip'],
 hist=False)
```

## Visualization

## Seaborn: Distributions (II)



```
sns.distplot(tips['tip'],
 rug=True)
```

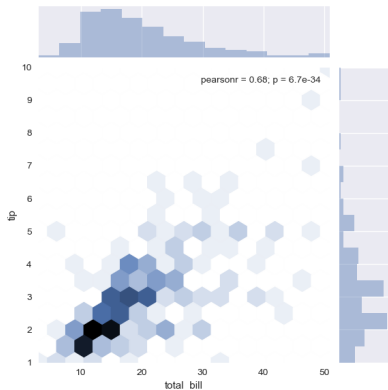


```
sns.kdeplot(tips['tip'])
sns.kdeplot(tips['total_bill'], shade=True)
```





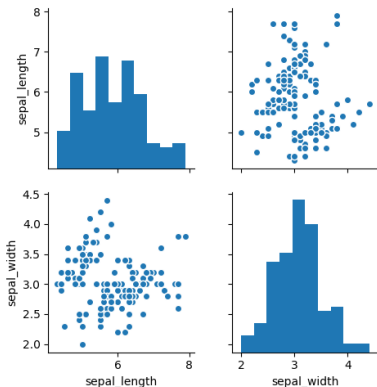
## Seaborn: Relationships (II)



```
sns.jointplot("total_bill", "tip", tips, kind="hex")
```



## Seaborn: Relationships (IV)



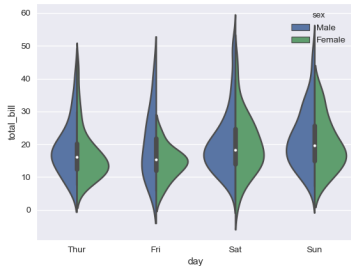
```
sns.pairplot(iris, hue="species", palette="husl",
 markers=["o", "s", "D"], diag_kind='kde')
```

```
sns.pairplot(iris, vars=["sepal_length", "sepal_width"])
```

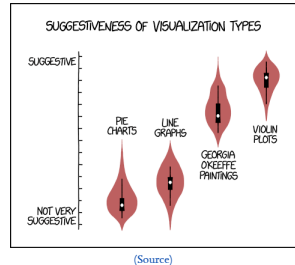


## Visualization

## Seaborn: Comparisons (II)

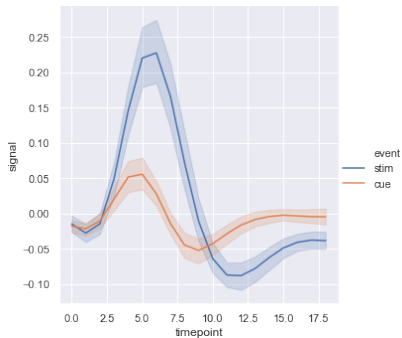


```
sns.violinplot(x="day", y="total_bill", hue="sex",
 data=tips, split=True)
```





## Seaborn: Continuity

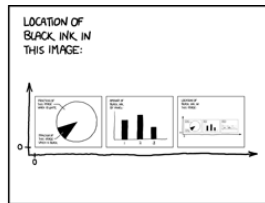
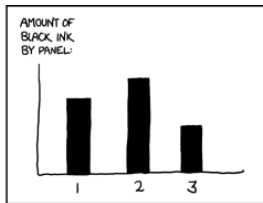
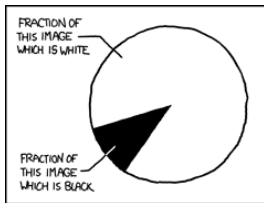


```
sns.relplot(x="timepoint", y="signal", hue="event",
 kind="line", data=fmri)
```

Seaborn &gt;= 0.9







(Source)