

# Statistical Machine Learning

Code in Python

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## INTRODUCTION

### 1.1 Python ecosystem for data-science

#### 1.1.1 Python language

- Interpreted
- Garbage collector (do not prevent from memory leak)
- Dynamically-typed language (Java is statically typed)

#### 1.1.2 Anaconda

Anaconda is a python distribution that ships most of python tools and libraries

##### Installation

1. Download anaconda (Python 3.x) <http://continuum.io/downloads>
2. Install it, on Linux

```
bash Anaconda3-2.4.1-Linux-x86_64.sh
```

3. Add anaconda path in your PATH variable in your .bashrc file:

```
export PATH="${HOME}/anaconda3/bin:$PATH"
```

##### Managing with “conda”

Update conda package and environment manager to current version

```
conda update conda
```

Install additional packages. Those commands install qt back-end (Fix a temporary issue to run spyder)

```
conda install pyqt
conda install PyOpenGL
conda update --all
```

Install seaborn for graphics

```
conda install seaborn
# install a specific version from anaconda channel
conda install -c anaconda pyqt=4.11.4
```

List installed packages

```
conda list
```

Search available packages

```
conda search pyqt
conda search scikit-learn
```

### Environments

- A conda environment is a directory that contains a specific collection of conda packages that you have installed.
- Control packages environment for a specific purpose: collaborating with someone else, delivering an application to your client,
- Switch between environments

List of all environments

```
:: conda info --envs
1. Create new environment
2. Activate
3. Install new package
```

```
conda create --name test
# Or
conda env create -f environment.yml
source activate test
conda info --envs
conda list
conda search -f numpy
conda install numpy
```

### Miniconda

Anaconda without the collection of (>700) packages. With Miniconda you download only the packages you want with the conda command: `conda install PACKAGENAME`

1. Download anaconda (Python 3.x) <https://conda.io/miniconda.html>
2. Install it, on Linux

```
bash Miniconda3-latest-Linux-x86_64.sh
```

3. Add anaconda path in your PATH variable in your .bashrc file:

```
export PATH=${HOME}/miniconda3/bin:$PATH
```

4. Install required packages

```
conda install -y scipy
conda install -y pandas
conda install -y matplotlib
conda install -y statsmodels
conda install -y scikit-learn
conda install -y sqlite
conda install -y spyder
conda install -y jupyter
```

### 1.1.3 Commands

**python**: python interpreter. On the dos/unix command line execute wholes file:

```
python file.py
```

Interactive mode:

```
python
```

Quite with CTL-D

**ipython**: advanced interactive python interpreter:

```
ipython
```

Quite with CTL-D

**pip** alternative for packages management (update -U in user directory --user):

```
pip install -U --user seaborn
```

For neuroimaging:

```
pip install -U --user nibabel
pip install -U --user nilearn
```

**spyder**: IDE (integrated development environment):

- Syntax highlighting.
- Code introspection for code completion (use TAB).
- Support for multiple Python consoles (including IPython).
- Explore and edit variables from a GUI.
- Debugging.
- Navigate in code (go to function definition) CTL.

3 or 4 panels:

text editor	help/variable explorer
	ipython interpreter

Shortcuts: - F9 run line/selection

### 1.1.4 Libraries

scipy.org: <https://www.scipy.org/docs.html>

**Numpy:** Basic numerical operation. Matrix operation plus some basic solvers.:

```
import numpy as np
X = np.array([[1, 2], [3, 4]])
#v = np.array([1, 2]).reshape((2, 1))
v = np.array([1, 2])
np.dot(X, v) # no broadcasting
X * v # broadcasting
np.dot(v, X)
X - X.mean(axis=0)
```

**Scipy:** general scientific libraries with advanced solver:

```
import scipy
import scipy.linalg
scipy.linalg.svd(X, full_matrices=False)
```

**Matplotlib:** visualization:

```
import numpy as np
import matplotlib.pyplot as plt
#%matplotlib qt
x = np.linspace(0, 10, 50)
sinus = np.sin(x)
plt.plot(x, sinus)
plt.show()
```

**Pandas:** Manipulation of structured data (tables). input/output excel files, etc.

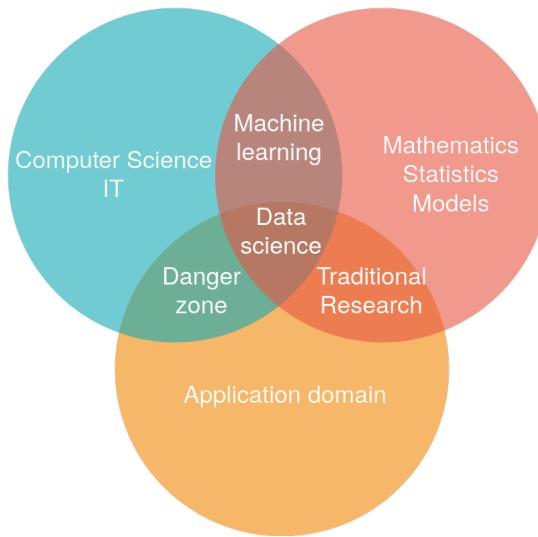
**Statsmodel:** Advanced statistics

**Scikit-learn:** Machine learning

li-brary	Arrays Num. I/O	data, comp,	Structured data, I/O	Solvers: basic	Solvers: advanced	Stats: basic	Stats: ad-vanced	Machine learning
Numpy	X			X				
Scipy				X	X	X		
Pan-das			X					
Stat-mod-els						X	X	
Scikit-learn								X

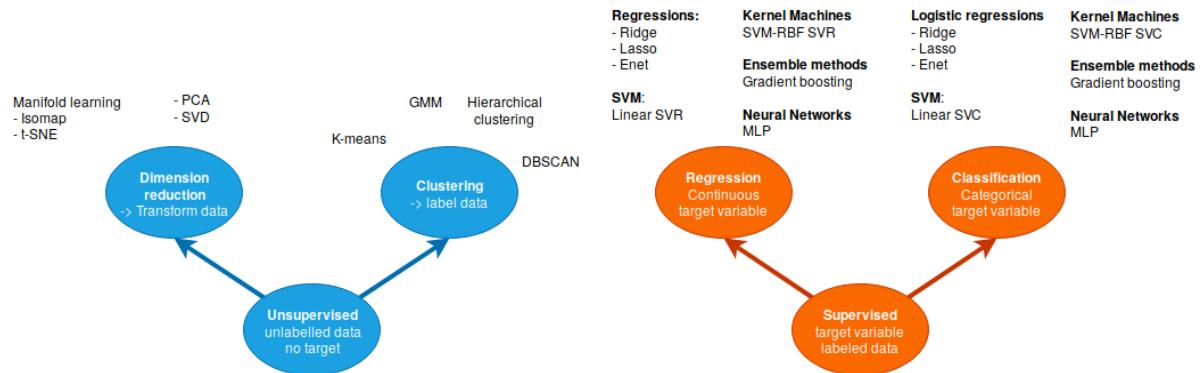
## 1.2 Introduction to Machine Learning

### 1.2.1 Machine learning within data science



Machine learning covers two main types of data analysis:

1. Exploratory analysis: **Unsupervised learning**. Discover the structure within the data. E.g.: Experience (in years in a company) and salary are correlated.
2. Predictive analysis: **Supervised learning**. This is sometimes described as “**learn from the past to predict the future**”. Scenario: a company wants to detect potential future clients among a base of prospects. Retrospective data analysis: we go through the data constituted of previous prospected companies, with their characteristics (size, domain, localization, etc...). Some of these companies became clients, others did not. The question is, can we possibly predict which of the new companies are more likely to become clients, based on their characteristics based on previous observations? In this example, the training data consists of a set of  $n$  training samples. Each sample,  $x_i$ , is a vector of  $p$  input features (company characteristics) and a target feature ( $y_i \in \{Yes, No\}$ ) (whether they became a client or not).



### 1.2.2 IT/computing science tools

- High Performance Computing (HPC)
- Data flow, data base, file I/O, etc.

- Python: the programming language.
- Numpy: python library particularly useful for handling of raw numerical data (matrices, mathematical operations).
- Pandas: input/output, manipulation structured data (tables).

### 1.2.3 Statistics and applied mathematics

- Linear model.
- Non parametric statistics.
- Linear algebra: matrix operations, inversion, eigenvalues.

## 1.3 Data analysis methodology

### 1. Formalize customer's needs into a learning problem:

- **A target variable: supervised problem.**
  - Target is qualitative: classification.
  - Target is quantitative: regression.
- **No target variable: unsupervised problem**
  - Vizualisation of high-dimensional samples: PCA, manifolds learning, etc.
  - Finding groups of samples (hidden structure): clustering.

### 2. Ask question about the datasets

- Number of samples
- Number of variables, types of each variable.

### 3. Define the sample

- For prospective study formalize the experimental design: inclusion/exclusion criteria. The conditions that define the acquisition of the dataset.
- For retrospective study formalize the experimental design: inclusion/exclusion criteria. The conditions that define the selection of the dataset.

### 4. In a document formalize (i) the project objectives; (ii) the required learning dataset (more specifically the input data and the target variables); (iii) The conditions that define the acquisition of the dataset. In this document, warn the customer that the learned algorithms may not work on new data acquired under different condition.

### 5. Read the learning dataset.

### 6. (i) Sanity check (basic descriptive statistics); (ii) data cleaning (impute missing data, recoding); Final Quality Control (QC) perform descriptive statistics and think ! (remove possible confounding variable, etc.).

### 7. Explore data (visualization, PCA) and perform basic univariate statistics for association between the target an input variables.

### 8. Perform more complex multivariate-machine learning.

9. Model validation using a left-out-sample strategy (cross-validation, etc.).
10. Apply on new data.



---

## CHAPTER TWO

---

# PYTHON LANGUAGE

---

**Note:** Click [here](#) to download the full example code

---

**Source** Kevin Markham <https://github.com/justmarkham/python-reference> Import libraries

---

```
# 'generic import' of math module
import math
math.sqrt(25)

# import a function
from math import sqrt
sqrt(25)      # no longer have to reference the module

# import multiple functions at once
from math import cos, floor

# import all functions in a module (generally discouraged)
# from os import *

# define an alias
import numpy as np

# show all functions in math module
content = dir(math)
```

## 2.1 Basic operations

```
# Numbers
10 + 4          # add (returns 14)
10 - 4          # subtract (returns 6)
10 * 4          # multiply (returns 40)
10 ** 4         # exponent (returns 10000)
10 / 4          # divide (returns 2 because both types are 'int')
10 / float(4)   # divide (returns 2.5)
5 % 4           # modulo (returns 1) - also known as the remainder

10 / 4          # true division (returns 2.5)
10 // 4         # floor division (returns 2)
```

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```
# Boolean operations
# comparisons (these return True)
5 > 3
5 >= 3
5 != 3
5 == 5

# boolean operations (these return True)
5 > 3 and 6 > 3
5 > 3 or 5 < 3
not False
False or not False and True      # evaluation order: not, and, or
```

## 2.2 Data types

```
# determine the type of an object
type(2)          # returns 'int'
type(2.0)        # returns 'float'
type('two')      # returns 'str'
type(True)       # returns 'bool'
type(None)        # returns 'NoneType'

# check if an object is of a given type
isinstance(2.0, int)        # returns False
isinstance(2.0, (int, float)) # returns True

# convert an object to a given type
float(2)
int(2.9)
str(2.9)

# zero, None, and empty containers are converted to False
bool(0)
bool(None)
bool('')
bool([])
bool({})           # empty dictionary

# non-empty containers and non-zeros are converted to True
bool(2)
bool('two')
bool([2])
```

### 2.2.1 Lists

Different objects categorized along a certain ordered sequence, lists are ordered, iterable, mutable (adding or removing objects changes the list size), can contain multiple data types ..  
chunk-chap13-001

```

# create an empty list (two ways)
empty_list = []
empty_list = list()

# create a list
simpsons = ['homer', 'marge', 'bart']

# examine a list
simpsons[0]      # print element 0 ('homer')
len(simpsons)    # returns the length (3)

# modify a list (does not return the list)
simpsons.append('lisa')          # append element to end
simpsons.extend(['itchy', 'scratchy']) # append multiple elements to end
simpsons.insert(0, 'maggie')       # insert element at index 0 (shifts everything_
                                ↪right)
simpsons.remove('bart')          # searches for first instance and removes it
simpsons.pop(0)                 # removes element 0 and returns it
del simpsons[0]                 # removes element 0 (does not return it)
simpsons[0] = 'krusty'          # replace element 0

# concatenate lists (slower than 'extend' method)
neighbors = simpsons + ['ned', 'rod', 'todd']

# find elements in a list
simpsons.count('lisa')          # counts the number of instances
simpsons.index('itchy')         # returns index of first instance

# list slicing [start:end:stride]
weekdays = ['mon', 'tues', 'wed', 'thurs', 'fri']
weekdays[0]          # element 0
weekdays[0:3]        # elements 0, 1, 2
weekdays[:3]         # elements 0, 1, 2
weekdays[3:]         # elements 3, 4
weekdays[-1]         # last element (element 4)
weekdays[::-2]        # every 2nd element (0, 2, 4)
weekdays[::-1]        # backwards (4, 3, 2, 1, 0)

# alternative method for returning the list backwards
list(reversed(weekdays))

# sort a list in place (modifies but does not return the list)
simpsons.sort()
simpsons.sort(reverse=True)     # sort in reverse
simpsons.sort(key=len)         # sort by a key

# return a sorted list (but does not modify the original list)
sorted(simpsons)
sorted(simpsons, reverse=True)
sorted(simpsons, key=len)

# create a second reference to the same list
num = [1, 2, 3]
same_num = num
same_num[0] = 0                # modifies both 'num' and 'same_num'

# copy a list (three ways)

```

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```
new_num = num.copy()
new_num = num[:]
new_num = list(num)

# examine objects
id(num) == id(same_num) # returns True
id(num) == id(new_num) # returns False
num is same_num          # returns True
num is new_num            # returns False
num == same_num           # returns True
num == new_num             # returns True (their contents are equivalent)

# concatenate +, replicate *
[1, 2, 3] + [4, 5, 6]
["a"] * 2 + ["b"] * 3
```

## 2.2.2 Tuples

Like lists, but their size cannot change: ordered, iterable, immutable, can contain multiple data types

```
# create a tuple
digits = (0, 1, 'two')           # create a tuple directly
digits = tuple([0, 1, 'two'])    # create a tuple from a list
zero = (0,)                      # trailing comma is required to indicate it's a tuple

# examine a tuple
digits[2]                      # returns 'two'
len(digits)                     # returns 3
digits.count(0)                 # counts the number of instances of that value (1)
digits.index(1)                  # returns the index of the first instance of that value (1)

# elements of a tuple cannot be modified
# digits[2] = 2                  # throws an error

# concatenate tuples
digits = digits + (3, 4)

# create a single tuple with elements repeated (also works with lists)
(3, 4) * 2                      # returns (3, 4, 3, 4)

# tuple unpacking
bart = ('male', 10, 'simpson') # create a tuple
```

## 2.2.3 Strings

A sequence of characters, they are iterable, immutable

```
# create a string
s = str(42)                      # convert another data type into a string
s = 'I like you'
```

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```

# examine a string
s[0]          # returns 'I'
len(s)         # returns 10

# string slicing like lists
s[:6]          # returns 'I like'
s[7:]          # returns 'you'
s[-1]          # returns 'u'

# basic string methods (does not modify the original string)
s.lower()      # returns 'i like you'
s.upper()      # returns 'I LIKE YOU'
s.startswith('I') # returns True
s.endswith('you') # returns True
s.isdigit()    # returns False (returns True if every character in the string is a_
               ↵digit)
s.find('like')   # returns index of first occurrence (2), but doesn't support regex
s.find('hate')    # returns -1 since not found
s.replace('like','love') # replaces all instances of 'like' with 'love'

# split a string into a list of substrings separated by a delimiter
s.split(' ')    # returns ['I','like','you']
s.split()        # same thing
s2 = 'a, an, the'
s2.split(',')    # returns ['a',' an',' the']

# join a list of strings into one string using a delimiter
stooges = ['larry','curly','moe']
' '.join(stooges) # returns 'larry curly moe'

# concatenate strings
s3 = 'The meaning of life is'
s4 = '42'
s3 + ' ' + s4    # returns 'The meaning of life is 42'
s3 + ' ' + str(42) # same thing

# remove whitespace from start and end of a string
s5 = ' ham and cheese '
s5.strip()       # returns 'ham and cheese'

# string substitutions: all of these return 'raining cats and dogs'
'raining %s and %s' % ('cats','dogs')           # old way
'raining {} and {}'.format('cats','dogs')        # new way
'raining {arg1} and {arg2}'.format(arg1='cats',arg2='dogs') # named arguments

# string formatting
# more examples: http://mkaz.com/2012/10/10/python-string-format/
'pi is {:.2f}'.format(3.14159)      # returns 'pi is 3.14'

```

## 2.2.4 Strings 2/2

Normal strings allow for escaped characters

```
print('first line\nsecond line')
```

Out:

```
first line
second line
```

raw strings treat backslashes as literal characters

```
print(r'first line\nfirst line')
```

Out:

```
first line\nfirst line
```

sequence of bytes are not strings, should be decoded before some operations

```
s = b'first line\nsecond line'
print(s)

print(s.decode('utf-8').split())
```

Out:

```
b'first line\nsecond line'
['first', 'line', 'second', 'line']
```

## 2.2.5 Dictionaries

Dictionaries are structures which can contain multiple data types, and is ordered with key-value pairs: for each (unique) key, the dictionary outputs one value. Keys can be strings, numbers, or tuples, while the corresponding values can be any Python object. Dictionaries are: unordered, iterable, mutable

```
# create an empty dictionary (two ways)
empty_dict = {}
empty_dict = dict()

# create a dictionary (two ways)
family = {'dad':'homer', 'mom':'marge', 'size':6}
family = dict(dad='homer', mom='marge', size=6)

# convert a list of tuples into a dictionary
list_of_tuples = [('dad', 'homer'), ('mom', 'marge'), ('size', 6)]
family = dict(list_of_tuples)

# examine a dictionary
family['dad']      # returns 'homer'
len(family)        # returns 3
family.keys()       # returns list: ['dad', 'mom', 'size']
family.values()     # returns list: ['homer', 'marge', 6]
family.items()      # returns list of tuples:
                   #   [ ('dad', 'homer'), ('mom', 'marge'), ('size', 6) ]
'mom' in family    # returns True
'marge' in family   # returns False (only checks keys)

# modify a dictionary (does not return the dictionary)
```

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```

family['cat'] = 'snowball'           # add a new entry
family['cat'] = 'snowball ii'        # edit an existing entry
del family['cat']                  # delete an entry
family['kids'] = ['bart', 'lisa']    # value can be a list
family.pop('dad')                  # removes an entry and returns the value ('homer')
family.update({'baby':'maggie', 'grandpa':'abe'})  # add multiple entries

# accessing values more safely with 'get'
family['mom']                      # returns 'marge'
family.get('mom')                  # same thing
try:
    family['grandma']              # throws an error
except KeyError as e:
    print("Error", e)

family.get('grandma')              # returns None
family.get('grandma', 'not found') # returns 'not found' (the default)

# accessing a list element within a dictionary
family['kids'][0]                  # returns 'bart'
family['kids'].remove('lisa')       # removes 'lisa'

# string substitution using a dictionary
'youngest child is %(baby)s' % family # returns 'youngest child is maggie'

```

Out:

Error 'grandma'

## 2.2.6 Sets

Like dictionaries, but with unique keys only (no corresponding values). They are: unordered, iterable, mutable, can contain multiple data types made up of unique elements (strings, numbers, or tuples)

```

# create an empty set
empty_set = set()

# create a set
languages = {'python', 'r', 'java'}          # create a set directly
snakes = set(['cobra', 'viper', 'python'])    # create a set from a list

# examine a set
len(languages)                # returns 3
'python' in languages         # returns True

# set operations
languages & snakes          # returns intersection: {'python'}
languages | snakes             # returns union: {'cobra', 'r', 'java', 'viper', 'python'}
languages - snakes            # returns set difference: {'r', 'java'}
snakes - languages            # returns set difference: {'cobra', 'viper'}

# modify a set (does not return the set)
languages.add('sql')          # add a new element

```

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```
languages.add('r')          # try to add an existing element (ignored, no error)
languages.remove('java')    # remove an element
try:
    languages.remove('c')    # try to remove a non-existing element (throws an error)
except KeyError as e:
    print("Error", e)
languages.discard('c')     # removes an element if present, but ignored otherwise
languages.pop()             # removes and returns an arbitrary element
languages.clear()           # removes all elements
languages.update('go', 'spark') # add multiple elements (can also pass a list or set)

# get a sorted list of unique elements from a list
sorted(set([9, 0, 2, 1, 0])) # returns [0, 1, 2, 9]
```

Out:

```
Error 'c'
```

## 2.3 Execution control statements

### 2.3.1 Conditional statements

```
x = 3
# if statement
if x > 0:
    print('positive')

# if/else statement
if x > 0:
    print('positive')
else:
    print('zero or negative')

# if/elif/else statement
if x > 0:
    print('positive')
elif x == 0:
    print('zero')
else:
    print('negative')

# single-line if statement (sometimes discouraged)
if x > 0: print('positive')

# single-line if/else statement (sometimes discouraged)
# known as a 'ternary operator'
'positive' if x > 0 else 'zero or negative'
```

Out:

```
positive
positive
```

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```
positive
positive
```

## 2.3.2 Loops

Loops are a set of instructions which repeat until termination conditions are met. This can include iterating through all values in an object, go through a range of values, etc

```
# range returns a list of integers
range(0, 3)      # returns [0, 1, 2]: includes first value but excludes second value
range(3)         # same thing: starting at zero is the default
range(0, 5, 2)   # returns [0, 2, 4]: third argument specifies the 'stride'

# for loop (not recommended)
fruits = ['apple', 'banana', 'cherry']
for i in range(len(fruits)):
    print(fruits[i].upper())

# alternative for loop (recommended style)
for fruit in fruits:
    print(fruit.upper())

# use range when iterating over a large sequence to avoid actually creating the integer_
# list in memory
for i in range(10**6):
    pass

# iterate through two things at once (using tuple unpacking)
family = {'dad':'homer', 'mom':'marge', 'size':6}
for key, value in family.items():
    print(key, value)

# use enumerate if you need to access the index value within the loop
for index, fruit in enumerate(fruits):
    print(index, fruit)

# for/else loop
for fruit in fruits:
    if fruit == 'banana':
        print("Found the banana!")
        break    # exit the loop and skip the 'else' block
    else:
        # this block executes ONLY if the for loop completes without hitting 'break'
        print("Can't find the banana")

# while loop
count = 0
while count < 5:
    print("This will print 5 times")
    count += 1      # equivalent to 'count = count + 1'
```

Out:

```
APPLE
BANANA
CHERRY
APPLE
BANANA
CHERRY
dad homer
mom marge
size 6
0 apple
1 banana
2 cherry
Can't find the banana
Found the banana!
This will print 5 times
```

### 2.3.3 Exceptions handling

```
dct = dict(a=[1, 2], b=[4, 5])

key = 'c'
try:
    dct[key]
except:
    print("Key %s is missing. Add it with empty value" % key)
    dct['c'] = []

print(dct)
```

Out:

```
Key c is missing. Add it with empty value
{'a': [1, 2], 'b': [4, 5], 'c': []}
```

## 2.4 Functions

Functions are sets of instructions launched when called upon, they can have multiple input values and a return value

```
# define a function with no arguments and no return values
def print_text():
    print('this is text')

# call the function
print_text()

# define a function with one argument and no return values
def print_this(x):
```

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```
print(x)

# call the function
print_this(3)      # prints 3
n = print_this(3)  # prints 3, but doesn't assign 3 to n
                   # because the function has no return statement

# define a function with one argument and one return value
def square_this(x):
    return x ** 2

# include an optional docstring to describe the effect of a function
def square_this(x):
    """Return the square of a number."""
    return x ** 2

# call the function
square_this(3)      # prints 9
var = square_this(3) # assigns 9 to var, but does not print 9

# default arguments
def power_this(x, power=2):
    return x ** power

power_this(2)       # 4
power_this(2, 3)   # 8

# use 'pass' as a placeholder if you haven't written the function body
def stub():
    pass

# return two values from a single function
def min_max(nums):
    return min(nums), max(nums)

# return values can be assigned to a single variable as a tuple
nums = [1, 2, 3]
min_max_num = min_max(nums)          # min_max_num = (1, 3)

# return values can be assigned into multiple variables using tuple unpacking
min_num, max_num = min_max(nums)    # min_num = 1, max_num = 3
```

Out:

```
this is text
3
3
```

## 2.5 List comprehensions, iterators, etc.

### 2.5.1 List comprehensions

Process which affects whole lists without iterating through loops. For more: <http://python-3-patterns-idioms-test.readthedocs.io/en/latest/Comprehensions.html>

```
# for loop to create a list of cubes
nums = [1, 2, 3, 4, 5]
cubes = []
for num in nums:
    cubes.append(num**3)

# equivalent list comprehension
cubes = [num**3 for num in nums]      # [1, 8, 27, 64, 125]

# for loop to create a list of cubes of even numbers
cubes_of_even = []
for num in nums:
    if num % 2 == 0:
        cubes_of_even.append(num**3)

# equivalent list comprehension
# syntax: [expression for variable in iterable if condition]
cubes_of_even = [num**3 for num in nums if num % 2 == 0]      # [8, 64]

# for loop to cube even numbers and square odd numbers
cubes_and_squares = []
for num in nums:
    if num % 2 == 0:
        cubes_and_squares.append(num**3)
    else:
        cubes_and_squares.append(num**2)

# equivalent list comprehension (using a ternary expression)
# syntax: [true_condition if condition else false_condition for variable in iterable]
cubes_and_squares = [num**3 if num % 2 == 0 else num**2 for num in nums]      # [1, 8, 9, ↵64, 25]

# for loop to flatten a 2d-matrix
matrix = [[1, 2], [3, 4]]
items = []
for row in matrix:
    for item in row:
        items.append(item)

# equivalent list comprehension
items = [item for row in matrix
          for item in row]      # [1, 2, 3, 4]

# set comprehension
fruits = ['apple', 'banana', 'cherry']
unique_lengths = {len(fruit) for fruit in fruits}  # {5, 6}

# dictionary comprehension
fruit_lengths = {fruit:len(fruit) for fruit in fruits}      # {'apple': 5, 'banana' ↵: 6, 'cherry': 6}
```

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## 2.6 Regular expression

### 1. Compile Regular expression with a pattern

```
import re

# 1. compile Regular expression with a pattern
regex = re.compile("^(sub-.+)_ses-(.+)_(mod-.+)$")
```

### 2. Match compiled RE on string

Capture the pattern `anyprefixsub-<subj id>\_ses-<session id>\_<modality>`

```
strings = ["abcsub-033_ses-01_mod-mri", "defsub-044_ses-01_mod-mri", "ghisub-055_ses-02_mod-ctscan"]
print([regex.findall(s)[0] for s in strings])
```

Out:

```
[('sub-033', 'ses-01', 'mod-mri'), ('sub-044', 'ses-01', 'mod-mri'), ('sub-055', 'ses-02',
    ↪ 'mod-ctscan')]
```

Match methods on compiled regular expression

Method/Attribute	Purpose
match(string)	Determine if the RE matches at the beginning of the string.
search(string)	Scan through a string, looking for any location where this RE matches.
findall(string)	Find all substrings where the RE matches, and returns them as a list.
finditer(string)	Find all substrings where the RE matches, and returns them as an iterator.

### 2. Replace compiled RE on string

```
regex = re.compile("(sub-[^_]+)") # match (sub-...)
print([regex.sub("SUB-", s) for s in strings])

regex.sub("SUB-", "toto")
```

Out:

```
['abcSUB-_ses-01_mod-mri', 'defSUB-_ses-01_mod-mri', 'ghiSUB-_ses-02_mod-ctscan']
```

Replace all non-alphanumeric characters in a string

```
re.sub('[^0-9a-zA-Z]+', '', 'h&ell`.,|o w]{+orld')
```

## 2.7 System programming

### 2.7.1 Operating system interfaces (os)

```
import os
```

Current working directory

```
# Get the current working directory
cwd = os.getcwd()
print(cwd)

# Set the current working directory
os.chdir(cwd)
```

Out:

```
/home/edouard/git/pystatsml/python_lang
```

Temporary directory

```
import tempfile

tmpdir = tempfile.gettempdir()
```

Join paths

```
mytmpdir = os.path.join(tmpdir, "foobar")

# list containing the names of the entries in the directory given by path.
os.listdir(tmpdir)
```

Create a directory

```
if not os.path.exists(mytmpdir):
    os.mkdir(mytmpdir)

os.makedirs(os.path.join(tmpdir, "foobar", "plop", "toto"), exist_ok=True)
```

### 2.7.2 File input/output

```
filename = os.path.join(mytmpdir, "myfile.txt")
print(filename)

# Write
lines = ["Dans python tout est bon", "Enfin, presque"]

## write line by line
fd = open(filename, "w")
fd.write(lines[0] + "\n")
fd.write(lines[1]+ "\n")
fd.close()
```

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```

## use a context manager to automatically close your file
with open(filename, 'w') as f:
    for line in lines:
        f.write(line + '\n')

# Read
## read one line at a time (entire file does not have to fit into memory)
f = open(filename, "r")
f.readline()    # one string per line (including newlines)
f.readline()    # next line
f.close()

## read one line at a time (entire file does not have to fit into memory)
f = open(filename, 'r')
f.readline()    # one string per line (including newlines)
f.readline()    # next line
f.close()

## read the whole file at once, return a list of lines
f = open(filename, 'r')
f.readlines()    # one list, each line is one string
f.close()

## use list comprehension to duplicate readlines without reading entire file at once
f = open(filename, 'r')
[line for line in f]
f.close()

## use a context manager to automatically close your file
with open(filename, 'r') as f:
    lines = [line for line in f]

```

Out:

```
/tmp/foobar/myfile.txt
```

### 2.7.3 Explore, list directories

Walk

```

import os

WD = os.path.join(os.environ["HOME"], "git", "pystatsml", "datasets")

for dirname, dirnames, filenames in os.walk(WD):
    print(dirname, dirnames, filenames)

```

Out:

```

/home/edouard/git/pystatsml/datasets ['brain_volumes'] ['multiTimeline.csv', 'Advertising.
↳csv', 'salary_table.csv', 'birthwt.txt', 'default of credit card clients.xls',
↳ 'eurodist.csv', 'birthwt.csv', 'iris.csv', 'readme.rst', 's_curve.csv']
/home/edouard/git/pystatsml/datasets/brain_volumes [] ['brain_volumes.xlsx', 'gm.csv',
↳ 'brain_volumes.csv', 'wm.csv', 'demo.csv', 'csf.csv']

```

glob, basename and file extension

```
import glob

filenames = glob.glob(os.path.join(os.environ["HOME"], "git", "pystatsml",
                                  "datasets", "*", "tissue-*.*.csv"))

# take basename then remove extension
basenames = [os.path.splitext(os.path.basename(f))[0] for f in filenames]
print(basenames)
```

Out:

```
[]
```

shutil - High-level file operations

```
import shutil

src = os.path.join(tmpdir, "foobar", "myfile.txt")
dst = os.path.join(tmpdir, "foobar", "plop", "myfile.txt")
print("copy %s to %s" % (src, dst))

shutil.copy(src, dst)

print("File %s exists ?" % dst, os.path.exists(dst))

src = os.path.join(tmpdir, "foobar", "plop")
dst = os.path.join(tmpdir, "plop2")
print("copy tree %s under %s" % (src, dst))

try:
    shutil.copytree(src, dst)

    shutil.rmtree(dst)

    shutil.move(src, dst)
except (FileExistsError, FileNotFoundError) as e:
    pass
```

Out:

```
copy /tmp/foobar/myfile.txt to /tmp/foobar/plop/myfile.txt
File /tmp/foobar/plop/myfile.txt exists ? True
copy tree /tmp/foobar/plop under /tmp/plop2
```

## 2.7.4 Command execution with subprocess

- For more advanced use cases, the underlying Popen interface can be used directly.
- Run the command described by args.
- Wait for command to complete
- return a CompletedProcess instance.

- Does not capture stdout or stderr by default. To do so, pass PIPE for the stdout and/or stderr arguments.

```
import subprocess

# doesn't capture output
p = subprocess.run(["ls", "-l"])
print(p.returncode)

# Run through the shell.
subprocess.run("ls -l", shell=True)

# Capture output
out = subprocess.run(["ls", "-a", "/"], stdout=subprocess.PIPE, stderr=subprocess.STDOUT)
# out.stdout is a sequence of bytes that should be decoded into a utf-8 string
print(out.stdout.decode('utf-8').split("\n")[:5])
```

Out:

```
0
[ '.', '..', 'bin', 'boot', 'cdrom']
```

## 2.7.5 Multiprocessing and multithreading

### Process

A process is a name given to a program instance that has been loaded into memory and managed by the operating system.

Process = address space + execution context (thread of control)

Process address space (segments):

- Code.
- Data (static/global).
- Heap (dynamic memory allocation).
- Stack.

Execution context:

- Data registers.
- Stack pointer (SP).
- Program counter (PC).
- Working Registers.

OS Scheduling of processes: context switching (ie. save/load Execution context)

Pros/cons

- Context switching expensive.
- (potentially) complex data sharing (not necessarily true).
- Cooperating processes - no need for memory protection (separate address spaces).

- Relevant for parallel computation with memory allocation.

### Threads

- Threads share the same address space (Data registers): access to code, heap and (global) data.
- Separate execution stack, PC and Working Registers.

### Pros/cons

- Faster context switching only SP, PC and Working Registers.
- Can exploit fine-grain concurrency
- Simple data sharing through the shared address space.
- Precautions have to be taken or two threads will write to the same memory at the same time. This is what the **global interpreter lock (GIL)** is for.
- Relevant for GUI, I/O (Network, disk) concurrent operation

### In Python

- The `threading` module uses threads.
- The `multiprocessing` module uses processes.

### Multithreading

```
import time
import threading

def list_append(count, sign=1, out_list=None):
    if out_list is None:
        out_list = list()
    for i in range(count):
        out_list.append(sign * i)
        sum(out_list) # do some computation
    return out_list

size = 10000 # Number of numbers to add

out_list = list() # result is a simple list
thread1 = threading.Thread(target=list_append, args=(size, 1, out_list, ))
thread2 = threading.Thread(target=list_append, args=(size, -1, out_list, ))

starttime = time.time()
# Will execute both in parallel
thread1.start()
thread2.start()
# Joins threads back to the parent process
thread1.join()
thread2.join()
print("Threading elapsed time ", time.time() - starttime)

print(out_list[:10])
```

Out:

```
Threading elapsed time 1.685194492340088
[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
```

## Multiprocessing

```
import multiprocessing

# Sharing requires specific mechanism
out_list1 = multiprocessing.Manager().list()
p1 = multiprocessing.Process(target=list_append, args=(size, 1, None))
out_list2 = multiprocessing.Manager().list()
p2 = multiprocessing.Process(target=list_append, args=(size, -1, None))

starttime = time.time()
p1.start()
p2.start()
p1.join()
p2.join()
print("Multiprocessing elapsed time ", time.time() - starttime)

# print(out_list[:10]) is not available
```

Out:

```
Multiprocessing elapsed time 0.38483119010925293
```

## Sharing object between process with Managers

Managers provide a way to create data which can be shared between different processes, including sharing over a network between processes running on different machines. A manager object controls a server process which manages shared objects.

```
import multiprocessing
import time

size = int(size / 100) # Number of numbers to add

# Sharing requires specific mechanism
out_list = multiprocessing.Manager().list()
p1 = multiprocessing.Process(target=list_append, args=(size, 1, out_list))
p2 = multiprocessing.Process(target=list_append, args=(size, -1, out_list))

starttime = time.time()

p1.start()
p2.start()

p1.join()
p2.join()

print(out_list[:10])

print("Multiprocessing with shared object elapsed time ", time.time() - starttime)
```

Out:

```
[0, 0, 1, -1, 2, -2, 3, -3, 4, -4]
Multiprocessing with shared object elapsed time 1.1143779754638672
```

## 2.8 Scripts and argument parsing

Example, the word count script

```
import os
import os.path
import argparse
import re
import pandas as pd

if __name__ == "__main__":
    # parse command line options
    output = "word_count.csv"
    parser = argparse.ArgumentParser()
    parser.add_argument('-i', '--input',
                        help='list of input files.',
                        nargs='+', type=str)
    parser.add_argument('-o', '--output',
                        help='output csv file (default %s)' % output,
                        type=str, default=output)
    options = parser.parse_args()

    if options.input is None :
        parser.print_help()
        raise SystemExit("Error: input files are missing")
    else:
        filenames = [f for f in options.input if os.path.isfile(f)]

    # Match words
    regex = re.compile("[a-zA-Z]+")

    count = dict()
    for filename in filenames:
        fd = open(filename, "r")
        for line in fd:
            for word in regex.findall(line.lower()):
                if not word in count:
                    count[word] = 1
                else:
                    count[word] += 1

        fd = open(options.output, "w")

    # Pandas
    df = pd.DataFrame([[k, count[k]] for k in count], columns=["word", "count"])
    df.to_csv(options.output, index=False)
```

## 2.9 Networking

```
# TODO
```

### 2.9.1 FTP

```
# Full FTP features with ftplib
import ftplib
ftp = ftplib.FTP("ftp.cea.fr")
ftp.login()
ftp.cwd('/pub/unati/people/educhesnay/pystatml')
ftp.retrlines('LIST')

fd = open(os.path.join(tmpdir, "README.md"), "wb")
ftp.retrbinary('RETR README.md', fd.write)
fd.close()
ftp.quit()

# File download urllib
import urllib.request
ftp_url = 'ftp://ftp.cea.fr/pub/unati/people/educhesnay/pystatml/README.md'
urllib.request.urlretrieve(ftp_url, os.path.join(tmpdir, "README2.md"))
```

Out:

```
-rw-r--r--    1 ftp      ftp          1282 Apr 15 22:33 README.md
-rw-r--r--    1 ftp      ftp        6301451 Mar 14 00:29_
↪StatisticsMachineLearningPythonDraft.pdf
```

### 2.9.2 HTTP

```
# TODO
```

### 2.9.3 Sockets

```
# TODO
```

### 2.9.4 xmlrpc

```
# TODO
```

## 2.10 Modules and packages

A module is a Python file. A package is a directory which MUST contain a special file called `__init__.py`

To import, extend variable `PYTHONPATH`:

```
export PYTHONPATH=path_to_parent_python_module:${PYTHONPATH}
```

Or

```
import sys
sys.path.append("path_to_parent_python_module")
```

The `__init__.py` file can be empty. But you can set which modules the package exports as the API, while keeping other modules internal, by overriding the `__all__` variable, like so:

parentmodule/`__init__.py` file:

```
from . import submodule1
from . import submodule2

from .submodule3 import function1
from .submodule3 import function2

__all__ = ["submodule1", "submodule2",
           "function1", "function2"]
```

User can import:

```
import parentmodule.submodule1
import parentmodule.function1
```

Python Unit Testing

## 2.11 Object Oriented Programming (OOP)

### Sources

- [http://python-textbook.readthedocs.org/en/latest/Object\\_Oriented\\_Programming.html](http://python-textbook.readthedocs.org/en/latest/Object_Oriented_Programming.html)

### Principles

- **Encapsulate** data (attributes) and code (methods) into objects.
- **Class** = template or blueprint that can be used to create objects.
- An **object** is a specific instance of a class.
- **Inheritance**: OOP allows classes to inherit commonly used state and behaviour from other classes. Reduce code duplication
- **Polymorphism**: (usually obtained through polymorphism) calling code is agnostic as to whether an object belongs to a parent class or one of its descendants (abstraction, modularity). The same method called on 2 objects of 2 different classes will behave differently.

```
import math

class Shape2D:
    def area(self):
        raise NotImplementedError()

# __init__ is a special method called the constructor
```

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```
# Inheritance + Encapsulation
class Square(Shape2D):
    def __init__(self, width):
        self.width = width

    def area(self):
        return self.width ** 2

class Disk(Shape2D):
    def __init__(self, radius):
        self.radius = radius

    def area(self):
        return math.pi * self.radius ** 2

shapes = [Square(2), Disk(3)]

# Polymorphism
print([s.area() for s in shapes])

s = Shape2D()
try:
    s.area()
except NotImplementedError as e:
    print("NotImplementedError")
```

Out:

```
[4, 28.27433882308138]
NotImplementedError
```

## 2.12 Exercises

### 2.12.1 Exercise 1: functions

Create a function that acts as a simple calculator. If the operation is not specified, default to addition. If the operation is misspecified, return an error message. Ex: calc(4,5,"multiply") returns 20. Ex: calc(3,5) returns 8. Ex: calc(1, 2, "something") returns error message.

### 2.12.2 Exercise 2: functions + list + loop

Given a list of numbers, return a list where all adjacent duplicate elements have been reduced to a single element. Ex: [1, 2, 2, 3, 2] returns [1, 2, 3, 2]. You may create a new list or modify the passed in list.

Remove all duplicate values (adjacent or not) Ex: [1, 2, 2, 3, 2] returns [1, 2, 3]

### 2.12.3 Exercise 3: File I/O

1. Copy/paste the BSD 4 clause license ([https://en.wikipedia.org/wiki/BSD\\_licenses](https://en.wikipedia.org/wiki/BSD_licenses)) into a text file. Read, the file and count the occurrences of each word within the file. Store the words' occurrence number in a dictionary.
2. Write an executable python command `count_words.py` that parse a list of input files provided after `--input` parameter. The dictionary of occurrence is save in a csv file provides by `--output`. with default value `word_count.csv`. Use: - open - regular expression - argparse (<https://docs.python.org/3/howto/argparse.html>)

### 2.12.4 Exercise 4: OOP

1. Create a class `Employee` with 2 attributes provided in the constructor: `name`, `years_of_service`. With one method `salary` which is obtained by  $1500 + 100 * \text{years\_of\_service}$ .
2. Create a subclass `Manager` which redefine `salary` method  $2500 + 120 * \text{years\_of\_service}$ .
3. Create a small dictionary-nosed database where the key is the employee's name. Populate the database with: `samples = Employee('lucy', 3), Employee('john', 1), Manager('julie', 10), Manager('paul', 3)`
4. Return a table of made name, salary rows, i.e. a list of list `[[name, salary]]`
5. Compute the average salary

**Total running time of the script:** ( 0 minutes 4.315 seconds)

## SCIENTIFIC PYTHON

---

**Note:** Click [here](#) to download the full example code

---

### 3.1 Numpy: arrays and matrices

NumPy is an extension to the Python programming language, adding support for large, multi-dimensional (numerical) arrays and matrices, along with a large library of high-level mathematical functions to operate on these arrays.

Sources:

- Kevin Markham: <https://github.com/justmarkham>

```
import numpy as np
```

#### 3.1.1 Create arrays

Create ndarrays from lists. note: every element must be the same type (will be converted if possible)

```
data1 = [1, 2, 3, 4, 5]          # list
arr1 = np.array(data1)           # 1d array
data2 = [range(1, 5), range(5, 9)] # list of lists
arr2 = np.array(data2)           # 2d array
arr2.tolist()                   # convert array back to list
```

create special arrays

```
np.zeros(10)
np.zeros((3, 6))
np.ones(10)
np.linspace(0, 1, 5)           # 0 to 1 (inclusive) with 5 points
np.logspace(0, 3, 4)           # 10^0 to 10^3 (inclusive) with 4 points
```

arange is like range, except it returns an array (not a list)

```
int_array = np.arange(5)
float_array = int_array.astype(float)
```

### 3.1.2 Examining arrays

```
arr1.dtype      # float64
arr2.dtype      # int32
arr2.ndim       # 2
arr2.shape      # (2, 4) - axis 0 is rows, axis 1 is columns
arr2.size       # 8 - total number of elements
len(arr2)       # 2 - size of first dimension (aka axis)
```

### 3.1.3 Reshaping

```
arr = np.arange(10, dtype=float).reshape((2, 5))
print(arr.shape)
print(arr.reshape(5, 2))
```

Out:

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

Add an axis

```
a = np.array([0, 1])
a_col = a[:, np.newaxis]
print(a_col)
#or
a_col = a[:, None]
```

Out:

```
[[0]
 [1]]
```

Transpose

```
print(a_col.T)
```

Out:

```
[[0 1]]
```

Flatten: always returns a flat copy of the original array

```
arr_flt = arr.flatten()
arr_flt[0] = 33
print(arr_flt)
print(arr)
```

Out:

```
[33.  1.  2.  3.  4.  5.  6.  7.  8.  9.]  
[[0.  1.  2.  3.  4.]  
 [5.  6.  7.  8.  9.]]
```

Ravel: returns a view of the original array whenever possible.

```
arr_flt = arr.ravel()  
arr_flt[0] = 33  
print(arr_flt)  
print(arr)
```

Out:

```
[33.  1.  2.  3.  4.  5.  6.  7.  8.  9.]  
[[33.  1.  2.  3.  4.]  
 [ 5.  6.  7.  8.  9.]]
```

### 3.1.4 Stack arrays

Stack flat arrays in columns

```
a = np.array([0, 1])  
b = np.array([2, 3])  
  
ab = np.stack((a, b)).T  
print(ab)  
  
# or  
np.hstack((a[:, None], b[:, None]))
```

Out:

```
[[0 2]  
 [1 3]]
```

### 3.1.5 Selection

Single item

```
arr = np.arange(10, dtype=float).reshape((2, 5))  
  
arr[0]      # 0th element (slices like a list)  
arr[0, 3]    # row 0, column 3: returns 4  
arr[0][3]    # alternative syntax
```

### Slicing

Syntax: start:stop:step with start (*default 0*) stop (*default last*) step (*default 1*)

```
arr[0, :]      # row 0: returns 1d array ([1, 2, 3, 4])
arr[:, 0]       # column 0: returns 1d array ([1, 5])
arr[:, :2]      # columns strictly before index 2 (2 first columns)
arr[:, 2:]      # columns after index 2 included
arr2 = arr[:, 1:4]    # columns between index 1 (included) and 4 (excluded)
print(arr2)
```

Out:

```
[[1. 2. 3.]
 [6. 7. 8.]]
```

Slicing returns a view (not a copy)

```
arr2[0, 0] = 33
print(arr2)
print(arr)
```

Out:

```
[[33. 2. 3.]
 [ 6. 7. 8.]]
[[ 0. 33. 2. 3. 4.]
 [ 5. 6. 7. 8. 9.]]
```

Row 0: reverse order

```
print(arr[0, ::-1])

# The rule of thumb here can be: in the context of lvalue indexing (i.e. the indices are_
# placed in the left hand side value of an assignment), no view or copy of the array is_
# created (because there is no need to). However, with regular values, the above rules_
# for creating views does apply.
```

Out:

```
[ 4. 3. 2. 33. 0.]
```

### Fancy indexing: Integer or boolean array indexing

Fancy indexing returns a copy not a view.

Integer array indexing

```
arr2 = arr[:, [1,2,3]]  # return a copy
print(arr2)
arr2[0, 0] = 44
print(arr2)
print(arr)
```

Out:

```
[[33. 2. 3.]
 [ 6. 7. 8.]]
```

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```
[[44.  2.  3.]
 [ 6.  7.  8.]]
[[ 0.  33.  2.  3.  4.]
 [ 5.  6.  7.  8.  9.]]
```

Boolean arrays indexing

```
arr2 = arr[arr > 5] # return a copy

print(arr2)
arr2[0] = 44
print(arr2)
print(arr)
```

Out:

```
[33.  6.  7.  8.  9.]
[44.  6.  7.  8.  9.]
[[ 0.  33.  2.  3.  4.]
 [ 5.  6.  7.  8.  9.]]
```

However, In the context of lvalue indexing (left hand side value of an assignment) Fancy authorizes the modification of the original array

```
arr[arr > 5] = 0
print(arr)
```

Out:

```
[[0.  0.  2.  3.  4.]
 [5.  0.  0.  0.  0.]]
```

Boolean arrays indexing continues

```
names = np.array(['Bob', 'Joe', 'Will', 'Bob'])
names == 'Bob'                      # returns a boolean array
names[names != 'Bob']                # logical selection
(names == 'Bob') | (names == 'Will') # keywords "and/or" don't work with boolean arrays
names[names != 'Bob'] = 'Joe'        # assign based on a logical selection
np.unique(names)                    # set function
```

### 3.1.6 Vectorized operations

```
nums = np.arange(5)
nums * 10                           # multiply each element by 10
nums = np.sqrt(nums)                 # square root of each element
np.ceil(nums)                       # also floor, rint (round to nearest int)
np.isnan(nums)                      # checks for NaN
nums + np.arange(5)                 # add element-wise
np.maximum(nums, np.array([1, -2, 3, -4, 5])) # compare element-wise

# Compute Euclidean distance between 2 vectors
vec1 = np.random.randn(10)
```

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```
vec2 = np.random.randn(10)
dist = np.sqrt(np.sum((vec1 - vec2) ** 2))

# math and stats
rnd = np.random.randn(4, 2) # random normals in 4x2 array
rnd.mean()
rnd.std()
rnd.argmin()             # index of minimum element
rnd.sum()
rnd.sum(axis=0)          # sum of columns
rnd.sum(axis=1)          # sum of rows

# methods for boolean arrays
(rnd > 0).sum()          # counts number of positive values
(rnd > 0).any()           # checks if any value is True
(rnd > 0).all()           # checks if all values are True

# random numbers
np.random.seed(12234)      # Set the seed
np.random.rand(2, 3)        # 2 x 3 matrix in [0, 1]
np.random.randn(10)         # random normals (mean 0, sd 1)
np.random.randint(0, 2, 10)  # 10 randomly picked 0 or 1
```

### 3.1.7 Broadcasting

Sources: <https://docs.scipy.org/doc/numpy-1.13.0/user/basics.broadcasting.html> Implicit conversion to allow operations on arrays of different sizes.

- The smaller array is stretched or “broadcasted” across the larger array so that they have compatible shapes.
- Fast vectorized operation in C instead of Python.
- No needless copies.

#### Rules

Starting with the trailing axis and working backward, Numpy compares arrays dimensions.

- If two dimensions are equal then continues
- If one of the operand has dimension 1 stretches it to match the largest one
- When one of the shapes runs out of dimensions (because it has less dimensions than the other shape), Numpy will use 1 in the comparison process until the other shape's dimensions run out as well.

```
a = np.array([[ 0,  0,  0],
              [10, 10, 10],
              [20, 20, 20],
              [30, 30, 30]])

b = np.array([0, 1, 2])

print(a + b)
```

Out:

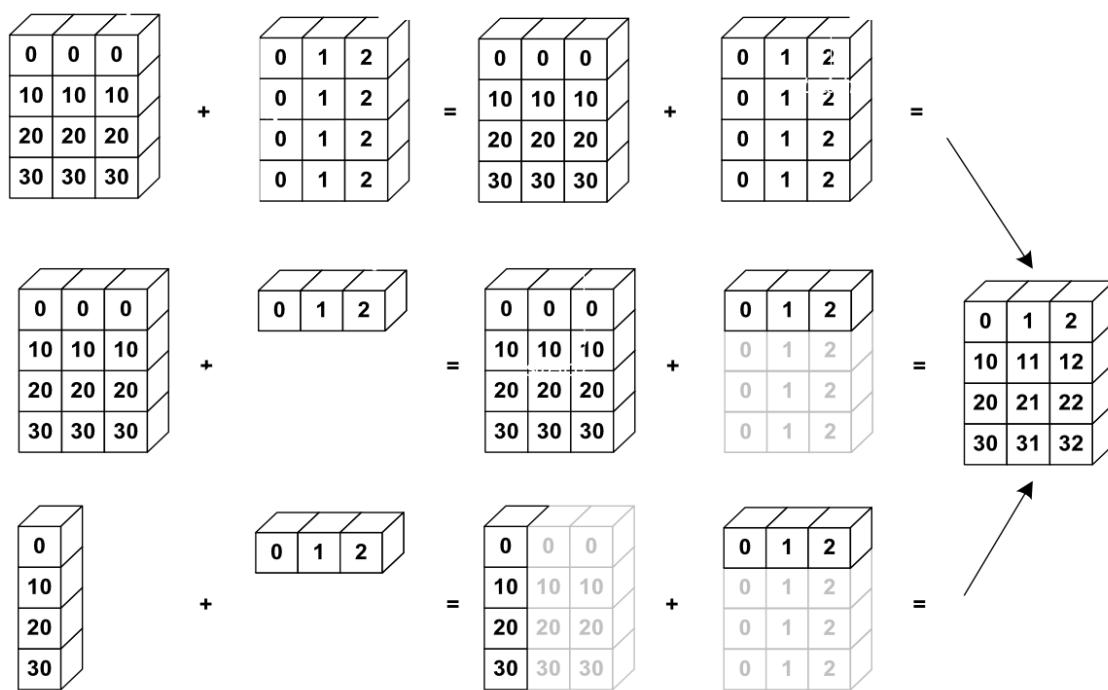


Fig. 1: Source: <http://www.scipy-lectures.org>

```
[[ 0  1  2]
 [10 11 12]
 [20 21 22]
 [30 31 32]]
```

## Examples

Shapes of operands A, B and result:

```
A      (2d array):  5 x 4
B      (1d array):    1
Result (2d array):  5 x 4

A      (2d array):  5 x 4
B      (1d array):    4
Result (2d array):  5 x 4

A      (3d array):  15 x 3 x 5
B      (3d array):  15 x 1 x 5
Result (3d array):  15 x 3 x 5

A      (3d array):  15 x 3 x 5
B      (2d array):    3 x 5
Result (3d array):  15 x 3 x 5

A      (3d array):  15 x 3 x 5
B      (2d array):    3 x 1
Result (3d array):  15 x 3 x 5
```

### 3.1.8 Exercises

Given the array:

```
X = np.random.randn(4, 2) # random normals in 4x2 array
```

- For each column find the row index of the minimum value.
- Write a function `standardize(X)` that return an array whose columns are centered and scaled (by std-dev).

**Total running time of the script:** ( 0 minutes 0.037 seconds)

---

**Note:** Click [here](#) to download the full example code

---

## 3.2 Pandas: data manipulation

It is often said that 80% of data analysis is spent on the cleaning and small, but important, aspect of data manipulation and cleaning with Pandas.

**Sources:**

- Kevin Markham: <https://github.com/justmarkham>

- Pandas doc: <http://pandas.pydata.org/pandas-docs/stable/index.html>

## Data structures

- Series** is a one-dimensional labeled array capable of holding any data type (integers, strings, floating point numbers, Python objects, etc.). The axis labels are collectively referred to as the index. The basic method to create a Series is to call `pd.Series([1,3,5,np.nan,6,8])`
- DataFrame** is a 2-dimensional labeled data structure with columns of potentially different types. You can think of it like a spreadsheet or SQL table, or a dict of Series objects. It stems from the R `data.frame()` object.

```
from __future__ import print_function

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

### 3.2.1 Create DataFrame

```
columns = ['name', 'age', 'gender', 'job']

user1 = pd.DataFrame([['alice', 19, "F", "student"],
                      ['john', 26, "M", "student"]],
                      columns=columns)

user2 = pd.DataFrame([['eric', 22, "M", "student"],
                      ['paul', 58, "F", "manager"]],
                      columns=columns)

user3 = pd.DataFrame(dict(name=['peter', 'julie'],
                           age=[33, 44], gender=['M', 'F'],
                           job=['engineer', 'scientist']))

print(user3)
```

Out:

	name	age	gender	job
0	peter	33	M	engineer
1	julie	44	F	scientist

### 3.2.2 Combining DataFrames

#### Concatenate DataFrame

```
user1.append(user2)
users = pd.concat([user1, user2, user3])
print(users)
```

Out:

```
name  age  gender      job
0   alice  19       F  student
1   john   26       M  student
0   eric   22       M  student
1   paul   58       F  manager
0   peter   33       M  engineer
1   julie   44       F  scientist
```

### Join DataFrame

```
user4 = pd.DataFrame(dict(name=['alice', 'john', 'eric', 'julie'],
                           height=[165, 180, 175, 171]))
print(user4)
```

Out:

```
name  height
0   alice    165
1   john     180
2   eric     175
3   julie    171
```

Use intersection of keys from both frames

```
merge_inter = pd.merge(users, user4, on="name")
print(merge_inter)
```

Out:

```
name  age  gender      job  height
0   alice  19       F  student    165
1   john   26       M  student    180
2   eric   22       M  student    175
3   julie   44       F  scientist  171
```

Use union of keys from both frames

```
users = pd.merge(users, user4, on="name", how='outer')
print(users)
```

Out:

```
name  age  gender      job  height
0   alice  19       F  student    165.0
1   john   26       M  student    180.0
2   eric   22       M  student    175.0
3   paul   58       F  manager     NaN
4   peter   33       M  engineer    NaN
5   julie   44       F  scientist   171.0
```

### Reshaping by pivoting

“Unpivots” a DataFrame from wide format to long (stacked) format,

```
staked = pd.melt(users, id_vars="name", var_name="variable", value_name="value")
print(staked)
```

Out:

	name	variable	value
0	alice	age	19
1	john	age	26
2	eric	age	22
3	paul	age	58
4	peter	age	33
5	julie	age	44
6	alice	gender	F
7	john	gender	M
8	eric	gender	M
9	paul	gender	F
10	peter	gender	M
11	julie	gender	F
12	alice	job	student
13	john	job	student
14	eric	job	student
15	paul	job	manager
16	peter	job	engineer
17	julie	job	scientist
18	alice	height	165
19	john	height	180
20	eric	height	175
21	paul	height	NaN
22	peter	height	NaN
23	julie	height	171

“pivots” a DataFrame from long (stacked) format to wide format,

```
print(staked.pivot(index='name', columns='variable', values='value'))
```

Out:

name	age	gender	height	job
alice	19	F	165	student
eric	22	M	175	student
john	26	M	180	student
julie	44	F	171	scientist
paul	58	F	NaN	manager
peter	33	M	NaN	engineer

### 3.2.3 Summarizing

```
# examine the users data

users           # print the first 30 and last 30 rows
type(users)     # DataFrame
users.head()    # print the first 5 rows
users.tail()    # print the last 5 rows
```

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```
users.index          # "the index" (aka "the labels")
users.columns        # column names (which is "an index")
users.dtypes         # data types of each column
users.shape          # number of rows and columns
users.values         # underlying numpy array
users.info()         # concise summary (includes memory usage as of pandas 0.15.0)
```

Out:

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 6 entries, 0 to 5
Data columns (total 5 columns):
name      6 non-null object
age       6 non-null int64
gender    6 non-null object
job       6 non-null object
height    4 non-null float64
dtypes: float64(1), int64(1), object(3)
memory usage: 288.0+ bytes
```

### 3.2.4 Columns selection

```
users['gender']      # select one column
type(users['gender']) # Series
users.gender         # select one column using the DataFrame

# select multiple columns
users[['age', 'gender']] # select two columns
my_cols = ['age', 'gender'] # or, create a list...
users[my_cols]           # ...and use that list to select columns
type(users[my_cols])    # DataFrame
```

### 3.2.5 Rows selection (basic)

iloc is strictly integer position based

```
df = users.copy()
df.iloc[0]      # first row
df.iloc[0, 0]   # first item of first row
df.iloc[0, 0] = 55

for i in range(users.shape[0]):
    row = df.iloc[i]
    row.age *= 100 # setting a copy, and not the original frame data.

print(df) # df is not modified
```

Out:

	name	age	gender	job	height
0	55	19	F	student	165.0
1	john	26	M	student	180.0
2	eric	22	M	student	175.0
3	paul	58	F	manager	NaN
4	peter	33	M	engineer	NaN
5	julie	44	F	scientist	171.0

ix supports mixed integer and label based access.

```
df = users.copy()
df.ix[0]          # first row
df.ix[0, "age"]   # first item of first row
df.ix[0, "age"] = 55

for i in range(df.shape[0]):
    df.ix[i, "age"] *= 10

print(df) # df is modified
```

Out:

	name	age	gender	job	height
0	alice	550	F	student	165.0
1	john	260	M	student	180.0
2	eric	220	M	student	175.0
3	paul	580	F	manager	NaN
4	peter	330	M	engineer	NaN
5	julie	440	F	scientist	171.0

### 3.2.6 Rows selection (filtering)

simple logical filtering

```
users[users.age < 20]      # only show users with age < 20
young_bool = users.age < 20 # or, create a Series of booleans...
young = users[young_bool]   # ...and use that Series to filter rows
users[users.age < 20].job   # select one column from the filtered results
print(young)
```

Out:

	name	age	gender	job	height
0	alice	19	F	student	165.0

Advanced logical filtering

```
users[users.age < 20][['age', 'job']]      # select multiple columns
users[(users.age > 20) & (users.gender == 'M')] # use multiple conditions
users[users.job.isin(['student', 'engineer'])] # filter specific values
```

### 3.2.7 Sorting

```
df = users.copy()

df.age.sort_values()                      # only works for a Series
df.sort_values(by='age')                   # sort rows by a specific column
df.sort_values(by='age', ascending=False)   # use descending order instead
df.sort_values(by=['job', 'age'])          # sort by multiple columns
df.sort_values(by=['job', 'age'], inplace=True) # modify df

print(df)
```

Out:

```
name  age  gender      job  height
4    peter    33       M  engineer     NaN
3    paul     58       F  manager     NaN
5    julie    44       F  scientist  171.0
0    alice    19       F  student   165.0
2    eric     22       M  student   175.0
1    john     26       M  student   180.0
```

### 3.2.8 Descriptive statistics

Summarize all numeric columns

```
print(df.describe())
```

Out:

```
age      height
count   6.000000  4.000000
mean   33.666667 172.750000
std    14.895189  6.344289
min    19.000000 165.000000
25%   23.000000 169.500000
50%   29.500000 173.000000
75%   41.250000 176.250000
max    58.000000 180.000000
```

Summarize all columns

```
print(df.describe(include='all'))
print(df.describe(include=['object'])) # limit to one (or more) types
```

Out:

```
name      age  gender      job      height
count      6  6.000000      6       6  4.000000
unique      6      NaN      2       4      NaN
top    john      NaN      F  student      NaN
freq      1      NaN      3       3      NaN
mean      NaN  33.666667      NaN      NaN  172.750000
std      NaN  14.895189      NaN      NaN  6.344289
```

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min	NaN	19.000000	NaN	NaN	165.000000
25%	NaN	23.000000	NaN	NaN	169.500000
50%	NaN	29.500000	NaN	NaN	173.000000
75%	NaN	41.250000	NaN	NaN	176.250000
max	NaN	58.000000	NaN	NaN	180.000000
	name	gender	job		
count	6	6	6		
unique	6	2	4		
top	john	F	student		
freq	1	3	3		

Statistics per group (groupby)

```
print(df.groupby("job").mean())

print(df.groupby("job")["age"].mean())

print(df.groupby("job").describe(include='all'))
```

Out:

age	height	
job		
engineer	33.000000	NaN
manager	58.000000	NaN
scientist	44.000000	171.000000
student	22.333333	173.333333
job		
engineer	33.000000	
manager	58.000000	
scientist	44.000000	
student	22.333333	
Name: age, dtype: float64		
	name	age
↳ ... gender	height	
↳ count	unique	top freq mean std min 25% 50% 75% max count unique top
↳ freq	... 25% 50% 75% max count unique top freq	mean std min
↳ 25%	50% 75% max	
job		
↳ ...		
engineer	1 1 peter 1 NaN NaN NaN NaN NaN NaN NaN 1.0 NaN NaN	
↳ NaN ...	NaN NaN NaN NaN 0.0 NaN NaN NaN NaN NaN NaN	
↳ NaN ...	NaN NaN NaN NaN	
manager	1 1 paul 1 NaN NaN NaN NaN NaN NaN 1.0 NaN NaN	
↳ NaN ...	NaN NaN NaN NaN 0.0 NaN NaN NaN NaN NaN NaN	
↳ NaN ...	NaN NaN NaN NaN	
scientist	1 1 julie 1 NaN NaN NaN NaN NaN NaN 1.0 NaN NaN	
↳ NaN ...	NaN NaN NaN NaN 1.0 NaN NaN NaN 171.000000 NaN 171.0 171.	
↳ 0 171.0 171.0 171.0		
student	3 3 john 1 NaN NaN NaN NaN NaN NaN 3.0 NaN NaN	
↳ NaN ...	NaN NaN NaN NaN 3.0 NaN NaN NaN 173.333333 7.637626 165.0 170.	
↳ 0 175.0 177.5 180.0		
[4 rows x 44 columns]		

Groupby in a loop

```
for grp, data in df.groupby("job"):
    print(grp, data)
```

Out:

	name	age	gender	job	height
4	peter	33	M	engineer	NaN
manager					
3	paul	58	F	manager	NaN
scientist					
5	julie	44	F	scientist	171.0
student					
0	alice	19	F	student	165.0
2	eric	22	M	student	175.0
1	john	26	M	student	180.0

### 3.2.9 Quality check

#### Remove duplicate data

```
df = users.append(df.iloc[0], ignore_index=True)

print(df.duplicated())                      # Series of booleans
# (True if a row is identical to a previous row)
df.duplicated().sum()                      # count of duplicates
df[df.duplicated()]                        # only show duplicates
df.age.duplicated()                        # check a single column for duplicates
df.duplicated(['age', 'gender']).sum()      # specify columns for finding duplicates
df = df.drop_duplicates()                  # drop duplicate rows
```

Out:

0	False
1	False
2	False
3	False
4	False
5	False
6	True
	dtype: bool

#### Missing data

```
# Missing values are often just excluded
df = users.copy()

df.describe(include='all')                  # excludes missing values

# find missing values in a Series
df.height.isnull()                         # True if NaN, False otherwise
df.height.notnull()                         # False if NaN, True otherwise
df[df.height.notnull()]                     # only show rows where age is not NaN
```

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```
df.height.isnull().sum()      # count the missing values

# find missing values in a DataFrame
df.isnull()                  # DataFrame of booleans
df.isnull().sum()             # calculate the sum of each column
```

Strategy 1: drop missing values

```
df.dropna()                  # drop a row if ANY values are missing
df.dropna(how='all')          # drop a row only if ALL values are missing
```

Strategy 2: fill in missing values

```
df.height.mean()
df = users.copy()
df.ix[df.height.isnull(), "height"] = df["height"].mean()

print(df)
```

Out:

	name	age	gender	job	height
0	alice	19	F	student	165.00
1	john	26	M	student	180.00
2	eric	22	M	student	175.00
3	paul	58	F	manager	172.75
4	peter	33	M	engineer	172.75
5	julie	44	F	scientist	171.00

### 3.2.10 Rename values

```
df = users.copy()
print(df.columns)
df.columns = ['age', 'genre', 'travail', 'nom', 'taille']

df.travail = df.travail.map({ 'student':'etudiant', 'manager':'manager',
                             'engineer':'ingenieur', 'scientist':'scientific'})
# assert df.travail.isnull().sum() == 0

df['travail'].str.contains("etu|inge")
```

Out:

```
Index(['name', 'age', 'gender', 'job', 'height'], dtype='object')
```

### 3.2.11 Dealing with outliers

```
size = pd.Series(np.random.normal(loc=175, size=20, scale=10))
# Corrupt the first 3 measures
size[:3] += 500
```

### Based on parametric statistics: use the mean

Assume random variable follows the normal distribution. Exclude data outside 3 standard-deviations:  
- Probability that a sample lies within 1 sd: 68.27%  
- Probability that a sample lies within 3 sd: 99.73% ( $68.27 + 2 * 15.73$ )

```
size_outlr_mean = size.copy()  
size_outlr_mean[((size - size.mean()).abs() > 3 * size.std())] = size.mean()  
print(size_outlr_mean.mean())
```

Out:

```
248.48963819938044
```

### Based on non-parametric statistics: use the median

Median absolute deviation (MAD), based on the median, is a robust non-parametric statistics.  
[https://en.wikipedia.org/wiki/Median\\_absolute\\_deviation](https://en.wikipedia.org/wiki/Median_absolute_deviation)

```
mad = 1.4826 * np.median(np.abs(size - size.median()))  
size_outlr_mad = size.copy()  
  
size_outlr_mad[((size - size.median()).abs() > 3 * mad)] = size.median()  
print(size_outlr_mad.mean(), size_outlr_mad.median())
```

Out:

```
173.80000467192673 178.7023568870694
```

## 3.2.12 File I/O

### CSV

```
import tempfile, os.path  
tmpdir = tempfile.gettempdir()  
csv_filename = os.path.join(tmpdir, "users.csv")  
users.to_csv(csv_filename, index=False)  
other = pd.read_csv(csv_filename)
```

### Read csv from url

```
url = 'https://raw.github.com/neurospin/pystatsml/master/datasets/salary_table.csv'  
salary = pd.read_csv(url)
```

### Excel

```

xls_filename = os.path.join(tmpdir, "users.xlsx")
users.to_excel(xls_filename, sheet_name='users', index=False)

pd.read_excel(xls_filename, sheetname='users')

# Multiple sheets
with pd.ExcelWriter(xls_filename) as writer:
    users.to_excel(writer, sheet_name='users', index=False)
    df.to_excel(writer, sheet_name='salary', index=False)

pd.read_excel(xls_filename, sheetname='users')
pd.read_excel(xls_filename, sheetname='salary')

```

## SQL (SQLite)

```

import pandas as pd
import sqlite3

db_filename = os.path.join(tmpdir, "users.db")

```

Connect

```
conn = sqlite3.connect(db_filename)
```

Creating tables with pandas

```

url = 'https://raw.github.com/neurospin/pystatsml/master/datasets/salary_table.csv'
salary = pd.read_csv(url)

salary.to_sql("salary", conn, if_exists="replace")

```

Push modifications

```

cur = conn.cursor()
values = (100, 14000, 5, 'Bachelor', 'N')
cur.execute("insert into salary values (?, ?, ?, ?, ?)", values)
conn.commit()

```

Reading results into a pandas DataFrame

```

salary_sql = pd.read_sql_query("select * from salary;", conn)
print(salary_sql.head())

pd.read_sql_query("select * from salary;", conn).tail()
pd.read_sql_query('select * from salary where salary>25000;', conn)
pd.read_sql_query('select * from salary where experience=16;', conn)
pd.read_sql_query('select * from salary where education="Master";', conn)

```

Out:

index	salary	experience	education	management
0	0	13876	1 Bachelor	Y
1	1	11608	1 Ph.D	N
2	2	18701	1 Ph.D	Y

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3	3	11283	1	Master	N
4	4	11767	1	Ph.D	N

### 3.2.13 Exercises

#### Data Frame

1. Read the iris dataset at '<https://github.com/neurospin/pystatsml/tree/master/datasets/iris.csv>'
2. Print column names
3. Get numerical columns
4. For each species compute the mean of numerical columns and store it in a stats table like:

	species	sepal_length	sepal_width	petal_length	petal_width
0	setosa	5.006	3.428	1.462	0.246
1	versicolor	5.936	2.770	4.260	1.326
2	virginica	6.588	2.974	5.552	2.026

#### Missing data

Add some missing data to the previous table users:

```
df = users.copy()
df.ix[[0, 2], "age"] = None
df.ix[[1, 3], "gender"] = None
```

1. Write a function `fillmissing_with_mean(df)` that fill all missing value of numerical column with the mean of the current columns.
2. Save the original users and “imputed” frame in a single excel file “users.xlsx” with 2 sheets: original, imputed.

**Total running time of the script:** ( 0 minutes 1.826 seconds)

## 3.3 Matplotlib: data visualization

**Sources** - Nicolas P. Rougier: <http://www.labri.fr/perso/nrougier/teaching/matplotlib> - <https://www.kaggle.com/benhamner/d/uciml/iris/python-data-visualizations>

### 3.3.1 Basic plots

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

# inline plot (for jupyter)
```

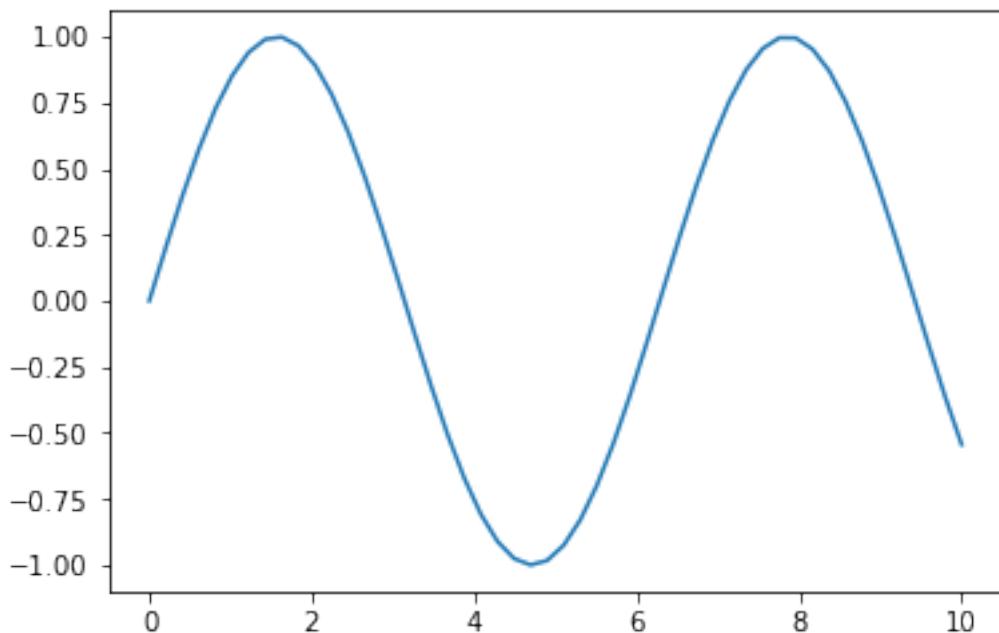
(continues on next page)

(continued from previous page)

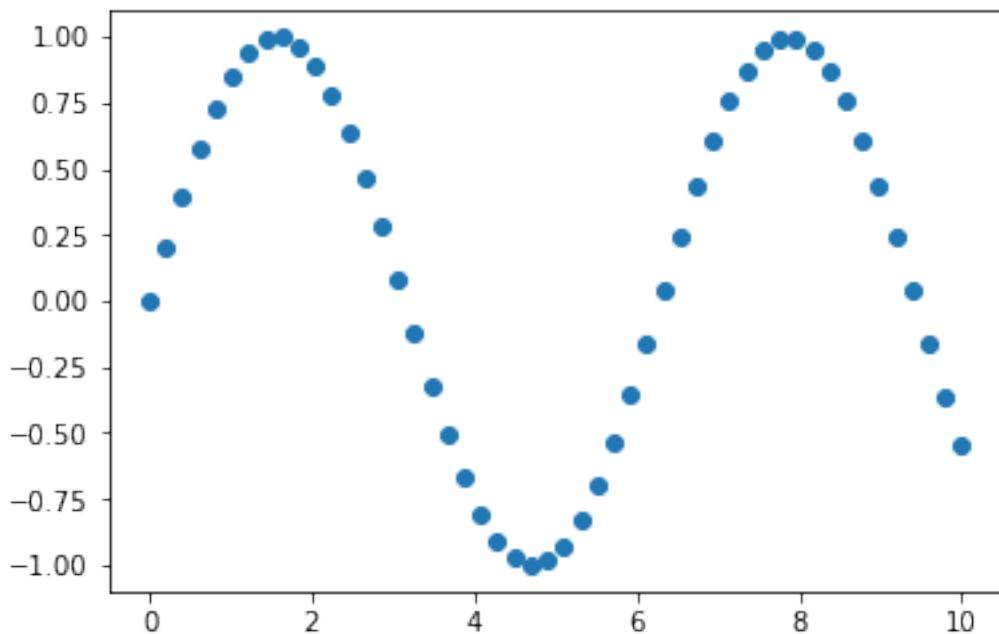
```
%matplotlib inline

x = np.linspace(0, 10, 50)
sinus = np.sin(x)

plt.plot(x, sinus)
plt.show()
```

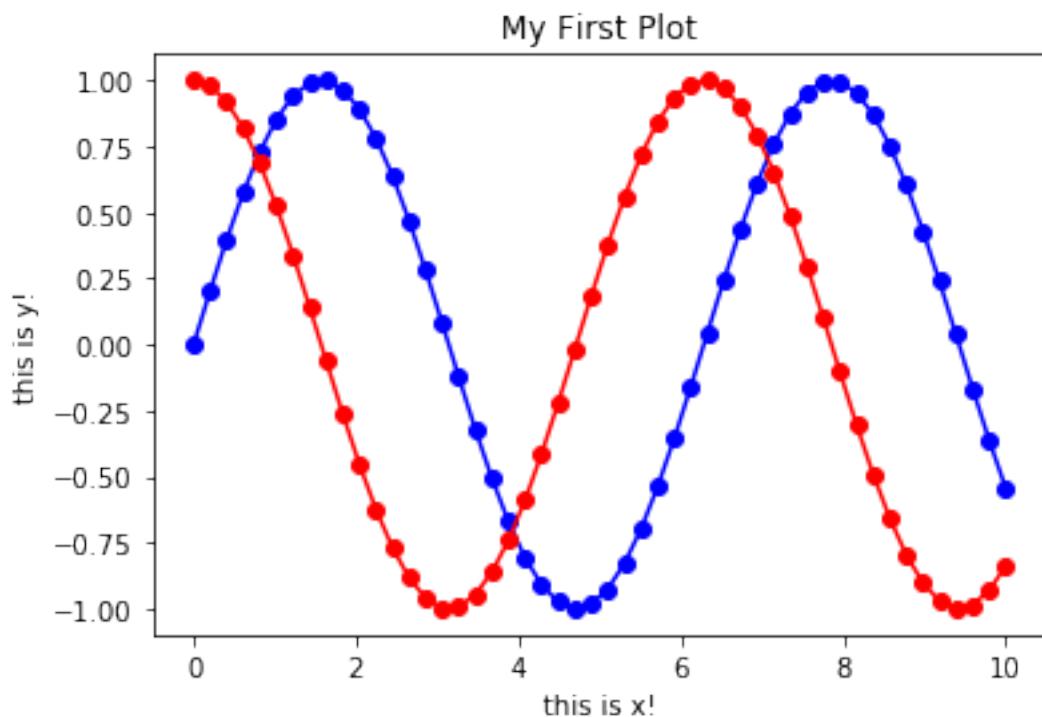


```
plt.plot(x, sinus, "o")
plt.show()
# use plt.plot to get color / marker abbreviations
```

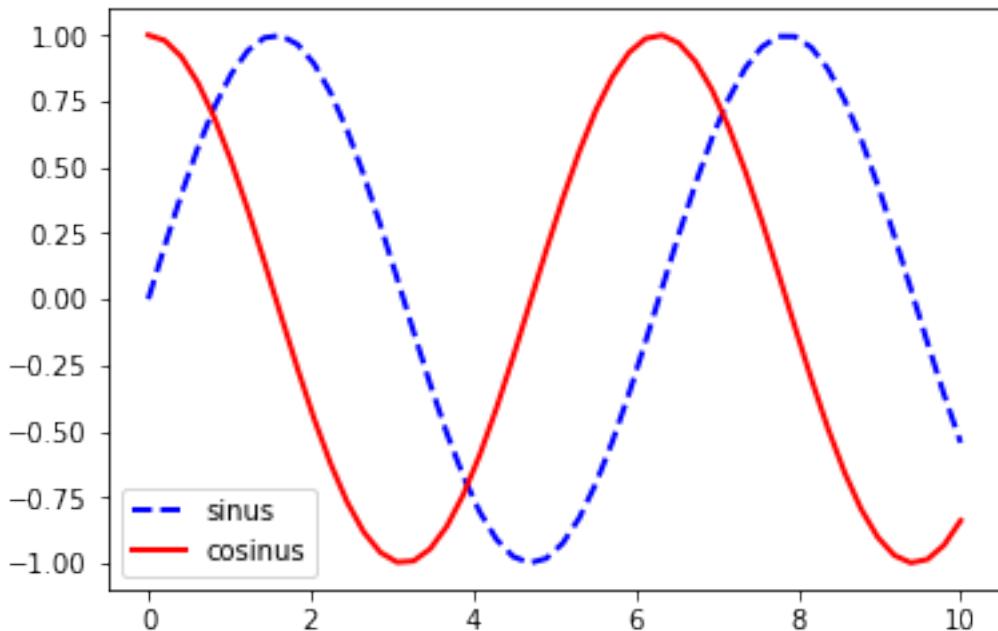


```
# Rapid multiplot

cosinus = np.cos(x)
plt.plot(x, sinus, "-b", x, sinus, "ob", x, cosinus, "-r", x, cosinus, "or")
plt.xlabel('this is x!')
plt.ylabel('this is y!')
plt.title('My First Plot')
plt.show()
```



```
# Step by step
plt.plot(x, sinus, label='sinus', color='blue', linestyle='--', linewidth=2)
plt.plot(x, cosinus, label='cosinus', color='red', linestyle='-', linewidth=2)
plt.legend()
plt.show()
```



### 3.3.2 Scatter (2D) plots

Load dataset

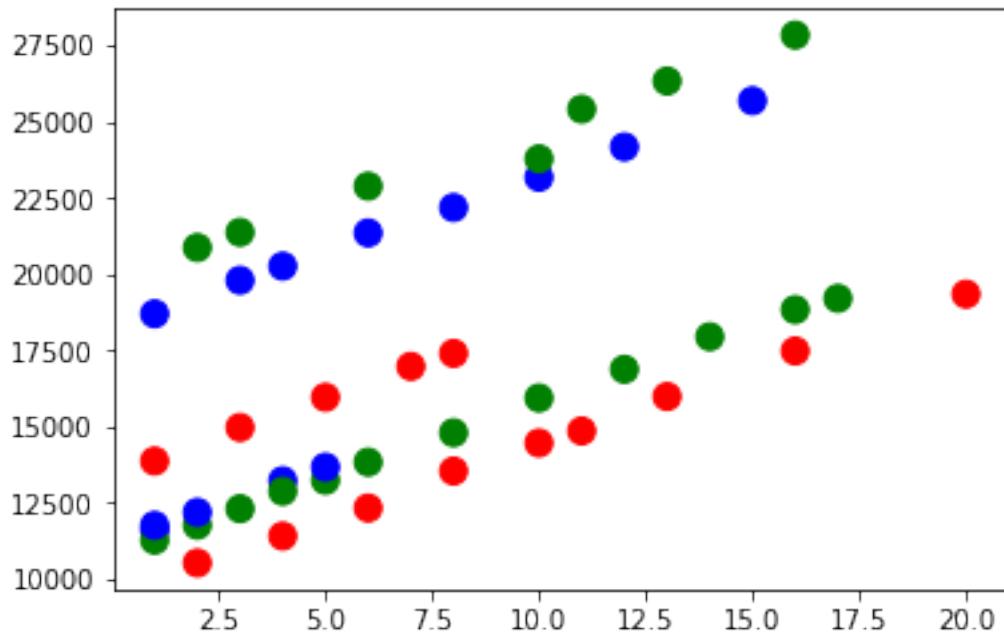
```
import pandas as pd
try:
    salary = pd.read_csv("../datasets/salary_table.csv")
except:
    url = 'https://raw.github.com/neurospin/pystatsml/master/datasets/salary_table.csv'
    salary = pd.read_csv(url)

df = salary
```

#### Simple scatter with colors

```
colors = colors_edu = {'Bachelor':'r', 'Master':'g', 'Ph.D':'blue'}
plt.scatter(df['experience'], df['salary'], c=df['education'].apply(lambda x: colors[x]), s=100)
```

```
<matplotlib.collections.PathCollection at 0x7fa627ddb438>
```



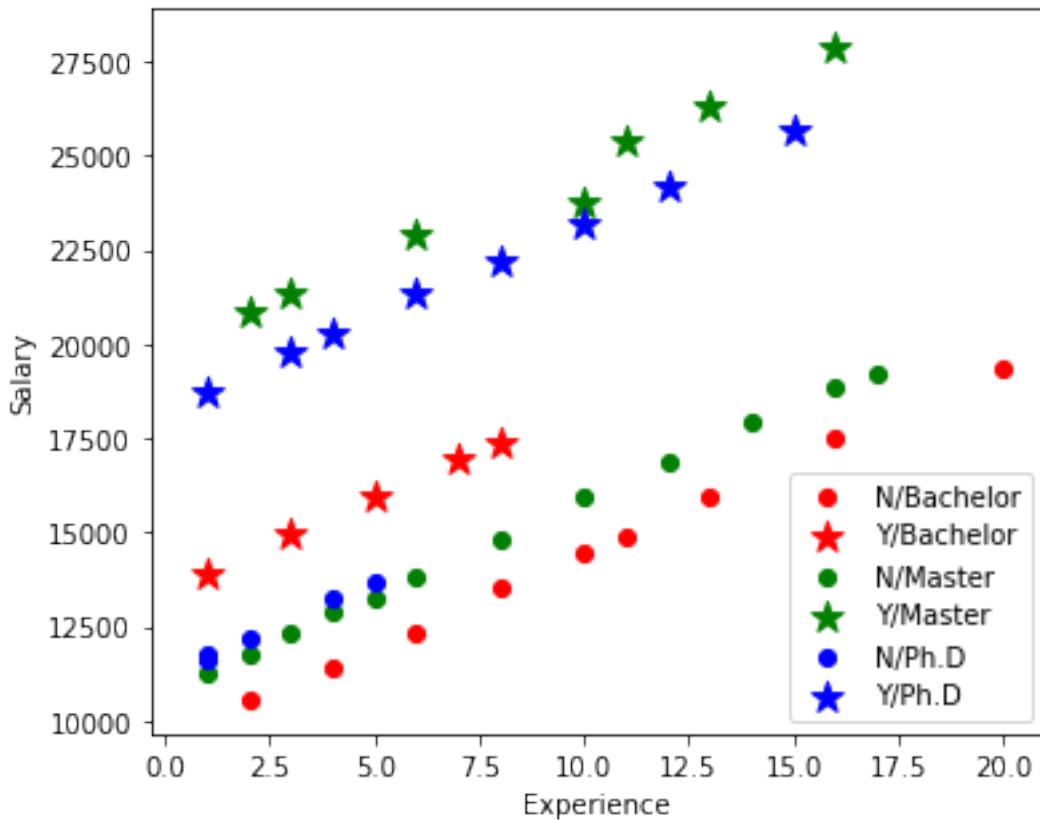
Scatter plot with colors and symbols

```
## Figure size
plt.figure(figsize=(6,5))

## Define colors / symbols manually
symbols_manag = dict(Y='*', N='.')
colors_edu = {'Bachelor':'r', 'Master':'g', 'Ph.D':'blue'}

## group by education x management => 6 groups
for values, d in salary.groupby(['education','management']):
    edu, manager = values
    plt.scatter(d['experience'], d['salary'], marker=symbols_manag[manager], color=colors_
    ↪edu[edu],
                s=150, label=manager+"/"+edu)

## Set labels
plt.xlabel('Experience')
plt.ylabel('Salary')
plt.legend(loc=4) # lower right
plt.show()
```



### 3.3.3 Saving Figures

```
### bitmap format
plt.plot(x, sinus)
plt.savefig("sinus.png")
plt.close()

# Prefer vectorial format (SVG: Scalable Vector Graphics) can be edited with
# Inkscape, Adobe Illustrator, Blender, etc.
plt.plot(x, sinus)
plt.savefig("sinus.svg")
plt.close()

# Or pdf
plt.plot(x, sinus)
plt.savefig("sinus.pdf")
plt.close()
```

### 3.3.4 Seaborn

**Sources:** - <http://stanford.edu/~mwaskom/software/seaborn> - <https://elitedatascience.com/python-seaborn-tutorial>

If needed, install using: pip install -U --user seaborn

## Boxplot

Box plots are non-parametric: they display variation in samples of a statistical population without making any assumptions of the underlying statistical distribution.

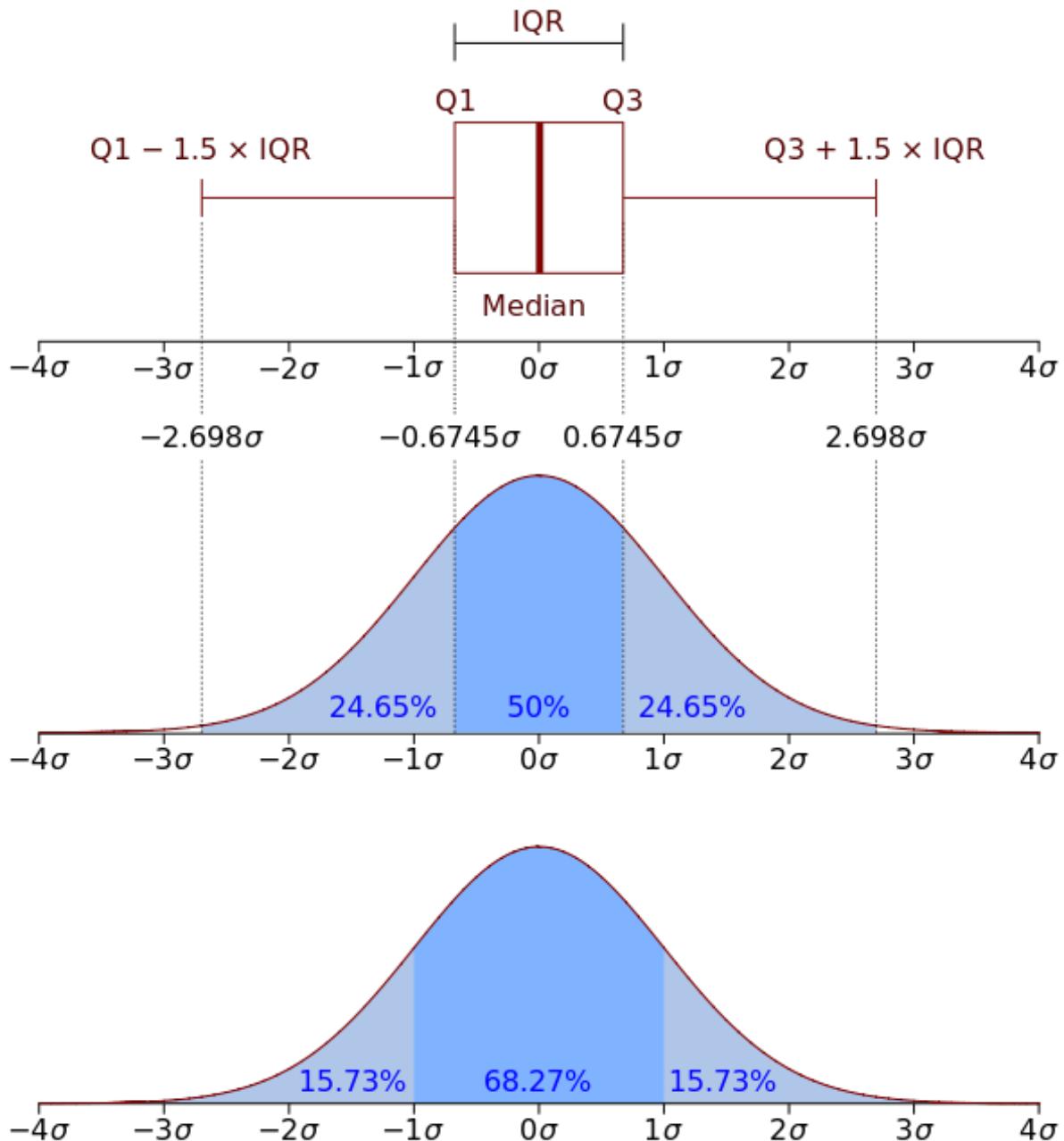
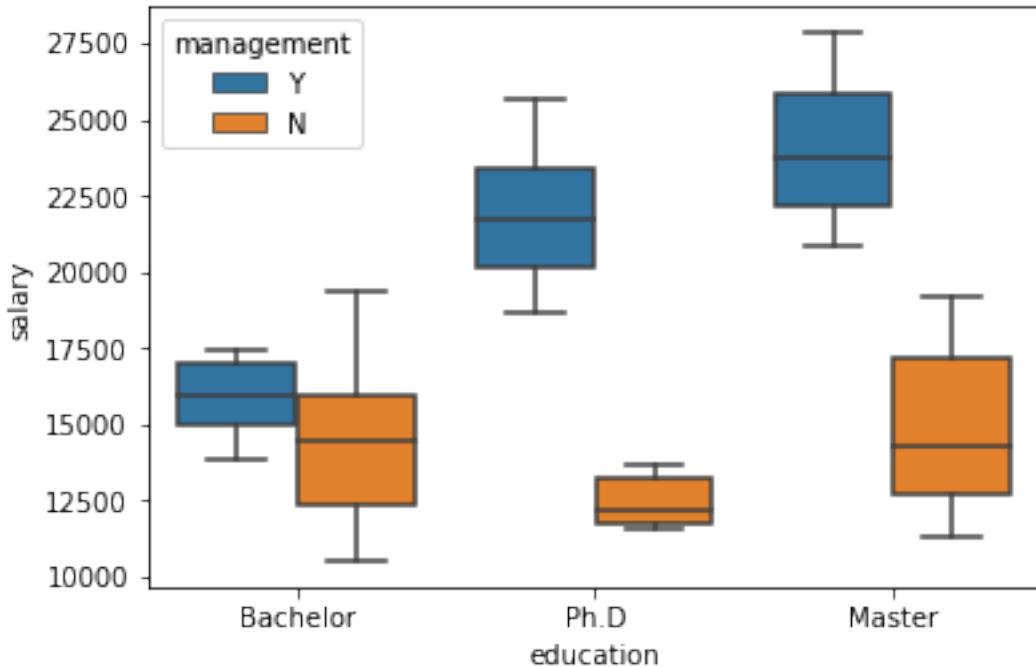


Fig. 2: title

```
import seaborn as sns
sns.boxplot(x="education", y="salary", hue="management", data=salary)
```

```
<matplotlib.axes._subplots.AxesSubplot at 0x7fa62372cb70>
```

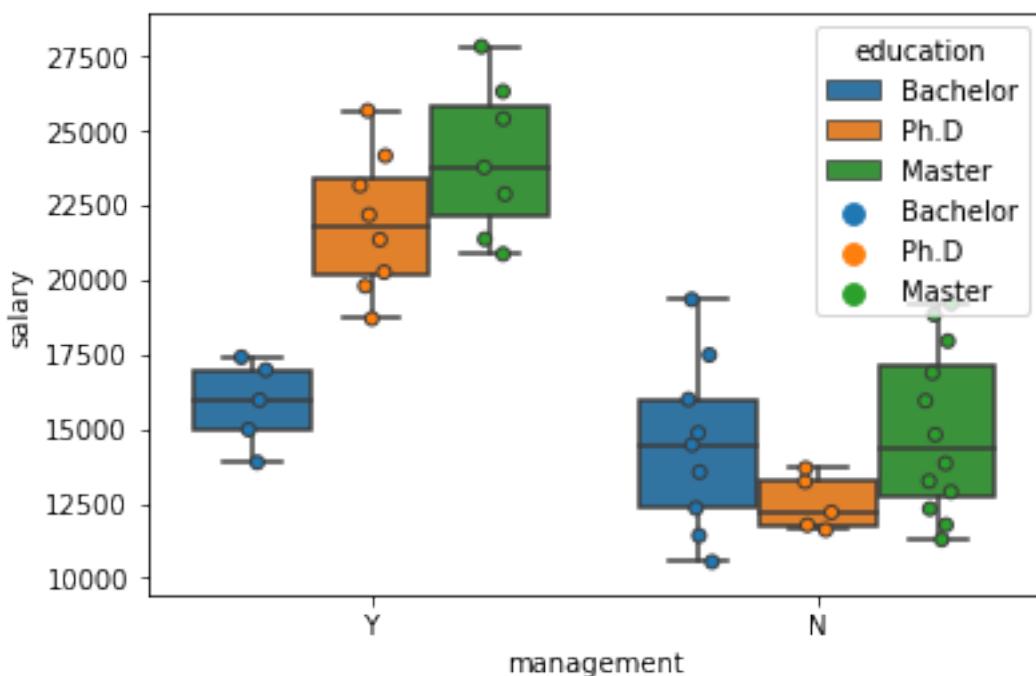


```

sns.boxplot(x="management", y="salary", hue="education", data=salary)
sns.stripplot(x="management", y="salary", hue="education", data=salary, jitter=True,
              dodge=True, linewidth=1)# Jitter and split options separate datapoints according to group

```

```
<matplotlib.axes._subplots.AxesSubplot at 0x7fa623680780>
```



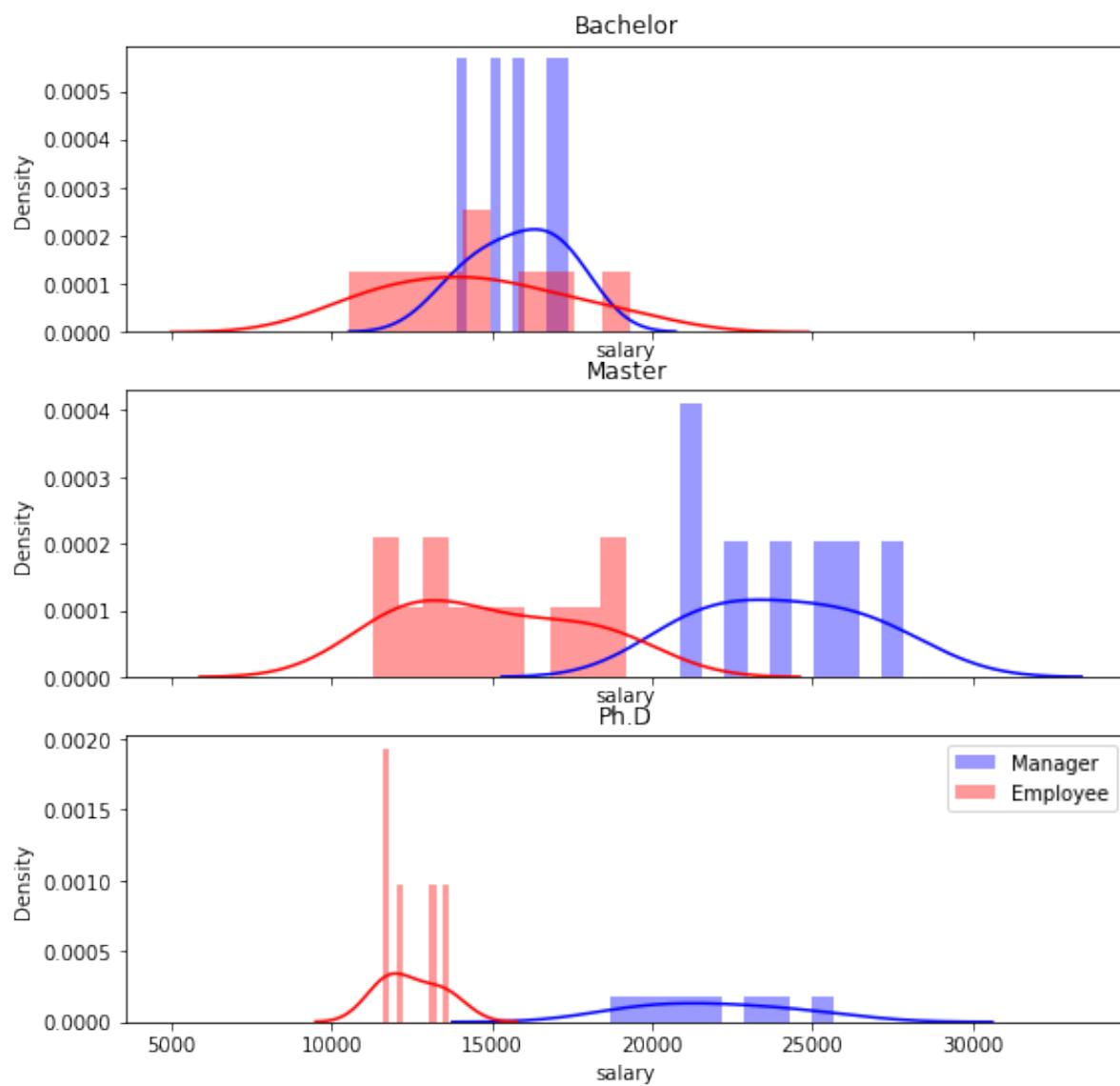
### Density plot with one figure containing multiple axis

One figure can contain several axis, whose contain the graphic elements

```
# Set up the matplotlib figure: 3 x 1 axis

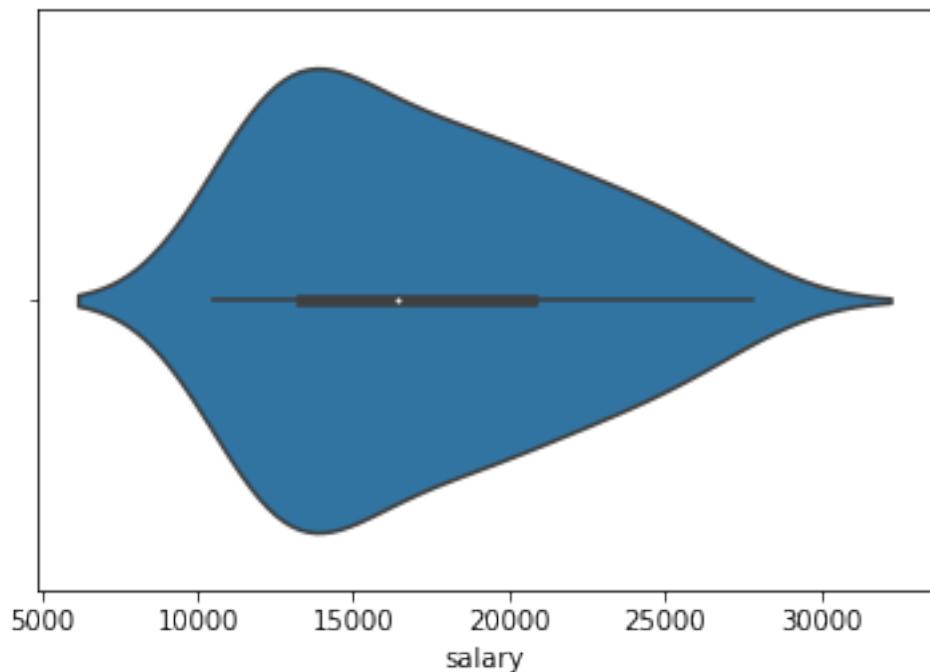
f, axes = plt.subplots(3, 1, figsize=(9, 9), sharex=True)

i = 0
for edu, d in salary.groupby(['education']):
    sns.distplot(d.salary[d.management == "Y"], color="b", bins=10, label="Manager", ax=axes[i])
    sns.distplot(d.salary[d.management == "N"], color="r", bins=10, label="Employee", ax=axes[i])
    axes[i].set_title(edu)
    axes[i].set_ylabel('Density')
    i += 1
ax = plt.legend()
```



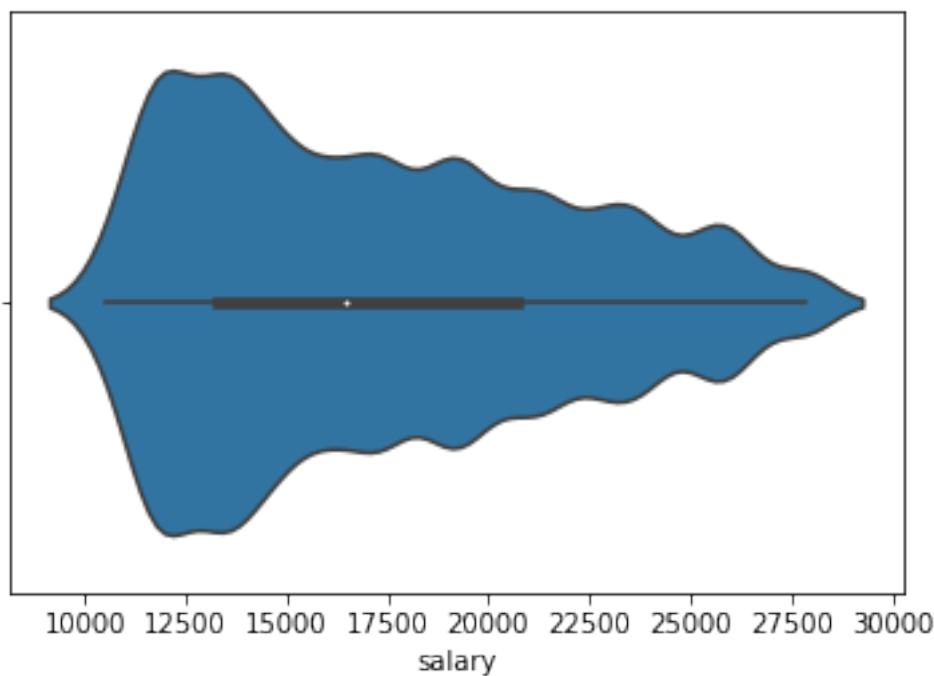
### Violin plot (distribution)

```
ax = sns.violinplot(x="salary", data=salary)
```

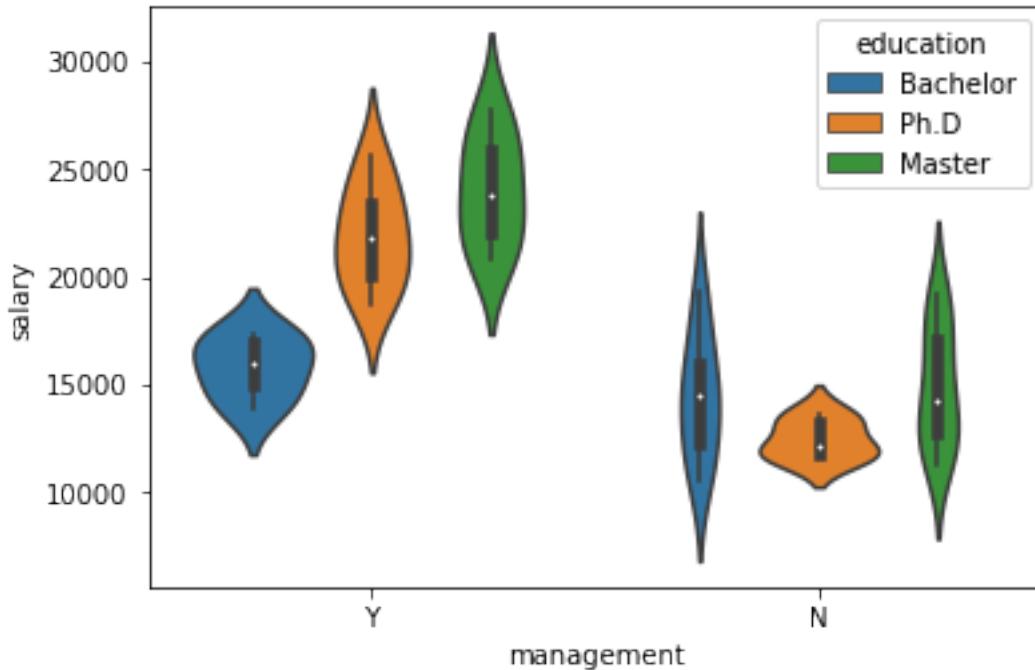


Tune bandwidth

```
ax = sns.violinplot(x="salary", data=salary, bw=.15)
```



```
ax = sns.violinplot(x="management", y="salary", hue="education", data=salary)
```

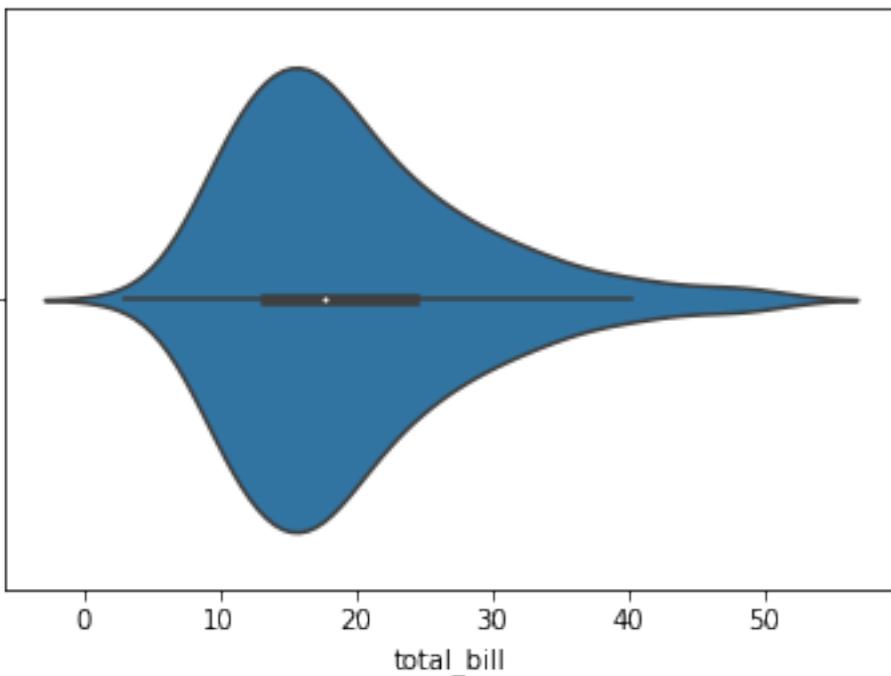


Tips dataset One waiter recorded information about each tip he received over a period of a few months working in one restaurant. He collected several variables:

```
import seaborn as sns
sns.set(style="whitegrid")
tips = sns.load_dataset("tips")
print(tips.head())

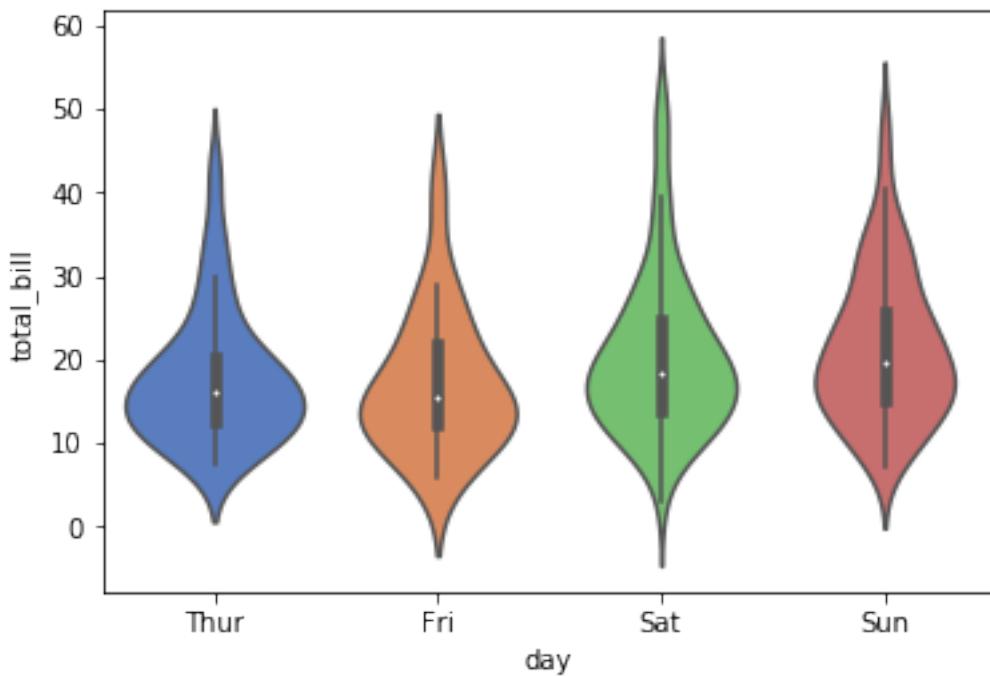
ax = sns.violinplot(x=tips["total_bill"])
```

	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



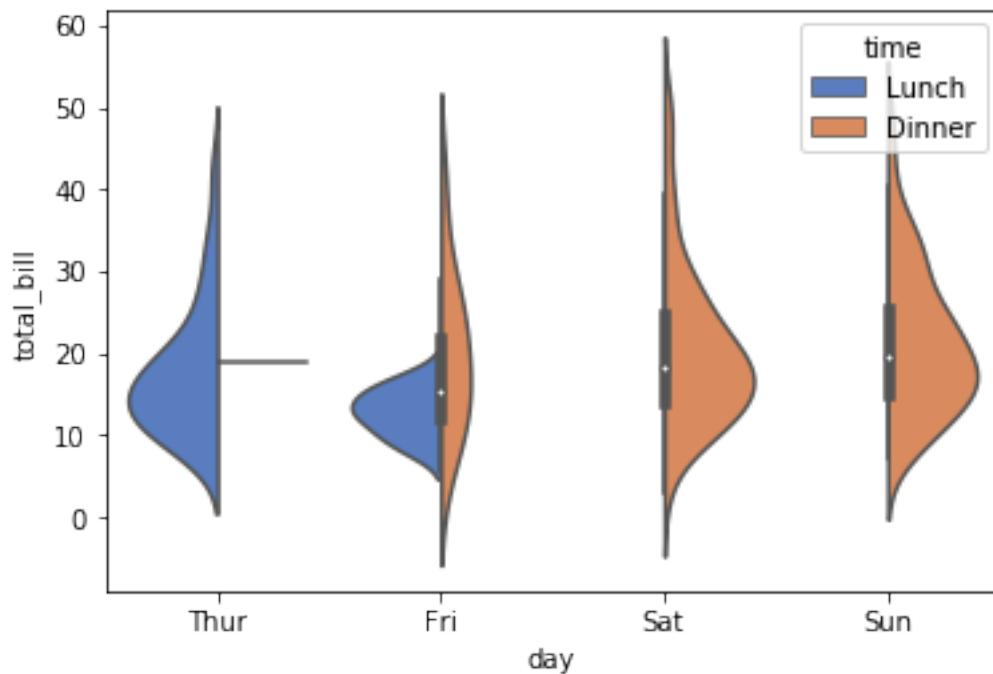
Group by day

```
ax = sns.violinplot(x="day", y="total_bill", data=tips, palette="muted")
```



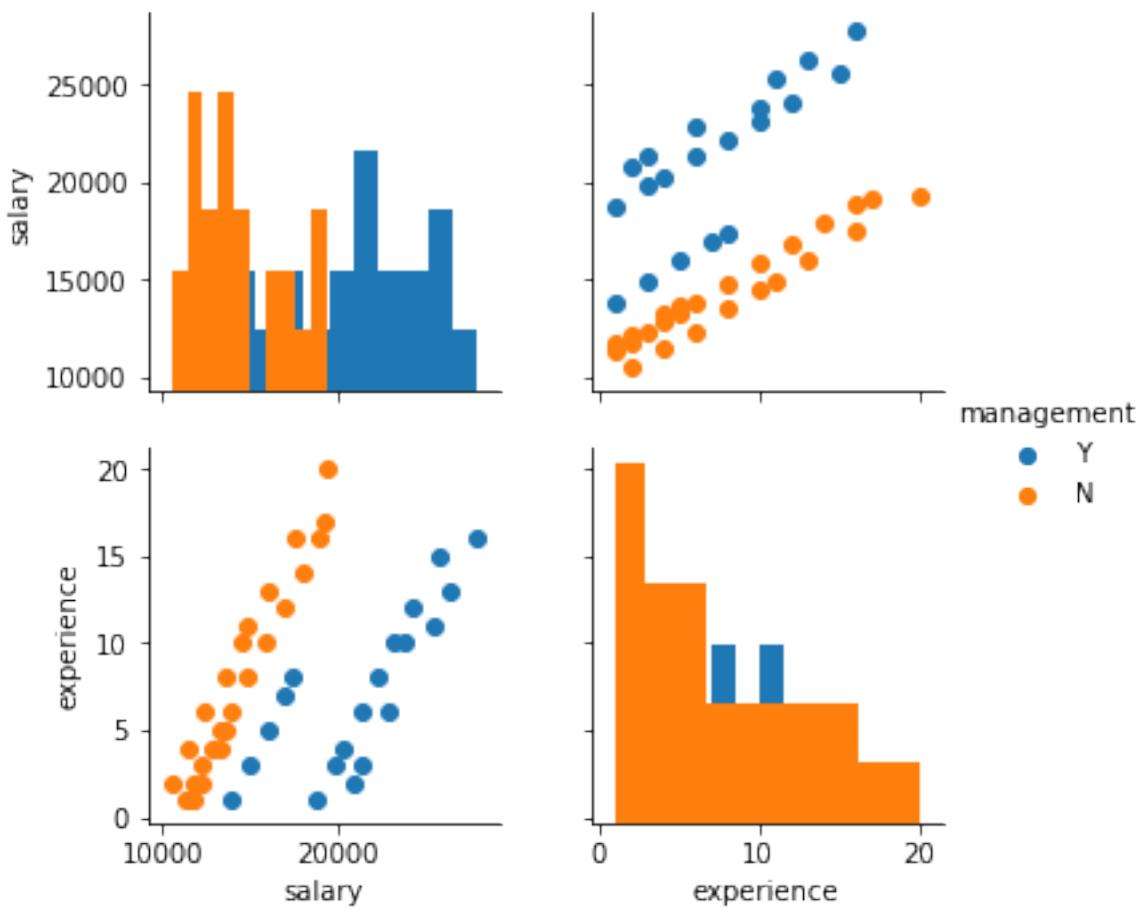
Group by day and color by time (lunch vs dinner)

```
ax = sns.violinplot(x="day", y="total_bill", hue="time", data=tips, palette="muted",  
split=True)
```



### Pairwise scatter plots

```
g = sns.PairGrid(salary, hue="management")
g.map_diag(plt.hist)
g.map_offdiag(plt.scatter)
ax = g.add_legend()
```



### 3.3.5 Time series

```

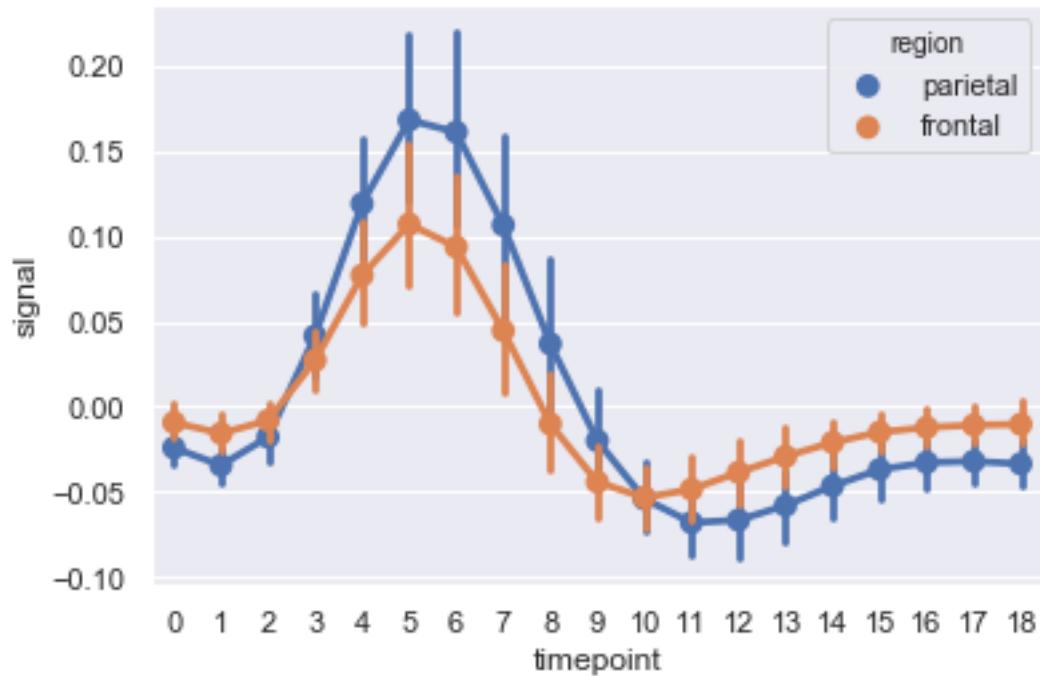
import seaborn as sns
sns.set(style="darkgrid")

# Load an example dataset with long-form data
fmri = sns.load_dataset("fmri")

# Plot the responses for different events and regions

ax = sns.pointplot(x="timepoint", y="signal",
                    hue="region", style="event",
                    data=fmri)
# version 0.9
# sns.lineplot(x="timepoint", y="signal",
#             hue="region", style="event",
#             data=fmri)

```



## 4.1 Univariate statistics

Basics univariate statistics are required to explore dataset:

- Discover associations between a variable of interest and potential predictors. It is strongly recommended to start with simple univariate methods before moving to complex multi-variate predictors.
- Assess the prediction performances of machine learning predictors.
- Most of the univariate statistics are based on the linear model which is one of the main model in machine learning.

### 4.1.1 Estimators of the main statistical measures

#### Mean

Properties of the expected value operator  $E(\cdot)$  of a random variable  $X$

$$E(X + c) = E(X) + c \quad (4.1)$$

$$E(X + Y) = E(X) + E(Y) \quad (4.2)$$

$$E(aX) = aE(X) \quad (4.3)$$

The estimator  $\bar{x}$  on a sample of size  $n$ :  $x = x_1, \dots, x_n$  is given by

$$\bar{x} = \frac{1}{n} \sum_i x_i$$

$\bar{x}$  is itself a random variable with properties:

- $E(\bar{x}) = \bar{x}$ ,
- $Var(\bar{x}) = \frac{Var(X)}{n}$ .

#### Variance

$$Var(X) = E((X - E(X))^2) = E(X^2) - (E(X))^2$$

The estimator is

$$\sigma_x^2 = \frac{1}{n-1} \sum_i (x_i - \bar{x})^2$$

Note here the subtracted 1 degree of freedom (df) in the divisor. In standard statistical practice,  $df = 1$  provides an unbiased estimator of the variance of a hypothetical infinite population. With  $df = 0$  it instead provides a maximum likelihood estimate of the variance for normally distributed variables.

### Standard deviation

$$Std(X) = \sqrt{Var(X)}$$

The estimator is simply  $\sigma_x = \sqrt{\sigma_x^2}$ .

### Covariance

$$Cov(X, Y) = E((X - E(X))(Y - E(Y))) = E(XY) - E(X)E(Y).$$

Properties:

$$\begin{aligned} \text{Cov}(X, X) &= \text{Var}(X) \\ \text{Cov}(X, Y) &= \text{Cov}(Y, X) \\ \text{Cov}(cX, Y) &= c \text{Cov}(X, Y) \\ \text{Cov}(X + c, Y) &= \text{Cov}(X, Y) \end{aligned}$$

The estimator with  $df = 1$  is

$$\sigma_{xy} = \frac{1}{n-1} \sum_i (x_i - \bar{x})(y_i - \bar{y}).$$

### Correlation

$$Cor(X, Y) = \frac{Cov(X, Y)}{Std(X)Std(Y)}$$

The estimator is

$$\rho_{xy} = \frac{\sigma_{xy}}{\sigma_x \sigma_y}.$$

### Standard Error (SE)

The standard error (SE) is the standard deviation (of the sampling distribution) of a statistic:

$$SE(X) = \frac{Std(X)}{\sqrt{n}}.$$

It is most commonly considered for the mean with the estimator \$

$$SE(\bar{x}) = \sigma_{\bar{x}} \tag{4.4}$$

$$= \frac{\sigma_x}{\sqrt{n}}. \tag{4.5}$$

## Exercises

- Generate 2 random samples:  $x \sim N(1.78, 0.1)$  and  $y \sim N(1.66, 0.1)$ , both of size 10.
- Compute  $\bar{x}, \sigma_x, \sigma_{xy}$  (`xbar`, `xvar`, `xcov`) using only the `np.sum()` operation. Explore the `np.` module to find out which numpy functions performs the same computations and compare them (using `assert`) with your previous results.

### 4.1.2 Main distributions

#### Normal distribution

The normal distribution, noted  $\mathcal{N}(\mu, \sigma)$  with parameters:  $\mu$  mean (location) and  $\sigma > 0$  std-dev. Estimators:  $\bar{x}$  and  $\sigma_x$ .

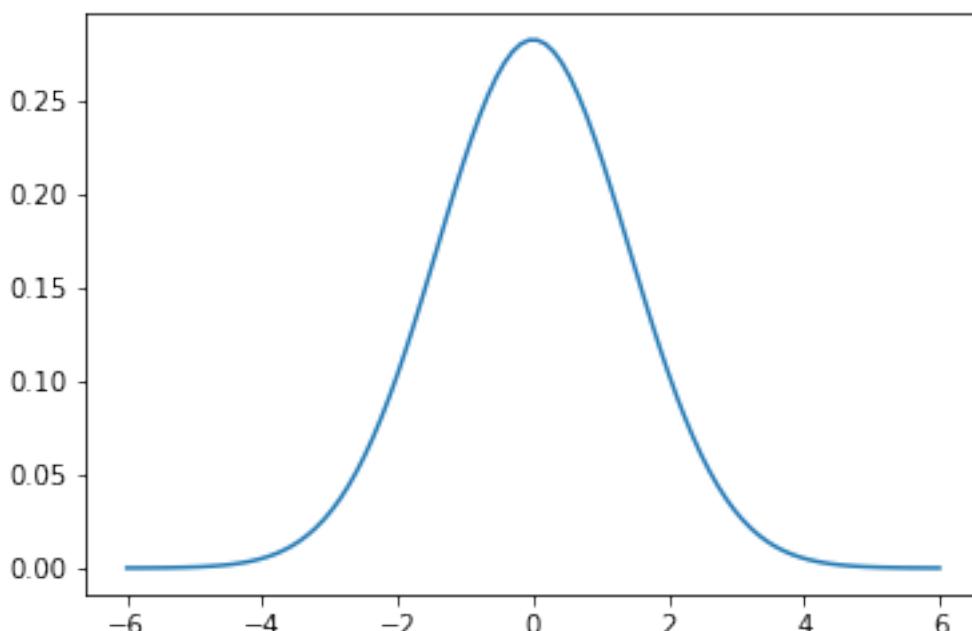
The normal distribution, noted

$\mathcal{N}$ , is useful because of the central limit theorem (CLT) which states that: given certain conditions, the arithmetic mean of a sufficiently large number of iterates of independent random variables, each with a well-defined expected value and well-defined variance, will be approximately normally distributed, regardless of the underlying distribution.

```
import numpy as np
import matplotlib.pyplot as plt
from scipy.stats import norm
%matplotlib inline

mu = 0 # mean
variance = 2 #variance
sigma = np.sqrt(variance) #standard deviation\n",
x = np.linspace(mu-3*variance,mu+3*variance, 100)
plt.plot(x, norm.pdf(x, mu, sigma))
```

[<matplotlib.lines.Line2D at 0x7f6f2a4dae48>]



## The Chi-Square distribution

The chi-square or  $\chi_n^2$  distribution with  $n$  degrees of freedom (df) is the distribution of a sum of the squares of  $n$  independent standard normal random variables  $\mathcal{N}(0, 1)$ . Let  $X \sim \mathcal{N}(\mu, \sigma^2)$ , then,  $Z = (X - \mu)/\sigma \sim \mathcal{N}(0, 1)$ , then:

- The squared standard  $Z^2 \sim \chi_1^2$  (one df).
- **The distribution of sum of squares** of  $n$  normal random variables:  $\sum_i^n Z_i^2 \sim \chi_n^2$

The sum of two  $\chi^2$  RV with  $p$  and  $q$  df is a  $\chi^2$  RV with  $p + q$  df. This is useful when summing/subtracting sum of squares.

The  $\chi^2$ -distribution is used to model **errors** measured as **sum of squares** or the distribution of the sample **variance**.

## The Fisher's F-distribution

The  $F$ -distribution,  $F_{n,p}$ , with  $n$  and  $p$  degrees of freedom is the ratio of two independent  $\chi^2$  variables. Let  $X \sim \chi_n^2$  and  $Y \sim \chi_p^2$  then:

$$F_{n,p} = \frac{X/n}{Y/p}$$

The  $F$ -distribution plays a central role in hypothesis testing answering the question: **Are two variances equals?, is the ratio or two errors significantly large ?**

```
import numpy as np
from scipy.stats import f
import matplotlib.pyplot as plt
%matplotlib inline

fvalues = np.linspace(.1, 5, 100)

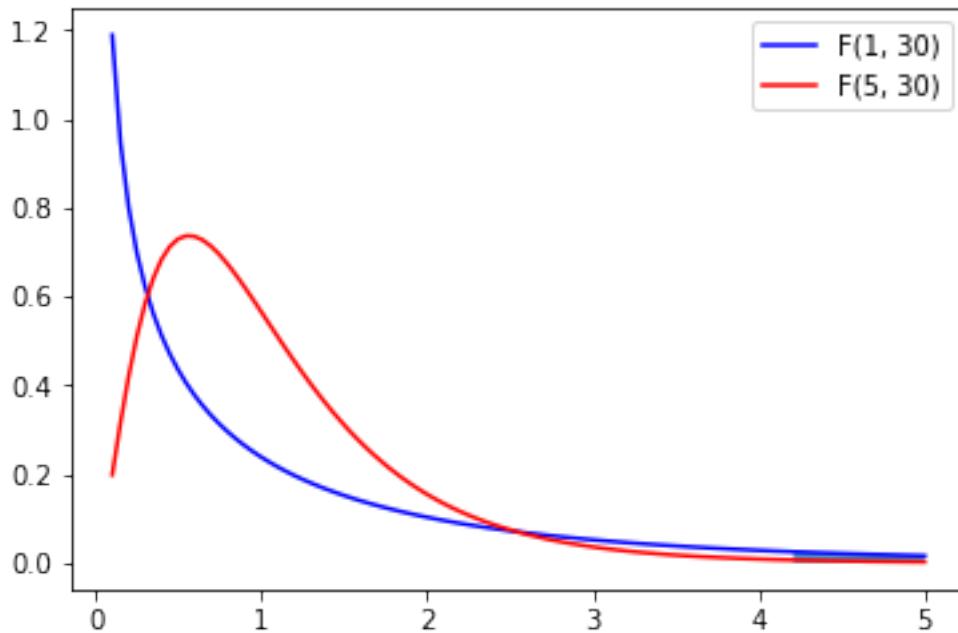
# pdf(x, df1, df2): Probability density function at x of F.
plt.plot(fvalues, f.pdf(fvalues, 1, 30), 'b-', label="F(1, 30)")
plt.plot(fvalues, f.pdf(fvalues, 5, 30), 'r-', label="F(5, 30)")
plt.legend()

# cdf(x, df1, df2): Cumulative distribution function of F.
# ie.
proba_at_f_inf_3 = f.cdf(3, 1, 30) # P(F(1,30) < 3)

# ppf(q, df1, df2): Percent point function (inverse of cdf) at q of F.
f_at_proba_inf_95 = f.ppf(.95, 1, 30) # q such P(F(1,30) < .95)
assert f.cdf(f_at_proba_inf_95, 1, 30) == .95

# sf(x, df1, df2): Survival function (1 - cdf) at x of F.
proba_at_f_sup_3 = f.sf(3, 1, 30) # P(F(1,30) > 3)
assert proba_at_f_inf_3 + proba_at_f_sup_3 == 1

# p-value: P(F(1, 30)) < 0.05
low_proba_fvalues = fvalues[fvalues > f_at_proba_inf_95]
plt.fill_between(low_proba_fvalues, 0, f.pdf(low_proba_fvalues, 1, 30),
                 alpha=.8, label="P < 0.05")
plt.show()
```



### The Student's $t$ -distribution

Let  $M \sim \mathcal{N}(0, 1)$  and  $V \sim \chi_n^2$ . The  $t$ -distribution,  $T_n$ , with  $n$  degrees of freedom is the ratio:

$$T_n = \frac{M}{\sqrt{V/n}}$$

The distribution of the difference between an estimated parameter and its true (or assumed) value divided by the standard deviation of the estimated parameter (standard error) follow a  $t$ -distribution. **Is this parameters different from a given value?**

#### 4.1.3 Hypothesis Testing

##### Examples

- Test a proportion: Biased coin ? 200 heads have been found over 300 flips, is it coins biased ?
- Test the association between two variables.
  - Exemple height and sex: In a sample of 25 individuals (15 females, 10 males), is female height is different from male height ?
  - Exemple age and arterial hypertension: In a sample of 25 individuals is age height correlated with arterial hypertension ?

##### Steps

1. Model the data
2. Fit: estimate the model parameters (frequency, mean, correlation, regression coefficient)
3. Compute a test statistic from model the parameters.
4. Formulate the null hypothesis: What would be the (distribution of the) test statistic if the observations are the result of pure chance.

5. Compute the probability ( $p$ -value) to obtain a larger value for the test statistic by chance (under the null hypothesis).

### Flip coin: Simplified example

Biased coin ? 2 heads have been found over 3 flips, is it coins biased ?

1. Model the data: number of heads follow a Binomial distribution.
2. Compute model parameters:  $N=3$ ,  $P = \text{the frequency of number of heads over the number of flip: } 2/3$ .
3. Compute a test statistic, same as frequency.
4. Under the null hypothesis the distribution of the number of tail is:

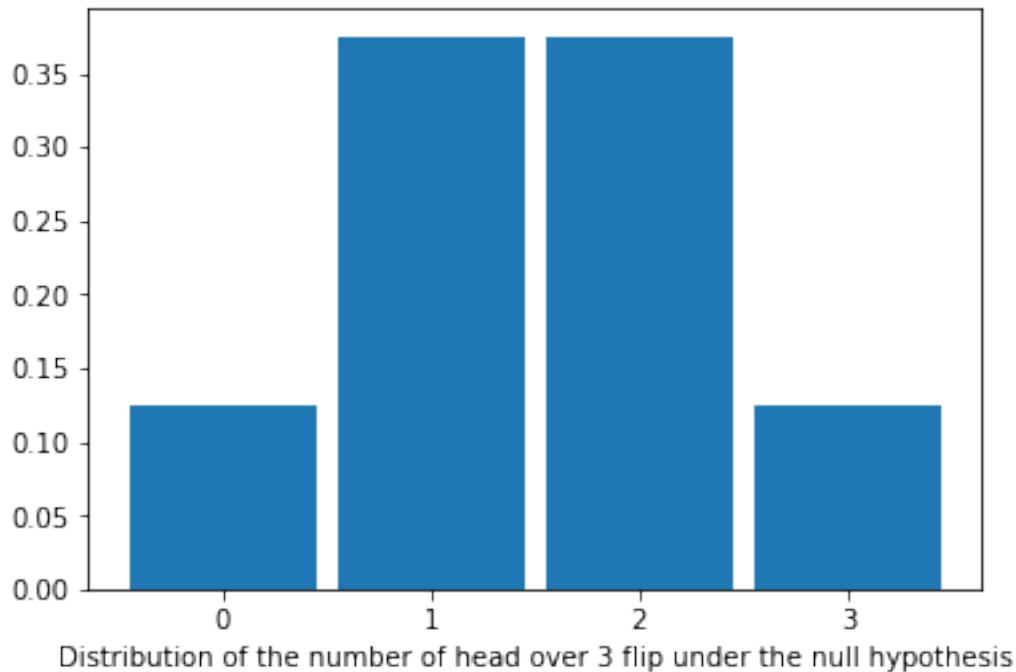
1	2	3	count #heads
			0
H			1
	H		1
		H	1
H	H		2
H		H	2
	H	H	2
H	H	H	3

8 possibles configurations, probabilities of differents values for  $p$  are:  $x$  measure the number of success.

- $P(x = 0) = 1/8$
- $P(x = 1) = 3/8$
- $P(x = 2) = 3/8$
- $P(x = 3) = 1/8$

```
plt.bar([0, 1, 2, 3], [1/8, 3/8, 3/8, 1/8], width=0.9)
_ = plt.xticks([0, 1, 2, 3], [0, 1, 2, 3])
plt.xlabel("Distribution of the number of head over 3 flip under the null hypothesis")
```

```
Text(0.5, 0, 'Distribution of the number of head over 3 flip under the null hypothesis')
```



3. Compute the probability (*p*-value) to observe a value larger or equal than 2 under the null hypothesis ? This probability is the *p*-value:

$$P(x \geq 2|H_0) = P(x = 2) + P(x = 3) = 3/8 + 1/8 = 4/8 = 1/2$$

### Flip coin: Real Example

Biased coin ? 60 heads have been found over 100 flips, is it coins biased ?

1. Model the data: number of heads follow a Binomial distribution.
2. Compute model parameters: N=100, P=60/100.
3. Compute a test statistic, same as frequency.
4. Compute a test statistic: 60/100.
5. Under the null hypothesis the distribution of the number of tail (*k*) follow the **binomial distribution** of parameters N=100, P=0.5:

$$Pr(X = k|H_0) = Pr(X = k|n = 100, p = 0.5) = \binom{100}{k} 0.5^k (1 - 0.5)^{(100-k)}.$$

$$\begin{aligned} Pr(X = k \geq 60|H_0) &= \sum_{k=60}^{100} \binom{100}{k} 0.5^k (1 - 0.5)^{(100-k)} \\ &= 1 - \sum_{k=1}^{60} \binom{100}{k} 0.5^k (1 - 0.5)^{(100-k)}, \text{ the cumulative distribution function.} \end{aligned}$$

### Use tabulated binomial distribution

```

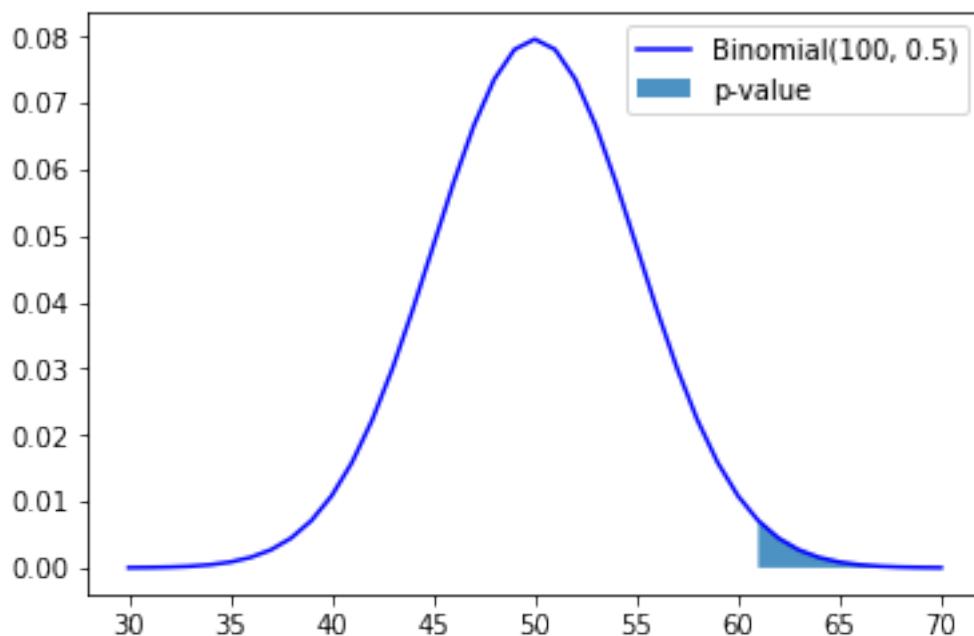
import scipy.stats
import matplotlib.pyplot as plt

#tobs = 2.39687663116 # assume the t-value
succes = np.linspace(30, 70, 41)
plt.plot(succes, scipy.stats.binom.pmf(succes, 100, 0.5), 'b-', label="Binomial(100, 0.5")
upper_succes_tvalues = succes[succes > 60]
plt.fill_between(upper_succes_tvalues, 0, scipy.stats.binom.pmf(upper_succes_tvalues, 100,
                                                               0.5), alpha=.8, label="p-value")
_ = plt.legend()

pval = 1 - scipy.stats.binom.cdf(60, 100, 0.5)
print(pval)

```

0.01760010010885238



### Random sampling of the Binomial distribution under the null hypothesis

```

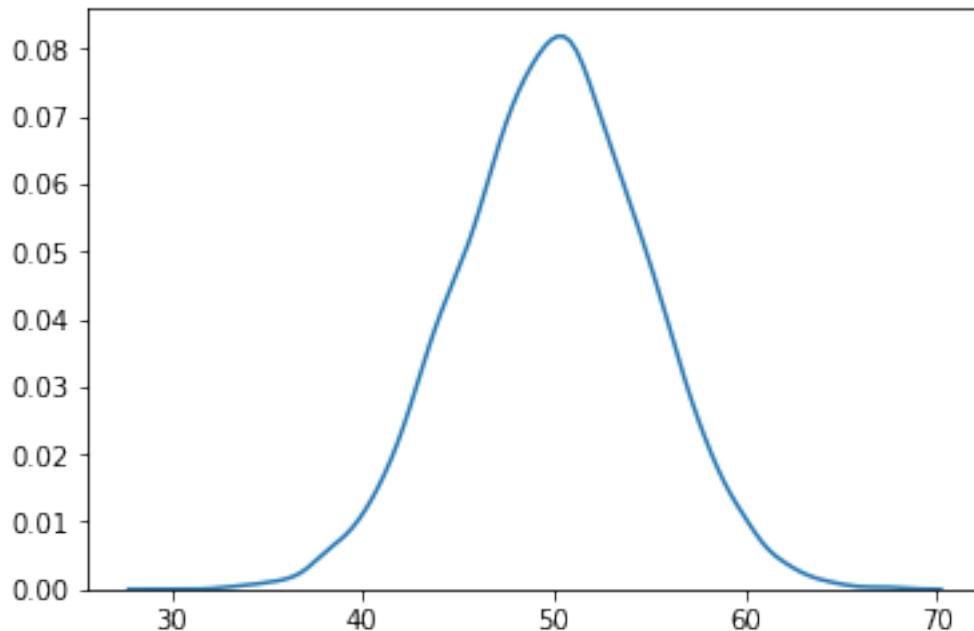
sccess_h0 = scipy.stats.binom.rvs(100, 0.5, size=10000, random_state=4)

#sccess_h0 = np.array([0 for i in range(5000)])
import seaborn as sns
_ = sns.distplot(sccess_h0, hist=False)

pval_rnd = np.sum(sccess_h0 >= 60) / (len(sccess_h0) + 1)
print("P-value using monte-carlo sampling of the Binomial distribution under H0=", pval_
      _rnd)

```

P-value using monte-carlo sampling of the Binomial distribution under H0= 0.  
025897410258974102



### One sample $t$ -test

The one-sample  $t$ -test is used to determine whether a sample comes from a population with a specific mean. For example you want to test if the average height of a population is 1.75 m.

1 Model the data

Assume that height is normally distributed:  $X \sim \mathcal{N}(\mu, \sigma)$ , ie:

$$\text{height}_i = \text{average height over the population} + \text{error}_i \quad (4.6)$$

$$x_i = \bar{x} + \varepsilon_i \quad (4.7)$$

The  $\varepsilon_i$  are called the residuals

2 Fit: estimate the model parameters

$\bar{x}, s_x$  are the estimators of  $\mu, \sigma$ .

3 Compute a test statistic

In testing the null hypothesis that the population mean is equal to a specified value  $\mu_0 = 1.75$ , one uses the statistic:

$$t = \frac{\bar{x} - \mu_0}{s_x / \sqrt{n}}$$

Remarks: Although the parent population does not need to be normally distributed, the distribution of the population of sample means,  $\bar{x}$ , is assumed to be normal. By the central limit theorem, if the sampling of the parent population is independent then the sample means will be approximately normal.

4 Compute the probability of the test statistic under the null hypothesis. This require to have the distribution of the  $t$  statistic under  $H_0$ .

## Example

Given the following samples, we will test whether its true mean is 1.75.

Warning, when computing the std or the variance, set ddof=1. The default value, ddof=0, leads to the biased estimator of the variance.

```
import numpy as np

x= [ 1.83,  1.83,  1.73,  1.82,  1.83,  1.73,  1.99,  1.85,  1.68,  1.87]

xbar = np.mean(x) # sample mean
mu0 = 1.75 # hypothesized value
s = np.std(x, ddof=1) # sample standard deviation
n = len(x) # sample size

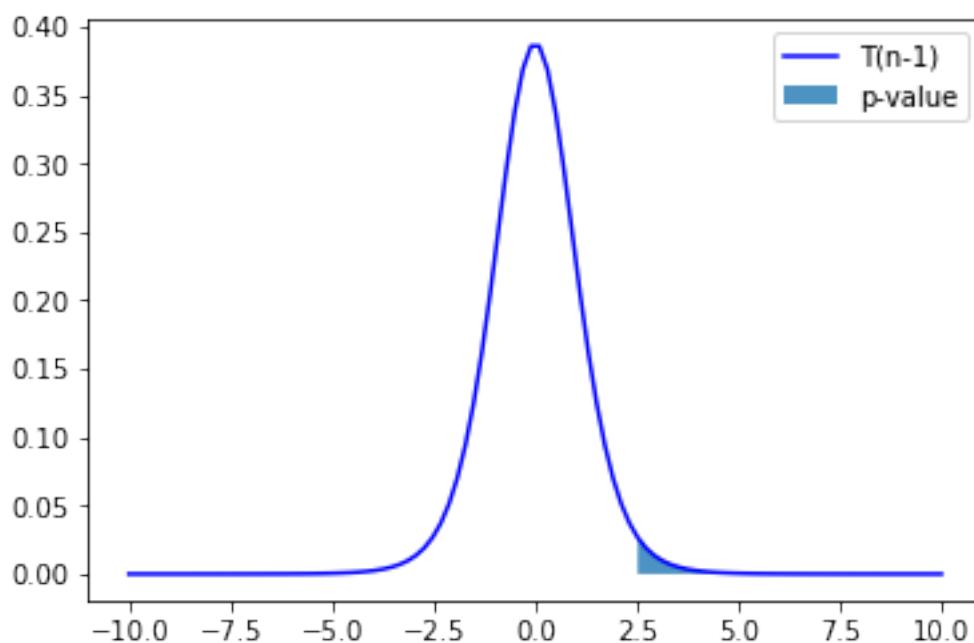
tobs = (xbar - mu0) / (s / np.sqrt(n))
print(tobs)
```

```
2.3968766311585883
```

The :math:`p`-value is the probability to observe a value  $t$  more extreme than the observed one  $t_{obs}$  under the null hypothesis  $H_0$ :  $P(t > t_{obs} | H_0)$

```
import scipy.stats as stats
import matplotlib.pyplot as plt

#tobs = 2.39687663116 # assume the t-value
tvalues = np.linspace(-10, 10, 100)
plt.plot(tvalues, stats.t.pdf(tvalues, n-1), 'b-', label="T(n-1)")
upper_tval_tvalues = tvalues[tvalues > tobs]
plt.fill_between(upper_tval_tvalues, 0, stats.t.pdf(upper_tval_tvalues, n-1), alpha=.8, color='red', label="p-value")
_ = plt.legend()
```



#### 4.1.4 Testing pairwise associations

Univariate statistical analysis: explore association between pairs of variables.

- In statistics, a **categorical variable or factor** is a variable that can take on one of a limited, and usually fixed, number of possible values, thus assigning each individual to a particular group or “category”. The levels are the possible values of the variable. Number of levels = 2: binomial; Number of levels > 2: multinomial. There is no intrinsic ordering to the categories. For example, gender is a categorical variable having two categories (male and female) and there is no intrinsic ordering to the categories. For example, Sex (Female, Male), Hair color (blonde, brown, etc.).
- An **ordinal variable** is a categorical variable with a clear ordering of the levels. For example: drinks per day (none, small, medium and high).
- A **continuous or quantitative variable**  $x \in \mathbb{R}$  is one that can take any value in a range of possible values, possibly infinite. E.g.: salary, experience in years, weight.

What statistical test should I use?

See: [http://www.ats.ucla.edu/stat/mult\\_pkg/whatstat/](http://www.ats.ucla.edu/stat/mult_pkg/whatstat/)

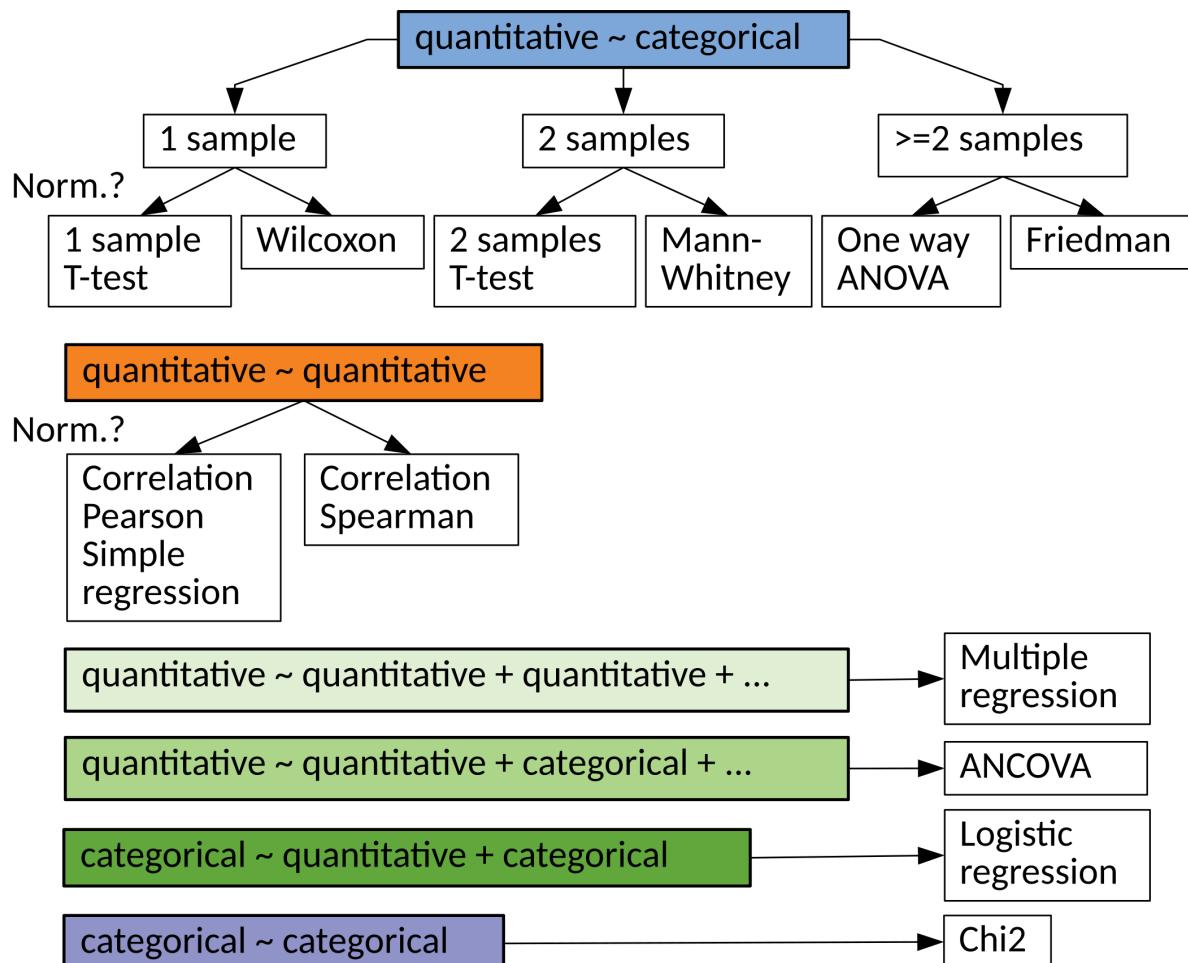


Fig. 1: Statistical tests

### Pearson correlation test: test association between two quantitative variables

Test the correlation coefficient of two quantitative variables. The test calculates a Pearson correlation coefficient and the  $p$ -value for testing non-correlation.

Let  $x$  and  $y$  two quantitative variables, where  $n$  samples were observed. The linear correlation coefficient is defined as :

$$r = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^n (y_i - \bar{y})^2}}.$$

Under  $H_0$ , the test statistic  $t = \sqrt{n-2} \frac{r}{\sqrt{1-r^2}}$  follow Student distribution with  $n - 2$  degrees of freedom.

```
import numpy as np
import scipy.stats as stats
n = 50
x = np.random.normal(size=n)
y = 2 * x + np.random.normal(size=n)

# Compute with scipy
cor, pval = stats.pearsonr(x, y)
```

## Two sample (Student) $t$ -test: compare two means

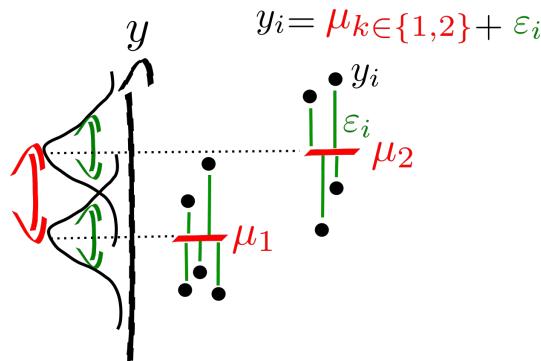


Fig. 2: Two-sample model

The two-sample  $t$ -test (Snedecor and Cochran, 1989) is used to determine if two population means are equal. There are several variations on this test. If data are paired (e.g. 2 measures, before and after treatment for each individual) use the one-sample  $t$ -test of the difference. The variances of the two samples may be assumed to be equal (a.k.a. homoscedasticity) or unequal (a.k.a. heteroscedasticity).

### 1. Model the data

Assume that the two random variables are normally distributed:  $y_1 \sim \mathcal{N}(\mu_1, \sigma_1)$ ,  $y_2 \sim \mathcal{N}(\mu_2, \sigma_2)$ .

### 2. Fit: estimate the model parameters

Estimate means and variances:  $\bar{y}_1, s_{y_1}^2, \bar{y}_2, s_{y_2}^2$ .

### 3. t-test

The general principle is

$$t = \frac{\text{difference of means}}{\text{its standard error}} \quad (4.8)$$

$$= \frac{\bar{y}_1 - \bar{y}_2}{s_{\bar{y}_1 - \bar{y}_2}} \quad (4.9)$$

Since  $y_1$  and  $y_2$  are independant:

$$s_{\bar{y}_1 - \bar{y}_2}^2 = s_{\bar{y}_1}^2 + s_{\bar{y}_2}^2 = \frac{s_{y_1}^2}{n_1} + \frac{s_{y_2}^2}{n_2} \quad (4.10)$$

$$\text{thus} \quad (4.11)$$

$$s_{\bar{y}_1 - \bar{y}_2} = \sqrt{\frac{s_{y_1}^2}{n_1} + \frac{s_{y_2}^2}{n_2}} \quad (4.12)$$

#### Equal or unequal sample sizes, unequal variances (Welch's t-test)

Welch's t-test defines the  $t$  statistic as

$$t = \frac{\bar{y}_1 - \bar{y}_2}{\sqrt{\frac{s_{y_1}^2}{n_1} + \frac{s_{y_2}^2}{n_2}}}.$$

To compute the  $p$ -value one needs the degrees of freedom associated with this variance estimate. It is approximated using the Welch–Satterthwaite equation:

$$\nu \approx \frac{\left( \frac{s_{y_1}^2}{n_1} + \frac{s_{y_2}^2}{n_2} \right)^2}{\frac{s_{y_1}^4}{n_1^2(n_1-1)} + \frac{s_{y_2}^4}{n_2^2(n_2-1)}}.$$

#### Equal or unequal sample sizes, equal variances

If we assume equal variance (ie,  $s_{y_1}^2 = s_{y_2}^2 = s^2$ ), where  $s^2$  is an estimator of the common variance of the two samples:

$$s^2 = \frac{s_{y_1}^2(n_1 - 1) + s_{y_2}^2(n_2 - 1)}{n_1 + n_2 - 2} \quad (4.13)$$

$$= \frac{\sum_i^{n_1} (y_{1i} - \bar{y}_1)^2 + \sum_j^{n_2} (y_{2j} - \bar{y}_2)^2}{(n_1 - 1) + (n_2 - 1)} \quad (4.14)$$

then

$$s_{\bar{y}_1 - \bar{y}_2} = \sqrt{\frac{s^2}{n_1} + \frac{s^2}{n_2}} = s \sqrt{\frac{1}{n_1} + \frac{1}{n_2}}$$

Therefore, the  $t$  statistic, that is used to test whether the means are different is:

$$t = \frac{\bar{y}_1 - \bar{y}_2}{s \cdot \sqrt{\frac{1}{n_1} + \frac{1}{n_2}}},$$

### Equal sample sizes, equal variances

If we simplify the problem assuming equal samples of size  $n_1 = n_2 = n$  we get

$$t = \frac{\bar{y}_1 - \bar{y}_2}{s\sqrt{2}} \cdot \sqrt{n} \quad (4.15)$$

$$\approx \text{effect size} \cdot \sqrt{n} \quad (4.16)$$

$$\approx \frac{\text{difference of means}}{\text{standard deviation of the noise}} \cdot \sqrt{n} \quad (4.17)$$

### Example

Given the following two samples, test whether their means are equal using the **standard t-test, assuming equal variance**.

```
import scipy.stats as stats

height = np.array([ 1.83,  1.83,  1.73,  1.82,  1.83,  1.73,  1.99,  1.85,  1.68,  1.87,
                   1.66,  1.71,  1.73,  1.64,  1.70,  1.60,  1.79,  1.73,  1.62,  1.77])

grp = np.array(["M"] * 10 + ["F"] * 10)

# Compute with scipy
print(stats.ttest_ind(height[grp == "M"], height[grp == "F"], equal_var=True))
```

```
Ttest_indResult(statistic=3.5511519888466885, pvalue=0.00228208937112721)
```

### ANOVA F-test (quantitative ~ categorial (>2 levels))

Analysis of variance (ANOVA) provides a statistical test of whether or not the means of several groups are equal, and therefore generalizes the  $t$ -test to more than two groups. ANOVAs are useful for comparing (testing) three or more means (groups or variables) for statistical significance. It is conceptually similar to multiple two-sample  $t$ -tests, but is less conservative.

Here we will consider one-way ANOVA with one independent variable, ie one-way anova.

[Wikipedia](#):

- Test if any group is on average superior, or inferior, to the others versus the null hypothesis that all four strategies yield the same mean response
- Detect any of several possible differences.
- The advantage of the ANOVA  $F$ -test is that we do not need to pre-specify which strategies are to be compared, and we do not need to adjust for making multiple comparisons.

- The disadvantage of the ANOVA  $F$ -test is that if we reject the null hypothesis, we do not know which strategies can be said to be significantly different from the others.

## 1. Model the data

A company has applied three marketing strategies to three samples of customers in order increase their business volume. The marketing is asking whether the strategies led to different increases of business volume. Let  $y_1, y_2$  and  $y_3$  be the three samples of business volume increase.

Here we assume that the three populations were sampled from three random variables that are normally distributed. I.e.,  $Y_1 \sim N(\mu_1, \sigma_1)$ ,  $Y_2 \sim N(\mu_2, \sigma_2)$  and  $Y_3 \sim N(\mu_3, \sigma_3)$ .

## 2. Fit: estimate the model parameters

Estimate means and variances:  $\bar{y}_i, \sigma_i, \forall i \in \{1, 2, 3\}$ .

## 3. $F$ -test

The formula for the one-way ANOVA  $F$ -test statistic is

$$F = \frac{\text{Explained variance}}{\text{Unexplained variance}} \quad (4.18)$$

$$= \frac{\text{Between-group variability}}{\text{Within-group variability}} = \frac{s_B^2}{s_W^2}. \quad (4.19)$$

The “explained variance”, or “between-group variability” is

$$s_B^2 = \sum_i n_i (\bar{y}_i - \bar{y})^2 / (K - 1),$$

where  $\bar{y}_i$  denotes the sample mean in the  $i$ th group,  $n_i$  is the number of observations in the  $i$ th group,  $\bar{y}$  denotes the overall mean of the data, and  $K$  denotes the number of groups.

The “unexplained variance”, or “within-group variability” is

$$s_W^2 = \sum_{ij} (y_{ij} - \bar{y}_i)^2 / (N - K),$$

where  $y_{ij}$  is the  $j$ th observation in the  $i$ th out of  $K$  groups and  $N$  is the overall sample size. This  $F$ -statistic follows the  $F$ -distribution with  $K - 1$  and  $N - K$  degrees of freedom under the null hypothesis. The statistic will be large if the between-group variability is large relative to the within-group variability, which is unlikely to happen if the population means of the groups all have the same value.

Note that when there are only two groups for the one-way ANOVA  $F$ -test,  $F = t^2$  where  $t$  is the Student's  $t$  statistic.

### Chi-square, $\chi^2$ (categorical ~ categorical)

Computes the chi-square,  $\chi^2$ , statistic and  $p$ -value for the hypothesis test of independence of frequencies in the observed contingency table (cross-table). The observed frequencies are tested against an expected contingency table obtained by computing expected frequencies based on the marginal sums under the assumption of independence.

Example: 20 participants: 10 exposed to some chemical product and 10 non exposed (exposed = 1 or 0). Among the 20 participants 10 had cancer 10 not (cancer = 1 or 0).  $\chi^2$  tests the association between those two variables.

```
import numpy as np
import pandas as pd
import scipy.stats as stats

# Dataset:
# 15 samples:
# 10 first exposed
exposed = np.array([1] * 10 + [0] * 10)
# 8 first with cancer, 10 without, the last two with.
cancer = np.array([1] * 8 + [0] * 10 + [1] * 2)

crosstab = pd.crosstab(exposed, cancer, rownames=['exposed'],
                       colnames=['cancer'])
print("Observed table:")
print("-----")
print(crosstab)

chi2, pval, dof, expected = stats.chi2_contingency(crosstab)
print("Statistics:")
print("-----")
print("Chi2 = %f, pval = %f" % (chi2, pval))
print("Expected table:")
print("-----")
print(expected)
```

```
Observed table:
-----
cancer   0   1
exposed
0        8   2
1        2   8
Statistics:
-----
Chi2 = 5.000000, pval = 0.025347
Expected table:
-----
[[5.  5.]
 [5.  5.]]
```

Computing expected cross-table

```
# Compute expected cross-table based on proportion
exposed_marg = crosstab.sum(axis=0)
exposed_freq = exposed_marg / exposed_marg.sum()
```

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```
cancer_marg = crosstab.sum(axis=1)
cancer_freq = cancer_marg / cancer_marg.sum()

print('Exposed frequency? Yes: %.2f' % exposed_freq[0],
      'No: %.2f' % exposed_freq[1])
print('Cancer frequency? Yes: %.2f' % cancer_freq[0],
      'No: %.2f' % cancer_freq[1])

print('Expected frequencies:')
print(np.outer(exposed_freq, cancer_freq))

print('Expected cross-table (frequencies * N): ')
print(np.outer(exposed_freq, cancer_freq) * len(exposed))
```

```
Exposed frequency? Yes: 0.50 No: 0.50
Cancer frequency? Yes: 0.50 No: 0.50
Expected frequencies:
[[0.25 0.25]
 [0.25 0.25]]
Expected cross-table (frequencies * N):
[[5. 5.]
 [5. 5.]]
```

#### 4.1.5 Non-parametric test of pairwise associations

```
### Spearman rank-order correlation (quantitative ~ quantitative)
```

The Spearman correlation is a non-parametric measure of the monotonicity of the relationship between two datasets.

When to use it? Observe the data distribution: - presence of **outliers** - the distribution of the residuals is not Gaussian.

Like other correlation coefficients, this one varies between -1 and +1 with 0 implying no correlation. Correlations of -1 or +1 imply an exact monotonic relationship. Positive correlations imply that as  $x$  increases, so does  $y$ . Negative correlations imply that as  $x$  increases,  $y$  decreases.

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

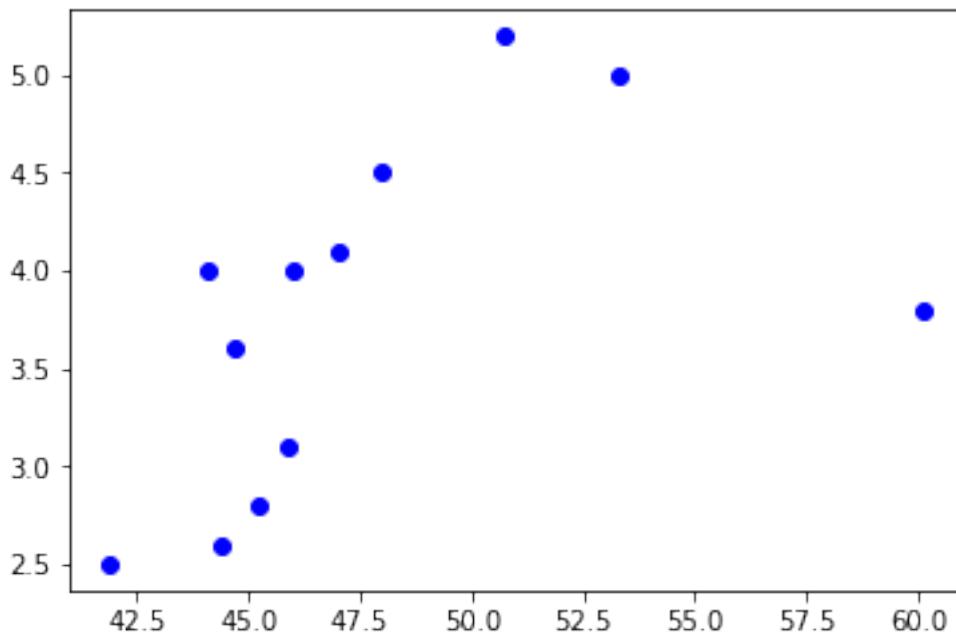
x = np.array([44.4, 45.9, 41.9, 53.3, 44.7, 44.1, 50.7, 45.2, 46, 47, 48, 60.1])
y = np.array([2.6, 3.1, 2.5, 5.0, 3.6, 4.0, 5.2, 2.8, 4, 4.1, 4.5, 3.8])

plt.plot(x, y, "bo")

# Non-Parametric Spearman
cor, pval = stats.spearmanr(x, y)
print("Non-Parametric Spearman cor test, cor: %.4f, pval: %.4f" % (cor, pval))

# Parametric Pearson cor test
cor, pval = stats.pearsonr(x, y)
print("Parametric Pearson cor test: cor: %.4f, pval: %.4f" % (cor, pval))
```

```
Non-Parametric Spearman cor test, cor: 0.7110, pval: 0.0095
Parametric Pearson cor test: cor: 0.5263, pval: 0.0788
```



### Wilcoxon signed-rank test (quantitative ~ cte)

Source: [https://en.wikipedia.org/wiki/Wilcoxon\\_signed-rank\\_test](https://en.wikipedia.org/wiki/Wilcoxon_signed-rank_test)

The Wilcoxon signed-rank test is a non-parametric statistical hypothesis test used when comparing two related samples, matched samples, or repeated measurements on a single sample to assess whether their population mean ranks differ (i.e. it is a paired difference test). It is equivalent to one-sample test of the difference of paired samples.

It can be used as an alternative to the paired Student's  $t$ -test,  $t$ -test for matched pairs, or the  $t$ -test for dependent samples when the population cannot be assumed to be normally distributed.

When to use it? Observe the data distribution: - presence of outliers - the distribution of the residuals is not Gaussian

It has a lower sensitivity compared to  $t$ -test. May be problematic to use when the sample size is small.

Null hypothesis  $H_0$ : difference between the pairs follows a symmetric distribution around zero.

```
import scipy.stats as stats
n = 20
# Buisness Volume time 0
bv0 = np.random.normal(loc=3, scale=.1, size=n)
# Buisness Volume time 1
bv1 = bv0 + 0.1 + np.random.normal(loc=0, scale=.1, size=n)

# create an outlier
bv1[0] -= 10

# Paired t-test
```

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```
print(stats.ttest_rel(bv0, bv1))

# Wilcoxon
print(stats.wilcoxon(bv0, bv1))
```

```
Ttest_relResult(statistic=0.7821450892478711, pvalue=0.4437681541620575)
WilcoxonResult(statistic=35.0, pvalue=0.008967599455194583)
```

### Mann–Whitney $U$ test (quantitative ~ categorial (2 levels))

In statistics, the Mann–Whitney  $U$  test (also called the Mann–Whitney–Wilcoxon, Wilcoxon rank-sum test or Wilcoxon–Mann–Whitney test) is a nonparametric test of the null hypothesis that two samples come from the same population against an alternative hypothesis, especially that a particular population tends to have larger values than the other.

It can be applied on unknown distributions contrary to e.g. a  $t$ -test that has to be applied only on normal distributions, and it is nearly as efficient as the  $t$ -test on normal distributions.

```
import scipy.stats as stats
n = 20
# Buismess Volume group 0
bv0 = np.random.normal(loc=1, scale=.1, size=n)

# Buismess Volume group 1
bv1 = np.random.normal(loc=1.2, scale=.1, size=n)

# create an outlier
bv1[0] -= 10

# Two-samples t-test
print(stats.ttest_ind(bv0, bv1))

# Wilcoxon
print(stats.mannwhitneyu(bv0, bv1))
```

```
Ttest_indResult(statistic=0.6725314683035514, pvalue=0.505314623871812)
MannwhitneyuResult(statistic=67.0, pvalue=0.0001690974050146689)
```

#### 4.1.6 Linear model

Given  $n$  random samples  $(y_i, x_{1i}, \dots, x_{pi})$ ,  $i = 1, \dots, n$ , the linear regression models the relation between the observations  $y_i$  and the independent variables  $x_i^p$  is formulated as

$$y_i = \beta_0 + \beta_1 x_{1i} + \dots + \beta_p x_{pi} + \varepsilon_i \quad i = 1, \dots, n$$

- The  $\beta$ 's are the model parameters, ie, the regression coefficients.
- $\beta_0$  is the intercept or the bias.
- $\varepsilon_i$  are the **residuals**.
- **An independent variable (IV)**. It is a variable that stands alone and isn't changed by the other variables you are trying to measure. For example, someone's age might be an

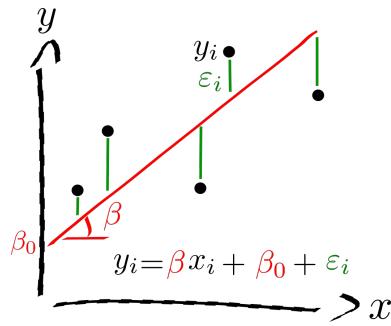


Fig. 3: Linear model

independent variable. Other factors (such as what they eat, how much they go to school, how much television they watch) aren't going to change a person's age. In fact, when you are looking for some kind of relationship between variables you are trying to see if the independent variable causes some kind of change in the other variables, or dependent variables. In Machine Learning, these variables are also called the **predictors**.

- **A dependent variable.** It is something that depends on other factors. For example, a test score could be a dependent variable because it could change depending on several factors such as how much you studied, how much sleep you got the night before you took the test, or even how hungry you were when you took it. Usually when you are looking for a relationship between two things you are trying to find out what makes the dependent variable change the way it does. In Machine Learning this variable is called a **target variable**.

### Simple regression: test association between two quantitative variables

Using the dataset "salary", explore the association between the dependant variable (e.g. Salary) and the independent variable (e.g.: Experience is quantitative).

```
import pandas as pd
import matplotlib.pyplot as plt
%matplotlib inline

url = 'https://raw.githubusercontent.com/neurospin/pystatsml/master/datasets/salary_table.csv'
salary = pd.read_csv(url)
```

#### 1. Model the data

Model the data on some **hypothesis** e.g.: salary is a linear function of the experience.

$$\text{salary}_i = \beta \text{ experience}_i + \beta_0 + \epsilon_i,$$

more generally

$$y_i = \beta x_i + \beta_0 + \epsilon_i$$

- $\beta$ : the slope or coefficient or parameter of the model,
- $\beta_0$ : the **intercept** or **bias** is the second parameter of the model,

- $\epsilon_i$ : is the  $i$ th error, or residual with  $\epsilon \sim \mathcal{N}(0, \sigma^2)$ .

The simple regression is equivalent to the Pearson correlation.

## 2. Fit: estimate the model parameters

The goal it so estimate  $\beta$ ,  $\beta_0$  and  $\sigma^2$ .

Minimizes the **mean squared error (MSE)** or the **Sum squared error (SSE)**. The so-called **Ordinary Least Squares (OLS)** finds  $\beta, \beta_0$  that minimizes the  $SSE = \sum_i \epsilon_i^2$

$$SSE = \sum_i (y_i - \beta x_i - \beta_0)^2$$

Recall from calculus that an extreme point can be found by computing where the derivative is zero, i.e. to find the intercept, we perform the steps:

$$\begin{aligned} \frac{\partial SSE}{\partial \beta_0} &= \sum_i (y_i - \beta x_i - \beta_0) = 0 \\ \sum_i y_i &= \beta \sum_i x_i + n \beta_0 \\ n \bar{y} &= n \beta \bar{x} + n \beta_0 \\ \beta_0 &= \bar{y} - \beta \bar{x} \end{aligned}$$

To find the regression coefficient, we perform the steps:

$$\frac{\partial SSE}{\partial \beta} = \sum_i x_i (y_i - \beta x_i - \beta_0) = 0$$

Plug in  $\beta_0$ :

$$\begin{aligned} \sum_i x_i (y_i - \beta x_i - \bar{y} + \beta \bar{x}) &= 0 \\ \sum_i x_i y_i - \bar{y} \sum_i x_i &= \beta \sum_i (x_i - \bar{x}) \end{aligned}$$

Divide both sides by  $n$ :

$$\begin{aligned} \frac{1}{n} \sum_i x_i y_i - \bar{y} \bar{x} &= \frac{1}{n} \beta \sum_i (x_i - \bar{x}) \\ \beta &= \frac{\frac{1}{n} \sum_i x_i y_i - \bar{y} \bar{x}}{\frac{1}{n} \sum_i (x_i - \bar{x})} = \frac{Cov(x, y)}{Var(x)}. \end{aligned}$$

```
from scipy import stats
import numpy as np
y, x = salary.salary, salary.experience
beta, beta0, r_value, p_value, std_err = stats.linregress(x,y)
print("y = %f x + %f,  r: %f, r-squared: %f,\np-value: %f, std_err: %f"
      % (beta, beta0, r_value, r_value**2, p_value, std_err))

print("Regression line with the scatterplot")
yhat = beta * x + beta0 # regression line
```

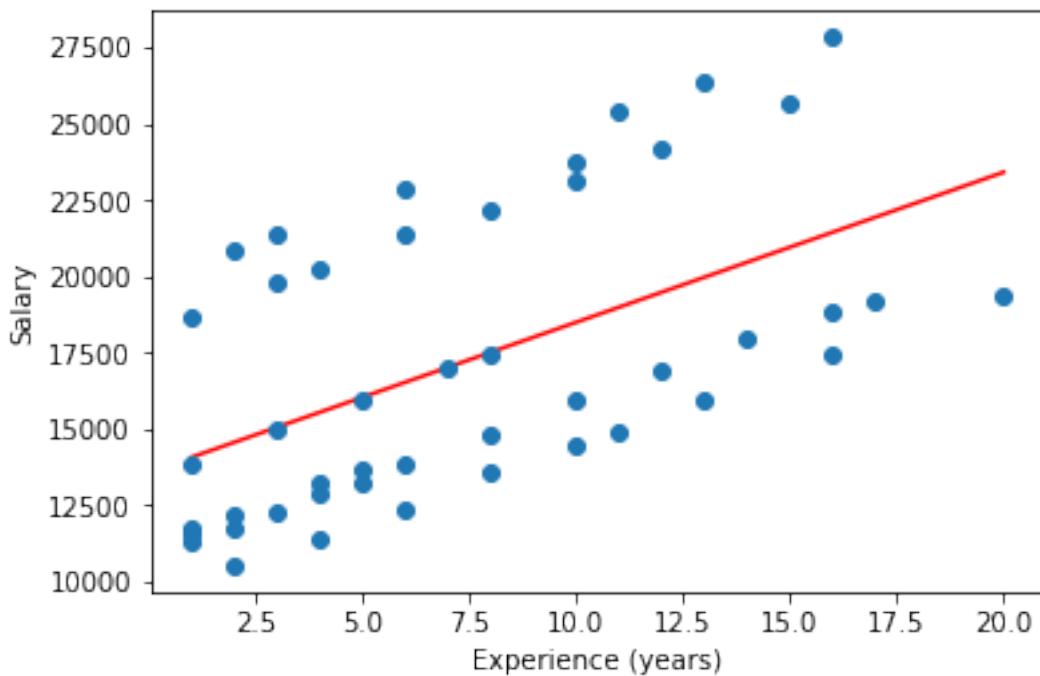
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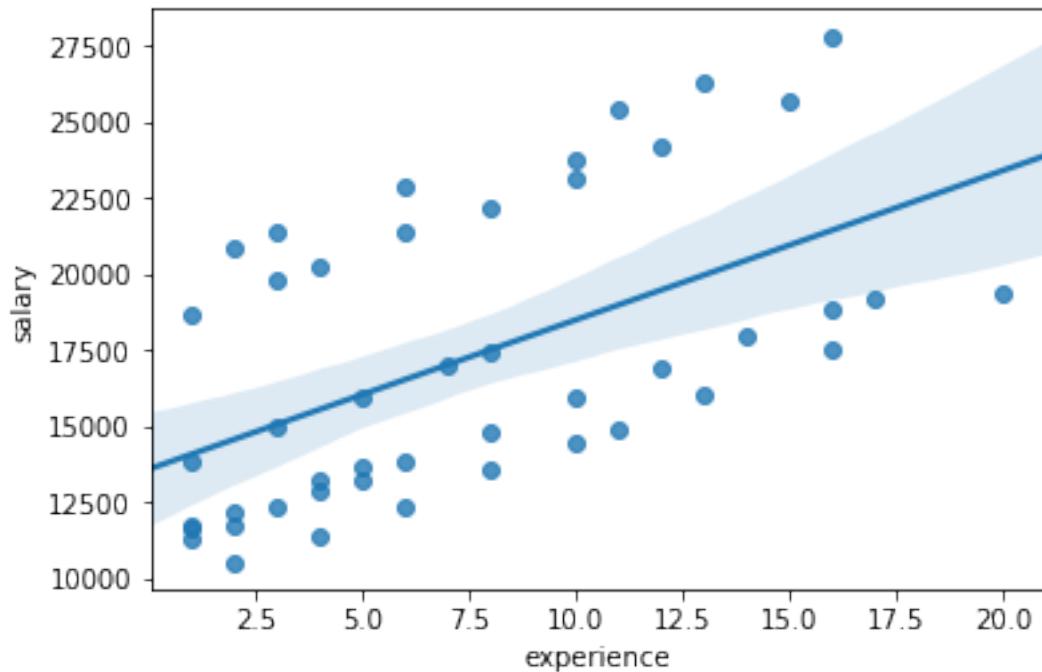
```
plt.plot(x, yhat, 'r-', x, y, 'o')
plt.xlabel('Experience (years)')
plt.ylabel('Salary')
plt.show()

print("Using seaborn")
import seaborn as sns
sns.regplot(x="experience", y="salary", data=salary);
```

```
y = 491.486913 x + 13584.043803, r: 0.538886, r-squared: 0.290398,
p-value: 0.000112, std_err: 115.823381
Regression line with the scatterplot
```



```
Using seaborn
```



### 3. F-Test

#### 3.1 Goodness of fit

The goodness of fit of a statistical model describes how well it fits a set of observations. Measures of goodness of fit typically summarize the discrepancy between observed values and the values expected under the model in question. We will consider the **explained variance** also known as the coefficient of determination, denoted  $R^2$  pronounced **R-squared**.

The total sum of squares,  $SS_{tot}$  is the sum of the sum of squares explained by the regression,  $SS_{reg}$ , plus the sum of squares of residuals unexplained by the regression,  $SS_{res}$ , also called the SSE, i.e. such that

$$SS_{tot} = SS_{reg} + SS_{res}$$

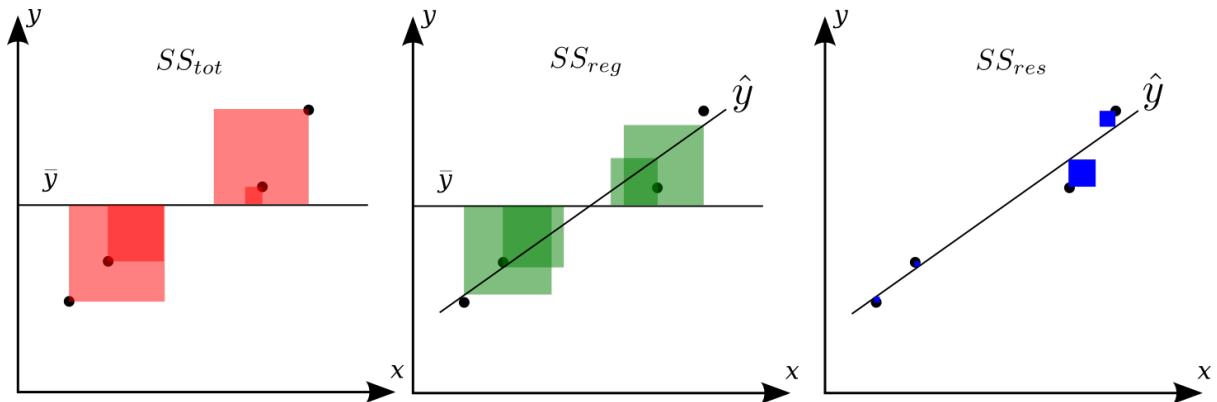


Fig. 4: title

The mean of  $y$  is

$$\bar{y} = \frac{1}{n} \sum_i y_i.$$

The total sum of squares is the total squared sum of deviations from the mean of  $y$ , i.e.

$$SS_{\text{tot}} = \sum_i (y_i - \bar{y})^2$$

The regression sum of squares, also called the explained sum of squares:

$$SS_{\text{reg}} = \sum_i (\hat{y}_i - \bar{y})^2,$$

where  $\hat{y}_i = \beta x_i + \beta_0$  is the estimated value of salary  $\hat{y}_i$  given a value of experience  $x_i$ .

The sum of squares of the residuals, also called the residual sum of squares (RSS) is:

$$SS_{\text{res}} = \sum_i (y_i - \hat{y}_i)^2.$$

$R^2$  is the explained sum of squares of errors. It is the variance explain by the regression divided by the total variance, i.e.

$$R^2 = \frac{\text{explained SS}}{\text{total SS}} = \frac{SS_{\text{reg}}}{SS_{\text{tot}}} = 1 - \frac{SS_{\text{res}}}{SS_{\text{tot}}}.$$

## 3.2 Test

Let  $\hat{\sigma}^2 = SS_{\text{res}}/(n - 2)$  be an estimator of the variance of  $\epsilon$ . The 2 in the denominator stems from the 2 estimated parameters: intercept and coefficient.

- **Unexplained variance:**  $\frac{SS_{\text{res}}}{\hat{\sigma}^2} \sim \chi^2_{n-2}$
- **Explained variance:**  $\frac{SS_{\text{reg}}}{\hat{\sigma}^2} \sim \chi^2_1$ . The single degree of freedom comes from the difference between  $\frac{SS_{\text{tot}}}{\hat{\sigma}^2} (\sim \chi^2_{n-1})$  and  $\frac{SS_{\text{res}}}{\hat{\sigma}^2} (\sim \chi^2_{n-2})$ , i.e.  $(n - 1) - (n - 2)$  degree of freedom.

The Fisher statistics of the ratio of two variances:

$$F = \frac{\text{Explained variance}}{\text{Unexplained variance}} = \frac{SS_{\text{reg}}/1}{SS_{\text{res}}/(n - 2)} \sim F(1, n - 2)$$

Using the  $F$ -distribution, compute the probability of observing a value greater than  $F$  under  $H_0$ , i.e.:  $P(x > F|H_0)$ , i.e. the survival function (1 – Cumulative Distribution Function) at  $x$  of the given  $F$ -distribution.

## Multiple regression

### Theory

Multiple Linear Regression is the most basic supervised learning algorithm.

Given: a set of training data  $\{x_1, \dots, x_N\}$  with corresponding targets  $\{y_1, \dots, y_N\}$ .

In linear regression, we assume that the model that generates the data involves only a linear combination of the input variables, i.e.

$$y(x_i, \beta) = \beta^0 + \beta^1 x_i^1 + \dots + \beta^P x_i^P,$$

or, simplified

$$y(x_i, \beta) = \beta_0 + \sum_{j=1}^{P-1} \beta_j x_i^j.$$

Extending each sample with an intercept,  $x_i := [1, x_i] \in R^{P+1}$  allows us to use a more general notation based on linear algebra and write it as a simple dot product:

$$y(x_i, \beta) = x_i^T \beta,$$

where  $\beta \in R^{P+1}$  is a vector of weights that define the  $P + 1$  parameters of the model. From now we have  $P$  regressors + the intercept.

Minimize the Mean Squared Error MSE loss:

$$MSE(\beta) = \frac{1}{N} \sum_{i=1}^N (y_i - y(x_i, \beta))^2 = \frac{1}{N} \sum_{i=1}^N (y_i - x_i^T \beta)^2$$

Let  $X = [x_0^T, \dots, x_N^T]$  be a  $N \times P + 1$  matrix of  $N$  samples of  $P$  input features with one column of one and let be  $y = [y_1, \dots, y_N]$  be a vector of the  $N$  targets. Then, using linear algebra, the **mean squared error (MSE) loss can be rewritten**:

$$MSE(\beta) = \frac{1}{N} \|y - X\beta\|_2^2.$$

The  $\beta$  that minimises the MSE can be found by:

$$\nabla_\beta \left( \frac{1}{N} \|y - X\beta\|_2^2 \right) = 0 \quad (4.20)$$

$$\frac{1}{N} \nabla_\beta (y - X\beta)^T (y - X\beta) = 0 \quad (4.21)$$

$$\frac{1}{N} \nabla_\beta (y^T y - 2\beta^T X^T y + \beta X^T X \beta) = 0 \quad (4.22)$$

$$-2X^T y + 2X^T X \beta = 0 \quad (4.23)$$

$$X^T X \beta = X^T y \quad (4.24)$$

$$\beta = (X^T X)^{-1} X^T y, \quad (4.25)$$

where  $(X^T X)^{-1} X^T$  is a pseudo inverse of  $X$ .

## Fit with numpy

```
import numpy as np
from scipy import linalg
np.random.seed(seed=42) # make the example reproducible
```

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```
# Dataset
N, P = 50, 4
X = np.random.normal(size= N * P).reshape((N, P))
## Our model needs an intercept so we add a column of 1s:
X[:, 0] = 1
print(X[:5, :])

betastar = np.array([10, 1., .5, 0.1])
e = np.random.normal(size=N)
y = np.dot(X, betastar) + e

# Estimate the parameters
Xpinv = linalg.pinv2(X)
betahat = np.dot(Xpinv, y)
print("Estimated beta:\n", betahat)
```

```
[[ 1.      -0.1382643   0.64768854  1.52302986]
 [ 1.      -0.23413696  1.57921282  0.76743473]
 [ 1.      0.54256004 -0.46341769 -0.46572975]
 [ 1.     -1.91328024 -1.72491783 -0.56228753]
 [ 1.      0.31424733 -0.90802408 -1.4123037 ]]
Estimated beta:
[10.14742501  0.57938106  0.51654653  0.17862194]
```

#### 4.1.7 Linear model with statsmodels

Sources: <http://statsmodels.sourceforge.net/devel/examples/>

##### Multiple regression

##### Interface with Numpy

```
import statsmodels.api as sm

## Fit and summary:
model = sm.OLS(y, X).fit()
print(model.summary())

# prediction of new values
ypred = model.predict(X)

# residuals + prediction == true values
assert np.all(ypred + model.resid == y)
```

OLS Regression Results			
=====			
Dep. Variable:	y	R-squared:	0.363
Model:	OLS	Adj. R-squared:	0.322
Method:	Least Squares	F-statistic:	8.748
Date:	Thu, 16 May 2019	Prob (F-statistic):	0.000106

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Time:	20:15:04	Log-Likelihood:	-71.271			
No. Observations:	50	AIC:	150.5			
Df Residuals:	46	BIC:	158.2			
Df Model:	3					
Covariance Type:	nonrobust					
<hr/>						
	coef	std err	t	P> t	[0.025	0.975]
const	10.1474	0.150	67.520	0.000	9.845	10.450
x1	0.5794	0.160	3.623	0.001	0.258	0.901
x2	0.5165	0.151	3.425	0.001	0.213	0.820
x3	0.1786	0.144	1.240	0.221	-0.111	0.469
<hr/>						
Omnibus:	2.493	Durbin-Watson:	2.369			
Prob(Omnibus):	0.288	Jarque-Bera (JB):	1.544			
Skew:	0.330	Prob(JB):	0.462			
Kurtosis:	3.554	Cond. No.	1.27			
<hr/>						
Warnings:						
[1] Standard Errors assume that the covariance matrix of the errors <b>is</b> correctly → specified.						

## Interface with Pandas

Use R language syntax for data.frame. For an additive model:  $y_i = \beta^0 + x_i^1\beta^1 + x_i^2\beta^2 + \epsilon_i \equiv y \sim x_1 + x_2$ .

```
import statsmodels.formula.api as smfrmla

df = pd.DataFrame(np.column_stack([X, y]), columns=['inter', 'x1','x2', 'x3', 'y'])
print(df.columns, df.shape)
# Build a model excluding the intercept, it is implicit
model = smfrmla.ols("y~x1 + x2 + x3", df).fit()
print(model.summary())
```

Index(['inter', 'x1', 'x2', 'x3', 'y'], dtype='object')	(50, 5)					
OLS Regression Results						
Dep. Variable:	y					
Model:	OLS					
Method:	Least Squares					
Date:	Thu, 16 May 2019					
Time:	20:15:04					
No. Observations:	50					
Df Residuals:	46					
Df Model:	3					
Covariance Type:	nonrobust					
<hr/>						
	coef	std err	t	P> t	[0.025	0.975]
Intercept	10.1474	0.150	67.520	0.000	9.845	10.450
x1	0.5794	0.160	3.623	0.001	0.258	0.901

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x2	0.5165	0.151	3.425	0.001	0.213	0.820
x3	0.1786	0.144	1.240	0.221	-0.111	0.469
<hr/>						
Omnibus:	2.493	Durbin-Watson:	2.369			
Prob(Omnibus):	0.288	Jarque-Bera (JB):	1.544			
Skew:	0.330	Prob(JB):	0.462			
Kurtosis:	3.554	Cond. No.	1.27			
<hr/>						
Warnings:						
[1] Standard Errors assume that the covariance matrix of the errors <b>is</b> correctly →specified.						

## Multiple regression with categorical independent variables or factors: Analysis of covariance (ANCOVA)

Analysis of covariance (ANCOVA) is a linear model that blends ANOVA and linear regression. ANCOVA evaluates whether population means of a dependent variable (DV) are equal across levels of a categorical independent variable (IV) often called a treatment, while statistically controlling for the effects of other quantitative or continuous variables that are not of primary interest, known as covariates (CV).

```
import pandas as pd
import matplotlib.pyplot as plt
%matplotlib inline

try:
    salary = pd.read_csv("../datasets/salary_table.csv")
except:
    url = 'https://raw.githubusercontent.com/neurospin/pystatsml/master/datasets/salary_table.csv'
    salary = pd.read_csv(url)
```

### One-way AN(C)OVA

- ANOVA: one categorical independent variable, i.e. one factor.
- ANCOVA: ANOVA with some covariates.

```
import statsmodels.formula.api as smfrmla

oneway = smfrmla.ols('salary ~ management + experience', salary).fit()
print(oneway.summary())
aov = sm.stats.anova_lm(oneway, typ=2) # Type 2 ANOVA DataFrame
print(aov)
```

OLS Regression Results				
<hr/>				
Dep. Variable:	salary	R-squared:	0.865	
Model:	OLS	Adj. R-squared:	0.859	
Method:	Least Squares	F-statistic:	138.2	
Date:	Thu, 16 May 2019	Prob (F-statistic):	1.90e-19	

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Time:	20:15:04	Log-Likelihood:	-407.76			
No. Observations:	46	AIC:	821.5			
Df Residuals:	43	BIC:	827.0			
Df Model:	2					
Covariance Type:	nonrobust					
<hr/>						
	coef	std err	t	P> t	[0.025	0.975]
Intercept	1.021e+04	525.999	19.411	0.000	9149.578	1.13e+04
management[T.Y]	7145.0151	527.320	13.550	0.000	6081.572	8208.458
experience	527.1081	51.106	10.314	0.000	424.042	630.174
<hr/>						
Omnibus:	11.437	Durbin-Watson:	2.193			
Prob(Omnibus):	0.003	Jarque-Bera (JB):	11.260			
Skew:	-1.131	Prob(JB):	0.00359			
Kurtosis:	3.872	Cond. No.	22.4			
<hr/>						
Warnings:						
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.						
	sum_sq	df	F	PR(>F)		
management	5.755739e+08	1.0	183.593466	4.054116e-17		
experience	3.334992e+08	1.0	106.377768	3.349662e-13		
Residual	1.348070e+08	43.0	NaN	NaN		

## Two-way AN(C)OVA

Ancova with two categorical independent variables, i.e. two factors.

```
import statsmodels.formula.api as smfrmla

twoway = smfrmla.ols('salary ~ education + management + experience', salary).fit()
print(twoway.summary())
aov = sm.stats.anova_lm(twoway, typ=2) # Type 2 ANOVA DataFrame
print(aov)
```

OLS Regression Results						
Dep. Variable:	salary	R-squared:	0.957			
Model:	OLS	Adj. R-squared:	0.953			
Method:	Least Squares	F-statistic:	226.8			
Date:	Thu, 16 May 2019	Prob (F-statistic):	2.23e-27			
Time:	20:15:04	Log-Likelihood:	-381.63			
No. Observations:	46	AIC:	773.3			
Df Residuals:	41	BIC:	782.4			
Df Model:	4					
Covariance Type:	nonrobust					
<hr/>						
	coef	std err	t	P> t	[0.025	0.975]
Intercept	8035.5976	386.689	20.781	0.000	7254.663	8816.532
education[T.Master]	3144.0352	361.968	8.686	0.000	2413.025	3875.045

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education[T.Ph.D]	2996.2103	411.753	7.277	0.000	2164.659	3827.762
management[T.Y]	6883.5310	313.919	21.928	0.000	6249.559	7517.503
experience	546.1840	30.519	17.896	0.000	484.549	607.819
<hr/>						
Omnibus:	2.293	Durbin-Watson:	2.237			
Prob(Omnibus):	0.318	Jarque-Bera (JB):	1.362			
Skew:	-0.077	Prob(JB):	0.506			
Kurtosis:	2.171	Cond. No.	33.5			
<hr/>						
Warnings:						
[1] Standard Errors assume that the covariance matrix of the errors <b>is</b> correctly specified.						
sum_sq	df	F	PR(>F)			
education	9.152624e+07	2.0	43.351589	7.672450e-11		
management	5.075724e+08	1.0	480.825394	2.901444e-24		
experience	3.380979e+08	1.0	320.281524	5.546313e-21		
Residual	4.328072e+07	41.0	NaN	NaN		

## Comparing two nested models

oneway is nested within twoway. Comparing two nested models tells us if the additional predictors (i.e. education) of the full model significantly decrease the residuals. Such comparison can be done using an *F*-test on residuals:

```
print(twoway.compare_f_test(oneway)) # return F, pval, df
```

```
(43.35158945918107, 7.672449570495418e-11, 2.0)
```

## Factor coding

See <http://statsmodels.sourceforge.net/devel/contrasts.html>

By default Pandas use “dummy coding”. Explore:

```
print(twoway.model.data.param_names)
print(twoway.model.data.exog[:10, :])
```

```
['Intercept', 'education[T.Master]', 'education[T.Ph.D]', 'management[T.Y]', 'experience']
[[1. 0. 0. 1. 1.]
 [1. 0. 1. 0. 1.]
 [1. 0. 1. 1. 1.]
 [1. 1. 0. 0. 1.]
 [1. 0. 1. 0. 1.]
 [1. 1. 0. 1. 2.]
 [1. 1. 0. 0. 2.]
 [1. 0. 0. 0. 2.]
 [1. 0. 1. 0. 2.]
 [1. 1. 0. 0. 3.]]
```

## Contrasts and post-hoc tests

```
# t-test of the specific contribution of experience:
ttest_exp = twoway.t_test([0, 0, 0, 0, 1])
ttest_exp.pvalue, ttest_exp.tvalue
print(ttest_exp)

# Alternatively, you can specify the hypothesis tests using a string
twoway.t_test('experience')

# Post-hoc is salary of Master different salary of Ph.D?
# ie. t-test salary of Master = salary of Ph.D.
print(twoway.t_test('education[T.Master] = education[T.Ph.D]'))
```

Test for Constraints						
	coef	std err	t	P> t	[0.025	0.975]
c0	546.1840	30.519	17.896	0.000	484.549	607.819

Test for Constraints						
	coef	std err	t	P> t	[0.025	0.975]
c0	147.8249	387.659	0.381	0.705	-635.069	930.719

### 4.1.8 Multiple comparisons

```
import numpy as np
np.random.seed(seed=42) # make example reproducible

# Dataset
n_samples, n_features = 100, 1000
n_info = int(n_features/10) # number of features with information
n1, n2 = int(n_samples/2), n_samples - int(n_samples/2)
snr = .5
Y = np.random.randn(n_samples, n_features)
grp = np.array(["g1"] * n1 + ["g2"] * n2)

# Add some group effect for Pinfo features
Y[grp=="g1", :n_info] += snr

#
import scipy.stats as stats
import matplotlib.pyplot as plt
tvals, pvals = np.full(n_features, np.NAN), np.full(n_features, np.NAN)
for j in range(n_features):
    tvals[j], pvals[j] = stats.ttest_ind(Y[grp=="g1", j], Y[grp=="g2", j],
                                         equal_var=True)

fig, axis = plt.subplots(3, 1)#, sharex='col')

axis[0].plot(range(n_features), tvals, 'o')
```

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```

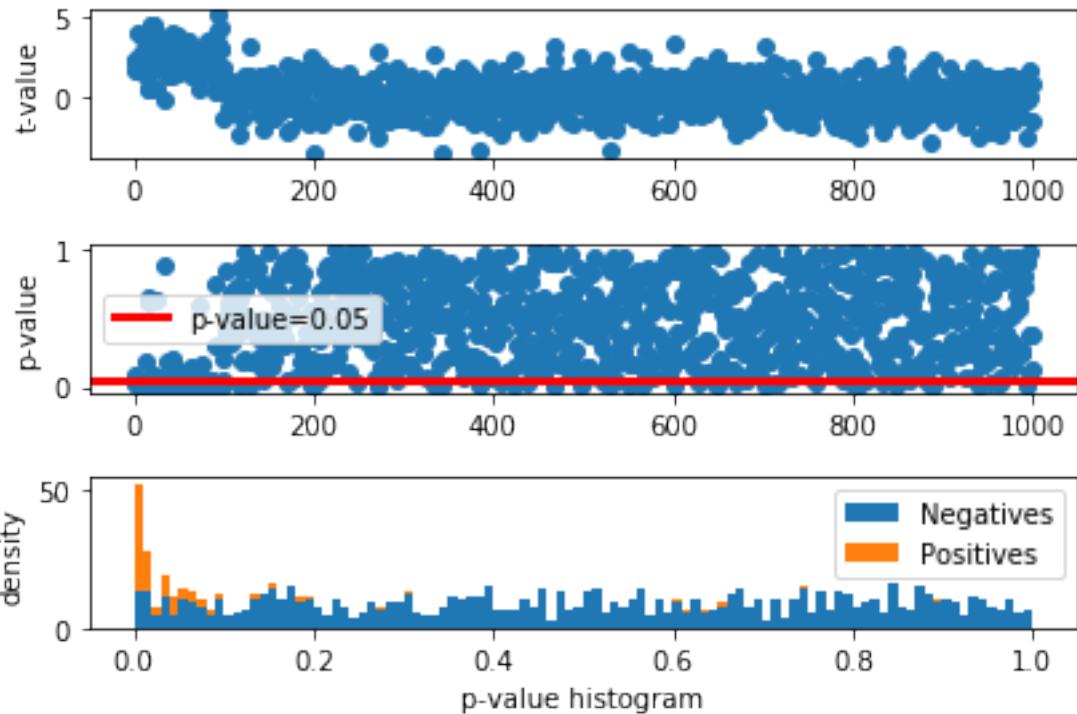
axis[0].set_ylabel("t-value")

axis[1].plot(range(n_features), pvals, 'o')
axis[1].axhline(y=0.05, color='red', linewidth=3, label="p-value=0.05")
#axis[1].axhline(y=0.05, label="toto", color='red')
axis[1].set_ylabel("p-value")
axis[1].legend()

axis[2].hist([pvals[n_info:], pvals[:n_info]], stacked=True, bins=100, label=["Negatives", "Positives"])
axis[2].set_xlabel("p-value histogram")
axis[2].set_ylabel("density")
axis[2].legend()

plt.tight_layout()

```



Note that under the null hypothesis the distribution of the  $p$ -values is uniform.

Statistical measures:

- **True Positive (TP)** equivalent to a hit. The test correctly concludes the presence of an effect.
- True Negative (TN). The test correctly concludes the absence of an effect.
- **False Positive (FP)** equivalent to a false alarm, **Type I error**. The test improperly concludes the presence of an effect. Thresholding at  $p$ -value  $< 0.05$  leads to 47 FP.
- False Negative (FN) equivalent to a miss, Type II error. The test improperly concludes the absence of an effect.

```

P, N = n_info, n_features - n_info # Positives, Negatives
TP = np.sum(pvals[:n_info] < 0.05) # True Positives

```

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```
FP = np.sum(pvals[n_info: ] < 0.05) # False Positives
print("No correction, FP: %i (expected: %.2f), TP: %i" % (FP, N * 0.05, TP))
```

```
No correction, FP: 47 (expected: 45.00), TP: 71
```

### Bonferroni correction for multiple comparisons

The Bonferroni correction is based on the idea that if an experimenter is testing  $P$  hypotheses, then one way of maintaining the familywise error rate (FWER) is to test each individual hypothesis at a statistical significance level of  $1/P$  times the desired maximum overall level.

So, if the desired significance level for the whole family of tests is  $\alpha$  (usually 0.05), then the Bonferroni correction would test each individual hypothesis at a significance level of  $\alpha/P$ . For example, if a trial is testing  $P = 8$  hypotheses with a desired  $\alpha = 0.05$ , then the Bonferroni correction would test each individual hypothesis at  $\alpha = 0.05/8 = 0.00625$ .

```
import statsmodels.sandbox.stats.multicomp as multicomp
_, pvals_fwer, _, _ = multicomp.multipletests(pvals, alpha=0.05,
                                              method='bonferroni')
TP = np.sum(pvals_fwer[:n_info] < 0.05) # True Positives
FP = np.sum(pvals_fwer[n_info:] < 0.05) # False Positives
print("FWER correction, FP: %i, TP: %i" % (FP, TP))
```

```
FWER correction, FP: 0, TP: 6
```

### The False discovery rate (FDR) correction for multiple comparisons

FDR-controlling procedures are designed to control the expected proportion of rejected null hypotheses that were incorrect rejections (“false discoveries”). FDR-controlling procedures provide less stringent control of Type I errors compared to the familywise error rate (FWER) controlling procedures (such as the Bonferroni correction), which control the probability of at least one Type I error. Thus, FDR-controlling procedures have greater power, at the cost of increased rates of Type I errors.

```
import statsmodels.sandbox.stats.multicomp as multicomp
_, pvals_fdr, _, _ = multicomp.multipletests(pvals, alpha=0.05,
                                              method='fdr_bh')
TP = np.sum(pvals_fdr[:n_info] < 0.05) # True Positives
FP = np.sum(pvals_fdr[n_info:] < 0.05) # False Positives

print("FDR correction, FP: %i, TP: %i" % (FP, TP))
```

```
FDR correction, FP: 3, TP: 20
```

### 4.1.9 Exercises

### Simple linear regression and correlation (application)

Load the dataset: birthwt Risk Factors Associated with Low Infant Birth Weight at <ftp://ftp.ceo.fr/pub/unati/people/educhesnay/pystatml/datasets/birthwt.csv>

1. Test the association of mother's age and birth weight using the correlation test and linear regression.
2. Test the association of mother's weight and birth weight using the correlation test and linear regression.
3. Produce two scatter plot of: (i) age by birth weight; (ii) mother's weight by birth weight.

Conclusion ?

### Simple linear regression (maths)

Considering the salary and the experience of the salary table.

[https://raw.githubusercontent.com/neurospin/pystatsml/master/datasets/salary\\_table.csv](https://raw.githubusercontent.com/neurospin/pystatsml/master/datasets/salary_table.csv)

Compute:

- Estimate the model parameters  $\beta, \beta_0$  using `scipy stats.linregress(x, y)`
- Compute the predicted values  $\hat{y}$

Compute:

- $\bar{y}$ : `y_mu`
- $SS_{\text{tot}}$ : `ss_tot`
- $SS_{\text{reg}}$ : `ss_reg`
- $SS_{\text{res}}$ : `ss_res`
- Check partition of variance formula based on sum of squares by using `assert np.allclose(val1, val2, atol=1e-05)`
- Compute  $R^2$  and compare it with the `r_value` above
- Compute the  $F$  score
- Compute the  $p$ -value:
- Plot the  $F(1, n)$  distribution for 100  $f$  values within  $[10, 25]$ . Draw  $P(F(1, n) > F)$ , i.e. color the surface defined by the  $x$  values larger than  $F$  below the  $F(1, n)$ .
- $P(F(1, n) > F)$  is the  $p$ -value, compute it.

### Multiple regression

Considering the simulated data used below:

1. What are the dimensions of  $\text{pinv}(X)$ ?
2. Compute the MSE between the predicted values and the true values.

```

import numpy as np
from scipy import linalg
np.random.seed(seed=42) # make the example reproducible

# Dataset
N, P = 50, 4
X = np.random.normal(size=N * P).reshape((N, P))
## Our model needs an intercept so we add a column of 1s:
X[:, 0] = 1
print(X[:5, :])

betastar = np.array([10, 1., .5, 0.1])
e = np.random.normal(size=N)
y = np.dot(X, betastar) + e

# Estimate the parameters
Xpinv = linalg.pinv2(X)
betahat = np.dot(Xpinv, y)
print("Estimated beta:\n", betahat)

```

```

[[ 1.      -0.1382643   0.64768854  1.52302986]
 [ 1.      -0.23413696  1.57921282  0.76743473]
 [ 1.      0.54256004 -0.46341769 -0.46572975]
 [ 1.     -1.91328024 -1.72491783 -0.56228753]
 [ 1.      0.31424733 -0.90802408 -1.4123037 ]]
Estimated beta:
[10.14742501  0.57938106  0.51654653  0.17862194]

```

## Two sample t-test (maths)

Given the following two sample, test whether their means are equals.

```

height = np.array([ 1.83,  1.83,  1.73,  1.82,  1.83,
                   1.73, 1.99,  1.85,  1.68,  1.87,
                   1.66,  1.71,  1.73,  1.64,  1.70,
                   1.60,  1.79,  1.73,  1.62,  1.77])
grp = np.array(["M"] * 10 + ["F"] * 10)

```

- Compute the means/std-dev per groups.
- Compute the  $t$ -value (standard two sample t-test with equal variances).
- Compute the  $p$ -value.
- The  $p$ -value is one-sided: a two-sided test would test  $P(T > tval)$  and  $P(T < -tval)$ . What would the two sided  $p$ -value be?
- Compare the two-sided  $p$ -value with the one obtained by `stats.ttest_ind` using `assert np.allclose(arr1, arr2)`.

## Two sample t-test (application)

Risk Factors Associated with Low Infant Birth Weight:

<https://raw.github.com/neurospin/pystatsml/master/datasets/birthwt.csv>

1. Explore the data
2. Recode smoke factor
3. Compute the means/std-dev per groups.
4. Plot birth weight by smoking (box plot, violin plot or histogram)
5. Test the effect of smoking on birth weight

### Two sample t-test and random permutations

Generate 100 samples following the model:

$$y = g + \varepsilon$$

Where the noise  $\varepsilon \sim N(1, 1)$  and  $g \in \{0, 1\}$  is a group indicator variable with 50 ones and 50 zeros.

- Write a function `tstat(y, g)` that compute the two samples t-test of `y` splited in two groups defined by `g`.
- Sample the t-statistic distribution under the null hypothesis using random permutations.
- Assess the p-value.

### Univariate associations (developpement)

Write a function `univar_stat(df, target, variables)` that computes the parametric statistics and *p*-values between the target variable (provided as a string) and all variables (provided as a list of string) of the pandas DataFrame `df`. The target is a quantitative variable but variables may be quantitative or qualitative. The function returns a DataFrame with four columns: `variable`, `test`, `value`, `p_value`.

Apply it to the salary dataset available at [https://raw.github.com/neurospin/pystatsml/master/datasets/salary\\_table.csv](https://raw.github.com/neurospin/pystatsml/master/datasets/salary_table.csv), with target being `S`: salaries for IT staff in a corporation.

### Multiple comparisons

This exercise has 2 goals: apply your knowledge of statistics using vectorized numpy operations. Given the dataset provided for multiple comparisons, compute the two-sample *t*-test (assuming equal variance) for each (column) feature of the `Y` array given the two groups defined by `grp` variable. You should return two vectors of size `n_features`: one for the *t*-values and one for the *p*-values.

### ANOVA

Perform an ANOVA dataset described below

- Compute between and within variances
- Compute *F*-value: `fval`
- Compare the *p*-value with the one obtained by `stats.f_oneway` using `assert np.allclose(arr1, arr2)`

```
# dataset
mu_k = np.array([1, 2, 3])      # means of 3 samples
sd_k = np.array([1, 1, 1])       # sd of 3 samples
n_k = np.array([10, 20, 30])     # sizes of 3 samples
grp = [0, 1, 2]                  # group labels
n = np.sum(n_k)
label = np.hstack([[k] * n_k[k] for k in [0, 1, 2]])

y = np.zeros(n)
for k in grp:
    y[label == k] = np.random.normal(mu_k[k], sd_k[k], n_k[k])

# Compute with scipy
fval, pval = stats.f_oneway(y[label == 0], y[label == 1], y[label == 2])
```

**Note:** Click [here](#) to download the full example code

## 4.2 Lab 1: Brain volumes study

The study provides the brain volumes of grey matter (gm), white matter (wm) and cerebrospinal fluid (csf) of 808 anatomical MRI scans. Manipulate data \_\_\_\_\_

Set the working directory within a directory called “brainvol”

Create 2 subdirectories: *data* that will contain downloaded data and *reports* for results of the analysis.

```
import os
import os.path
import pandas as pd
import tempfile
import urllib.request

WD = os.path.join(tempfile.gettempdir(), "brainvol")
os.makedirs(WD, exist_ok=True)
#os.chdir(WD)

# use cookiecutter file organization
# https://drivendata.github.io/cookiecutter-data-science/
os.makedirs(os.path.join(WD, "data"), exist_ok=True)
#os.makedirs("reports", exist_ok=True)
```

### Fetch data

- Demographic data *demo.csv* (columns: *participant\_id*, *site*, *group*, *age*, *sex*) and tissue volume data: *group* is Control or Patient. *site* is the recruiting site.
- Gray matter volume *gm.csv* (columns: *participant\_id*, *session*, *gm\_vol*)
- White matter volume *wm.csv* (columns: *participant\_id*, *session*, *wm\_vol*)
- Cerebrospinal Fluid *csf.csv* (columns: *participant\_id*, *session*, *csf\_vol*)

```
base_url = 'https://raw.github.com/neurospin/pystatsml/master/datasets/brain_volumes/%s'
data = dict()
for file in ["demo.csv", "gm.csv", "wm.csv", "csf.csv"]:
    urllib.request.urlretrieve(base_url % file, os.path.join(WD, "data", file))

demo = pd.read_csv(os.path.join(WD, "data", "demo.csv"))
gm = pd.read_csv(os.path.join(WD, "data", "gm.csv"))
wm = pd.read_csv(os.path.join(WD, "data", "wm.csv"))
csf = pd.read_csv(os.path.join(WD, "data", "csf.csv"))

print("tables can be merge using shared columns")
print(gm.head())
```

Out:

```
tables can be merge using shared columns
  participant_id session      gm_vol
0      sub-S1-0002  ses-01  0.672506
1      sub-S1-0002  ses-02  0.678772
2      sub-S1-0002  ses-03  0.665592
3      sub-S1-0004  ses-01  0.890714
4      sub-S1-0004  ses-02  0.881127
```

**Merge tables** according to *participant\_id*

```
brain_vol = pd.merge(pd.merge(demo, gm), wm), csf)
assert brain_vol.shape == (808, 9)
```

**Drop rows with missing values**

```
brain_vol = brain_vol.dropna()
assert brain_vol.shape == (766, 9)
```

**Compute Total Intra-cranial volume**  $tiv\_vol = gm\_vol + csf\_vol + wm\_vol$ .

```
brain_vol["tiv_vol"] = brain_vol["gm_vol"] + brain_vol["wm_vol"] + brain_vol["csf_vol"]
```

**Compute tissue fractions**  $gm_f = gm\_vol / tiv\_vol$ ,  $wm_f = wm\_vol / tiv\_vol$ .

```
brain_vol["gm_f"] = brain_vol["gm_vol"] / brain_vol["tiv_vol"]
brain_vol["wm_f"] = brain_vol["wm_vol"] / brain_vol["tiv_vol"]
```

**Save in a excel file** *brain\_vol.xlsx*

```
brain_vol.to_excel(os.path.join(WD, "data", "brain_vol.xlsx"),
                  sheet_name='data', index=False)
```

### 4.2.1 Descriptive Statistics

Load excel file *brain\_vol.xlsx*

```
import os
import pandas as pd
import seaborn as sns
```

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```
import statsmodels.formula.api as smfrmla
import statsmodels.api as sm

brain_vol = pd.read_excel(os.path.join(WD, "data", "brain_vol.xlsx"),
                         sheet_name='data')
# Round float at 2 decimals when printing
pd.options.display.float_format = '{:.2f}'.format
```

**Descriptive statistics** Most of participants have several MRI sessions (column *session*) Select on rows from session one “ses-01”

```
brain_vol1 = brain_vol[brain_vol.session == "ses-01"]
# Check that there are no duplicates
assert len(brain_vol1.participant_id.unique()) == len(brain_vol1.participant_id)
```

Global descriptives statistics of numerical variables

```
desc_glob_num = brain_vol1.describe()
print(desc_glob_num)
```

Out:

	age	gm_vol	wm_vol	csf_vol	tiv_vol	gm_f	wm_f
count	244.00	244.00	244.00	244.00	244.00	244.00	244.00
mean	34.54	0.71	0.44	0.31	1.46	0.49	0.30
std	12.09	0.08	0.07	0.08	0.17	0.04	0.03
min	18.00	0.48	0.05	0.12	0.83	0.37	0.06
25%	25.00	0.66	0.40	0.25	1.34	0.46	0.28
50%	31.00	0.70	0.43	0.30	1.45	0.49	0.30
75%	44.00	0.77	0.48	0.37	1.57	0.52	0.31
max	61.00	1.03	0.62	0.63	2.06	0.60	0.36

Global Descriptive statistics of categorical variable

```
desc_glob_cat = brain_vol1[["site", "group", "sex"]].describe(include='all')
print(desc_glob_cat)

print("Get count by level")
desc_glob_cat = pd.DataFrame({col: brain_vol1[col].value_counts().to_dict()
                               for col in ["site", "group", "sex"]})
print(desc_glob_cat)
```

Out:

	site	group	sex
count	244	244	244
unique	7	2	2
top	S7	Patient	M
freq	65	157	155

Get count by level

	site	group	sex
Control	nan	87.00	nan
F	nan	nan	89.00
M	nan	nan	155.00
Patient	nan	157.00	nan

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S1	13.00	nan	nan
S3	29.00	nan	nan
S4	15.00	nan	nan
S5	62.00	nan	nan
S6	1.00	nan	nan
S7	65.00	nan	nan
S8	59.00	nan	nan

Remove the single participant from site 6

```
brain_vol = brain_vol[brain_vol.site != "S6"]
brain_vol1 = brain_vol[brain_vol.session == "ses-01"]
desc_glob_cat = pd.DataFrame({col: brain_vol1[col].value_counts().to_dict()
                               for col in ["site", "group", "sex"]})
print(desc_glob_cat)
```

Out:

site	group	sex	
Control	nan	86.00	nan
F	nan	nan	88.00
M	nan	nan	155.00
Patient	nan	157.00	nan
S1	13.00	nan	nan
S3	29.00	nan	nan
S4	15.00	nan	nan
S5	62.00	nan	nan
S7	65.00	nan	nan
S8	59.00	nan	nan

Descriptives statistics of numerical variables per clinical status

```
desc_group_num = brain_vol1[["group", 'gm_vol']].groupby("group").describe()
print(desc_group_num)
```

Out:

gm_vol	count	mean	std	min	25%	50%	75%	max
<b>group</b>								
Control	86.00	0.72	0.09	0.48	0.66	0.71	0.78	1.03
Patient	157.00	0.70	0.08	0.53	0.65	0.70	0.76	0.90

## 4.2.2 Statistics

Objectives:

1. Site effect of gray matter atrophy
2. Test the association between the age and gray matter atrophy in the control and patient population independently.
3. Test for differences of atrophy between the patients and the controls
4. Test for interaction between age and clinical status, ie: is the brain atrophy process in patient population faster than in the control population.

5. The effect of the medication in the patient population.

```
import statsmodels.api as sm
import statsmodels.formula.api as smf
import scipy.stats
import seaborn as sns
```

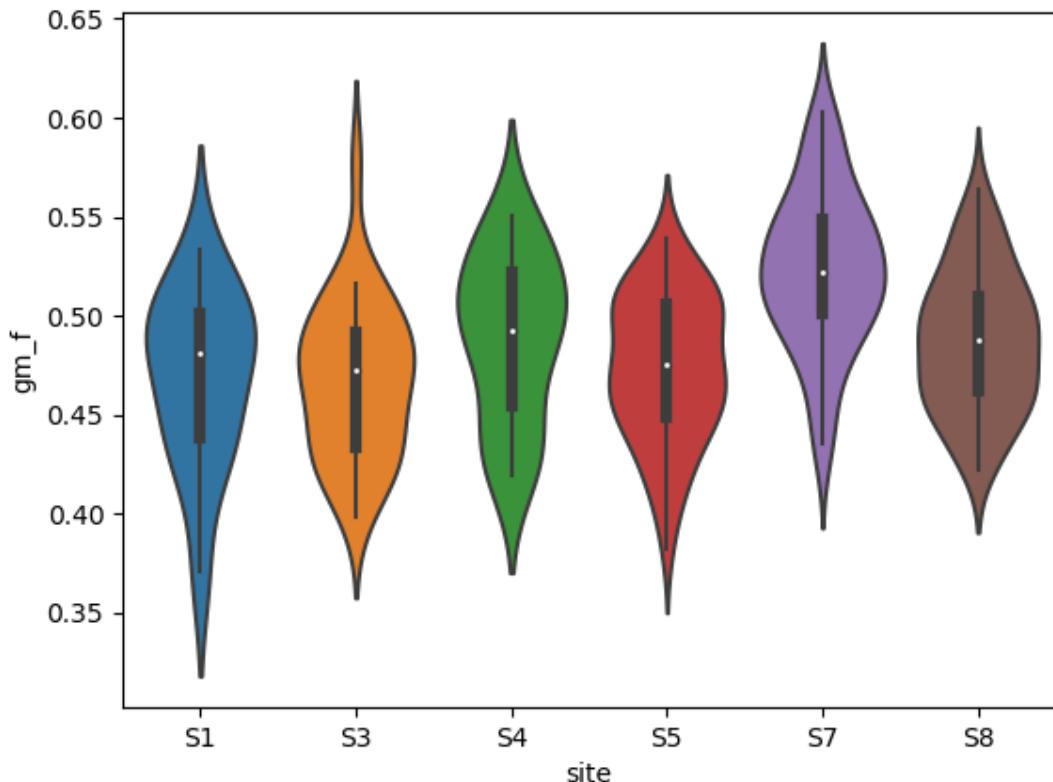
### 1 Site effect on Grey Matter atrophy

The model is Oneway Anova  $gm\_f \sim site$  The ANOVA test has important assumptions that must be satisfied in order for the associated p-value to be valid.

- The samples are independent.
- Each sample is from a normally distributed population.
- The population standard deviations of the groups are all equal. This property is known as homoscedasticity.

Plot

```
sns.violinplot("site", "gm_f", data=brain_vol1)
```



Stats with scipy

```
fstat, pval = scipy.stats.f_oneway(*[brain_vol1.gm_f[brain_vol1.site == s]
                                         for s in brain_vol1.site.unique()])
print("Oneway Anova gm_f ~ site F=% .2f, p-value=%E" % (fstat, pval))
```

Out:

```
Oneway Anova gm_f ~ site F=14.82, p-value=1.188136E-12
```

Stats with statsmodels

```
anova = smfrmla.ols("gm_f ~ site", data=brain_vol1).fit()  
# print(anova.summary())  
print("Site explains %.2f%% of the grey matter fraction variance" %  
      (anova.rsquared * 100))  
  
print(sm.stats.anova_lm(anova, typ=2))
```

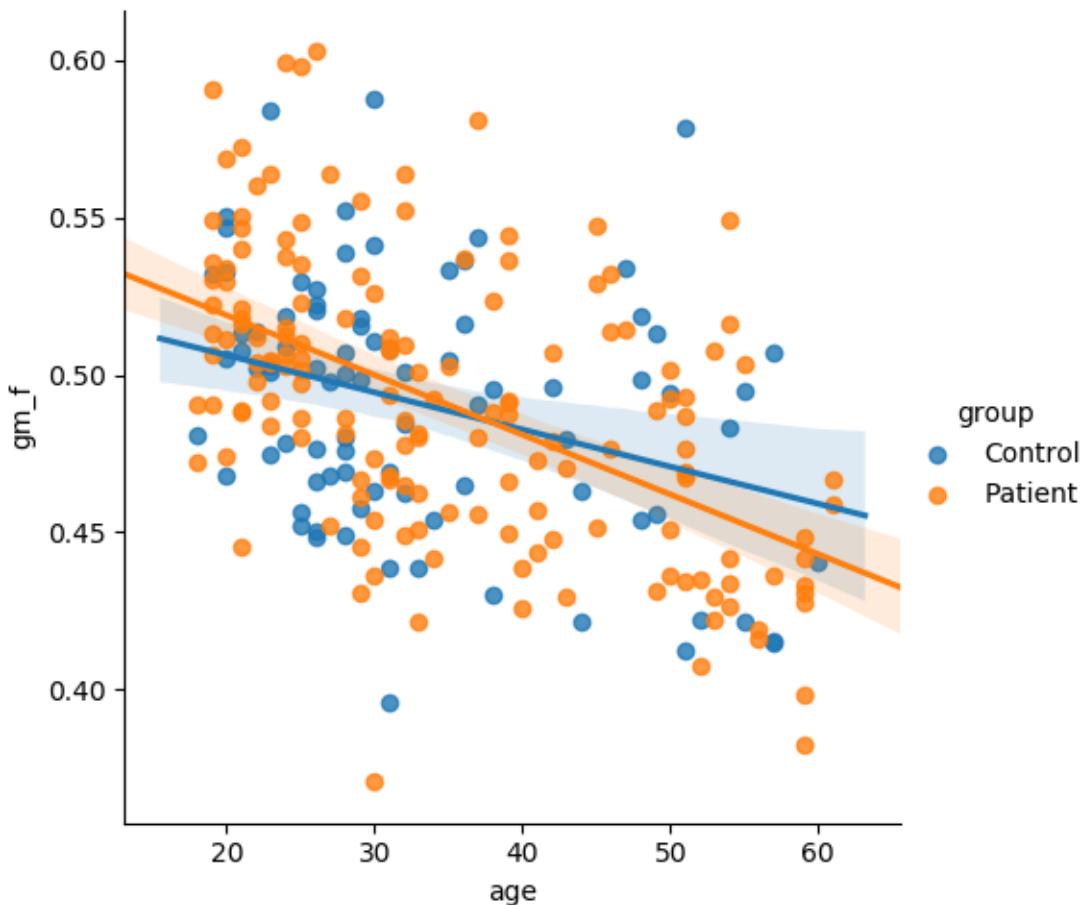
Out:

```
Site explains 23.82% of the grey matter fraction variance  
      sum_sq     df      F   PR(>F)  
site        0.11  5.00 14.82    0.00  
Residual    0.35 237.00    nan    nan
```

**2. Test the association between the age and gray matter atrophy in the control and patient population independently.**

Plot

```
sns.lmplot("age", "gm_f", hue="group", data=brain_vol1)  
  
brain_vol1_ctl = brain_vol1[brain_vol1.group == "Control"]  
brain_vol1_pat = brain_vol1[brain_vol1.group == "Patient"]
```



Stats with scipy

```
print("--- In control population ---")
beta, beta0, r_value, p_value, std_err = \
    scipy.stats.linregress(x=brain_vol1_ctl.age, y=brain_vol1_ctl.gm_f)

print("gm_f = %f * age + %f" % (beta, beta0))
print("Corr: %f, r-squared: %f, p-value: %f, std_err: %f" \
    % (r_value, r_value**2, p_value, std_err))

print("--- In patient population ---")
beta, beta0, r_value, p_value, std_err = \
    scipy.stats.linregress(x=brain_vol1_pat.age, y=brain_vol1_pat.gm_f)

print("gm_f = %f * age + %f" % (beta, beta0))
print("Corr: %f, r-squared: %f, p-value: %f, std_err: %f" \
    % (r_value, r_value**2, p_value, std_err))

print("Decrease seems faster in patient than in control population")
```

Out:

```
--- In control population ---
gm_f = -0.001181 * age + 0.529829
Corr: -0.325122, r-squared: 0.105704, p-value: 0.002255, std_err: 0.000375
--- In patient population ---
```

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```
gm_f = -0.001899 * age + 0.556886
Corr: -0.528765, r-squared: 0.279592, p-value: 0.000000, std_err: 0.000245
Decrease seems faster in patient than in control population
```

### Stats with statsmodels

```
print("--- In control population ---")
lr = smfrmla.ols("gm_f ~ age", data=brain_vol1_ctl).fit()
print(lr.summary())
print("Age explains %.2f%% of the grey matter fraction variance" %
      (lr.rsquared * 100))

print("--- In patient population ---")
lr = smfrmla.ols("gm_f ~ age", data=brain_vol1_pat).fit()
print(lr.summary())
print("Age explains %.2f%% of the grey matter fraction variance" %
      (lr.rsquared * 100))
```

Out:

```
--- In control population ---
OLS Regression Results
=====
Dep. Variable: gm_f R-squared: 0.106
Model: OLS Adj. R-squared: 0.095
Method: Least Squares F-statistic: 9.929
Date: jeu., 16 mai 2019 Prob (F-statistic): 0.00226
Time: 20:18:24 Log-Likelihood: 159.34
No. Observations: 86 AIC: -314.7
Df Residuals: 84 BIC: -309.8
Df Model: 1
Covariance Type: nonrobust
=====
            coef    std err        t     P>|t|    [0.025    0.975]
-----
Intercept  0.5298    0.013   40.350    0.000    0.504    0.556
age        -0.0012    0.000   -3.151    0.002   -0.002   -0.000
-----
Omnibus: 0.946 Durbin-Watson: 1.628
Prob(Omnibus): 0.623 Jarque-Bera (JB): 0.782
Skew: 0.233 Prob(JB): 0.676
Kurtosis: 2.962 Cond. No. 111.
```

### Warnings:

[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.

Age explains 10.57% of the grey matter fraction variance

--- In patient population ---

```
OLS Regression Results
=====
Dep. Variable: gm_f R-squared: 0.280
Model: OLS Adj. R-squared: 0.275
Method: Least Squares F-statistic: 60.16
Date: jeu., 16 mai 2019 Prob (F-statistic): 1.09e-12
Time: 20:18:24 Log-Likelihood: 289.38
```

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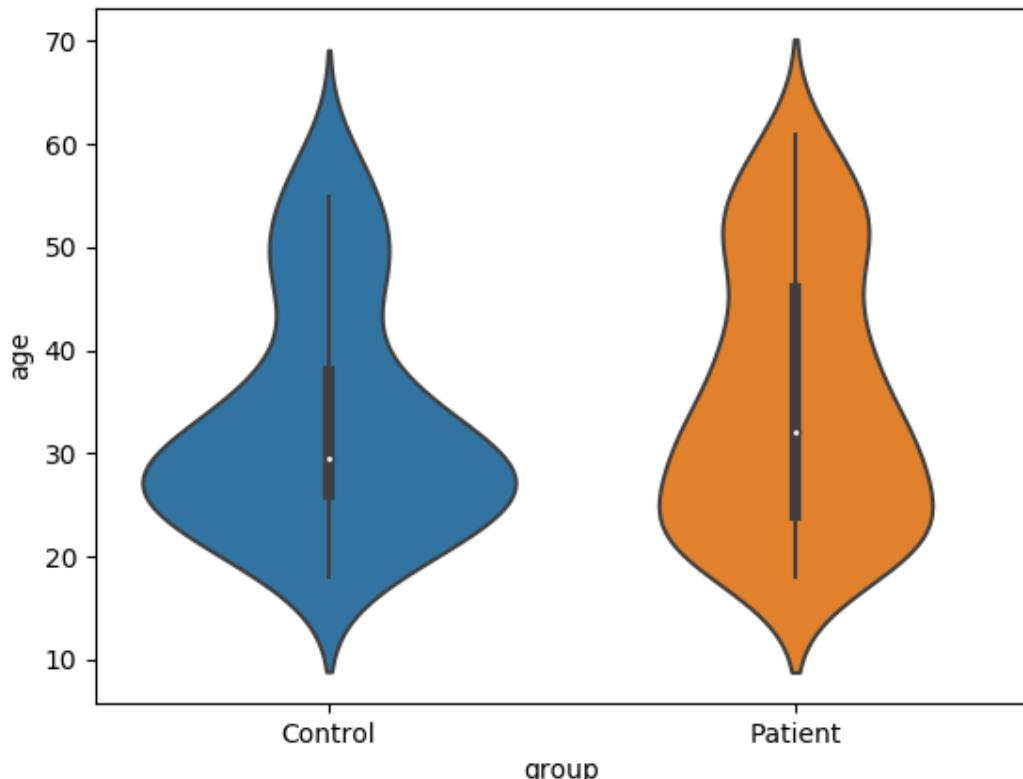
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No. Observations:	157	AIC:	-574.8			
Df Residuals:	155	BIC:	-568.7			
Df Model:	1					
Covariance Type:	nonrobust					
<hr/>						
	coef	std err	t	P> t	[0.025	0.975]
Intercept	0.5569	0.009	60.817	0.000	0.539	0.575
age	-0.0019	0.000	-7.756	0.000	-0.002	-0.001
<hr/>						
Omnibus:	2.310	Durbin-Watson:	1.325			
Prob(Omnibus):	0.315	Jarque-Bera (JB):	1.854			
Skew:	0.230	Prob(JB):	0.396			
Kurtosis:	3.268	Cond. No.	111.			
<hr/>						
Warnings:						
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.						
Age explains 27.96% of the grey matter fraction variance						

Before testing for differences of atrophy between the patients and the controls **Preliminary tests for age x group effect** (patients would be older or younger than Controls)

Plot

```
sns.violinplot("group", "age", data=brain_vol1)
```



### Stats with scipy

```
print(scipy.stats.ttest_ind(brain_vol1_ctl.age, brain_vol1_pat.age))
```

Out:

```
Ttest_indResult(statistic=-1.215557697674162, pvalue=0.225343592508479)
```

### Stats with statsmodels

```
print(smsfrmla.ols("age ~ group", data=brain_vol1).fit().summary())
print("No significant difference in age between patients and controls")
```

Out:

```
OLS Regression Results
=====
Dep. Variable: age R-squared: 0.006
Model: OLS Adj. R-squared: 0.002
Method: Least Squares F-statistic: 1.478
Date: jeu., 16 mai 2019 Prob (F-statistic): 0.225
Time: 20:18:24 Log-Likelihood: -949.69
No. Observations: 243 AIC: 1903.
Df Residuals: 241 BIC: 1910.
Df Model: 1
Covariance Type: nonrobust
=====
```

	coef	std err	t	P> t	[0.025	0.975]
Intercept	33.2558	1.305	25.484	0.000	30.685	35.826
group[T.Patient]	1.9735	1.624	1.216	0.225	-1.225	5.172

```
=====
Omnibus: 35.711 Durbin-Watson: 2.096
Prob(Omnibus): 0.000 Jarque-Bera (JB): 20.726
Skew: 0.569 Prob(JB): 3.16e-05
Kurtosis: 2.133 Cond. No. 3.12
=====
```

### Warnings:

[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.

No significant difference in age between patients and controls

### Preliminary tests for sex x group (more/less males in patients than in Controls)

```
crosstab = pd.crosstab(brain_vol1.sex, brain_vol1.group)
print("Observed contingency table")
print(crosstab)

chi2, pval, dof, expected = scipy.stats.chi2_contingency(crosstab)

print("Chi2 = %f, pval = %f" % (chi2, pval))
print("Expected contingency table under the null hypothesis")
print(expected)
print("No significant difference in sex between patients and controls")
```

Out:

```
Observed contingency table
group Control Patient
sex
F          33      55
M          53     102
Chi2 = 0.143253, pval = 0.705068
Expected contingency table under the null hypothesis
[[ 31.14403292  56.85596708]
 [ 54.85596708 100.14403292]]
No significant difference in sex between patients and controls
```

### 3. Test for differences of atrophy between the patients and the controls

```
print(sm.stats.anova_lm(smfrmla.ols("gm_f ~ group", data=brain_vol1).fit(), typ=2))
print("No significant difference in age between patients and controls")
```

Out:

sum_sq	df	F	PR(>F)
group	0.00	1.00	0.01
Residual	0.46	241.00	nan
No significant difference in age between patients and controls			

This model is simplistic we should adjust for age and site

```
print(sm.stats.anova_lm(smfrmla.ols(
    "gm_f ~ group + age + site", data=brain_vol1).fit(), typ=2))
print("No significant difference in age between patients and controls")
```

Out:

sum_sq	df	F	PR(>F)
group	0.00	1.00	1.82
site	0.11	5.00	19.79
age	0.09	1.00	86.86
Residual	0.25	235.00	nan
No significant difference in age between patients and controls			

### 4. Test for interaction between age and clinical status, ie: is the brain atrophy process in patient population faster than in the control population.

```
ancova = smfrmla.ols("gm_f ~ group:age + age + site", data=brain_vol1).fit()
print(sm.stats.anova_lm(ancova, typ=2))

print("= Parameters =")
print(ancova.params)

print("%.3f%% of grey matter loss per year (almost %.1f%% per decade)" %\
      (ancova.params.age * 100, ancova.params.age * 100 * 10))

print("grey matter loss in patients is accelerated by %.3f%% per decade" %
      (ancova.params['group[T.Patient]:age'] * 100 * 10))
```

Out:

```

sum_sq     df      F   PR(>F)
site        0.11  5.00 20.28    0.00
age         0.10  1.00 89.37    0.00
group:age   0.00  1.00  3.28    0.07
Residual    0.25 235.00    nan    nan
= Parameters =
Intercept          0.52
site[T.S3]          0.01
site[T.S4]          0.03
site[T.S5]          0.01
site[T.S7]          0.06
site[T.S8]          0.02
age                 -0.00
group[T.Patient]:age -0.00
dtype: float64
-0.148% of grey matter loss per year (almost -1.5% per decade)
grey matter loss in patients is accelerated by -0.232% per decade

```

Total running time of the script: ( 0 minutes 5.184 seconds)

## 4.3 Multivariate statistics

Multivariate statistics includes all statistical techniques for analyzing samples made of two or more variables. The data set (a  $N \times P$  matrix  $\mathbf{X}$ ) is a collection of  $N$  independent samples column **vectors**  $[\mathbf{x}_1, \dots, \mathbf{x}_i, \dots, \mathbf{x}_N]$  of length  $P$

$$\mathbf{X} = \begin{bmatrix} -\mathbf{x}_1^T - \\ \vdots \\ -\mathbf{x}_i^T - \\ \vdots \\ -\mathbf{x}_P^T - \end{bmatrix} = \begin{bmatrix} x_{11} & \cdots & x_{1j} & \cdots & x_{1P} \\ \vdots & & \vdots & & \vdots \\ x_{i1} & \cdots & x_{ij} & \cdots & x_{iP} \\ \vdots & & \vdots & & \vdots \\ x_{N1} & \cdots & x_{Nj} & \cdots & x_{NP} \end{bmatrix} = \begin{bmatrix} x_{11} & \cdots & x_{1P} \\ \vdots & & \vdots \\ \mathbf{x} \\ \vdots & & \vdots \\ x_{N1} & \cdots & x_{NP} \end{bmatrix}_{N \times P}.$$

### 4.3.1 Linear Algebra

#### Euclidean norm and distance

The Euclidean norm of a vector  $\mathbf{a} \in \mathbb{R}^P$  is denoted

$$\|\mathbf{a}\|_2 = \sqrt{\sum_i^P a_i^2}$$

The Euclidean distance between two vectors  $\mathbf{a}, \mathbf{b} \in \mathbb{R}^P$  is

$$\|\mathbf{a} - \mathbf{b}\|_2 = \sqrt{\sum_i^P (a_i - b_i)^2}$$

#### Dot product and projection

Source: [Wikipedia](#)

## Algebraic definition

The dot product, denoted “.” of two  $P$ -dimensional vectors  $\mathbf{a} = [a_1, a_2, \dots, a_P]$  and  $\mathbf{b} = [b_1, b_2, \dots, b_P]$  is defined as

$$\mathbf{a} \cdot \mathbf{b} = \mathbf{a}^T \mathbf{b} = \sum_i a_i b_i = [a_1 \ \dots \ \mathbf{a}^T \ \dots \ a_P] \begin{bmatrix} b_1 \\ \vdots \\ \mathbf{b} \\ \vdots \\ b_P \end{bmatrix}.$$

The Euclidean norm of a vector can be computed using the dot product, as

$$\|\mathbf{a}\|_2 = \sqrt{\mathbf{a} \cdot \mathbf{a}}.$$

## Geometric definition: projection

In Euclidean space, a Euclidean vector is a geometrical object that possesses both a magnitude and a direction. A vector can be pictured as an arrow. Its magnitude is its length, and its direction is the direction that the arrow points. The magnitude of a vector  $\mathbf{a}$  is denoted by  $\|\mathbf{a}\|_2$ . The dot product of two Euclidean vectors  $\mathbf{a}$  and  $\mathbf{b}$  is defined by

$$\mathbf{a} \cdot \mathbf{b} = \|\mathbf{a}\|_2 \|\mathbf{b}\|_2 \cos \theta,$$

where  $\theta$  is the angle between  $\mathbf{a}$  and  $\mathbf{b}$ .

In particular, if  $\mathbf{a}$  and  $\mathbf{b}$  are orthogonal, then the angle between them is  $90^\circ$  and

$$\mathbf{a} \cdot \mathbf{b} = 0.$$

At the other extreme, if they are codirectional, then the angle between them is  $0^\circ$  and

$$\mathbf{a} \cdot \mathbf{b} = \|\mathbf{a}\|_2 \|\mathbf{b}\|_2$$

This implies that the dot product of a vector  $\mathbf{a}$  by itself is

$$\mathbf{a} \cdot \mathbf{a} = \|\mathbf{a}\|_2^2.$$

The scalar projection (or scalar component) of a Euclidean vector  $\mathbf{a}$  in the direction of a Euclidean vector  $\mathbf{b}$  is given by

$$a_b = \|\mathbf{a}\|_2 \cos \theta,$$

where  $\theta$  is the angle between  $\mathbf{a}$  and  $\mathbf{b}$ .

In terms of the geometric definition of the dot product, this can be rewritten

$$a_b = \frac{\mathbf{a} \cdot \mathbf{b}}{\|\mathbf{b}\|_2},$$

```
import numpy as np
np.random.seed(42)

a = np.random.randn(10)
b = np.random.randn(10)

np.dot(a, b)
```

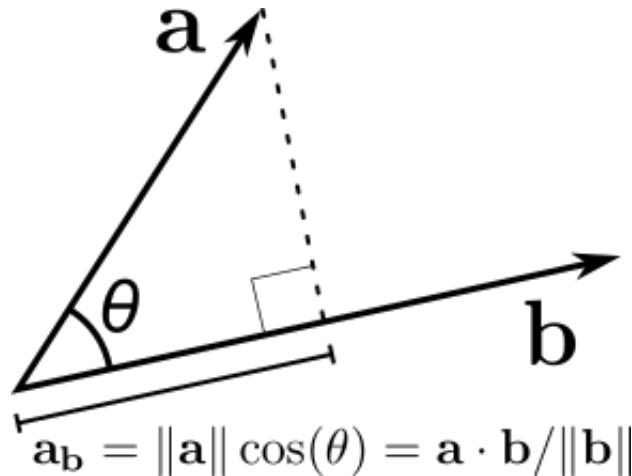


Fig. 5: Projection.

-4. 085788532659924

### 4.3.2 Mean vector

The mean ( $P \times 1$ ) column-vector  $\mu$  whose estimator is

$$\bar{\mathbf{x}} = \frac{1}{N} \sum_{i=1}^N \mathbf{x}_i = \frac{1}{N} \sum_{i=1}^N \begin{bmatrix} x_{i1} \\ \vdots \\ x_{ij} \\ \vdots \\ x_{iP} \end{bmatrix} = \begin{bmatrix} \bar{x}_1 \\ \vdots \\ \bar{x}_j \\ \vdots \\ \bar{x}_P \end{bmatrix}.$$

### 4.3.3 Covariance matrix

- The covariance matrix  $\Sigma_{\mathbf{X}\mathbf{X}}$  is a **symmetric** positive semi-definite matrix whose element in the  $j, k$  position is the covariance between the  $j^{th}$  and  $k^{th}$  elements of a random vector i.e. the  $j^{th}$  and  $k^{th}$  columns of  $\mathbf{X}$ .
- The covariance matrix generalizes the notion of covariance to multiple dimensions.
- The covariance matrix describe the shape of the sample distribution around the mean assuming an elliptical distribution:

$$\Sigma_{\mathbf{X}\mathbf{X}} = E(\mathbf{X} - E(\mathbf{X}))^T E(\mathbf{X} - E(\mathbf{X})),$$

whose estimator  $S_{\mathbf{X}\mathbf{X}}$  is a  $P \times P$  matrix given by

$$S_{\mathbf{X}\mathbf{X}} = \frac{1}{N-1} (\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}^T)^T (\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}^T).$$

If we assume that  $\mathbf{X}$  is centered, i.e.  $\mathbf{X}$  is replaced by  $\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}^T$  then the estimator is

$$S_{\mathbf{X}\mathbf{X}} = \frac{1}{N-1} \mathbf{X}^T \mathbf{X} = \frac{1}{N-1} \begin{bmatrix} x_{11} & \cdots & x_{N1} \\ x_{1j} & \cdots & x_{Nj} \\ \vdots & & \vdots \\ x_{1P} & \cdots & x_{NP} \end{bmatrix} \begin{bmatrix} x_{11} & \cdots & x_{1k} & x_{1P} \\ \vdots & & \vdots & \vdots \\ x_{N1} & \cdots & x_{Nk} & x_{NP} \end{bmatrix} = \begin{bmatrix} s_1 & \cdots & s_{1k} & s_{1P} \\ & \ddots & & \vdots \\ & & s_{jk} & \vdots \\ & & s_k & s_{kP} \\ & & & s_P \end{bmatrix},$$

where

$$s_{jk} = s_{kj} = \frac{1}{N-1} \mathbf{x_j}^T \mathbf{x_k} = \frac{1}{N-1} \sum_{i=1}^N x_{ij} x_{ik}$$

is an estimator of the covariance between the  $j^{th}$  and  $k^{th}$  variables.

```
## Avoid warnings and force inline plot
%matplotlib inline
import warnings
warnings.filterwarnings("ignore")
##
import numpy as np
import scipy
import matplotlib.pyplot as plt
import seaborn as sns
import pystatsml.plot_utils
import seaborn as sns # nice color

np.random.seed(42)
colors = sns.color_palette()

n_samples, n_features = 100, 2

mean, Cov, X = [None] * 4, [None] * 4, [None] * 4
mean[0] = np.array([-2.5, 2.5])
Cov[0] = np.array([[1, 0],
                  [0, 1]])

mean[1] = np.array([2.5, 2.5])
Cov[1] = np.array([[1, .5],
                  [.5, 1]])

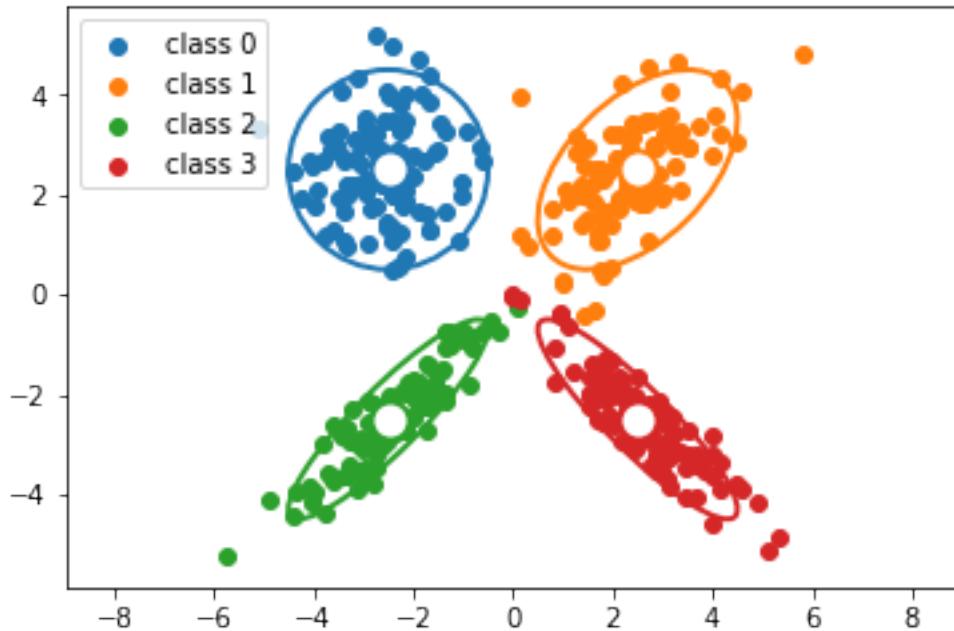
mean[2] = np.array([-2.5, -2.5])
Cov[2] = np.array([[1, .9],
                  [.9, 1]])

mean[3] = np.array([2.5, -2.5])
Cov[3] = np.array([[1, -.9],
                  [-.9, 1]])

# Generate dataset
for i in range(len(mean)):
    X[i] = np.random.multivariate_normal(mean[i], Cov[i], n_samples)

# Plot
for i in range(len(mean)):
    # Points
    plt.scatter(X[i][:, 0], X[i][:, 1], color=colors[i], label="class %i" % i)
    # Means
    plt.scatter(mean[i][0], mean[i][1], marker="o", s=200, facecolor='w',
                edgecolors=colors[i], linewidth=2)
    # Ellipses representing the covariance matrices
    pystatsml.plot_utils.plot_cov_ellipse(Cov[i], pos=mean[i], facecolor='none',
                                           linewidth=2, edgecolor=colors[i])

plt.axis('equal')
_ = plt.legend(loc='upper left')
```



#### 4.3.4 Correlation matrix

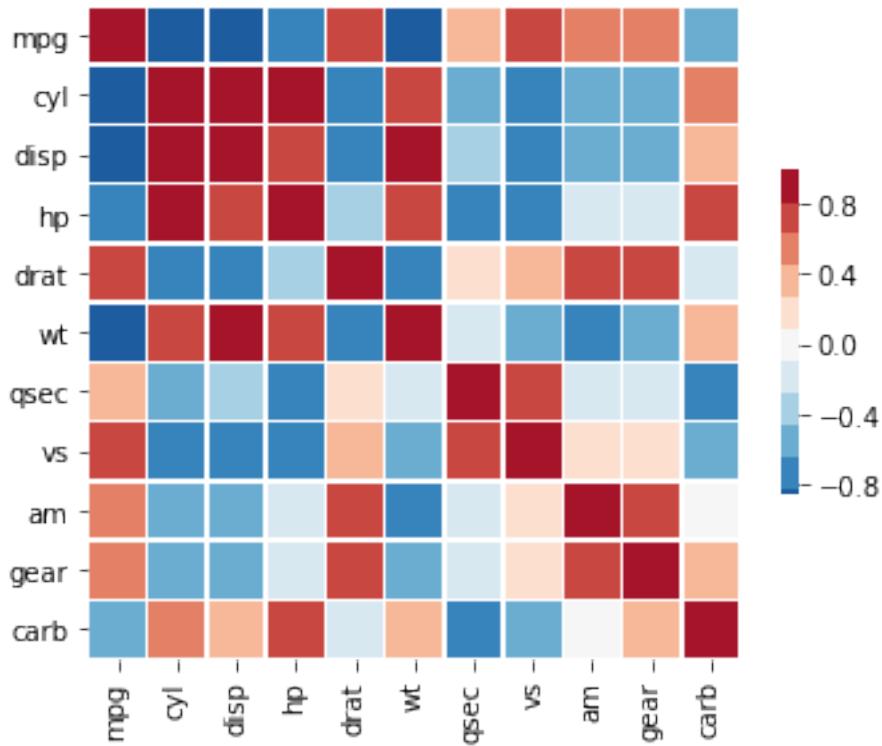
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns

url = 'https://python-graph-gallery.com/wp-content/uploads/mtcars.csv'
df = pd.read_csv(url)

# Compute the correlation matrix
corr = df.corr()

# Generate a mask for the upper triangle
mask = np.zeros_like(corr, dtype=np.bool)
mask[np.triu_indices_from(mask)] = True

f, ax = plt.subplots(figsize=(5.5, 4.5))
cmap = sns.color_palette("RdBu_r", 11)
# Draw the heatmap with the mask and correct aspect ratio
_ = sns.heatmap(corr, mask=mask, cmap=cmap, vmax=1, center=0,
                 square=True, linewidths=.5, cbar_kws={"shrink": .5})
```



Re-order correlation matrix using AgglomerativeClustering

```
# convert correlation to distances
d = 2 * (1 - np.abs(corr))

from sklearn.cluster import AgglomerativeClustering
clustering = AgglomerativeClustering(n_clusters=3, linkage='single', affinity="precomputed")
clustering.fit(d)
lab=0

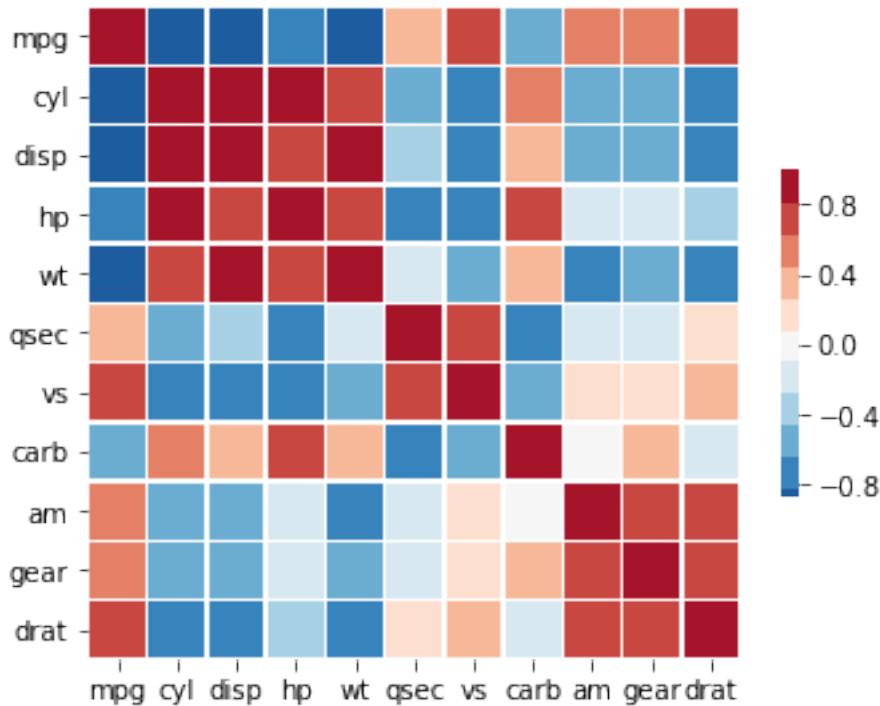
clusters = [list(corr.columns[clustering.labels_==lab]) for lab in set(clustering.labels_)]
print(clusters)

reordered = np.concatenate(clusters)

R = corr.loc(reordered, reordered)

f, ax = plt.subplots(figsize=(5.5, 4.5))
# Draw the heatmap with the mask and correct aspect ratio
sns.heatmap(R, mask=None, cmap=cmap, vmax=1, center=0,
            square=True, linewidths=.5, cbar_kws={"shrink": .5})
```

```
[['mpg', 'cyl', 'disp', 'hp', 'wt', 'qsec', 'vs', 'carb'], ['am', 'gear'], ['drat']]
```



### 4.3.5 Precision matrix

In statistics, precision is the reciprocal of the variance, and the precision matrix is the matrix inverse of the covariance matrix.

It is related to **partial correlations** that measures the degree of association between two variables, while controlling the effect of other variables.

```
import numpy as np

Cov = np.array([[1.0, 0.9, 0.9, 0.0, 0.0, 0.0],
                [0.9, 1.0, 0.9, 0.0, 0.0, 0.0],
                [0.9, 0.9, 1.0, 0.0, 0.0, 0.0],
                [0.0, 0.0, 0.0, 1.0, 0.9, 0.0],
                [0.0, 0.0, 0.0, 0.9, 1.0, 0.0],
                [0.0, 0.0, 0.0, 0.0, 0.0, 1.0]])

print("# Precision matrix:")
Prec = np.linalg.inv(Cov)
print(Prec.round(2))

print("# Partial correlations:")
Pcor = np.zeros(Prec.shape)
Pcor[:, :] = np.NaN

for i, j in zip(*np.triu_indices_from(Prec, 1)):
    Pcor[i, j] = - Prec[i, j] / np.sqrt(Prec[i, i] * Prec[j, j])

print(Pcor.round(2))
```

```
# Precision matrix:
[[ 6.79 -3.21 -3.21  0.    0.    0.   ]
 [-3.21  6.79 -3.21  0.    0.    0.   ]
 [-3.21 -3.21  6.79  0.    0.    0.   ]
 [ 0.    -0.    -0.    5.26 -4.74 -0.   ]
 [ 0.     0.    -4.74  5.26  0.    0.   ]
 [ 0.     0.    0.    0.    0.    1.   ]]

# Partial correlations:
[[ nan  0.47  0.47 -0.   -0.   -0.   ]
 [ nan  nan  0.47 -0.   -0.   -0.   ]
 [ nan  nan  nan -0.   -0.   -0.   ]
 [ nan  nan  nan  nan  0.9  0.   ]
 [ nan  nan  nan  nan  nan -0.   ]
 [ nan  nan  nan  nan  nan  nan ]]
```

### 4.3.6 Mahalanobis distance

- The Mahalanobis distance is a measure of the distance between two points  $\mathbf{x}$  and  $\mu$  where the dispersion (i.e. the covariance structure) of the samples is taken into account.
- The dispersion is considered through covariance matrix.

This is formally expressed as

$$D_M(\mathbf{x}, \mu) = \sqrt{(\mathbf{x} - \mu)^T \Sigma^{-1} (\mathbf{x} - \mu)}.$$

#### Intuitions

- Distances along the principal directions of dispersion are contracted since they correspond to likely dispersion of points.
- Distances orthogonal to the principal directions of dispersion are dilated since they correspond to unlikely dispersion of points.

For example

$$D_M(\mathbf{1}) = \sqrt{\mathbf{1}^T \Sigma^{-1} \mathbf{1}}.$$

```
ones  = np.ones(Cov.shape[0])
d_euc = np.sqrt(np.dot(ones, ones))
d_mah = np.sqrt(np.dot(np.dot(ones, Prec), ones))

print("Euclidean norm of ones=% .2f. Mahalanobis norm of ones=% .2f" % (d_euc, d_mah))
```

```
Euclidean norm of ones=2.45. Mahalanobis norm of ones=1.77
```

The first dot product that distances along the principal directions of dispersion are contracted:

```
print(np.dot(ones, Prec))
```

```
[0.35714286 0.35714286 0.35714286 0.52631579 0.52631579 1.]
```

```
import numpy as np
import scipy
import matplotlib.pyplot as plt
import seaborn as sns
import pystatsml.plot_utils
%matplotlib inline
np.random.seed(40)
colors = sns.color_palette()

mean = np.array([0, 0])
Cov = np.array([[1, .8],
               [.8, 1]])
samples = np.random.multivariate_normal(mean, Cov, 100)
x1 = np.array([0, 2])
x2 = np.array([2, 2])

plt.scatter(samples[:, 0], samples[:, 1], color=colors[0])
plt.scatter(mean[0], mean[1], color=colors[0], s=200, label="mean")
plt.scatter(x1[0], x1[1], color=colors[1], s=200, label="x1")
plt.scatter(x2[0], x2[1], color=colors[2], s=200, label="x2")

# plot covariance ellipsis
pystatsml.plot_utils.plot_cov_ellipse(Cov, pos=mean, facecolor='none',
                                       linewidth=2, edgecolor=colors[0])
# Compute distances
d2_m_x1 = scipy.spatial.distance.euclidean(mean, x1)
d2_m_x2 = scipy.spatial.distance.euclidean(mean, x2)

Covi = scipy.linalg.inv(Cov)
dm_m_x1 = scipy.spatial.distance.mahalanobis(mean, x1, Covi)
dm_m_x2 = scipy.spatial.distance.mahalanobis(mean, x2, Covi)

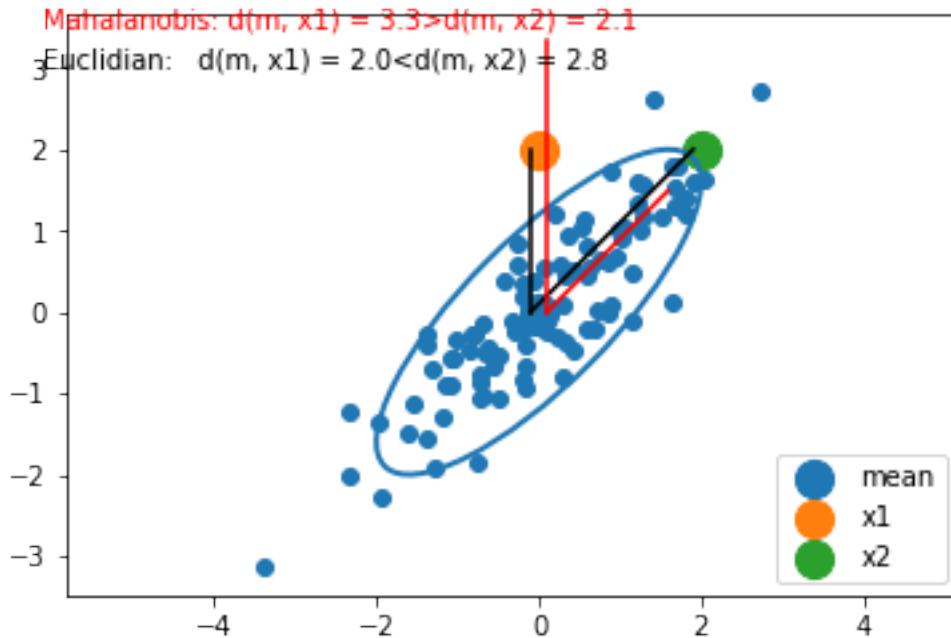
# Plot distances
vm_x1 = (x1 - mean) / d2_m_x1
vm_x2 = (x2 - mean) / d2_m_x2
jitter = .1
plt.plot([mean[0] - jitter, d2_m_x1 * vm_x1[0] - jitter],
         [mean[1], d2_m_x1 * vm_x1[1]], color='k')
plt.plot([mean[0] - jitter, d2_m_x2 * vm_x2[0] - jitter],
         [mean[1], d2_m_x2 * vm_x2[1]], color='k')

plt.plot([mean[0] + jitter, dm_m_x1 * vm_x1[0] + jitter],
         [mean[1], dm_m_x1 * vm_x1[1]], color='r')
plt.plot([mean[0] + jitter, dm_m_x2 * vm_x2[0] + jitter],
         [mean[1], dm_m_x2 * vm_x2[1]], color='r')

plt.legend(loc='lower right')
plt.text(-6.1, 3,
         'Euclidian: d(m, x1) = %.1f < d(m, x2) = %.1f' % (d2_m_x1, d2_m_x2), color='k')
plt.text(-6.1, 3.5,
         'Mahalanobis: d(m, x1) = %.1f > d(m, x2) = %.1f' % (dm_m_x1, dm_m_x2), color='r')

plt.axis('equal')
print('Euclidian d(m, x1) = %.2f < d(m, x2) = %.2f' % (d2_m_x1, d2_m_x2))
print('Mahalanobis d(m, x1) = %.2f > d(m, x2) = %.2f' % (dm_m_x1, dm_m_x2))
```

```
Euclidian d(m, x1) = 2.00 < d(m, x2) = 2.83
Mahalanobis d(m, x1) = 3.33 > d(m, x2) = 2.11
```



If the covariance matrix is the identity matrix, the Mahalanobis distance reduces to the Euclidean distance. If the covariance matrix is diagonal, then the resulting distance measure is called a normalized Euclidean distance.

More generally, the Mahalanobis distance is a measure of the distance between a point  $x$  and a distribution  $\mathcal{N}(x|\mu, \Sigma)$ . It is a multi-dimensional generalization of the idea of measuring how many standard deviations away  $x$  is from the mean. This distance is zero if  $x$  is at the mean, and grows as  $x$  moves away from the mean: along each principal component axis, it measures the number of standard deviations from  $x$  to the mean of the distribution.

#### 4.3.7 Multivariate normal distribution

The distribution, or probability density function (PDF) (sometimes just density), of a continuous random variable is a function that describes the relative likelihood for this random variable to take on a given value.

The multivariate normal distribution, or multivariate Gaussian distribution, of a  $P$ -dimensional random vector  $\mathbf{x} = [x_1, x_2, \dots, x_P]^T$  is

$$\mathcal{N}(\mathbf{x}|\mu, \Sigma) = \frac{1}{(2\pi)^{P/2}|\Sigma|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x} - \mu)^T \Sigma^{-1} (\mathbf{x} - \mu)\right\}.$$

```
import numpy as np
import matplotlib.pyplot as plt
import scipy.stats
from scipy.stats import multivariate_normal
from mpl_toolkits.mplot3d import Axes3D
```

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```
def multivariate_normal_pdf(X, mean, sigma):
    """Multivariate normal probability density function over X (n_samples x n_features)"""
    P = X.shape[1]
    det = np.linalg.det(sigma)
    norm_const = 1.0 / (((2*np.pi) ** (P/2)) * np.sqrt(det))
    X_mu = X - mu
    inv = np.linalg.inv(sigma)
    d2 = np.sum(np.dot(X_mu, inv) * X_mu, axis=1)
    return norm_const * np.exp(-0.5 * d2)

# mean and covariance
mu = np.array([0, 0])
sigma = np.array([[1, -.5],
                 [-.5, 1]])

# x, y grid
x, y = np.mgrid[-3:3:.1, -3:3:.1]
X = np.stack((x.ravel(), y.ravel())).T
norm = multivariate_normal_pdf(X, mean, sigma).reshape(x.shape)

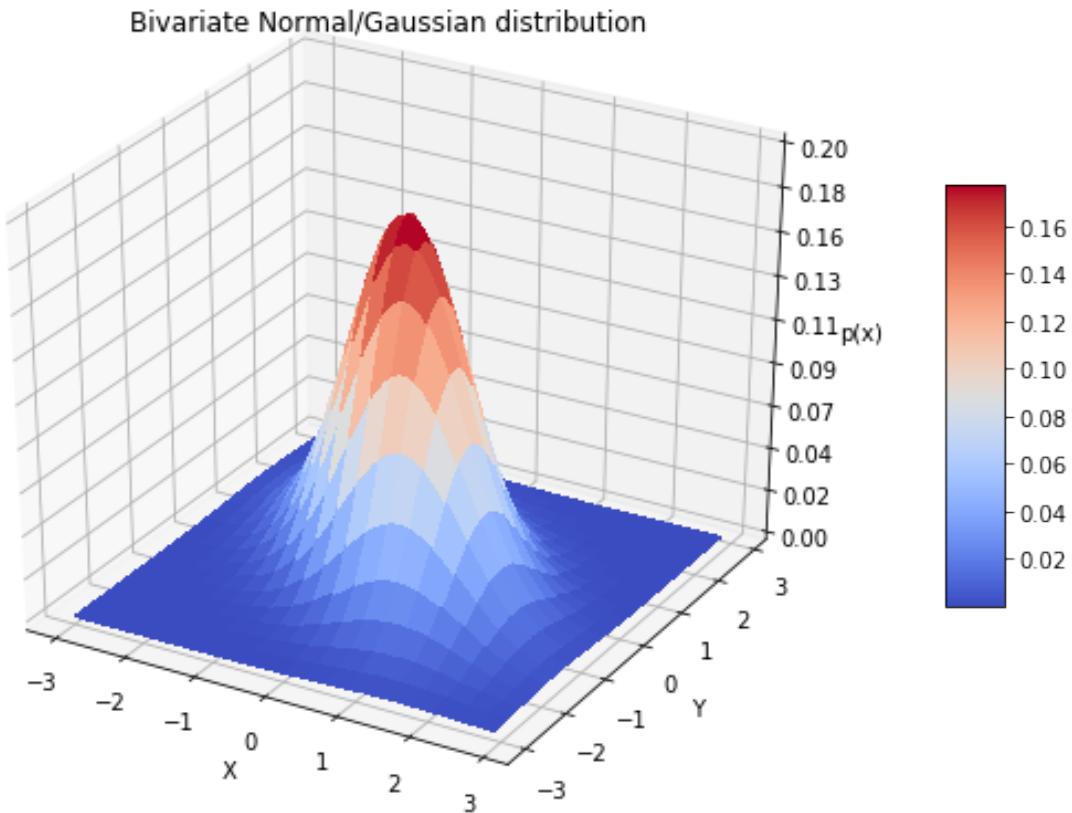
# Do it with scipy
norm_scp = multivariate_normal(mu, sigma).pdf(np.stack((x, y), axis=2))
assert np.allclose(norm, norm_scp)

# Plot
fig = plt.figure(figsize=(10, 7))
ax = fig.gca(projection='3d')
surf = ax.plot_surface(x, y, norm, rstride=3,
                       cstride=3, cmap=plt.cm.coolwarm,
                       linewidth=1, antialiased=False
                      )

ax.set_zlim(0, 0.2)
ax.xaxis.set_major_locator(plt.LinearLocator(10))
ax.xaxis.set_major_formatter(plt.FormatStrFormatter('%.02f'))

ax.set_xlabel('X')
ax.set_ylabel('Y')
ax.set_zlabel('p(x)')

plt.title('Bivariate Normal/Gaussian distribution')
fig.colorbar(surf, shrink=0.5, aspect=7, cmap=plt.cm.coolwarm)
plt.show()
```



### 4.3.8 Exercises

#### Dot product and Euclidean norm

Given  $\mathbf{a} = [2, 1]^T$  and  $\mathbf{b} = [1, 1]^T$

1. Write a function `euclidean(x)` that computes the Euclidean norm of vector,  $x$ .
2. Compute the Euclidean norm of  $\mathbf{a}$ .
3. Compute the Euclidean distance of  $\|\mathbf{a} - \mathbf{b}\|_2$ .
4. Compute the projection of  $\mathbf{b}$  in the direction of vector  $\mathbf{a}$ :  $b_a$ .
5. Simulate a dataset  $\mathbf{X}$  of  $N = 100$  samples of 2-dimensional vectors.
6. Project all samples in the direction of the vector  $\mathbf{a}$ .

#### Covariance matrix and Mahalanobis norm

1. Sample a dataset  $\mathbf{X}$  of  $N = 100$  samples of 2-dimensional vectors from the bivariate normal distribution  $\mathcal{N}(\mu, \Sigma)$  where  $\mu = [1, 1]^T$  and  $\Sigma = \begin{bmatrix} 1 & 0.8 \\ 0.8, 1 \end{bmatrix}$ .
2. Compute the mean vector  $\bar{\mathbf{x}}$  and center  $\mathbf{X}$ . Compare the estimated mean  $\bar{\mathbf{x}}$  to the true mean,  $\mu$ .
3. Compute the empirical covariance matrix  $\mathbf{S}$ . Compare the estimated covariance matrix  $\mathbf{S}$  to the true covariance matrix,  $\Sigma$ .

4. Compute  $S^{-1}$  ( $S_{inv}$ ) the inverse of the covariance matrix by using `scipy.linalg.inv(S)`.
5. Write a function `mahalanobis(x, xbar, Sinv)` that computes the Mahalanobis distance of a vector  $x$  to the mean,  $\bar{x}$ .
6. Compute the Mahalanobis and Euclidean distances of each sample  $x_i$  to the mean  $\bar{x}$ . Store the results in a  $100 \times 2$  data frame.

## 4.4 Time Series in python

Two libraries:

- Pandas: <https://pandas.pydata.org/pandas-docs/stable/timeseries.html>
- scipy <http://www.statsmodels.org/devel/tsa.html>

### 4.4.1 Stationarity

A TS is said to be stationary if its statistical properties such as mean, variance remain constant over time.

- constant mean
- constant variance
- an autocovariance that does not depend on time.

what is making a TS non-stationary. There are 2 major reasons behind non-stationaruty of a TS:

1. Trend – varying mean over time. For eg, in this case we saw that on average, the number of passengers was growing over time.
2. Seasonality – variations at specific time-frames. eg people might have a tendency to buy cars in a particular month because of pay increment or festivals.

### 4.4.2 Pandas Time Series Data Structure

A Series is similar to a list or an array in Python. It represents a series of values (numeric or otherwise) such as a column of data. It provides additional functionality, methods, and operators, which make it a more powerful version of a list.

```
import pandas as pd
import numpy as np

# Create a Series from a list
ser = pd.Series([1, 3])
print(ser)

# String as index
prices = {'apple': 4.99,
          'banana': 1.99,
          'orange': 3.99}
ser = pd.Series(prices)
```

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```
print(ser)

x = pd.Series(np.arange(1,3), index=[x for x in 'ab'])
print(x)
print(x['b'])
```

```
0    1
1    3
dtype: int64
apple    4.99
banana   1.99
orange   3.99
dtype: float64
a    1
b    2
dtype: int64
2
```

#### 4.4.3 Time Series Analysis of Google Trends

source: <https://www.datacamp.com/community/tutorials/time-series-analysis-tutorial>

Get Google Trends data of keywords such as ‘diet’ and ‘gym’ and see how they vary over time while learning about trends and seasonality in time series data.

In the Facebook Live code along session on the 4th of January, we checked out Google trends data of keywords ‘diet’, ‘gym’ and ‘finance’ to see how they vary over time. We asked ourselves if there could be more searches for these terms in January when we’re all trying to turn over a new leaf?

In this tutorial, you’ll go through the code that we put together during the session step by step. You’re not going to do much mathematics but you are going to do the following:

- Read data
- Recode data
- Exploratory Data Analysis

#### 4.4.4 Read data

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns

# Plot appears on its own windows
%matplotlib inline
# Tools / Preferences / Ipython Console / Graphics / Graphics Backend / Backend:_
# "automatic"
# Interactive Matplotlib Jupyter Notebook
# %matplotlib inline
```

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```

try:
    url = "https://raw.githubusercontent.com/databricks/databricks_mlflow_ny_
→resolution/master/datasets/multiTimeline.csv"
    df = pd.read_csv(url, skiprows=2)
except:
    df = pd.read_csv("../datasets/multiTimeline.csv", skiprows=2)

print(df.head())

# Rename columns
df.columns = ['month', 'diet', 'gym', 'finance']

# Describe
print(df.describe())

```

	Month	diet: (Worldwide)	gym: (Worldwide)	finance: (Worldwide)
0	2004-01	100	31	48
1	2004-02	75	26	49
2	2004-03	67	24	47
3	2004-04	70	22	48
4	2004-05	72	22	43
	diet	gym	finance	
count	168.000000	168.000000	168.000000	
mean	49.642857	34.690476	47.148810	
std	8.033080	8.134316	4.972547	
min	34.000000	22.000000	38.000000	
25%	44.000000	28.000000	44.000000	
50%	48.500000	32.500000	46.000000	
75%	53.000000	41.000000	50.000000	
max	100.000000	58.000000	73.000000	

#### 4.4.5 Recode data

Next, you'll turn the 'month' column into a DateTime data type and make it the index of the DataFrame.

Note that you do this because you saw in the result of the `.info()` method that the 'Month' column was actually an of data type object. Now, that generic data type encapsulates everything from strings to integers, etc. That's not exactly what you want when you want to be looking at time series data. That's why you'll use `.to_datetime()` to convert the 'month' column in your DataFrame to a DateTime.

Be careful! Make sure to include the `inplace` argument when you're setting the index of the DataFrame `df` so that you actually alter the original index and set it to the 'month' column.

```

df.month = pd.to_datetime(df.month)
df.set_index('month', inplace=True)

print(df.head())

```

	diet	gym	finance
month			
2004-01-01	100	31	48

(continues on next page)

(continued from previous page)

2004-02-01	75	26	49
2004-03-01	67	24	47
2004-04-01	70	22	48
2004-05-01	72	22	43

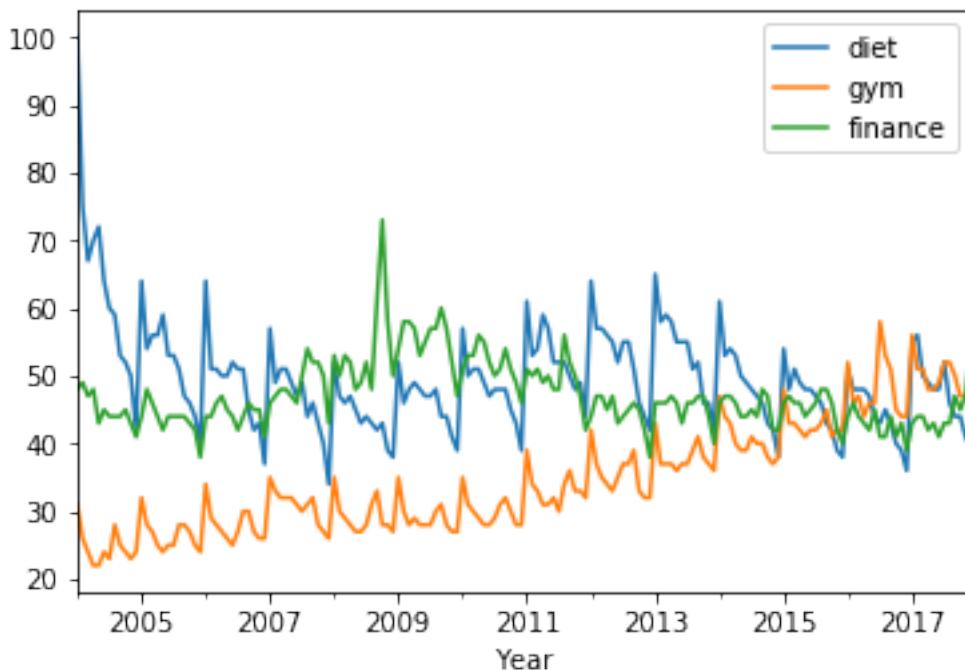
#### 4.4.6 Exploratory Data Analysis

You can use a built-in pandas visualization method `.plot()` to plot your data as 3 line plots on a single figure (one for each column, namely, ‘diet’, ‘gym’, and ‘finance’).

```
df.plot()
plt.xlabel('Year');

# change figure parameters
# df.plot(figsize=(20,10), linewidth=5, fontsize=20)

# Plot single column
# df[['diet']].plot(figsize=(20,10), linewidth=5, fontsize=20)
# plt.xlabel('Year', fontsize=20);
```



Note that this data is relative. As you can read on Google trends:

Numbers represent search interest relative to the highest point on the chart for the given region and time. A value of 100 is the peak popularity for the term. A value of 50 means that the term is half as popular. Likewise a score of 0 means the term was less than 1% as popular as the peak.

#### 4.4.7 Resampling, Smoothing, Windowing, Rolling average: Trends

Rolling average, for each time point, take the average of the points on either side of it. Note that the number of points is specified by a window size.

Remove Seasonality with pandas Series.

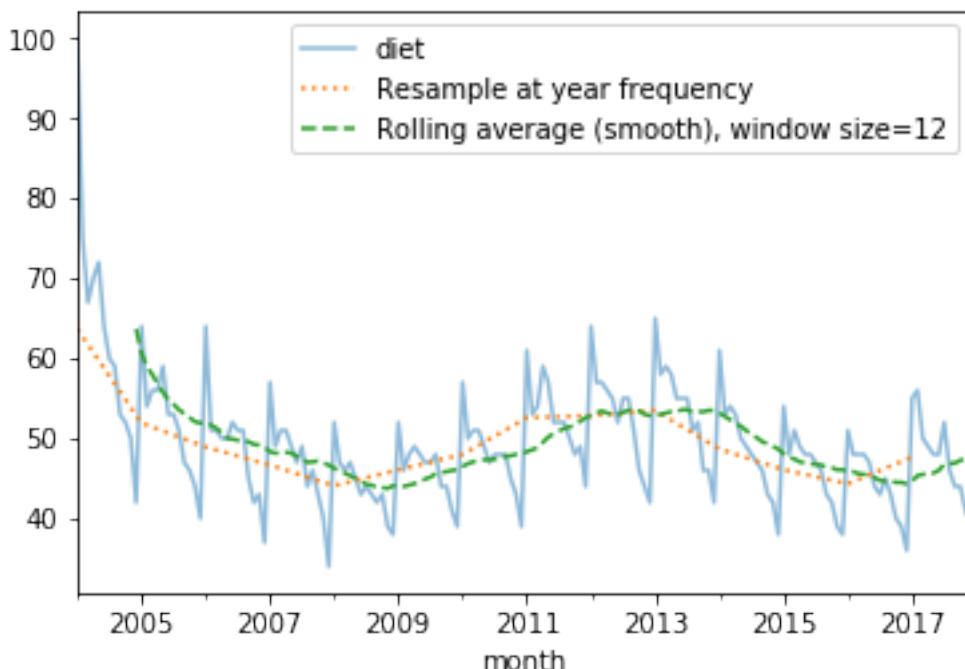
See: <http://pandas.pydata.org/pandas-docs/stable/timeseries.html> A: 'year end frequency' year frequency

```
diet = df['diet']

diet_resamp_yr = diet.resample('A').mean()
diet_roll_yr = diet.rolling(12).mean()

ax = diet.plot(alpha=0.5, style='-' ) # store axis (ax) for latter plots
diet_resamp_yr.plot(style=':', label='Resample at year frequency', ax=ax)
diet_roll_yr.plot(style='--', label='Rolling average (smooth), window size=12', ax=ax)
ax.legend()
```

```
<matplotlib.legend.Legend at 0x7f12ec1eec50>
```

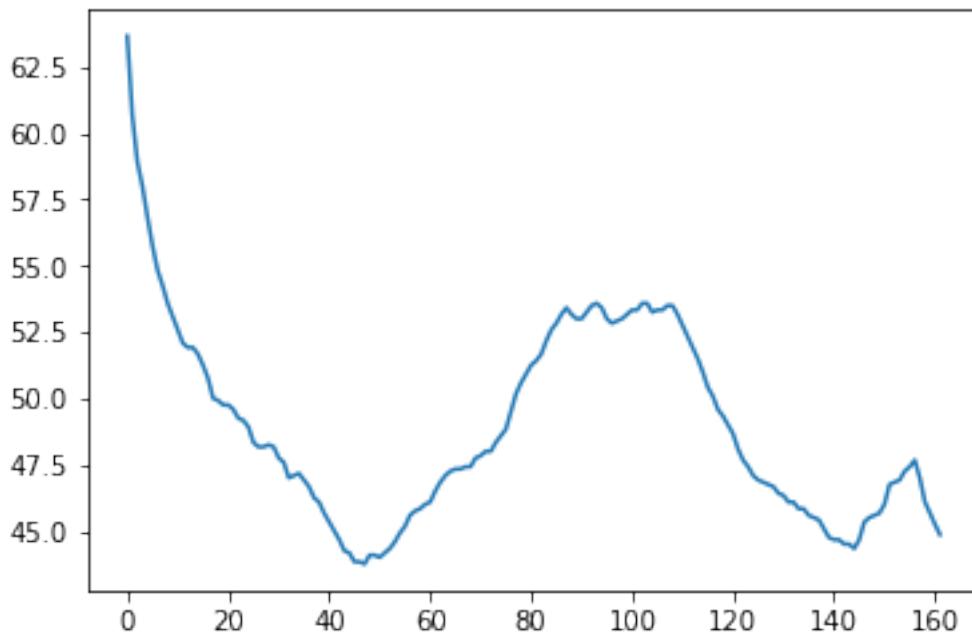


Rolling average (smoothing) with Numpy

```
x = np.asarray(df[['diet']])
win = 12
win_half = int(win / 2)
# print([(idx-win_half), (idx+win_half)) for idx in np.arange(win_half, len(x))])

diet_smooth = np.array([x[(idx-win_half):(idx+win_half)].mean() for idx in np.arange(win_
half, len(x))])
plt.plot(diet_smooth)
```

```
[<matplotlib.lines.Line2D at 0x7f12ec163f98>]
```



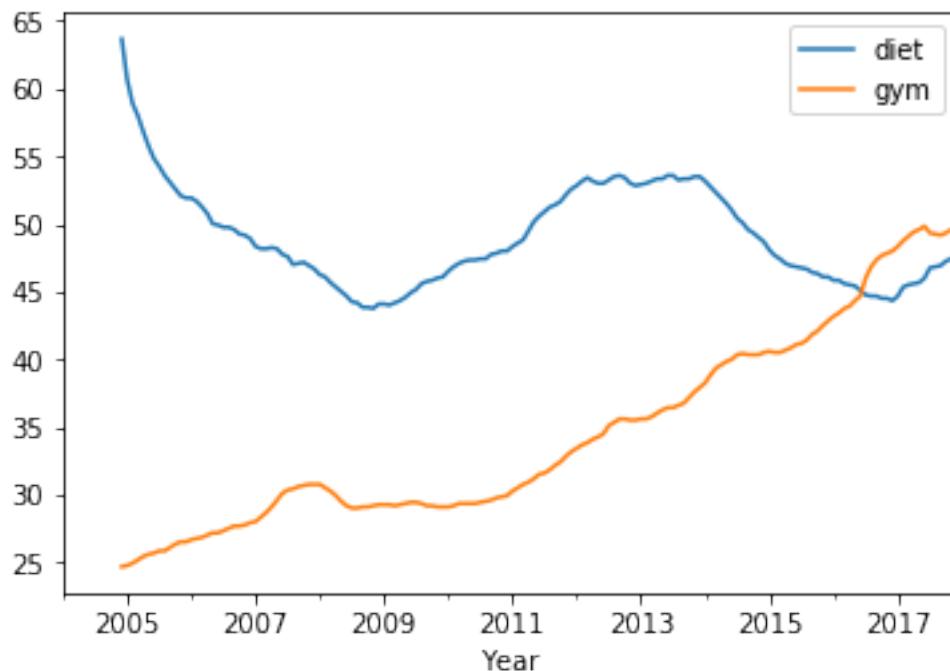
### Trends Plot Diet and Gym

Build a new DataFrame which is the concatenation diet and gym smoothed data

```
gym = df['gym']

df_avg = pd.concat([diet.rolling(12).mean(), gym.rolling(12).mean()], axis=1)
df_avg.plot()
plt.xlabel('Year')
```

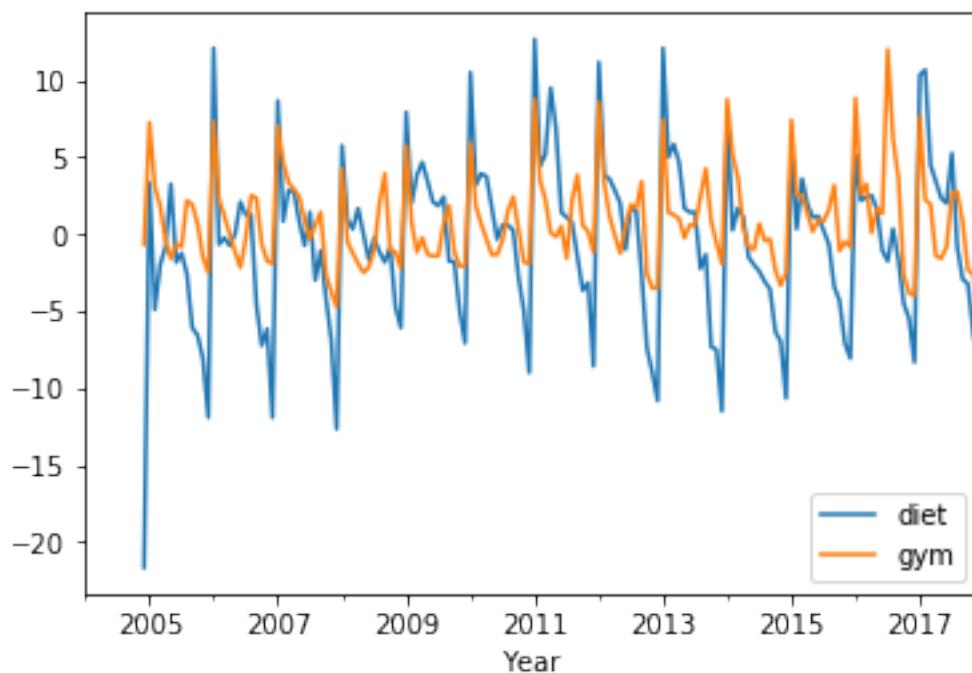
```
Text(0.5, 0, 'Year')
```



Detrending

```
df_dtrend = df[["diet", "gym"]] - df_avg  
df_dtrend.plot()  
plt.xlabel('Year')
```

```
Text(0.5, 0, 'Year')
```

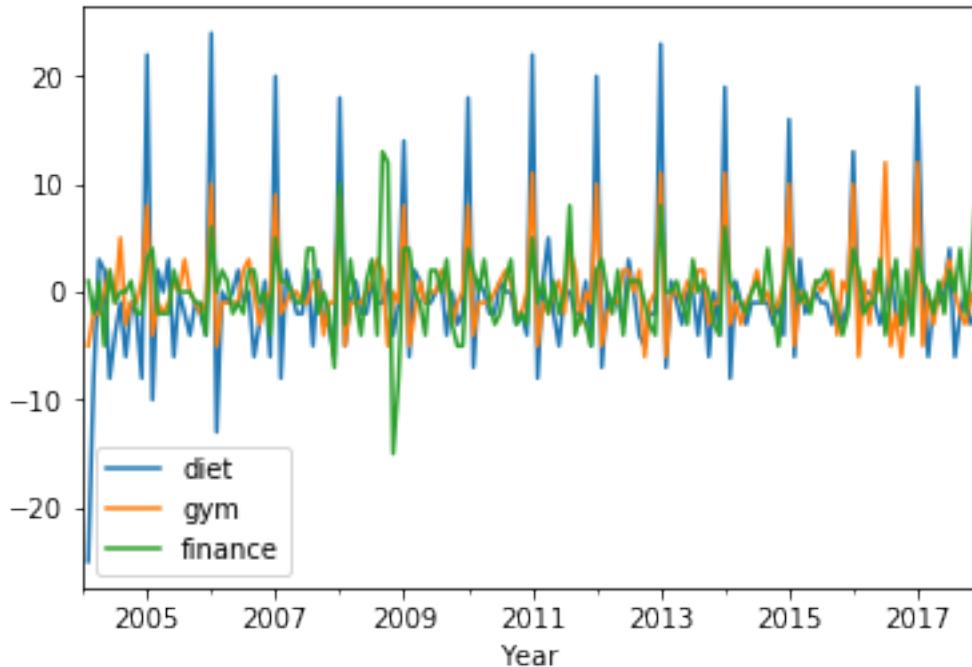


#### 4.4.8 First-order differencing: Seasonal Patterns

```
# diff = original - shifted data
# (exclude first term for some implementation details)
assert np.all((diet.diff() == diet - diet.shift())[1:])

df.diff().plot()
plt.xlabel('Year')
```

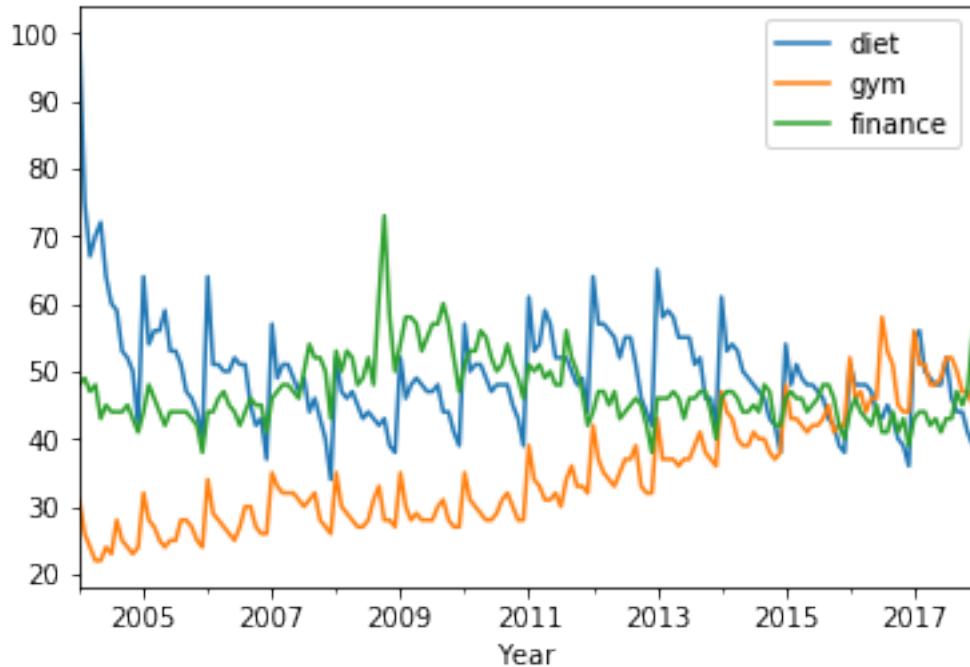
```
Text(0.5, 0, 'Year')
```



#### 4.4.9 Periodicity and Correlation

```
df.plot()
plt.xlabel('Year');
print(df.corr())
```

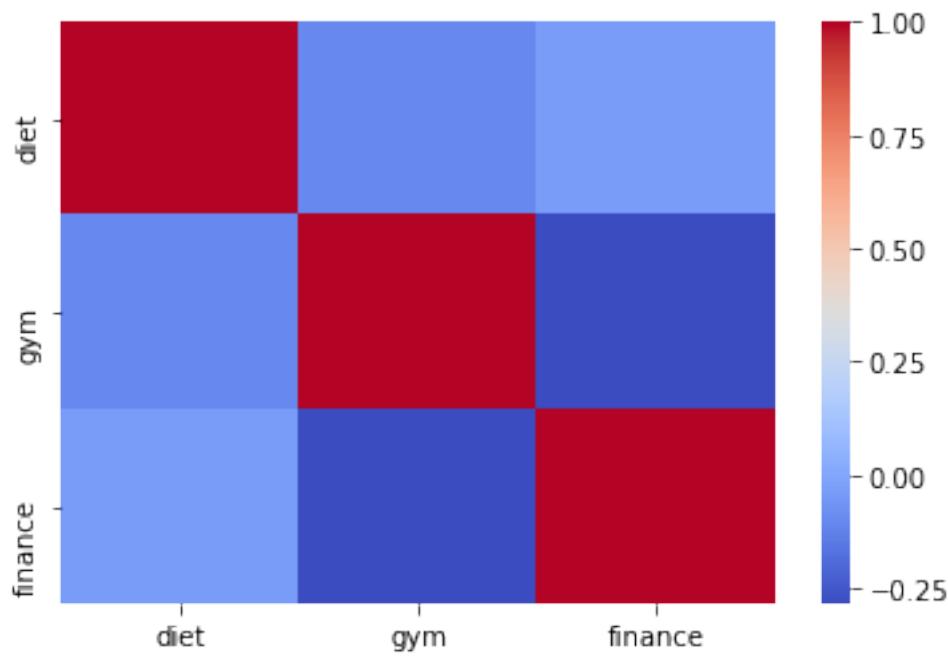
	diet	gym	finance
diet	1.000000	-0.100764	-0.034639
gym	-0.100764	1.000000	-0.284279
finance	-0.034639	-0.284279	1.000000



Plot correlation matrix

```
sns.heatmap(df.corr(), cmap="coolwarm")
```

```
<matplotlib.axes._subplots.AxesSubplot at 0x7f12e9e05a90>
```



'diet' and 'gym' are negatively correlated! Remember that you have a seasonal and a trend component. From the correlation coefficient, 'diet' and 'gym' are negatively correlated:

- trends components are negatively correlated.
- seasonal components would positively correlated and their

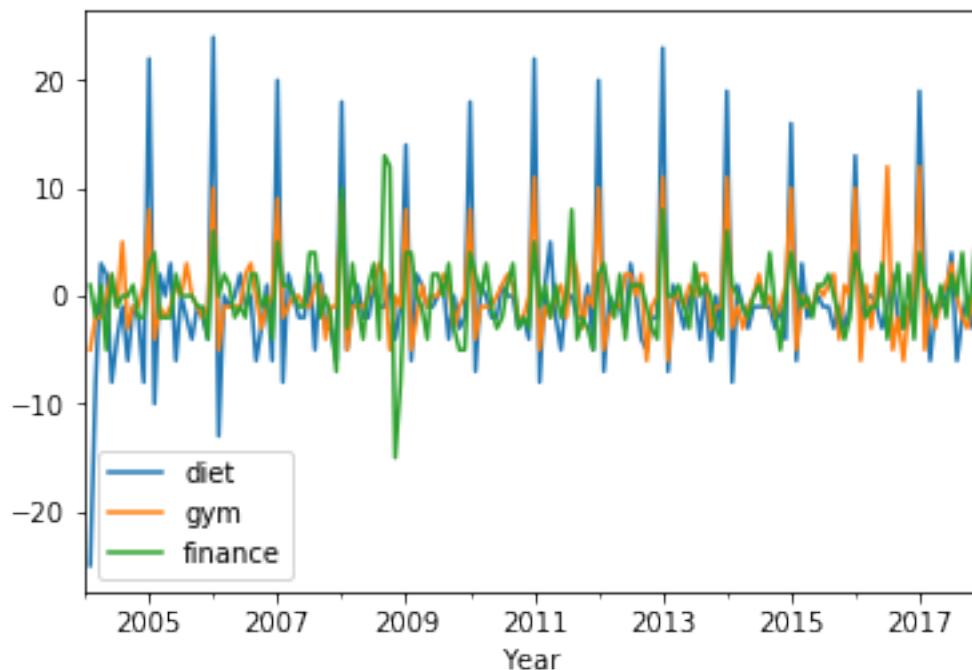
The actual correlation coefficient is actually capturing both of those.

Seasonal correlation: correlation of the first-order differences of these time series

```
df.diff().plot()
plt.xlabel('Year');

print(df.diff().corr())
```

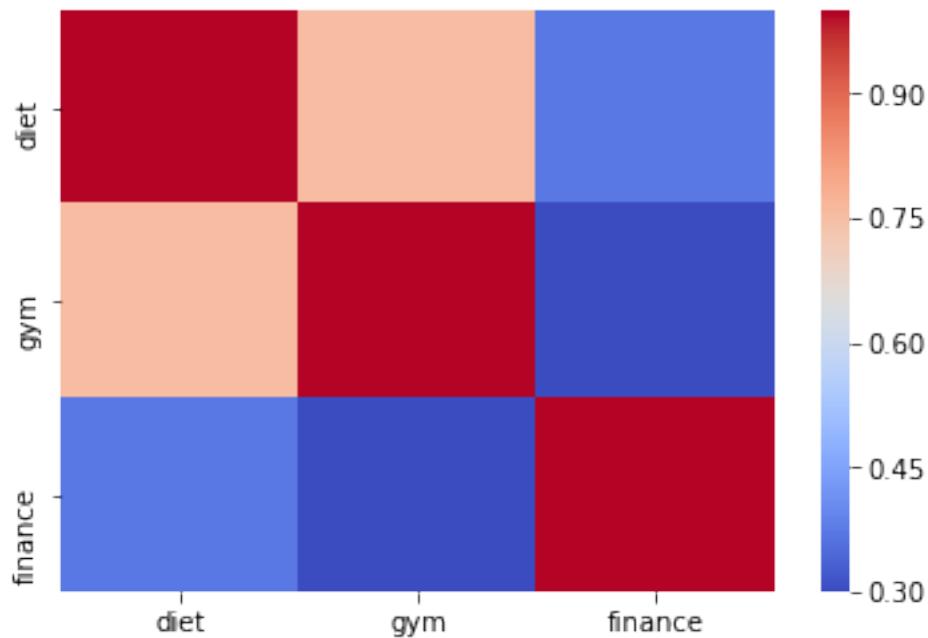
	diet	gym	finance
diet	1.000000	0.758707	0.373828
gym	0.758707	1.000000	0.301111
finance	0.373828	0.301111	1.000000



Plot correlation matrix

```
sns.heatmap(df.diff().corr(), cmap="coolwarm")
```

```
<matplotlib.axes._subplots.AxesSubplot at 0x7f12ec06c438>
```



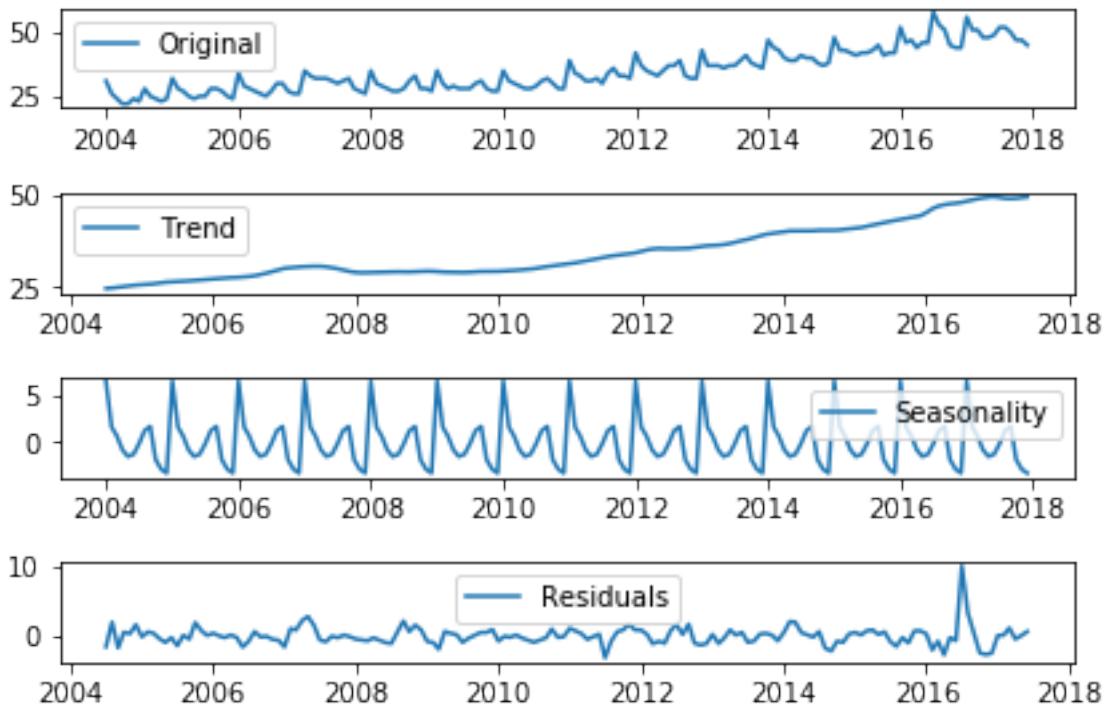
Decomposing time serie in trend, seasonality and residuals

```
from statsmodels.tsa.seasonal import seasonal_decompose

x = gym

x = x.astype(float) # force float
decomposition = seasonal_decompose(x)
trend = decomposition.trend
seasonal = decomposition.seasonal
residual = decomposition.resid

plt.subplot(411)
plt.plot(x, label='Original')
plt.legend(loc='best')
plt.subplot(412)
plt.plot(trend, label='Trend')
plt.legend(loc='best')
plt.subplot(413)
plt.plot(seasonal,label='Seasonality')
plt.legend(loc='best')
plt.subplot(414)
plt.plot(residual, label='Residuals')
plt.legend(loc='best')
plt.tight_layout()
```



#### 4.4.10 Autocorrelation

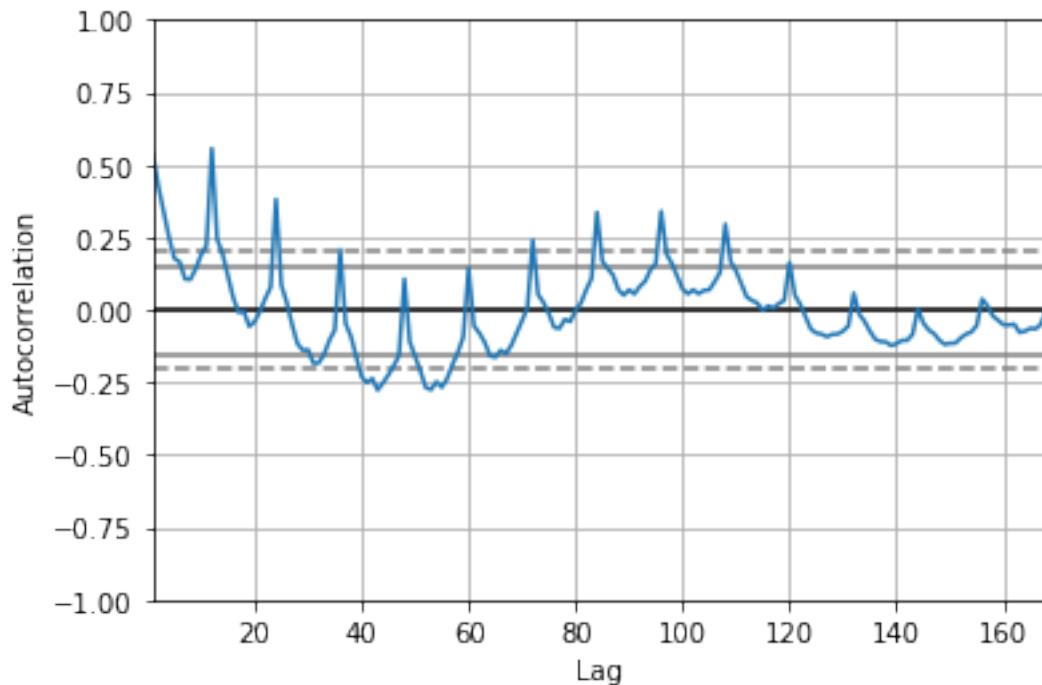
A time series is periodic if it repeats itself at equally spaced intervals, say, every 12 months. Autocorrelation Function (ACF): It is a measure of the correlation between the TS with a lagged version of itself. For instance at lag 5, ACF would compare series at time instant  $t_1 \dots t_2$  with series at instant  $t_{1-5} \dots t_{2-5}$  ( $t_{1-5}$  and  $t_2$  being end points).

Plot

```
# from pandas.plotting import autocorrelation_plot
from pandas.plotting import autocorrelation_plot

x = df["diet"].astype(float)
autocorrelation_plot(x)
```

```
<matplotlib.axes._subplots.AxesSubplot at 0x7f12e9a6d4e0>
```

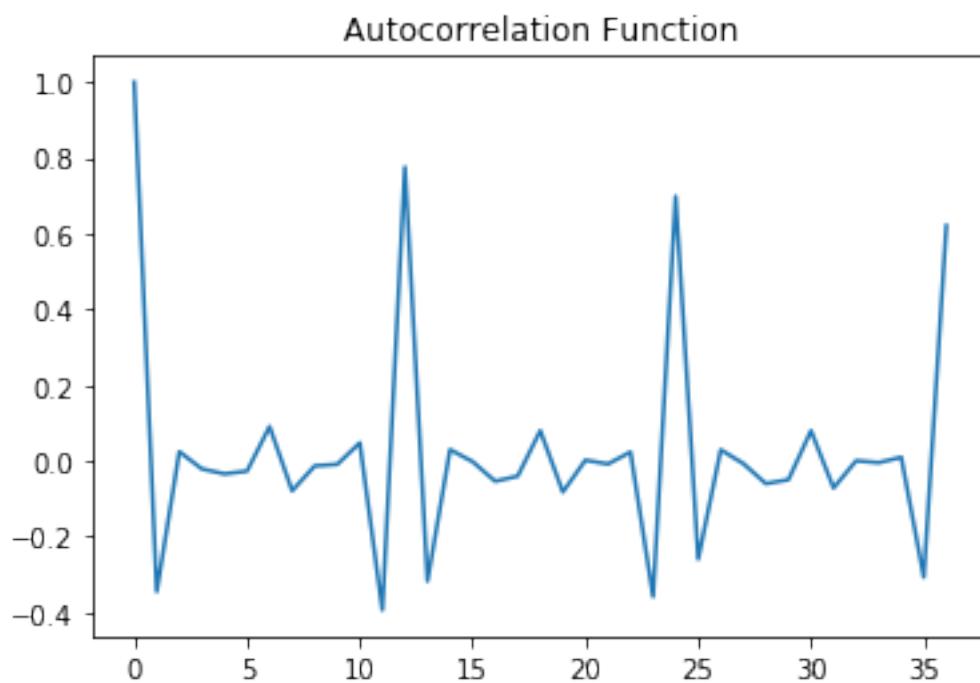


Compute Autocorrelation Function (ACF)

```
from statsmodels.tsa.stattools import acf

x_diff = x.diff().dropna() # first item is NA
lag_acf = acf(x_diff, nlags=36)
plt.plot(lag_acf)
plt.title('Autocorrelation Function')
```

```
Text(0.5, 1.0, 'Autocorrelation Function')
```



ACF peaks every 12 months: Time series is correlated with itself shifted by 12 months.

#### 4.4.11 Time Series Forecasting with Python using Autoregressive Moving Average (ARMA) models

Source:

- [https://www.packtpub.com/mapt/book/big\\_data\\_and\\_business\\_intelligence/9781783553358/7/ch07lvl1sec77/arma-models](https://www.packtpub.com/mapt/book/big_data_and_business_intelligence/9781783553358/7/ch07lvl1sec77/arma-models)
- [http://en.wikipedia.org/wiki/Autoregressive%20moving-average\\_model](http://en.wikipedia.org/wiki/Autoregressive%20moving-average_model)
- ARIMA: <https://www.analyticsvidhya.com/blog/2016/02/time-series-forecasting-codes-python/>

ARMA models are often used to forecast a time series. These models combine autoregressive and moving average models. In moving average models, we assume that a variable is the sum of the mean of the time series and a linear combination of noise components.

The autoregressive and moving average models can have different orders. In general, we can define an ARMA model with p autoregressive terms and q moving average terms as follows:

$$x_t = \sum_i^p a_i x_{t-i} + \sum_i^q b_i \varepsilon_{t-i} + \varepsilon_t$$

#### Choosing p and q

Plot the partial autocorrelation functions for an estimate of p, and likewise using the autocorrelation functions for an estimate of q.

Partial Autocorrelation Function (PACF): This measures the correlation between the TS with a lagged version of itself but after eliminating the variations already explained by the intervening comparisons. Eg at lag 5, it will check the correlation but remove the effects already explained by lags 1 to 4.

```
from statsmodels.tsa.stattools import acf, pacf

x = df["gym"].astype(float)

x_diff = x.diff().dropna() # first item is NA
# ACF and PACF plots:

lag_acf = acf(x_diff, nlags=20)
lag_pacf = pacf(x_diff, nlags=20, method='ols')

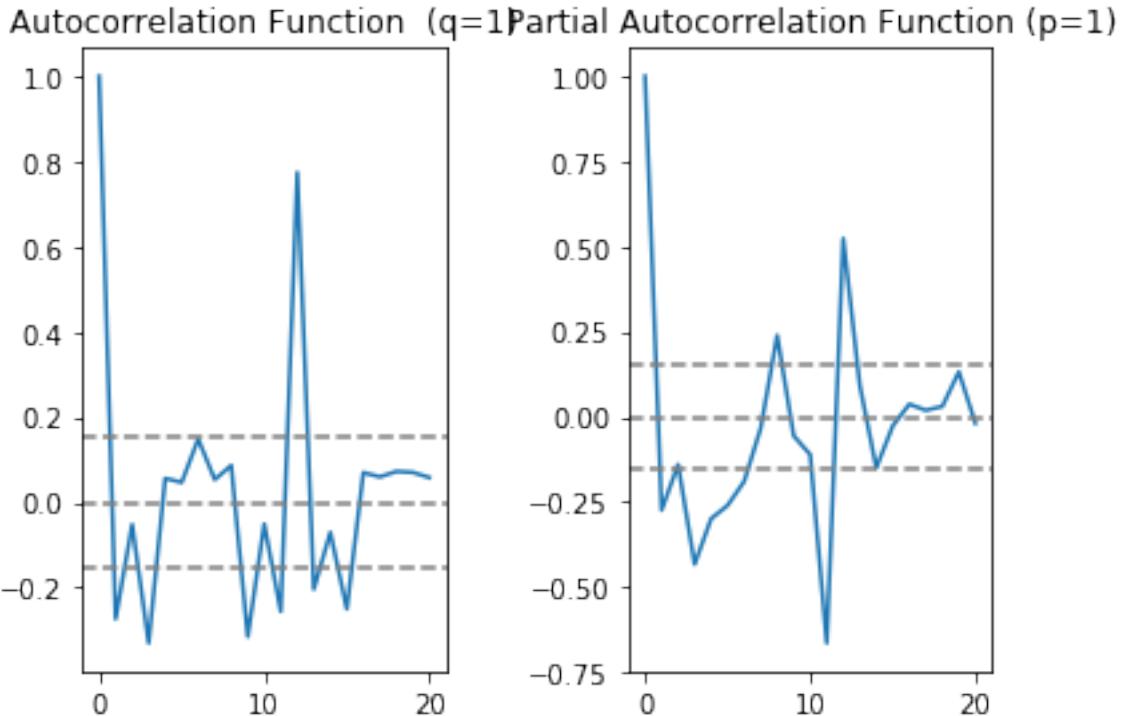
#Plot ACF:
plt.subplot(121)
plt.plot(lag_acf)
plt.axhline(y=0, linestyle='--', color='gray')
plt.axhline(y=-1.96/np.sqrt(len(x_diff)), linestyle='--', color='gray')
plt.axhline(y=1.96/np.sqrt(len(x_diff)), linestyle='--', color='gray')
plt.title('Autocorrelation Function (q=1)')

#Plot PACF:
plt.subplot(122)
plt.plot(lag_pacf)
plt.axhline(y=0, linestyle='--', color='gray')
```

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```
plt.axhline(y=-1.96/np.sqrt(len(x_diff)), linestyle='--', color='gray')
plt.axhline(y=1.96/np.sqrt(len(x_diff)), linestyle='--', color='gray')
plt.title('Partial Autocorrelation Function (p=1)')
plt.tight_layout()
```



In this plot, the two dotted lines on either sides of 0 are the confidence intervals. These can be used to determine the p and q values as:

- p: The lag value where the PACF chart crosses the upper confidence interval for the first time, in this case p=1.
- q: The lag value where the ACF chart crosses the upper confidence interval for the first time, in this case q=1.

### Fit ARMA model with statsmodels

1. Define the model by calling `ARMA()` and passing in the p and q parameters.
2. The model is prepared on the training data by calling the `fit()` function.
3. Predictions can be made by calling the `predict()` function and specifying the index of the time or times to be predicted.

```
from statsmodels.tsa.arima_model import ARMA

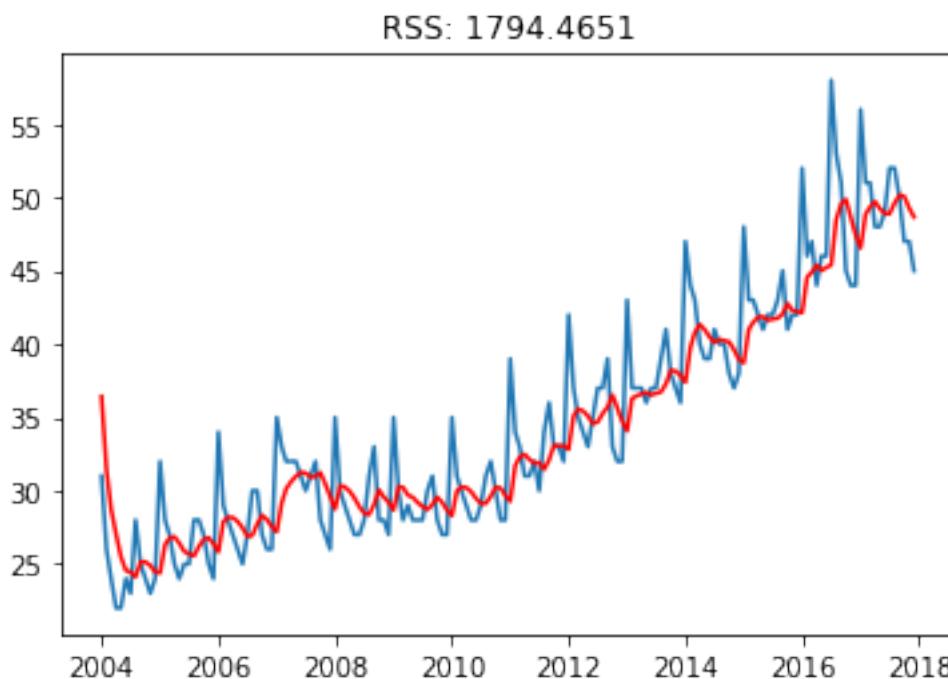
model = ARMA(x, order=(1, 1)).fit() # fit model

print(model.summary())
plt.plot(x)
plt.plot(model.predict(), color='red')
plt.title('RSS: %.4f' % sum((model.fittedvalues-x)**2))
```

```
/home/edouard/anaconda3/lib/python3.7/site-packages/statsmodels/tsa/base/tsa_
→model.py:171: ValueWarning: No frequency information was provided, so inferred_
→frequency MS will be used.
    % freq, ValueWarning)
/home/edouard/anaconda3/lib/python3.7/site-packages/statsmodels/tsa/base/
→tsa_model.py:191: FutureWarning: Creating a DatetimeIndex by passing range_
→endpoints is deprecated. Use pandas.date_range instead.
    start=index[0], end=index[-1], freq=freq)
```

ARMA Model Results						
Dep. Variable:	gym	No. Observations:	168			
Model:	ARMA(1, 1)	Log Likelihood	-436.852			
Method:	css-mle	S.D. of innovations	3.229			
Date:	Thu, 16 May 2019	AIC	881.704			
Time:	20:15:20	BIC	894.200			
Sample:	01-01-2004 - 12-01-2017	HQIC	886.776			
coef	std err	z	P> z	[0.025	0.975]	
const	36.4315	8.827	4.127	0.000	19.131	53.732
ar.L1.gym	0.9967	0.005	220.566	0.000	0.988	1.006
ma.L1.gym	-0.7494	0.054	-13.931	0.000	-0.855	-0.644
Roots						
Real	Imaginary	Modulus	Frequency			
AR.1	1.0033	+0.0000j	1.0033	0.0000		
MA.1	1.3344	+0.0000j	1.3344	0.0000		

Text(0.5, 1.0, 'RSS: 1794.4651')





## MACHINE LEARNING

### 5.1 Dimension reduction and feature extraction

#### 5.1.1 Introduction

In machine learning and statistics, dimensionality reduction or dimension reduction is the process of reducing the number of features under consideration, and can be divided into feature selection (not addressed here) and feature extraction.

Feature extraction starts from an initial set of measured data and builds derived values (features) intended to be informative and non-redundant, facilitating the subsequent learning and generalization steps, and in some cases leading to better human interpretations. Feature extraction is related to dimensionality reduction.

The input matrix  $\mathbf{X}$ , of dimension  $N \times P$ , is

$$\begin{bmatrix} x_{11} & \dots & x_{1P} \\ \vdots & \mathbf{X} & \vdots \\ x_{N1} & \dots & x_{NP} \end{bmatrix}$$

where the rows represent the samples and columns represent the variables.

The goal is to learn a transformation that extracts a few relevant features. This is generally done by exploiting the covariance  $\Sigma_{\mathbf{XX}}$  between the input features.

#### 5.1.2 Singular value decomposition and matrix factorization

##### Matrix factorization principles

Decompose the data matrix  $\mathbf{X}_{N \times P}$  into a product of a mixing matrix  $\mathbf{U}_{N \times K}$  and a dictionary matrix  $\mathbf{V}_{P \times K}$ .

$$\mathbf{X} = \mathbf{UV}^T,$$

If we consider only a subset of components  $K < \text{rank}(\mathbf{X}) < \min(P, N - 1)$ ,  $\mathbf{X}$  is approximated by a matrix  $\hat{\mathbf{X}}$ :

$$\mathbf{X} \approx \hat{\mathbf{X}} = \mathbf{UV}^T,$$

Each line of  $\mathbf{x}_i$  is a linear combination (mixing  $\mathbf{u}_i$ ) of dictionary items  $\mathbf{V}$ .

$N P$ -dimensional data points lie in a space whose dimension is less than  $N - 1$  (2 dots lie on a line, 3 on a plane, etc.).

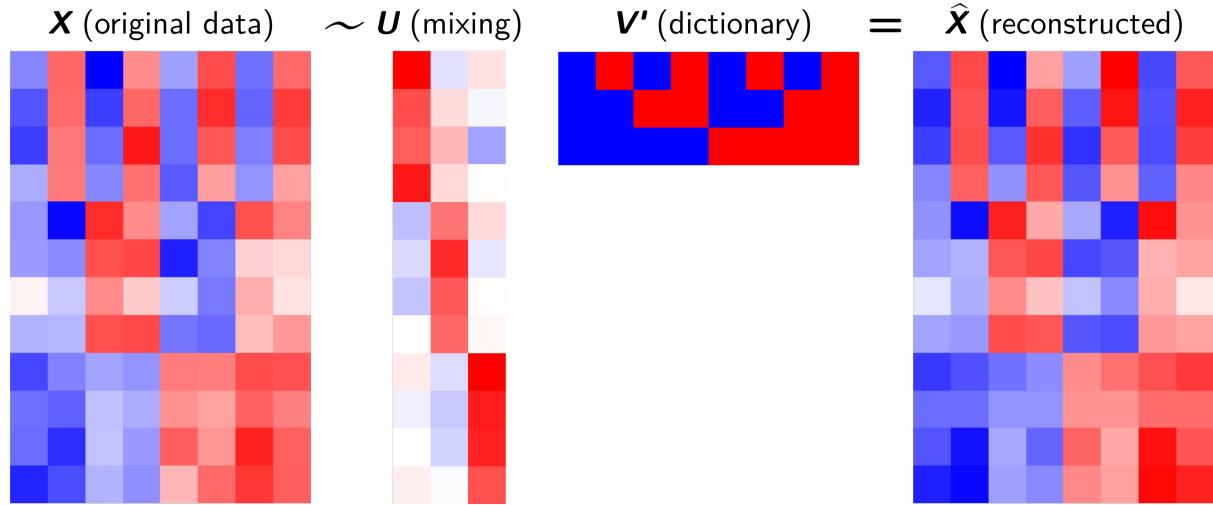


Fig. 1: Matrix factorization

### Singular value decomposition (SVD) principles

Singular-value decomposition (SVD) factorises the data matrix  $\mathbf{X}_{N \times P}$  into a product:

$$\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^T,$$

where

$$\begin{bmatrix} x_{11} & x_{1P} \\ \vdots & \vdots \\ x_{N1} & x_{NP} \end{bmatrix} = \begin{bmatrix} u_{11} & u_{1K} \\ \vdots & \vdots \\ u_{N1} & u_{NK} \end{bmatrix} \begin{bmatrix} d_1 & 0 \\ 0 & d_K \end{bmatrix} \begin{bmatrix} v_{11} & v_{1P} \\ \vdots & \vdots \\ v_{K1} & v_{KP} \end{bmatrix}.$$

#### U: right-singular

- $\mathbf{V} = [\mathbf{v}_1, \dots, \mathbf{v}_K]$  is a  $P \times K$  orthogonal matrix.
- It is a **dictionary** of patterns to be combined (according to the mixing coefficients) to reconstruct the original samples.
- $\mathbf{V}$  performs the initial **rotations (projection)** along the  $K = \min(N, P)$  **principal component directions**, also called **loadings**.
- Each  $\mathbf{v}_j$  performs the linear combination of the variables that has maximum sample variance, subject to being uncorrelated with the previous  $\mathbf{v}_{j-1}$ .

#### D: singular values

- $\mathbf{D}$  is a  $K \times K$  diagonal matrix made of the singular values of  $\mathbf{X}$  with  $d_1 \geq d_2 \geq \dots \geq d_K \geq 0$ .
- $\mathbf{D}$  scale the projection along the coordinate axes by  $d_1, d_2, \dots, d_K$ .

- Singular values are the square roots of the eigenvalues of  $\mathbf{X}^T \mathbf{X}$ .

### V: left-singular vectors

- $\mathbf{U} = [\mathbf{u}_1, \dots, \mathbf{u}_K]$  is an  $N \times K$  orthogonal matrix.
- Each row  $\mathbf{v}_i$  provides the **mixing coefficients** of dictionary items to reconstruct the sample  $\mathbf{x}_i$
- It may be understood as the coordinates on the new orthogonal basis (obtained after the initial rotation) called **principal components** in the PCA.

### SVD for variables transformation

$\mathbf{V}$  transforms correlated variables ( $\mathbf{X}$ ) into a set of uncorrelated ones ( $\mathbf{UD}$ ) that better expose the various relationships among the original data items.

$$\mathbf{X} = \mathbf{UDV}^T, \quad (5.1)$$

$$\mathbf{X}\mathbf{V} = \mathbf{UDV}^T\mathbf{V}, \quad (5.2)$$

$$\mathbf{X}\mathbf{V} = \mathbf{UDI}, \quad (5.3)$$

$$\mathbf{X}\mathbf{V} = \mathbf{UD} \quad (5.4)$$

At the same time, SVD is a method for identifying and ordering the dimensions along which data points exhibit the most variation.

```
import numpy as np
import scipy
from sklearn.decomposition import PCA
import matplotlib.pyplot as plt
import seaborn as sns
%matplotlib inline

np.random.seed(42)

# dataset
n_samples = 100
experience = np.random.normal(size=n_samples)
salary = 1500 + experience + np.random.normal(size=n_samples, scale=.5)
X = np.column_stack([experience, salary])

# PCA using SVD
X -= X.mean(axis=0) # Centering is required
U, s, Vh = scipy.linalg.svd(X, full_matrices=False)
# U : Unitary matrix having left singular vectors as columns.
#     Of shape (n_samples,n_samples) or (n_samples,n_comps), depending on
#     full_matrices.
#
# s : The singular values, sorted in non-increasing order. Of shape (n_comps,),
#     with n_comps = min(n_samples, n_features).
#
# Vh: Unitary matrix having right singular vectors as rows.
#     Of shape (n_features, n_features) or (n_comps, n_features) depending
#     on full_matrices.
```

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```

plt.figure(figsize=(9, 3))

plt.subplot(131)
plt.scatter(U[:, 0], U[:, 1], s=50)
plt.axis('equal')
plt.title("U: Rotated and scaled data")

plt.subplot(132)

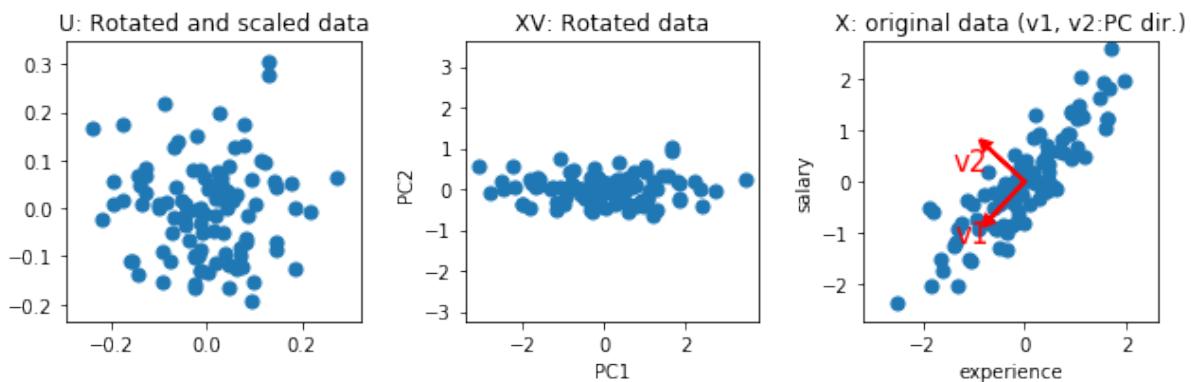
# Project data
PC = np.dot(X, Vh.T)
plt.scatter(PC[:, 0], PC[:, 1], s=50)
plt.axis('equal')
plt.title("XV: Rotated data")
plt.xlabel("PC1")
plt.ylabel("PC2")

plt.subplot(133)
plt.scatter(X[:, 0], X[:, 1], s=50)
for i in range(Vh.shape[0]):
    plt.arrow(x=0, y=0, dx=Vh[i, 0], dy=Vh[i, 1], head_width=0.2,
              head_length=0.2, linewidth=2, fc='r', ec='r')
    plt.text(Vh[i, 0], Vh[i, 1], 'v%i' % (i+1), color="r", fontsize=15,
             horizontalalignment='right', verticalalignment='top')
plt.axis('equal')
plt.ylim(-4, 4)

plt.title("X: original data (v1, v2:PC dir.)")
plt.xlabel("experience")
plt.ylabel("salary")

plt.tight_layout()

```



### 5.1.3 Principal components analysis (PCA)

Sources:

- C. M. Bishop *Pattern Recognition and Machine Learning*, Springer, 2006
- Everything you did and didn't know about PCA
- Principal Component Analysis in 3 Simple Steps

## Principles

- Principal components analysis is the main method used for linear dimension reduction.
- The idea of principal component analysis is to find the  $K$  **principal components directions** (called the **loadings**)  $\mathbf{V}_{K \times P}$  that capture the variation in the data as much as possible.
- It converts a set of  $N$   $P$ -dimensional observations  $\mathbf{N}_{N \times P}$  of possibly correlated variables into a set of  $N$   $K$ -dimensional samples  $\mathbf{C}_{N \times K}$ , where the  $K < P$ . The new variables are linearly uncorrelated. The columns of  $\mathbf{C}_{N \times K}$  are called the **principal components**.
- The dimension reduction is obtained by using only  $K < P$  components that exploit correlation (covariance) among the original variables.
- PCA is mathematically defined as an orthogonal linear transformation  $\mathbf{V}_{K \times P}$  that transforms the data to a new coordinate system such that the greatest variance by some projection of the data comes to lie on the first coordinate (called the first principal component), the second greatest variance on the second coordinate, and so on.

$$\mathbf{C}_{N \times K} = \mathbf{X}_{N \times P} \mathbf{V}_{P \times K}$$

- PCA can be thought of as fitting a  $P$ -dimensional ellipsoid to the data, where each axis of the ellipsoid represents a principal component. If some axis of the ellipse is small, then the variance along that axis is also small, and by omitting that axis and its corresponding principal component from our representation of the dataset, we lose only a commensurately small amount of information.
- Finding the  $K$  largest axes of the ellipse will permit to project the data onto a space having dimensionality  $K < P$  while maximizing the variance of the projected data.

## Dataset preprocessing

### Centering

Consider a data matrix,  $\mathbf{X}$ , with column-wise zero empirical mean (the sample mean of each column has been shifted to zero), ie.  $\mathbf{X}$  is replaced by  $\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}^T$ .

### Standardizing

Optionally, standardize the columns, i.e., scale them by their standard-deviation. Without standardization, a variable with a high variance will capture most of the effect of the PCA. The principal direction will be aligned with this variable. Standardization will, however, raise noise variables to the same level as informative variables.

The covariance matrix of centered standardized data is the correlation matrix.

### Eigendecomposition of the data covariance matrix

To begin with, consider the projection onto a one-dimensional space ( $K = 1$ ). We can define the direction of this space using a  $P$ -dimensional vector  $\mathbf{v}$ , which for convenience (and without loss of generality) we shall choose to be a unit vector so that  $\|\mathbf{v}\|_2 = 1$  (note that we are only

interested in the direction defined by  $\mathbf{v}$ , not in the magnitude of  $\mathbf{v}$  itself). PCA consists of two main steps:

### Projection in the directions that capture the greatest variance

Each  $P$ -dimensional data point  $\mathbf{x}_i$  is then projected onto  $\mathbf{v}$ , where the coordinate (in the coordinate system of  $\mathbf{v}$ ) is a scalar value, namely  $\mathbf{x}_i^T \mathbf{v}$ . I.e., we want to find the vector  $\mathbf{v}$  that maximizes these coordinates along  $\mathbf{v}$ , which we will see corresponds to maximizing the variance of the projected data. This is equivalently expressed as

$$\mathbf{v} = \arg \max_{\|\mathbf{v}\|=1} \frac{1}{N} \sum_i (\mathbf{x}_i^T \mathbf{v})^2.$$

We can write this in matrix form as

$$\mathbf{v} = \arg \max_{\|\mathbf{v}\|=1} \frac{1}{N} \|\mathbf{X}\mathbf{v}\|^2 = \frac{1}{N} \mathbf{v}^T \mathbf{X}^T \mathbf{X} \mathbf{v} = \mathbf{v}^T \mathbf{S}_{\mathbf{XX}} \mathbf{v},$$

where  $\mathbf{S}_{\mathbf{XX}}$  is a biased estimate of the covariance matrix of the data, i.e.

$$\mathbf{S}_{\mathbf{XX}} = \frac{1}{N} \mathbf{X}^T \mathbf{X}.$$

We now maximize the projected variance  $\mathbf{v}^T \mathbf{S}_{\mathbf{XX}} \mathbf{v}$  with respect to  $\mathbf{v}$ . Clearly, this has to be a constrained maximization to prevent  $\|\mathbf{v}_2\| \rightarrow \infty$ . The appropriate constraint comes from the normalization condition  $\|\mathbf{v}\|_2 \equiv \|\mathbf{v}\|_2^2 = \mathbf{v}^T \mathbf{v} = 1$ . To enforce this constraint, we introduce a Lagrange multiplier that we shall denote by  $\lambda$ , and then make an unconstrained maximization of

$$\mathbf{v}^T \mathbf{S}_{\mathbf{XX}} \mathbf{v} - \lambda(\mathbf{v}^T \mathbf{v} - 1).$$

By setting the gradient with respect to  $\mathbf{v}$  equal to zero, we see that this quantity has a stationary point when

$$\mathbf{S}_{\mathbf{XX}} \mathbf{v} = \lambda \mathbf{v}.$$

We note that  $\mathbf{v}$  is an eigenvector of  $\mathbf{S}_{\mathbf{XX}}$ .

If we left-multiply the above equation by  $\mathbf{v}^T$  and make use of  $\mathbf{v}^T \mathbf{v} = 1$ , we see that the variance is given by

$$\mathbf{v}^T \mathbf{S}_{\mathbf{XX}} \mathbf{v} = \lambda,$$

and so the variance will be at a maximum when  $\mathbf{v}$  is equal to the eigenvector corresponding to the largest eigenvalue,  $\lambda$ . This eigenvector is known as the first principal component.

We can define additional principal components in an incremental fashion by choosing each new direction to be that which maximizes the projected variance amongst all possible directions that are orthogonal to those already considered. If we consider the general case of a  $K$ -dimensional projection space, the optimal linear projection for which the variance of the projected data is maximized is now defined by the  $K$  eigenvectors,  $\mathbf{v}_1, \dots, \mathbf{v}_K$ , of the data covariance matrix  $\mathbf{S}_{\mathbf{XX}}$  that corresponds to the  $K$  largest eigenvalues,  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_K$ .

[Back to SVD](#)

The sample covariance matrix of **centered data**  $\mathbf{X}$  is given by

$$\mathbf{S}_{\mathbf{XX}} = \frac{1}{N-1} \mathbf{X}^T \mathbf{X}.$$

We rewrite  $\mathbf{X}^T \mathbf{X}$  using the SVD decomposition of  $\mathbf{X}$  as

$$\begin{aligned}\mathbf{X}^T \mathbf{X} &= (\mathbf{UDV}^T)^T (\mathbf{UDV}^T) \\ &= \mathbf{VD}^T \mathbf{U}^T \mathbf{UDV}^T \\ &= \mathbf{VD}^2 \mathbf{V}^T \\ \mathbf{V}^T \mathbf{X}^T \mathbf{X} \mathbf{V} &= \mathbf{D}^2 \\ \frac{1}{N-1} \mathbf{V}^T \mathbf{X}^T \mathbf{X} \mathbf{V} &= \frac{1}{N-1} \mathbf{D}^2 \\ \mathbf{V}^T \mathbf{S}_{\mathbf{XX}} \mathbf{V} &= \frac{1}{N-1} \mathbf{D}^2 \\ &\vdots\end{aligned}$$

Considering only the  $k^{th}$  right-singular vectors  $\mathbf{v}_k$  associated to the singular value  $d_k$

$$\mathbf{v}_k^T \mathbf{S}_{\mathbf{XX}} \mathbf{v}_k = \frac{1}{N-1} d_k^2,$$

It turns out that if you have done the singular value decomposition then you already have the Eigenvalue decomposition for  $\mathbf{X}^T \mathbf{X}$ . Where - The eigenvectors of  $\mathbf{S}_{\mathbf{XX}}$  are equivalent to the right singular vectors,  $\mathbf{V}$ , of  $\mathbf{X}$ . - The eigenvalues,  $\lambda_k$ , of  $\mathbf{S}_{\mathbf{XX}}$ , i.e. the variances of the components, are equal to  $\frac{1}{N-1}$  times the squared singular values,  $d_k$ .

Moreover computing PCA with SVD do not require to form the matrix  $\mathbf{X}^T \mathbf{X}$ , so computing the SVD is now the standard way to calculate a principal components analysis from a data matrix, unless only a handful of components are required.

## PCA outputs

The SVD or the eigendecomposition of the data covariance matrix provides three main quantities:

1. **Principal component directions or loadings** are the **eigenvectors** of  $\mathbf{X}^T \mathbf{X}$ . The  $\mathbf{V}_{K \times P}$  or the **right-singular vectors** of an SVD of  $\mathbf{X}$  are called principal component directions of  $\mathbf{X}$ . They are generally computed using the SVD of  $\mathbf{X}$ .
2. **Principal components** is the  $N \times K$  matrix  $\mathbf{C}$  which is obtained by projecting  $\mathbf{X}$  onto the principal components directions, i.e.

$$\mathbf{C}_{N \times K} = \mathbf{X}_{N \times P} \mathbf{V}_{P \times K}.$$

Since  $\mathbf{X} = \mathbf{UDV}^T$  and  $\mathbf{V}$  is orthogonal ( $\mathbf{V}^T \mathbf{V} = \mathbf{I}$ ):

$$\mathbf{C}_{N \times K} = \mathbf{U} \mathbf{D} \mathbf{V}_{N \times P}^T \mathbf{V}_{P \times K} \quad (5.5)$$

$$\mathbf{C}_{N \times K} = \mathbf{U} \mathbf{D}_{N \times K}^T \mathbf{I}_{K \times K} \quad (5.6)$$

$$\mathbf{C}_{N \times K} = \mathbf{U} \mathbf{D}_{N \times K}^T \quad (5.7)$$

$$(5.8)$$

Thus  $\mathbf{c}_j = \mathbf{X}\mathbf{v}_j = \mathbf{u}_j d_j$ , for  $j = 1, \dots, K$ . Hence  $\mathbf{u}_j$  is simply the projection of the row vectors of  $\mathbf{X}$ , i.e., the input predictor vectors, on the direction  $\mathbf{v}_j$ , scaled by  $d_j$ .

$$\mathbf{c}_1 = \begin{bmatrix} x_{1,1}v_{1,1} + \dots + x_{1,P}v_{1,P} \\ x_{2,1}v_{1,1} + \dots + x_{2,P}v_{1,P} \\ \vdots \\ x_{N,1}v_{1,1} + \dots + x_{N,P}v_{1,P} \end{bmatrix}$$

3. The **variance** of each component is given by the eigen values  $\lambda_k, k = 1, \dots, K$ . It can be obtained from the singular values:

$$var(\mathbf{c}_k) = \frac{1}{N-1} (\mathbf{X}\mathbf{v}_k)^2 \quad (5.9)$$

$$= \frac{1}{N-1} (\mathbf{u}_k d_k)^2 \quad (5.10)$$

$$= \frac{1}{N-1} d_k^2 \quad (5.11)$$

## Determining the number of PCs

We must choose  $K^* \in [1, \dots, K]$ , the number of required components. This can be done by calculating the explained variance ratio of the  $K^*$  first components and by choosing  $K^*$  such that the **cumulative explained variance** ratio is greater than some given threshold (e.g.,  $\approx 90\%$ ). This is expressed as

$$\text{cumulative explained variance}(\mathbf{c}_k) = \frac{\sum_j^{K^*} var(\mathbf{c}_k)}{\sum_j^K var(\mathbf{c}_k)}.$$

## Interpretation and visualization

### PCs

Plot the samples projected on first the principal components as e.g. PC1 against PC2.

### PC directions

Exploring the loadings associated with a component provides the contribution of each original variable in the component.

Remark: The loadings (PC directions) are the coefficients of multiple regression of PC on original variables:

$$\mathbf{c} = \mathbf{X}\mathbf{v} \quad (5.12)$$

$$\mathbf{X}^T\mathbf{c} = \mathbf{X}^T\mathbf{X}\mathbf{v} \quad (5.13)$$

$$(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{c} = \mathbf{v} \quad (5.14)$$

Another way to evaluate the contribution of the original variables in each PC can be obtained by computing the correlation between the PCs and the original variables, i.e. columns of  $\mathbf{X}$ , denoted  $\mathbf{x}_j$ , for  $j = 1, \dots, P$ . For the  $k^{th}$  PC, compute and plot the correlations with all original variables

$$\text{cor}(\mathbf{c}_k, \mathbf{x}_j), j = 1 \dots K, j = 1 \dots K.$$

These quantities are sometimes called the *correlation loadings*.

```
import numpy as np
from sklearn.decomposition import PCA
import matplotlib.pyplot as plt

np.random.seed(42)

# dataset
n_samples = 100
experience = np.random.normal(size=n_samples)
salary = 1500 + experience + np.random.normal(size=n_samples, scale=.5)
X = np.column_stack([experience, salary])

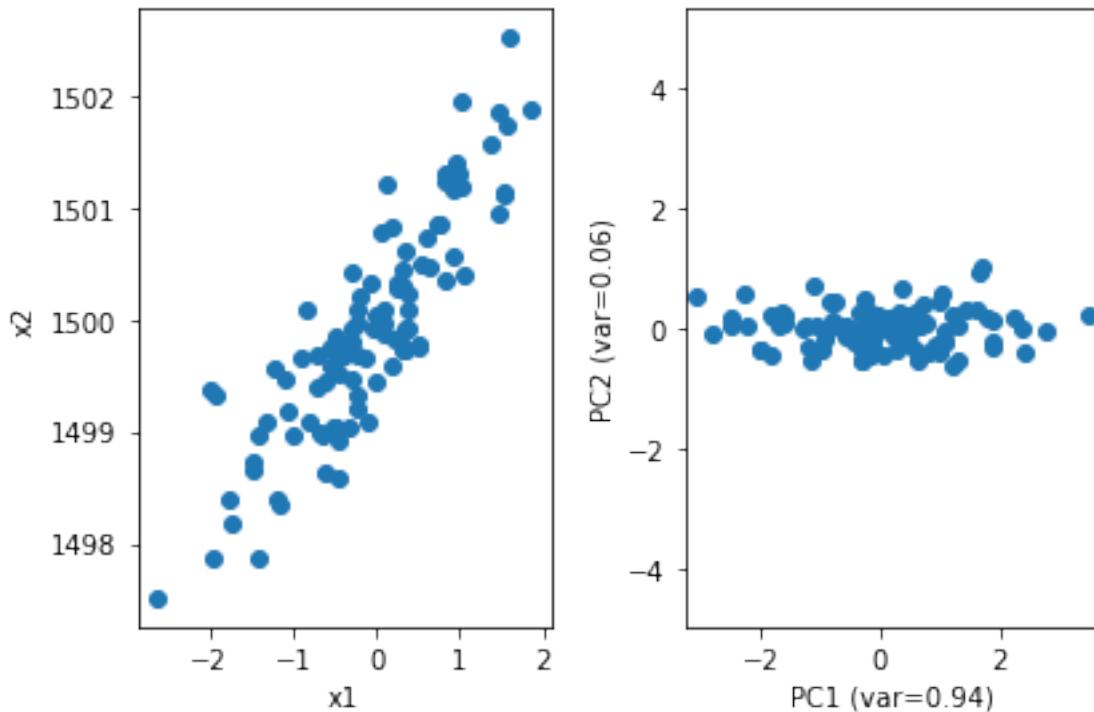
# PCA with scikit-learn
pca = PCA(n_components=2)
pca.fit(X)
print(pca.explained_variance_ratio_)

PC = pca.transform(X)

plt.subplot(121)
plt.scatter(X[:, 0], X[:, 1])
plt.xlabel("x1"); plt.ylabel("x2")

plt.subplot(122)
plt.scatter(PC[:, 0], PC[:, 1])
plt.xlabel("PC1 (var=%.2f)" % pca.explained_variance_ratio_[0])
plt.ylabel("PC2 (var=%.2f)" % pca.explained_variance_ratio_[1])
plt.axis('equal')
plt.tight_layout()
```

[0.93646607 0.06353393]



### 5.1.4 Multi-dimensional Scaling (MDS)

Resources:

- [http://www.stat.pitt.edu/sungkyu/course/2221Fall13/lec8\\_mds\\_combined.pdf](http://www.stat.pitt.edu/sungkyu/course/2221Fall13/lec8_mds_combined.pdf)
- [https://en.wikipedia.org/wiki/Multidimensional\\_scaling](https://en.wikipedia.org/wiki/Multidimensional_scaling)
- Hastie, Tibshirani and Friedman (2009). *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*. New York: Springer, Second Edition.

The purpose of MDS is to find a low-dimensional projection of the data in which the pairwise distances between data points is preserved, as closely as possible (in a least-squares sense).

- Let  $\mathbf{D}$  be the  $(N \times N)$  pairwise distance matrix where  $d_{ij}$  is a distance between points  $i$  and  $j$ .
- The MDS concept can be extended to a wide variety of data types specified in terms of a similarity matrix.

Given the dissimilarity (distance) matrix  $\mathbf{D}_{N \times N} = [d_{ij}]$ , MDS attempts to find  $K$ -dimensional projections of the  $N$  points  $\mathbf{x}_1, \dots, \mathbf{x}_N \in \mathbb{R}^K$ , concatenated in an  $\mathbf{X}_{N \times K}$  matrix, so that  $d_{ij} \approx \|\mathbf{x}_i - \mathbf{x}_j\|$  are as close as possible. This can be obtained by the minimization of a loss function called the **stress function**

$$\text{stress}(\mathbf{X}) = \sum_{i \neq j} (d_{ij} - \|\mathbf{x}_i - \mathbf{x}_j\|)^2.$$

This loss function is known as *least-squares* or *Kruskal-Shepard scaling*.

A modification of *least-squares* scaling is the *Sammon mapping*

$$\text{stress}_{\text{Sammon}}(\mathbf{X}) = \sum_{i \neq j} \frac{(d_{ij} - \|\mathbf{x}_i - \mathbf{x}_j\|)^2}{d_{ij}}.$$

The Sammon mapping performs better at preserving small distances compared to the *least-squares* scaling.

### Classical multidimensional scaling

Also known as *principal coordinates analysis*, PCoA.

- The distance matrix,  $\mathbf{D}$ , is transformed to a *similarity matrix*,  $\mathbf{B}$ , often using centered inner products.
- The loss function becomes

$$\text{stress}_{\text{classical}}(\mathbf{X}) = \sum_{i \neq j} (b_{ij} - \langle \mathbf{x}_i, \mathbf{x}_j \rangle)^2.$$

- The stress function in classical MDS is sometimes called *strain*.
- The solution for the classical MDS problems can be found from the eigenvectors of the similarity matrix.
- If the distances in  $\mathbf{D}$  are Euclidean and double centered inner products are used, the results are equivalent to PCA.

### Example

The eurodist dataset provides the road distances (in kilometers) between 21 cities in Europe. Given this matrix of pairwise (non-Euclidean) distances  $\mathbf{D} = [d_{ij}]$ , MDS can be used to recover the coordinates of the cities in some Euclidean referential whose orientation is arbitrary.

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

# Pairwise distance between European cities
try:
    url = '../datasets/eurodist.csv'
    df = pd.read_csv(url)
except:
    url = 'https://raw.githubusercontent.com/neurospin/pystatsml/master/datasets/eurodist.csv'
    df = pd.read_csv(url)

print(df.iloc[:5, :5])

city = df["city"]
D = np.array(df.iloc[:, 1:]) # Distance matrix

# Arbitrary choice of K=2 components
from sklearn.manifold import MDS
mds = MDS(dissimilarity='precomputed', n_components=2, random_state=40, max_iter=3000,
           eps=1e-9)
X = mds.fit_transform(D)
```

	city	Athens	Barcelona	Brussels	Calais
0	Athens	0	3313	2963	3175
1	Barcelona	3313	0	1318	1326

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2	Brussels	2963	1318	0	204
3	Calais	3175	1326	204	0
4	Cherbourg	3339	1294	583	460

Recover coordinates of the cities in Euclidean referential whose orientation is arbitrary:

```
from sklearn import metrics
Declidean = metrics.pairwise.pairwise_distances(X, metric='euclidean')
print(np.round(Declidean[:5, :5]))
```

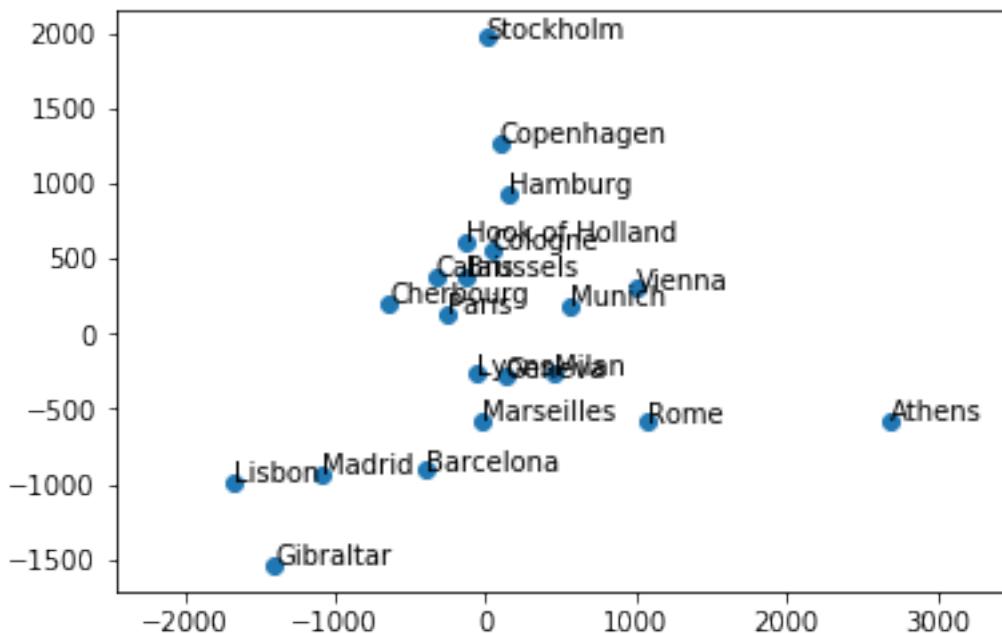
```
[[ 0. 3116. 2994. 3181. 3428.]
 [3116. 0. 1317. 1289. 1128.]
 [2994. 1317. 0. 198. 538.]
 [3181. 1289. 198. 0. 358.]
 [3428. 1128. 538. 358. 0.]]
```

Plot the results:

```
# Plot: apply some rotation and flip
theta = 80 * np.pi / 180.
rot = np.array([[np.cos(theta), -np.sin(theta)],
               [np.sin(theta), np.cos(theta)]])
Xr = np.dot(X, rot)
# flip x
Xr[:, 0] *= -1
plt.scatter(Xr[:, 0], Xr[:, 1])

for i in range(len(city)):
    plt.text(Xr[i, 0], Xr[i, 1], city[i])
plt.axis('equal')
```

```
(-1894.1017744377398,
 2914.3652937179477,
 -1712.9885463201906,
 2145.4522453884565)
```



### Determining the number of components

We must choose  $K^* \in \{1, \dots, K\}$  the number of required components. Plotting the values of the stress function, obtained using  $k \leq N - 1$  components. In general, start with  $1, \dots, K \leq 4$ . Choose  $K^*$  where you can clearly distinguish an *elbow* in the stress curve.

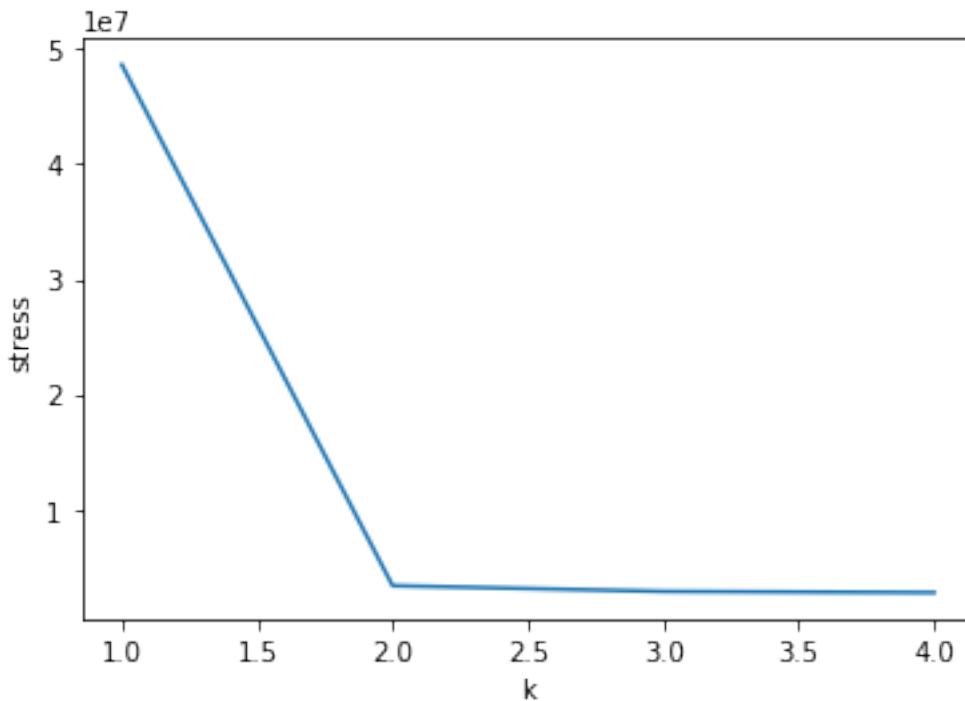
Thus, in the plot below, we choose to retain information accounted for by the first *two* components, since this is where the *elbow* is in the stress curve.

```
k_range = range(1, min(5, D.shape[0]-1))
stress = [MDS(dissimilarity='precomputed', n_components=k,
              random_state=42, max_iter=300, eps=1e-9).fit(D).stress_ for k in k_range]

print(stress)
plt.plot(k_range, stress)
plt.xlabel("k")
plt.ylabel("stress")
```

```
[48644495.28571428, 3356497.365752386, 2858455.495887962, 2756310.637628011]
```

```
Text(0, 0.5, 'stress')
```



### 5.1.5 Nonlinear dimensionality reduction

Sources:

- Scikit-learn documentation
- Wikipedia

Nonlinear dimensionality reduction or **manifold learning** cover unsupervised methods that attempt to identify low-dimensional manifolds within the original  $P$ -dimensional space that represent high data density. Then those methods provide a mapping from the high-dimensional space to the low-dimensional embedding.

#### Isomap

Isomap is a nonlinear dimensionality reduction method that combines a procedure to compute the distance matrix with MDS. The distances calculation is based on geodesic distances evaluated on neighborhood graph:

1. Determine the neighbors of each point. All points in some fixed radius or K nearest neighbors.
2. Construct a neighborhood graph. Each point is connected to other if it is a K nearest neighbor. Edge length equal to Euclidean distance.
3. Compute shortest path between pairwise of points  $d_{ij}$  to build the distance matrix  $\mathbf{D}$ .
4. Apply MDS on  $\mathbf{D}$ .

```
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from sklearn import manifold, datasets
```

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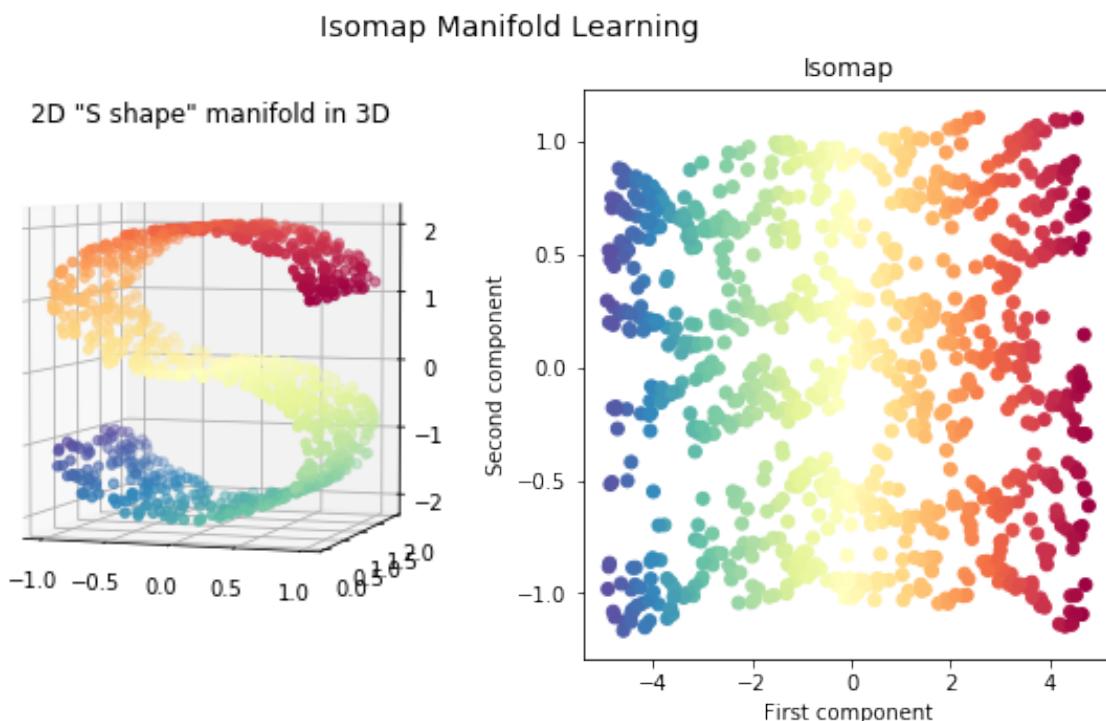
```
X, color = datasets.samples_generator.make_s_curve(1000, random_state=42)

fig = plt.figure(figsize=(10, 5))
plt.suptitle("Isomap Manifold Learning", fontsize=14)

ax = fig.add_subplot(121, projection='3d')
ax.scatter(X[:, 0], X[:, 1], X[:, 2], c=color, cmap=plt.cm.Spectral)
ax.view_init(4, -72)
plt.title('2D "S shape" manifold in 3D')

Y = manifold.Isomap(n_neighbors=10, n_components=2).fit_transform(X)
ax = fig.add_subplot(122)
plt.scatter(Y[:, 0], Y[:, 1], c=color, cmap=plt.cm.Spectral)
plt.title("Isomap")
plt.xlabel("First component")
plt.ylabel("Second component")
plt.axis('tight')
```

(-5.4164373180970316, 5.276311544714793, -1.2910940054965336, 1.23497771017066)



## 5.1.6 Exercises

### PCA

#### Write a basic PCA class

Write a class BasicPCA with two methods:

- `fit(X)` that estimates the data mean, principal components directions  $V$  and the explained variance of each component.
- `transform(X)` that projects the data onto the principal components.

Check that your BasicPCA gave similar results, compared to the results from sklearn.

### Apply your Basic PCA on the `iris` dataset

The data set is available at: <https://raw.github.com/neurospin/pystatsml/master/datasets/iris.csv>

- Describe the data set. Should the dataset been standardized?
- Describe the structure of correlations among variables.
- Compute a PCA with the maximum number of components.
- Compute the cumulative explained variance ratio. Determine the number of components  $K$  by your computed values.
- Print the  $K$  principal components directions and correlations of the  $K$  principal components with the original variables. Interpret the contribution of the original variables into the PC.
- Plot the samples projected into the  $K$  first PCs.
- Color samples by their species.

### MDS

Apply MDS from sklearn on the `iris` dataset available at:

<https://raw.github.com/neurospin/pystatsml/master/datasets/iris.csv>

- Center and scale the dataset.
- Compute Euclidean pairwise distances matrix.
- Select the number of components.
- Show that classical MDS on Euclidean pairwise distances matrix is equivalent to PCA.

## 5.2 Clustering

Wikipedia: Cluster analysis or clustering is the task of grouping a set of objects in such a way that objects in the same group (called a cluster) are more similar (in some sense or another) to each other than to those in other groups (clusters). Clustering is one of the main tasks of exploratory data mining, and a common technique for statistical data analysis, used in many fields, including machine learning, pattern recognition, image analysis, information retrieval, and bioinformatics.

Sources: <http://scikit-learn.org/stable/modules/clustering.html>

### 5.2.1 K-means clustering

Source: C. M. Bishop *Pattern Recognition and Machine Learning*, Springer, 2006

Suppose we have a data set  $X = \{x_1, \dots, x_N\}$  that consists of  $N$  observations of a random  $D$ -dimensional Euclidean variable  $x$ . Our goal is to partition the data set into some number,  $K$ , of clusters, where we shall suppose for the moment that the value of  $K$  is given. Intuitively, we might think of a cluster as comprising a group of data points whose inter-point distances are small compared to the distances to points outside of the cluster. We can formalize this notion by first introducing a set of  $D$ -dimensional vectors  $\mu_k$ , where  $k = 1, \dots, K$ , in which  $\mu_k$  is a **prototype** associated with the  $k^{\text{th}}$  cluster. As we shall see shortly, we can think of the  $\mu_k$  as representing the centres of the clusters. Our goal is then to find an assignment of data points to clusters, as well as a set of vectors  $\{\mu_k\}$ , such that the sum of the squares of the distances of each data point to its closest prototype vector  $\mu_k$ , is at a minimum.

It is convenient at this point to define some notation to describe the assignment of data points to clusters. For each data point  $x_i$ , we introduce a corresponding set of binary indicator variables  $r_{ik} \in \{0, 1\}$ , where  $k = 1, \dots, K$ , that describes which of the  $K$  clusters the data point  $x_i$  is assigned to, so that if data point  $x_i$  is assigned to cluster  $k$  then  $r_{ik} = 1$ , and  $r_{ij} = 0$  for  $j \neq k$ . This is known as the 1-of- $K$  coding scheme. We can then define an objective function, denoted **inertia**, as

$$J(r, \mu) = \sum_i^N \sum_k^K r_{ik} \|x_i - \mu_k\|_2^2$$

which represents the sum of the squares of the Euclidean distances of each data point to its assigned vector  $\mu_k$ . Our goal is to find values for the  $\{r_{ik}\}$  and the  $\{\mu_k\}$  so as to minimize the function  $J$ . We can do this through an iterative procedure in which each iteration involves two successive steps corresponding to successive optimizations with respect to the  $r_{ik}$  and the  $\mu_k$ . First we choose some initial values for the  $\mu_k$ . Then in the first phase we minimize  $J$  with respect to the  $r_{ik}$ , keeping the  $\mu_k$  fixed. In the second phase we minimize  $J$  with respect to the  $\mu_k$ , keeping  $r_{ik}$  fixed. This two-stage optimization process is then repeated until convergence. We shall see that these two stages of updating  $r_{ik}$  and  $\mu_k$  correspond respectively to the expectation (E) and maximization (M) steps of the expectation-maximisation (EM) algorithm, and to emphasize this we shall use the terms E step and M step in the context of the  $K$ -means algorithm.

Consider first the determination of the  $r_{ik}$ . Because  $J$  is a linear function of  $r_{ik}$ , this optimization can be performed easily to give a closed form solution. The terms involving different  $i$  are independent and so we can optimize for each  $i$  separately by choosing  $r_{ik}$  to be 1 for whichever value of  $k$  gives the minimum value of  $\|x_i - \mu_k\|^2$ . In other words, we simply assign the  $i$ th data point to the closest cluster centre. More formally, this can be expressed as

$$r_{ik} = \begin{cases} 1, & \text{if } k = \arg \min_j \|x_i - \mu_j\|^2 \\ 0, & \text{otherwise.} \end{cases} \quad (5.15)$$

Now consider the optimization of the  $\mu_k$  with the  $r_{ik}$  held fixed. The objective function  $J$  is a quadratic function of  $\mu_k$ , and it can be minimized by setting its derivative with respect to  $\mu_k$  to zero giving

$$2 \sum_i r_{ik} (x_i - \mu_k) = 0$$

which we can easily solve for  $\mu_k$  to give

$$\mu_k = \frac{\sum_i r_{ik} x_i}{\sum_i r_{ik}}.$$

The denominator in this expression is equal to the number of points assigned to cluster  $k$ , and so this result has a simple interpretation, namely set  $\mu_k$  equal to the mean of all of the data points  $x_i$  assigned to cluster  $k$ . For this reason, the procedure is known as the  $K$ -means algorithm.

The two phases of re-assigning data points to clusters and re-computing the cluster means are repeated in turn until there is no further change in the assignments (or until some maximum number of iterations is exceeded). Because each phase reduces the value of the objective function  $J$ , convergence of the algorithm is assured. However, it may converge to a local rather than global minimum of  $J$ .

```
from sklearn import cluster, datasets
import matplotlib.pyplot as plt
import seaborn as sns # nice color
%matplotlib inline

iris = datasets.load_iris()
X = iris.data[:, :2] # use only 'sepal length' and 'sepal width'
y_iris = iris.target

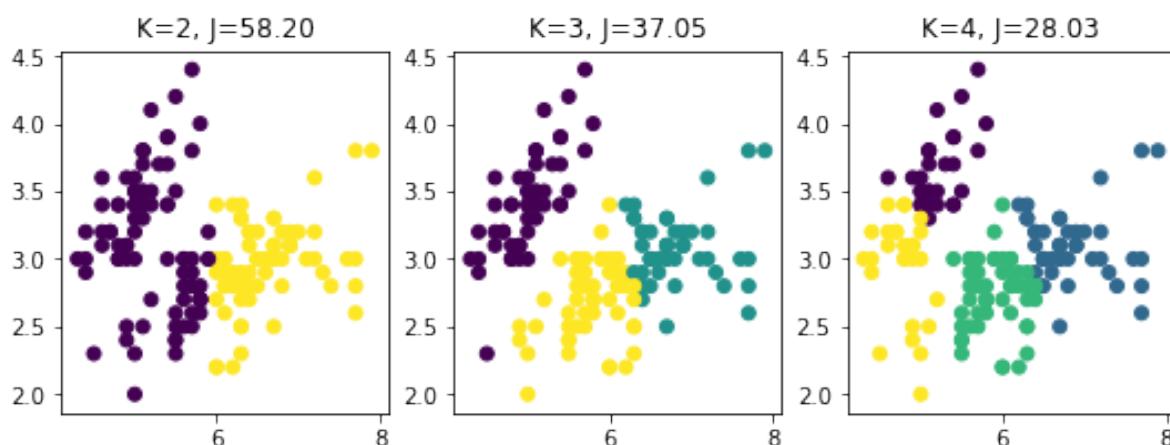
km2 = cluster.KMeans(n_clusters=2).fit(X)
km3 = cluster.KMeans(n_clusters=3).fit(X)
km4 = cluster.KMeans(n_clusters=4).fit(X)

plt.figure(figsize=(9, 3))
plt.subplot(131)
plt.scatter(X[:, 0], X[:, 1], c=km2.labels_)
plt.title("K=2, J=% .2f" % km2.inertia_)

plt.subplot(132)
plt.scatter(X[:, 0], X[:, 1], c=km3.labels_)
plt.title("K=3, J=% .2f" % km3.inertia_)

plt.subplot(133)
plt.scatter(X[:, 0], X[:, 1], c=km4.labels_.astype(np.float))
plt.title("K=4, J=% .2f" % km4.inertia_)
```

Text(0.5, 1.0, 'K=4, J=28.03')



## Exercises

### 1. Analyse clusters

- Analyse the plot above visually. What would a good value of  $K$  be?
- If you instead consider the inertia, the value of  $J$ , what would a good value of  $K$  be?
- Explain why there is such difference.
- For  $K = 2$  why did  $K$ -means clustering not find the two “natural” clusters? See the assumptions of  $K$ -means: [http://scikit-learn.org/stable/auto\\_examples/cluster/plot\\_kmeans\\_assumptions.html#example-cluster-plot-kmeans-assumptions-py](http://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_assumptions.html#example-cluster-plot-kmeans-assumptions-py)

### 2. Re-implement the $K$ -means clustering algorithm (homework)

Write a function `kmeans(X, K)` that return an integer vector of the samples' labels.

## 5.2.2 Hierarchical clustering

Hierarchical clustering is an approach to clustering that build hierarchies of clusters in two main approaches:

- **Agglomerative:** A *bottom-up* strategy, where each observation starts in their own cluster, and pairs of clusters are merged upwards in the hierarchy.
- **Divisive:** A *top-down* strategy, where all observations start out in the same cluster, and then the clusters are split recursively downwards in the hierarchy.

In order to decide which clusters to merge or to split, a measure of dissimilarity between clusters is introduced. More specific, this comprise a *distance* measure and a *linkage* criterion. The distance measure is just what it sounds like, and the linkage criterion is essentially a function of the distances between points, for instance the minimum distance between points in two clusters, the maximum distance between points in two clusters, the average distance between points in two clusters, etc. One particular linkage criterion, the Ward criterion, will be discussed next.

### Ward clustering

Ward clustering belongs to the family of agglomerative hierarchical clustering algorithms. This means that they are based on a “bottoms up” approach: each sample starts in its own cluster, and pairs of clusters are merged as one moves up the hierarchy.

In Ward clustering, the criterion for choosing the pair of clusters to merge at each step is the minimum variance criterion. Ward’s minimum variance criterion minimizes the total within-cluster variance by each merge. To implement this method, at each step: find the pair of clusters that leads to minimum increase in total within-cluster variance after merging. This increase is a weighted squared distance between cluster centers.

The main advantage of agglomerative hierarchical clustering over  $K$ -means clustering is that you can benefit from known neighborhood information, for example, neighboring pixels in an image.

```
from sklearn import cluster, datasets
import matplotlib.pyplot as plt
import seaborn as sns # nice color

iris = datasets.load_iris()
X = iris.data[:, :2] # 'sepal length (cm)' 'sepal width (cm)'
y_iris = iris.target

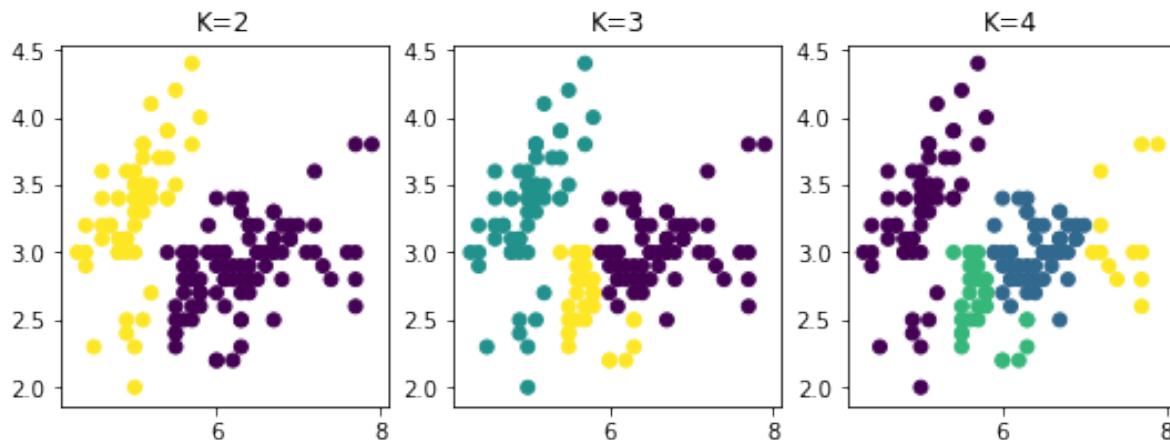
ward2 = cluster.AgglomerativeClustering(n_clusters=2, linkage='ward').fit(X)
ward3 = cluster.AgglomerativeClustering(n_clusters=3, linkage='ward').fit(X)
ward4 = cluster.AgglomerativeClustering(n_clusters=4, linkage='ward').fit(X)

plt.figure(figsize=(9, 3))
plt.subplot(131)
plt.scatter(X[:, 0], X[:, 1], c=ward2.labels_)
plt.title("K=2")

plt.subplot(132)
plt.scatter(X[:, 0], X[:, 1], c=ward3.labels_)
plt.title("K=3")

plt.subplot(133)
plt.scatter(X[:, 0], X[:, 1], c=ward4.labels_) # .astype(np.float))
plt.title("K=4")
```

```
Text(0.5, 1.0, 'K=4')
```



### 5.2.3 Gaussian mixture models

The Gaussian mixture model (GMM) is a simple linear superposition of Gaussian components over the data, aimed at providing a rich class of density models. We turn to a formulation of Gaussian mixtures in terms of discrete latent variables: the  $K$  hidden classes to be discovered.

Differences compared to  $K$ -means:

- Whereas the  $K$ -means algorithm performs a hard assignment of data points to clusters, in which each data point is associated uniquely with one cluster, the GMM algorithm makes a soft assignment based on posterior probabilities.
- Whereas the classic  $K$ -means is only based on Euclidean distances, classic GMM use a

Mahalanobis distances that can deal with non-spherical distributions. It should be noted that Mahalanobis could be plugged within an improved version of  $K$ -Means clustering. The Mahalanobis distance is unitless and scale-invariant, and takes into account the correlations of the data set.

The Gaussian mixture distribution can be written as a linear superposition of  $K$  Gaussians in the form:

$$p(x) = \sum_{k=1}^K \mathcal{N}(x | \mu_k, \Sigma_k) p(k),$$

where:

- The  $p(k)$  are the mixing coefficients also known as the class probability of class  $k$ , and they sum to one:  $\sum_{k=1}^K p(k) = 1$ .
- $\mathcal{N}(x | \mu_k, \Sigma_k) = p(x | k)$  is the conditional distribution of  $x$  given a particular class  $k$ . It is the multivariate Gaussian distribution defined over a  $P$ -dimensional vector  $x$  of continuous variables.

The goal is to maximize the log-likelihood of the GMM:

$$\ln \prod_{i=1}^N p(x_i) = \ln \prod_{i=1}^N \left\{ \sum_{k=1}^K \mathcal{N}(x_i | \mu_k, \Sigma_k) p(k) \right\} = \sum_{i=1}^N \ln \left\{ \sum_{k=1}^K \mathcal{N}(x_i | \mu_k, \Sigma_k) p(k) \right\}.$$

To compute the classes parameters:  $p(k), \mu_k, \Sigma_k$  we sum over all samples, by weighting each sample  $i$  by its responsibility or contribution to class  $k$ :  $p(k | x_i)$  such that for each point its contribution to all classes sum to one  $\sum_k p(k | x_i) = 1$ . This contribution is the conditional probability of class  $k$  given  $x$ :  $p(k | x)$  (sometimes called the posterior). It can be computed using Bayes' rule:

$$p(k | x) = \frac{p(x | k)p(k)}{p(x)} \tag{5.16}$$

$$= \frac{\mathcal{N}(x | \mu_k, \Sigma_k)p(k)}{\sum_{k=1}^K \mathcal{N}(x | \mu_k, \Sigma_k)p(k)} \tag{5.17}$$

Since the class parameters,  $p(k)$ ,  $\mu_k$  and  $\Sigma_k$ , depend on the responsibilities  $p(k | x)$  and the responsibilities depend on class parameters, we need a two-step iterative algorithm: the expectation-maximization (EM) algorithm. We discuss this algorithm next.

### The expectation-maximization (EM) algorithm for Gaussian mixtures

Given a Gaussian mixture model, the goal is to maximize the likelihood function with respect to the parameters (comprised of the means and covariances of the components and the mixing coefficients).

Initialize the means  $\mu_k$ , covariances  $\Sigma_k$  and mixing coefficients  $p(k)$

1. **E step.** For each sample  $i$ , evaluate the responsibilities for each class  $k$  using the current parameter values

$$p(k | x_i) = \frac{\mathcal{N}(x_i | \mu_k, \Sigma_k)p(k)}{\sum_{k=1}^K \mathcal{N}(x_i | \mu_k, \Sigma_k)p(k)}$$

2. **M step.** For each class, re-estimate the parameters using the current responsibilities

$$\mu_k^{\text{new}} = \frac{1}{N_k} \sum_{i=1}^N p(k|x_i) x_i \quad (5.18)$$

$$\Sigma_k^{\text{new}} = \frac{1}{N_k} \sum_{i=1}^N p(k|x_i) (x_i - \mu_k^{\text{new}})(x_i - \mu_k^{\text{new}})^T \quad (5.19)$$

$$p^{\text{new}}(k) = \frac{N_k}{N} \quad (5.20)$$

### 3. Evaluate the log-likelihood

$$\sum_{i=1}^N \ln \left\{ \sum_{k=1}^K \mathcal{N}(x|\mu_k, \Sigma_k) p(k) \right\},$$

and check for convergence of either the parameters or the log-likelihood. If the convergence criterion is not satisfied return to step 1.

```

import numpy as np
from sklearn import datasets
import matplotlib.pyplot as plt
import seaborn as sns # nice color
import sklearn
from sklearn.mixture import GaussianMixture

import pystatsml.plot_utils

colors = sns.color_palette()

iris = datasets.load_iris()
X = iris.data[:, :2] # 'sepal length (cm)' 'sepal width (cm)'
y_iris = iris.target

gmm2 = GaussianMixture(n_components=2, covariance_type='full').fit(X)
gmm3 = GaussianMixture(n_components=3, covariance_type='full').fit(X)
gmm4 = GaussianMixture(n_components=4, covariance_type='full').fit(X)

plt.figure(figsize=(9, 3))
plt.subplot(131)
plt.scatter(X[:, 0], X[:, 1], c=[colors[lab] for lab in gmm2.predict(X)])#, color=colors)
for i in range(gmm2.covariances_.shape[0]):
    pystatsml.plot_utils.plot_cov_ellipse(cov=gmm2.covariances_[i, :], pos=gmm2.means_[i, :],
                                          facecolor='none', linewidth=2, edgecolor=colors[i])
    plt.scatter(gmm2.means_[i, 0], gmm2.means_[i, 1], edgecolor=colors[i],
                marker="o", s=100, facecolor="w", linewidth=2)
plt.title("K=2")

plt.subplot(132)
plt.scatter(X[:, 0], X[:, 1], c=[colors[lab] for lab in gmm3.predict(X)])
for i in range(gmm3.covariances_.shape[0]):
    pystatsml.plot_utils.plot_cov_ellipse(cov=gmm3.covariances_[i, :], pos=gmm3.means_[i, :],
                                          facecolor='none', linewidth=2, edgecolor=colors[i])
    plt.scatter(gmm3.means_[i, 0], gmm3.means_[i, 1], edgecolor=colors[i],
                marker="o", s=100, facecolor="w", linewidth=2)

```

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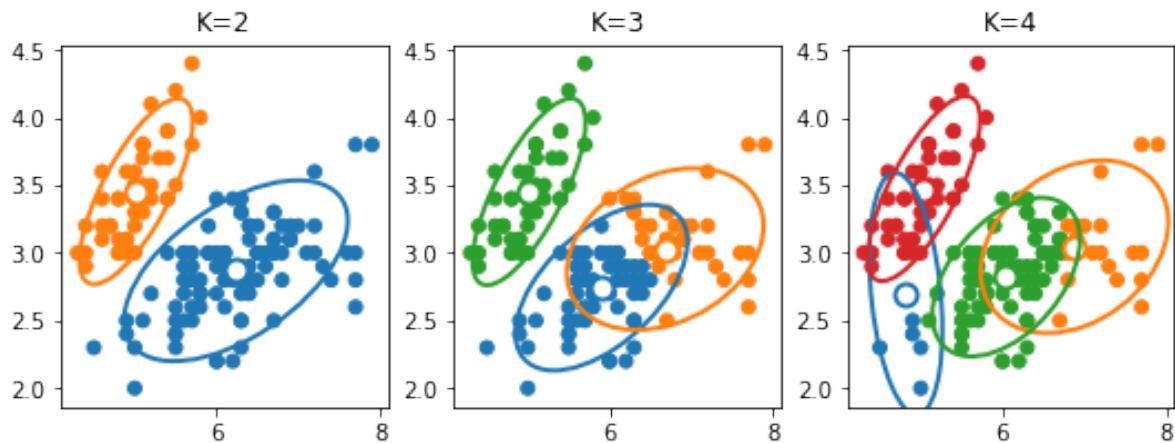
(continued from previous page)

```

plt.title("K=3")

plt.subplot(133)
plt.scatter(X[:, 0], X[:, 1], c=[colors[lab] for lab in gmm4.predict(X)]) # .astype(np.
#float)
for i in range(gmm4.covariances_.shape[0]):
    pystatsml.plot_utils.plot_cov_ellipse(cov=gmm4.covariances_[i, :], pos=gmm4.means_[i, :],
                                          facecolor='none', linewidth=2, edgecolor=colors[i])
    plt.scatter(gmm4.means_[i, 0], gmm4.means_[i, 1], edgecolor=colors[i],
                marker="o", s=100, facecolor="w", linewidth=2)
_ = plt.title("K=4")

```



## 5.2.4 Model selection

```
### Bayesian information criterion
```

In statistics, the Bayesian information criterion (BIC) is a criterion for model selection among a finite set of models; the model with the lowest BIC is preferred. It is based, in part, on the likelihood function and it is closely related to the Akaike information criterion (AIC).

```

X = iris.data
y_iris = iris.target

bic = list()
#print(X)

ks = np.arange(1, 10)

for k in ks:
    gmm = GaussianMixture(n_components=k, covariance_type='full')
    gmm.fit(X)
    bic.append(gmm.bic(X))

k_chosen = ks[np.argmin(bic)]

plt.plot(ks, bic)
plt.xlabel("k")
plt.ylabel("BIC")

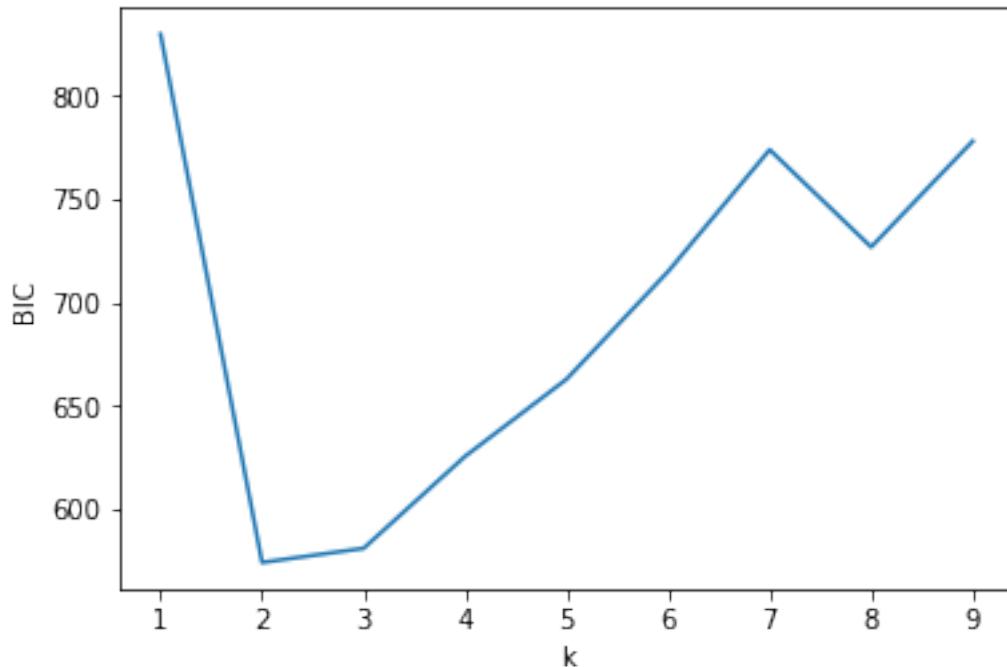
```

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```
print("Choose k=", k_chosen)
```

```
Choose k= 2
```



### 5.2.5 Exercises

Perform clustering of the iris dataset based on all variables using Gaussian mixture models. Use PCA to visualize clusters.

## 5.3 Linear methods for regression

### 5.3.1 Ordinary least squares

Linear regression models the **output**, or **target** variable  $y \in \mathbb{R}$  as a linear combination of the  $(P - 1)$ -dimensional input  $x \in \mathbb{R}^{(P-1)}$ . Let  $\mathbf{X}$  be the  $N \times P$  matrix with each row an input vector (with a 1 in the first position), and similarly let  $y$  be the  $N$ -dimensional vector of outputs in the **training set**, the linear model will predict the  $y$  given  $\mathbf{X}$  using the **parameter vector**, or **weight vector**  $\beta \in \mathbb{R}^P$  according to

$$\mathbf{y} = \mathbf{X}\beta + \varepsilon,$$

where  $\varepsilon \in \mathbb{R}^N$  are the **residuals**, or the errors of the prediction. The  $\beta$  is found by minimizing an **objective function**, which is the **loss function**,  $\mathcal{L}(\beta)$ , i.e. the error measured on the data. This error is the **sum of squared errors (SSE) loss**. Minimizing the SSE is the Ordinary Least Square **OLS** regression as objective function.

$$\text{OLS}(\boldsymbol{\beta}) = \mathcal{L}(\boldsymbol{\beta}) \quad (5.21)$$

$$= \text{SSE}(\boldsymbol{\beta}) \quad (5.22)$$

$$= \sum_i^N (y_i - \mathbf{x}_i^T \boldsymbol{\beta})^2 \quad (5.23)$$

$$= (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) \quad (5.24)$$

$$= \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2, \quad (5.25)$$

which is a simple **ordinary least squares (OLS)** minimization.

### 5.3.2 Linear regression with scikit-learn

Scikit learn offer many models for supervised learning, and they all follow the same application programming interface (API), namely:

```
model = Estimator()
model.fit(X, y)
predictions = model.predict(X)
```

```
%matplotlib inline
import warnings
warnings.filterwarnings(action='once')
```

```
from mpl_toolkits.mplot3d import Axes3D
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
import sklearn.linear_model as lm
import sklearn.metrics as metrics
%matplotlib inline

# Fit Ordinary Least Squares: OLS
csv = pd.read_csv('https://raw.githubusercontent.com/neurospin/pystatsml/master/datasets/
                   ↪Advertising.csv', index_col=0)
X = csv[['TV', 'Radio']]
y = csv['Sales']

lr = lm.LinearRegression().fit(X, y)
y_pred = lr.predict(X)
print("R-squared =", metrics.r2_score(y, y_pred))

print("Coefficients =", lr.coef_)

# Plot
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')

ax.scatter(csv['TV'], csv['Radio'], csv['Sales'], c='r', marker='o')

xx1, xx2 = np.meshgrid(
    np.linspace(csv['TV'].min(), csv['TV'].max(), num=10),
```

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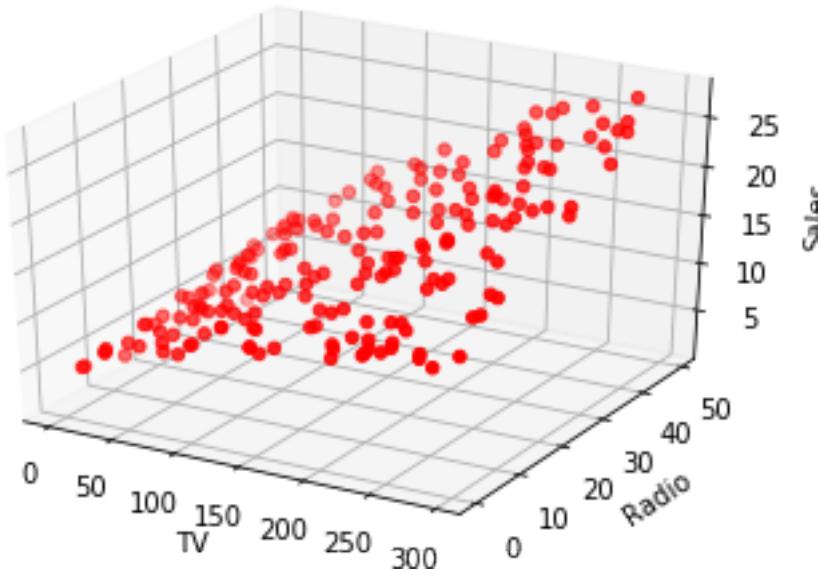
```
np.linspace(csv['Radio'].min(), csv['Radio'].max(), num=10))

XX = np.column_stack([xx1.ravel(), xx2.ravel()])

yy = lr.predict(XX)
ax.plot_surface(xx1, xx2, yy.reshape(xx1.shape), color='None')
ax.set_xlabel('TV')
ax.set_ylabel('Radio')
_ = ax.set_zlabel('Sales')
```

```
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
    ↪ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
    ↪got 216 from PyObject
    ↪return f(*args, **kwds)
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
    ↪ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
    ↪got 216 from PyObject
    ↪return f(*args, **kwds)
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
    ↪ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
    ↪got 216 from PyObject
    ↪return f(*args, **kwds)
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
    ↪ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
    ↪got 216 from PyObject
    ↪return f(*args, **kwds)
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
    ↪ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
    ↪got 216 from PyObject
    ↪return f(*args, **kwds)
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
    ↪ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
    ↪got 216 from PyObject
    ↪return f(*args, **kwds)
```

```
R-squared = 0.8971942610828956
Coefficients = [0.04575482 0.18799423]
```



### 5.3.3 Overfitting

In statistics and machine learning, overfitting occurs when a statistical model describes random errors or noise instead of the underlying relationships. Overfitting generally occurs when a model is **excessively complex**, such as having **too many parameters relative to the number of observations**. A model that has been overfit will generally have poor predictive performance, as it can exaggerate minor fluctuations in the data.

A learning algorithm is trained using some set of training samples. If the learning algorithm has the capacity to overfit the training samples the performance on the **training sample set** will improve while the performance on unseen **test sample set** will decline.

The overfitting phenomenon has three main explanations: - excessively complex models, - multicollinearity, and - high dimensionality.

#### Model complexity

Complex learners with too many parameters relative to the number of observations may overfit the training dataset.

#### Multicollinearity

Predictors are highly correlated, meaning that one can be linearly predicted from the others. In this situation the coefficient estimates of the multiple regression may change erratically in response to small changes in the model or the data. Multicollinearity does not reduce the predictive power or reliability of the model as a whole, at least not within the sample data set; it only affects computations regarding individual predictors. That is, a multiple regression model with correlated predictors can indicate how well the entire bundle of predictors predicts the outcome variable, but it may not give valid results about any individual predictor, or about which predictors are redundant with respect to others. In case of perfect multicollinearity the predictor matrix is singular and therefore cannot be inverted. Under these circumstances, for a

general linear model  $\mathbf{y} = \mathbf{X}\beta + \varepsilon$ , the ordinary least-squares estimator,  $\beta_{OLS} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$ , does not exist.

An example where correlated predictor may produce an unstable model follows:

```

import numpy as np
from mpl_toolkits.mplot3d import Axes3D
import matplotlib.pyplot as plt

bv = np.array([10, 20, 30, 40, 50])           # business volume
tax = .2 * bv                                # Tax
bp = .1 * bv + np.array([-1, .2, .1, -.2, .1]) # business potential

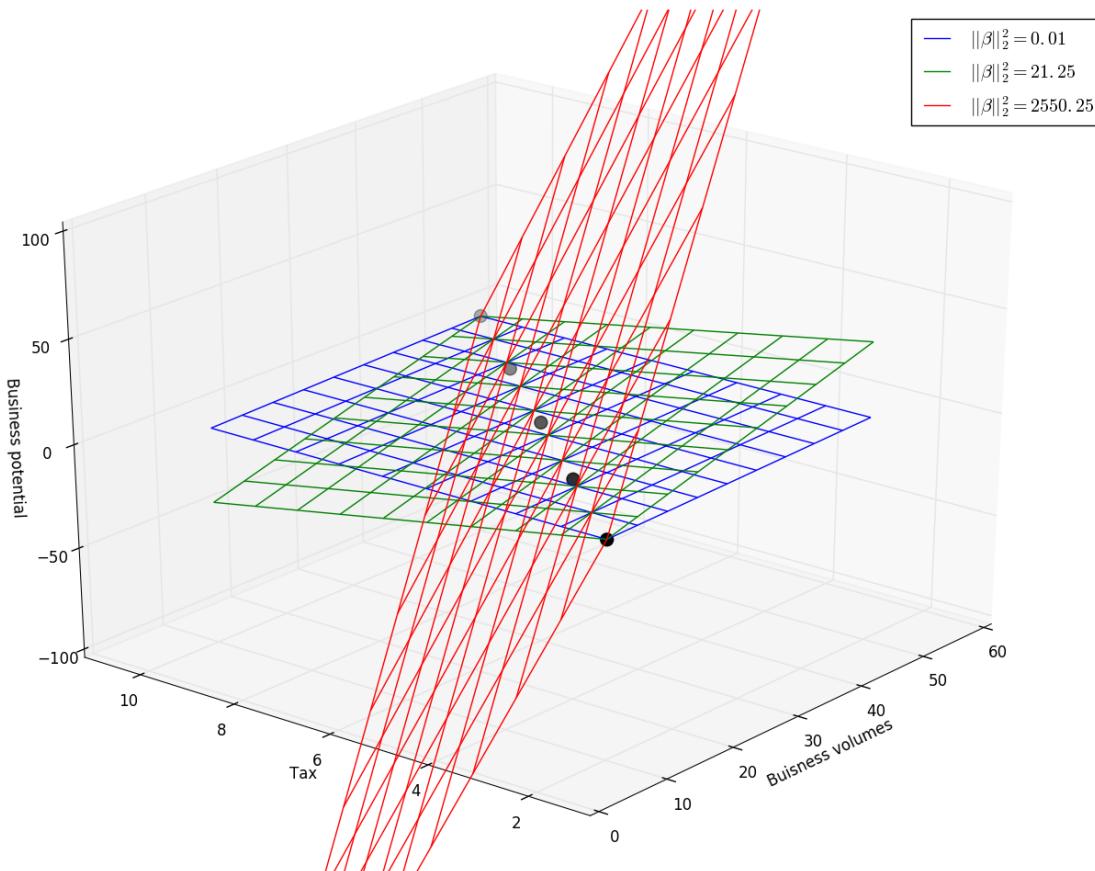
X = np.column_stack([bv, tax])
beta_star = np.array([.1, 0]) # true solution
...
Since tax and bv are correlated, there is an infinite number of linear combinations
leading to the same prediction.
"""

# 10 times the bv then subtract it 9 times using the tax variable:
beta_medium = np.array([.1 * 10, -.1 * 9 * (1/.2)])
# 100 times the bv then subtract it 99 times using the tax variable:
beta_large = np.array([.1 * 100, -.1 * 99 * (1/.2)])

# Check that all model lead to the same result
assert np.all(np.dot(X, beta_star) == np.dot(X, beta_medium))
assert np.all(np.dot(X, beta_star) == np.dot(X, beta_large))

```

Multicollinearity between the predictors: business volumes and tax produces unstable models with arbitrary large coefficients.



Dealing with multicollinearity:

- Regularisation by e.g.  $\ell_2$  shrinkage: Introduce a bias in the solution by making  $(X^T X)^{-1}$  non-singular. See  $\ell_2$  shrinkage.
- Feature selection: select a small number of features. See: Isabelle Guyon and André Elisseeff *An introduction to variable and feature selection* The Journal of Machine Learning Research, 2003.
- Feature selection: select a small number of features using  $\ell_1$  shrinkage.
- Extract few independent (uncorrelated) features using e.g. principal components analysis (PCA), partial least squares regression (PLS-R) or regression methods that cut the number of predictors to a smaller set of uncorrelated components.

## High dimensionality

High dimensions means a large number of input features. Linear predictor associate one parameter to each input feature, so a high-dimensional situation ( $P$ , number of features, is large) with a relatively small number of samples  $N$  (so-called large  $P$  small  $N$  situation) generally lead to an overfit of the training data. Thus it is generally a bad idea to add many input features into the learner. This phenomenon is called the **curse of dimensionality**.

One of the most important criteria to use when choosing a learning algorithm is based on the relative size of  $P$  and  $N$ .

- Remember that the “covariance” matrix  $\mathbf{X}^T \mathbf{X}$  used in the linear model is a  $P \times P$  matrix of rank  $\min(N, P)$ . Thus if  $P > N$  the equation system is overparameterized and admit an

infinity of solutions that might be specific to the learning dataset. See also ill-conditioned or singular matrices.

- The sampling density of  $N$  samples in an  $P$ -dimensional space is proportional to  $N^{1/P}$ . Thus a high-dimensional space becomes very sparse, leading to poor estimations of samples densities.
- Another consequence of the sparse sampling in high dimensions is that all sample points are close to an edge of the sample. Consider  $N$  data points uniformly distributed in a  $P$ -dimensional unit ball centered at the origin. Suppose we consider a nearest-neighbor estimate at the origin. The median distance from the origin to the closest data point is given by the expression

$$d(P, N) = \left(1 - \frac{1}{2}^N\right)^{1/P}.$$

A more complicated expression exists for the mean distance to the closest point. For  $N = 500$ ,  $P = 10$ ,  $d(P, N) \approx 0.52$ , more than halfway to the boundary. Hence most data points are closer to the boundary of the sample space than to any other data point. The reason that this presents a problem is that prediction is much more difficult near the edges of the training sample. One must extrapolate from neighboring sample points rather than interpolate between them. (Source: T Hastie, R Tibshirani, J Friedman. *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*. Second Edition, 2009.)

- Structural risk minimization provides a theoretical background of this phenomenon. (See VC dimension.)
- See also bias-variance trade-off.

```
import seaborn # nicer plots

def fit_on_increasing_size(model):
    n_samples = 100
    n_features_ = np.arange(10, 800, 20)
    r2_train, r2_test, snr = [], [], []
    for n_features in n_features_:
        # Sample the dataset (* 2 nb of samples)
        n_features_info = int(n_features/10)
        np.random.seed(42) # Make reproducible
        X = np.random.randn(n_samples * 2, n_features)
        beta = np.zeros(n_features)
        beta[:n_features_info] = 1
        Xbeta = np.dot(X, beta)
        eps = np.random.randn(n_samples * 2)
        y = Xbeta + eps
        # Split the dataset into train and test sample
        Xtrain, Xtest = X[:n_samples, :], X[n_samples:, :]
        ytrain, ytest = y[:n_samples], y[n_samples:]
        # fit/predict
        lr = model.fit(Xtrain, ytrain)
        y_pred_train = lr.predict(Xtrain)
        y_pred_test = lr.predict(Xtest)
        snr.append(Xbeta.std() / eps.std())
        r2_train.append(metrics.r2_score(ytrain, y_pred_train))
        r2_test.append(metrics.r2_score(ytest, y_pred_test))
    return n_features_, np.array(r2_train), np.array(r2_test), np.array(snr)
```

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```

def plot_r2_snr(n_features_, r2_train, r2_test, xvline, snr, ax):
    """
    Two scales plot. Left y-axis: train test r-squared. Right y-axis SNR.
    """
    ax.plot(n_features_, r2_train, label="Train r-squared", linewidth=2)
    ax.plot(n_features_, r2_test, label="Test r-squared", linewidth=2)
    ax.axvline(x=xvline, linewidth=2, color='k', ls='--')
    ax.axhline(y=0, linewidth=1, color='k', ls='--')
    ax.set_xlim(-0.2, 1.1)
    ax.set_xlabel("Number of input features")
    ax.set_ylabel("r-squared")
    ax.legend(loc='best')
    ax.set_title("Prediction perf.")
    ax_right = ax.twinx()
    ax_right.plot(n_features_, snr, 'r-', label="SNR", linewidth=1)
    ax_right.set_ylabel("SNR", color='r')
    for tl in ax_right.get_yticklabels():
        tl.set_color('r')

# Model = linear regression
mod = lm.LinearRegression()

# Fit models on dataset
n_features, r2_train, r2_test, snr = fit_on_increasing_size(model=mod)

argmax = n_features[np.argmax(r2_test)]

# plot
fig, axis = plt.subplots(1, 2, figsize=(9, 3))

# Left pane: all features
plot_r2_snr(n_features, r2_train, r2_test, argmax, snr, axis[0])

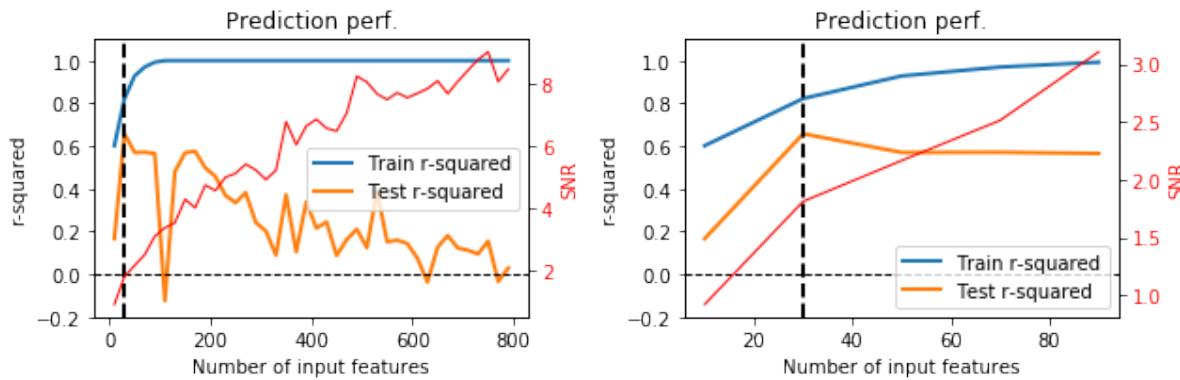
# Right pane: Zoom on 100 first features
plot_r2_snr(n_features[n_features <= 100],
            r2_train[n_features <= 100], r2_test[n_features <= 100],
            argmax,
            snr[n_features <= 100],
            axis[1])
plt.tight_layout()

```

```

/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
    ↵ufunc size changed, may indicate binary incompatibility. Expected 216, got 192
    return f(*args, **kwds)
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: ImportWarning: can't
    ↵resolve package from __spec__ or __package__, falling back on __name__ and __path__
    return f(*args, **kwds)
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
    ↵ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,
    ↵got 216 from PyObject
    return f(*args, **kwds)

```



## Exercises

Study the code above and:

- Describe the datasets:  $N$ : nb\_samples,  $P$ : nb\_features.
- What is n\_features\_info?
- Give the equation of the generative model.
- What is modified by the loop?
- What is the SNR?

Comment the graph above, in terms of training and test performances:

- How does the train and test performance changes as a function of  $x$ ?
- Is it the expected results when compared to the SNR?
- What can you conclude?

### 5.3.4 Ridge regression ( $\ell_2$ -regularization)

Overfitting generally leads to excessively complex weight vectors, accounting for noise or spurious correlations within predictors. To avoid this phenomenon the learning should **constrain the solution** in order to fit a global pattern. This constraint will reduce (bias) the capacity of the learning algorithm. Adding such a penalty will force the coefficients to be small, i.e. to shrink them toward zeros.

Therefore the **loss function**  $\mathcal{L}(\beta)$  (generally the SSE) is combined with a **penalty function**  $\Omega(\beta)$  leading to the general form:

$$\text{Penalized}(\beta) = \mathcal{L}(\beta) + \lambda\Omega(\beta)$$

The respective contribution of the loss and the penalty is controlled by the **regularization parameter**  $\lambda$ .

Ridge regression impose a  $\ell_2$  penalty on the coefficients, i.e. it penalizes with the Euclidean norm of the coefficients while minimizing SSE. The objective function becomes:

$$\text{Ridge}(\beta) = \|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \lambda\|\beta\|_2^2.$$

The  $\beta$  that minimises  $F_{\text{Ridge}}(\beta)$  can be found by the following derivation:

$$\nabla_{\beta} \text{Ridge}(\beta) = 0 \quad (5.26)$$

$$\nabla_{\beta}((y - X\beta)^T(y - X\beta) + \lambda\beta^T\beta) = 0 \quad (5.27)$$

$$\nabla_{\beta}((y^T y - 2\beta^T X^T y + \beta^T X^T X \beta + \lambda\beta^T\beta)) = 0 \quad (5.28)$$

$$-2X^T y + 2X^T X \beta + 2\lambda\beta = 0 \quad (5.29)$$

$$-X^T y + (X^T X + \lambda I)\beta = 0 \quad (5.30)$$

$$(X^T X + \lambda I)\beta = X^T y \quad (5.31)$$

$$\beta = (X^T X + \lambda I)^{-1} X^T y \quad (5.32)$$

- The solution adds a positive constant to the diagonal of  $X^T X$  before inversion. This makes the problem nonsingular, even if  $X^T X$  is not of full rank, and was the main motivation behind ridge regression.
- Increasing  $\lambda$  shrinks the  $\beta$  coefficients toward 0.
- This approach **penalizes** the objective function by the **Euclidian** (:math:`'ell\_2'` norm of the coefficients such that solutions with large coefficients become unattractive.

The ridge penalty shrinks the coefficients toward zero. The figure illustrates: the OLS solution on the left. The  $\ell_1$  and  $\ell_2$  penalties in the middle pane. The penalized OLS in the right pane. The right pane shows how the penalties shrink the coefficients toward zero. The black points are the minimum found in each case, and the white points represents the true solution used to generate the data.

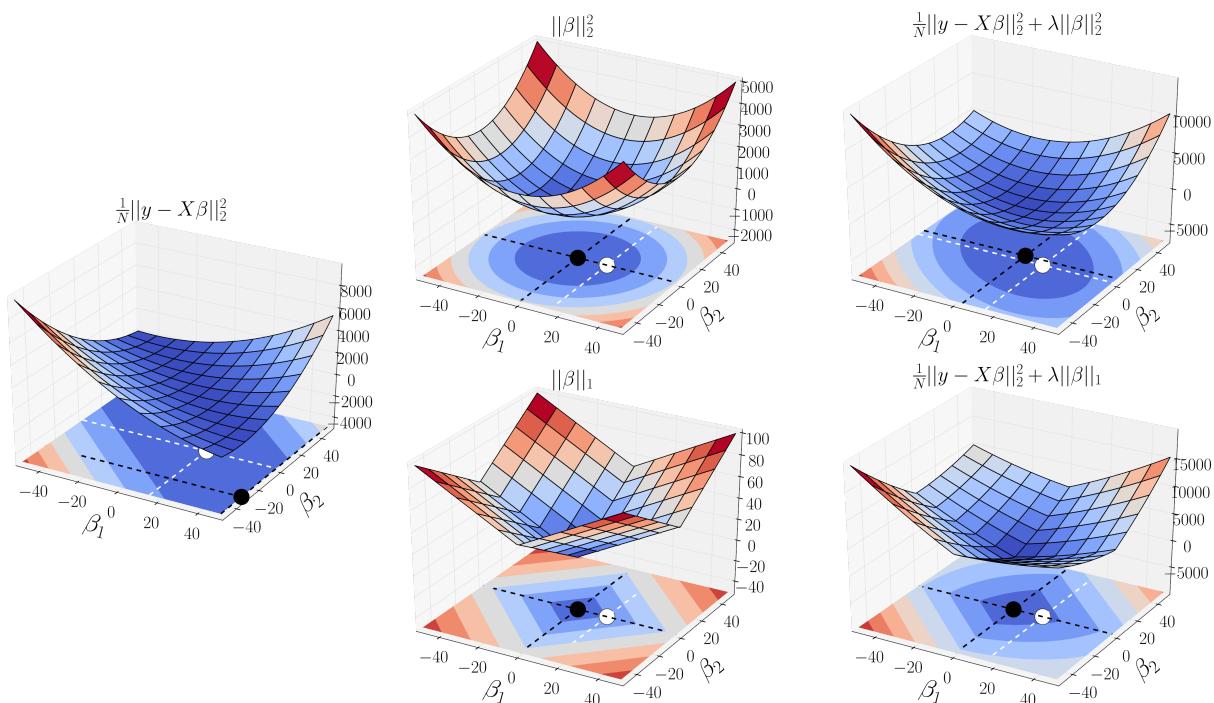


Fig. 2:  $\ell_1$  and  $\ell_2$  shrinkages

```
import matplotlib.pyplot as plt
import numpy as np
import sklearn.linear_model as lm
```

(continues on next page)

(continued from previous page)

```
# lambda is alpha!
mod = lm.Ridge(alpha=10)

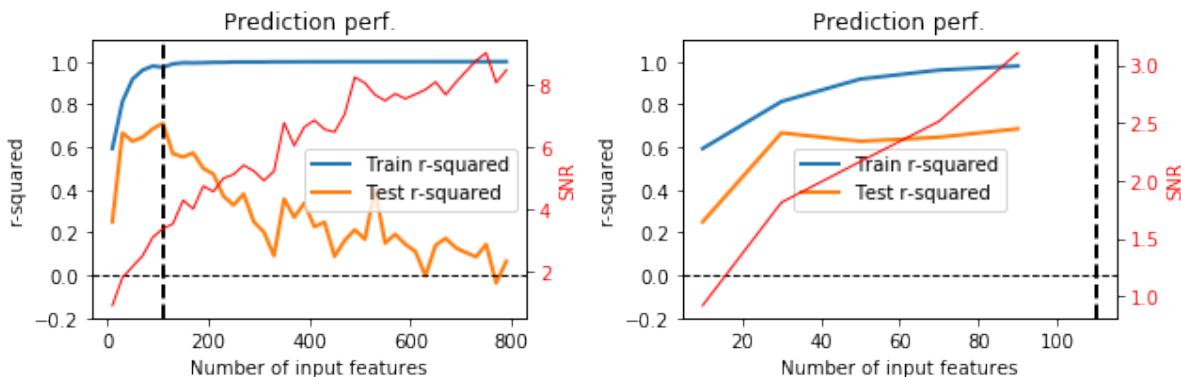
# Fit models on dataset
n_features, r2_train, r2_test, snr = fit_on_increasing_size(model=mod)

argmax = n_features[np.argmax(r2_test)]

# plot
fig, axis = plt.subplots(1, 2, figsize=(9, 3))

# Left pane: all features
plot_r2_snr(n_features, r2_train, r2_test, argmax, snr, axis[0])

# Right pane: Zoom on 100 first features
plot_r2_snr(n_features[n_features <= 100],
            r2_train[n_features <= 100], r2_test[n_features <= 100],
            argmax,
            snr[n_features <= 100],
            axis[1])
plt.tight_layout()
```



## Exercice

What benefit has been obtained by using  $\ell_2$  regularization?

### 5.3.5 Lasso regression ( $\ell_1$ -regularization)

Lasso regression penalizes the coefficients by the  $\ell_1$  norm. This constraint will reduce (bias) the capacity of the learning algorithm. To add such a penalty forces the coefficients to be small, i.e. it shrinks them toward zero. The objective function to minimize becomes:

$$\text{Lasso}(\beta) = \|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \lambda\|\beta\|_1. \quad (5.33)$$

This penalty forces some coefficients to be exactly zero, providing a feature selection property.

```

import matplotlib.pyplot as plt
import numpy as np
import sklearn.linear_model as lm

# lambda is alpha !
mod = lm.Lasso(alpha=.1)

# Fit models on dataset
n_features, r2_train, r2_test, snr = fit_on_increasing_size(model=mod)

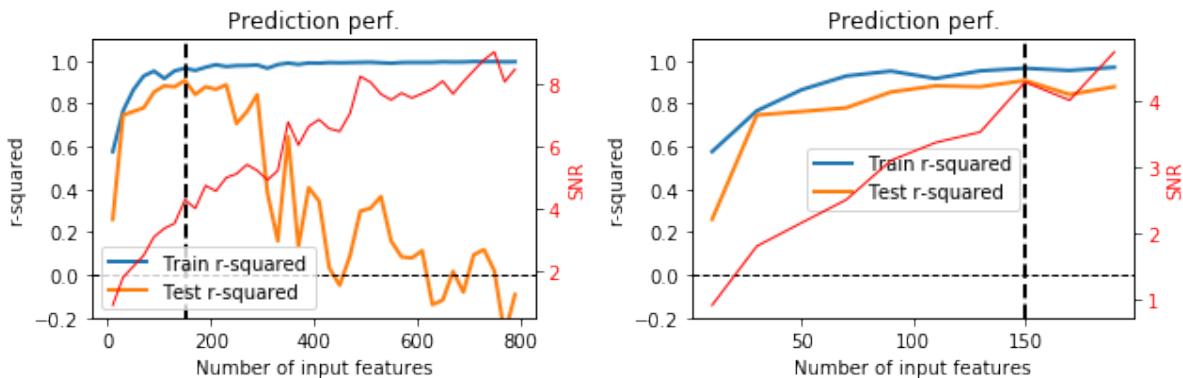
argmax = n_features[np.argmax(r2_test)]

# plot
fig, axis = plt.subplots(1, 2, figsize=(9, 3))

# Left pane: all features
plot_r2_snr(n_features, r2_train, r2_test, argmax, snr, axis[0])

# Right pane: Zoom on 200 first features
plot_r2_snr(n_features[n_features <= 200],
            r2_train[n_features <= 200], r2_test[n_features <= 200],
            argmax,
            snr[n_features <= 200],
            axis[1])
plt.tight_layout()

```



### Sparsity of the $\ell_1$ norm

#### Occam's razor

Occam's razor (also written as Ockham's razor, and **lex parsimoniae** in Latin, which means law of parsimony) is a problem solving principle attributed to William of Ockham (1287-1347), who was an English Franciscan friar and scholastic philosopher and theologian. The principle can be interpreted as stating that **among competing hypotheses, the one with the fewest assumptions should be selected**.

#### Principle of parsimony

The simplest of two competing theories is to be preferred. Definition of parsimony: Economy of explanation in conformity with Occam's razor.

Among possible models with similar loss, choose the simplest one:

- Choose the model with the smallest coefficient vector, i.e. smallest  $\ell_2$  ( $\|\beta\|_2$ ) or  $\ell_1$  ( $\|\beta\|_1$ ) norm of  $\beta$ , i.e.  $\ell_2$  or  $\ell_1$  penalty. See also bias-variance tradeoff.
- Choose the model that uses the smallest number of predictors. In other words, choose the model that has many predictors with zero weights. Two approaches are available to obtain this: (i) Perform a feature selection as a preprocessing prior to applying the learning algorithm, or (ii) embed the feature selection procedure within the learning process.

#### Sparsity-induced penalty or embedded feature selection with the  $\ell_1$  penalty

The penalty based on the  $\ell_1$  norm promotes **sparsity** (scattered, or not dense): it forces many coefficients to be exactly zero. This also makes the coefficient vector scattered.

The figure below illustrates the OLS loss under a constraint acting on the  $\ell_1$  norm of the coefficient vector. I.e., it illustrates the following optimization problem:

$$\begin{aligned} & \underset{\beta}{\text{minimize}} \quad \|\mathbf{y} - \mathbf{X}\beta\|_2^2 \\ & \text{subject to} \quad \|\beta\|_1 \leq 1. \end{aligned}$$

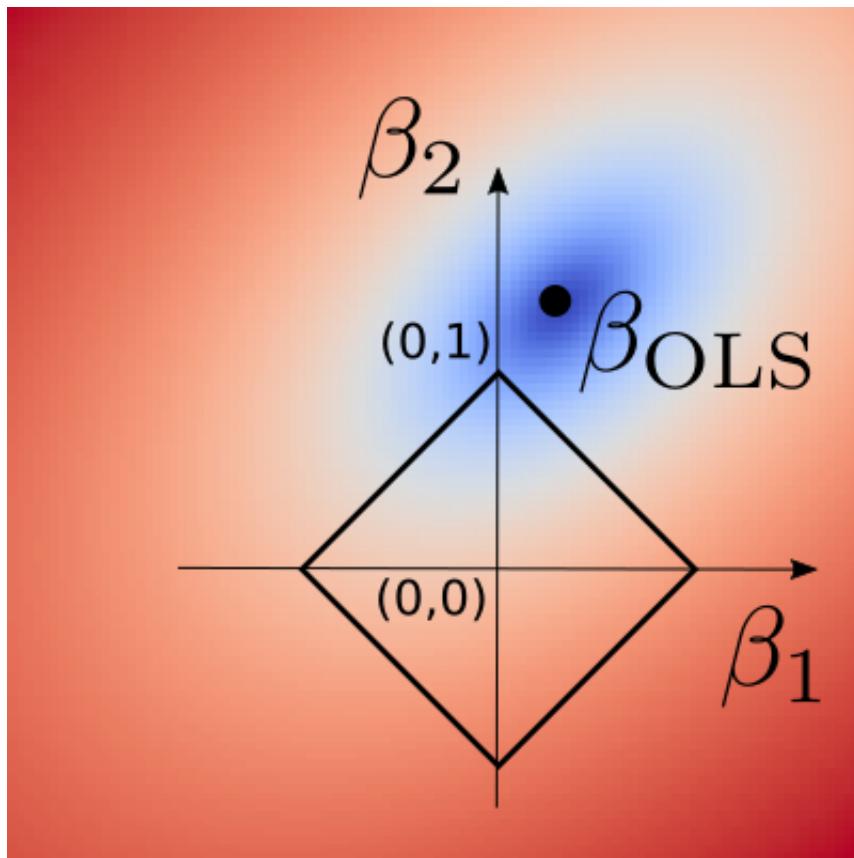


Fig. 3: Sparsity of L1 norm

## Optimization issues

*Section to be completed*

- No more closed-form solution.
- Convex but not differentiable.
- Requires specific optimization algorithms, such as the fast iterative shrinkage-thresholding algorithm (FISTA): Amir Beck and Marc Teboulle, *A Fast Iterative Shrinkage-Thresholding Algorithm for Linear Inverse Problems* SIAM J. Imaging Sci., 2009.

### 5.3.6 Elastic-net regression ( $\ell_2$ - $\ell_1$ -regularization)

The Elastic-net estimator combines the  $\ell_1$  and  $\ell_2$  penalties, and results in the problem to

$$\text{Enet}(\beta) = \|\mathbf{y} - \mathbf{X}^T \beta\|_2^2 + \alpha (\rho \|\beta\|_1 + (1 - \rho) \|\beta\|_2^2), \quad (5.34)$$

where  $\alpha$  acts as a global penalty and  $\rho$  as an  $\ell_1/\ell_2$  ratio.

#### ### Rationale

- If there are groups of highly correlated variables, Lasso tends to arbitrarily select only one from each group. These models are difficult to interpret because covariates that are strongly associated with the outcome are not included in the predictive model. Conversely, the elastic net encourages a grouping effect, where strongly correlated predictors tend to be in or out of the model together.
- Studies on real world data and simulation studies show that the elastic net often outperforms the lasso, while enjoying a similar sparsity of representation.

```
import matplotlib.pyplot as plt
import numpy as np
import sklearn.linear_model as lm

mod = lm.ElasticNet(alpha=.5, l1_ratio=.5)

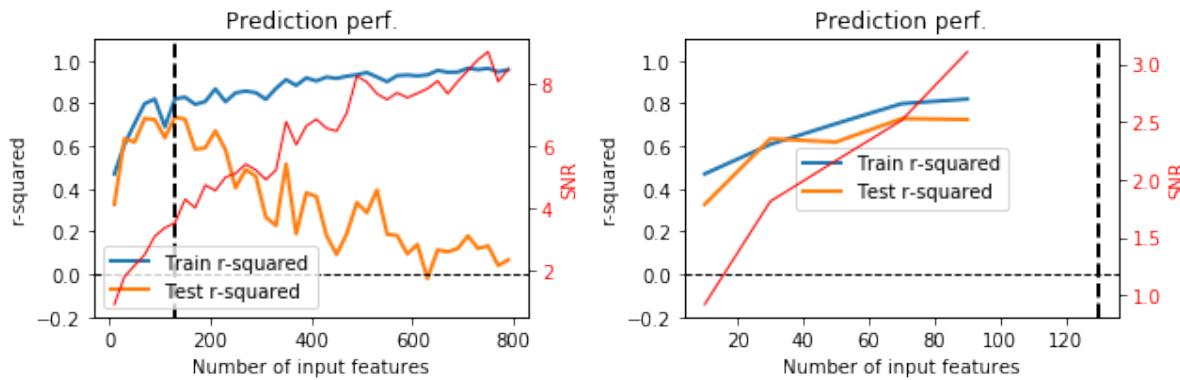
# Fit models on dataset
n_features, r2_train, r2_test, snr = fit_on_increasing_size(model=mod)

argmax = n_features[np.argmax(r2_test)]

# plot
fig, axis = plt.subplots(1, 2, figsize=(9, 3))

# Left pane: all features
plot_r2_snr(n_features, r2_train, r2_test, argmax, snr, axis[0])

# Right pane: Zoom on 100 first features
plot_r2_snr(n_features[n_features <= 100],
             r2_train[n_features <= 100], r2_test[n_features <= 100],
             argmax,
             snr[n_features <= 100],
             axis[1])
plt.tight_layout()
```



## 5.4 Linear classification

Given a training set of  $N$  samples,  $D = \{(x_1, y_1), \dots, (x_N, y_N)\}$ , where  $x_i$  is a multidimensional input vector with dimension  $P$  and class label (target or response)  $y_i \in \{0, 1\}$  (binary classification problem).

The vector of parameters  $w$  performs a linear combination of the input variables,  $x^T w$ . This step performs a **projection** or a **rotation** of input sample into a good discriminative one-dimensional sub-space.

This score (a.k.a decision function) is transformed, using the nonlinear activation function  $y(\cdot)$ , to a “posterior probabilities” of class 1

$$p(y = 1|x) = y(x^T w), \\ \text{where}$$

$$p(y = 1|x) = 1 - p(y = 0|x).$$

The decision surfaces correspond to  $y(x) = \text{constant}$ , so that  $x^T w = \text{constant}$  and hence the decision surfaces are linear functions of  $x$ , even if the function  $f(\cdot)$  is nonlinear.

A thresholding of the activation provides the predicted class label.

The vector of parameters, that defines the discriminative axis, minimizes an objective function  $f$  that is a sum of loss function  $\mathcal{L}(w)$  and some penalties on the weights vector  $\Omega(w)$ .

$$\min_w f = \sum_i \mathcal{L}(y_i, x_i^T w) + \Omega(w),$$

### 5.4.1 Fisher's linear discriminant with equal class covariance

This geometric method does not make any probabilistic assumptions, instead it relies on distances. It looks for the **linear projection** of the data points onto a vector,  $w$ , that maximizes the between/within variance ratio, denoted  $F(w)$ . Under a few assumptions, it will provide the same results as linear discriminant analysis (LDA), explained below.

Suppose two classes of observations,  $C_0$  and  $C_1$ , have means  $\mu_0$  and  $\mu_1$  and the same total within-class scatter (“covariance”) matrix,

$$S_W = \sum_{i \in C_0} (\mathbf{x}_i - \boldsymbol{\mu}_0)(\mathbf{x}_i - \boldsymbol{\mu}_0)^T + \sum_{j \in C_1} (\mathbf{x}_j - \boldsymbol{\mu}_1)(\mathbf{x}_j - \boldsymbol{\mu}_1)^T \quad (5.35)$$

$$= \mathbf{X}_c^T \mathbf{X}_c, \quad (5.36)$$

where  $\mathbf{X}_c$  is the  $(N \times P)$  matrix of data centered on their respective means:

$$\mathbf{X}_c = \begin{bmatrix} \mathbf{X}_0 - \boldsymbol{\mu}_0 \\ \mathbf{X}_1 - \boldsymbol{\mu}_1 \end{bmatrix},$$

where  $\mathbf{X}_0$  and  $\mathbf{X}_1$  are the  $(N_0 \times P)$  and  $(N_1 \times P)$  matrices of samples of classes  $C_0$  and  $C_1$ .

Let  $S_B$  being the scatter “between-class” matrix, given by

$$S_B = (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^T.$$

The linear combination of features  $\mathbf{w}^T \mathbf{x}$  have means  $\mathbf{w}^T \boldsymbol{\mu}_i$  for  $i = 0, 1$ , and variance  $\mathbf{w}^T \mathbf{X}_c^T \mathbf{X}_c \mathbf{w}$ . Fisher defined the separation between these two distributions to be the ratio of the variance between the classes to the variance within the classes:

$$F_{\text{Fisher}}(\mathbf{w}) = \frac{\sigma_{\text{between}}^2}{\sigma_{\text{within}}^2} \quad (5.37)$$

$$= \frac{(\mathbf{w}^T \boldsymbol{\mu}_1 - \mathbf{w}^T \boldsymbol{\mu}_0)^2}{\mathbf{w}^T \mathbf{X}_c^T \mathbf{X}_c \mathbf{w}} \quad (5.38)$$

$$= \frac{(\mathbf{w}^T (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0))^2}{\mathbf{w}^T \mathbf{X}_c^T \mathbf{X}_c \mathbf{w}} \quad (5.39)$$

$$= \frac{\mathbf{w}^T (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0) (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^T \mathbf{w}}{\mathbf{w}^T \mathbf{X}_c^T \mathbf{X}_c \mathbf{w}} \quad (5.40)$$

$$= \frac{\mathbf{w}^T S_B \mathbf{w}}{\mathbf{w}^T S_W \mathbf{w}}. \quad (5.41)$$

### The Fisher most discriminant projection

In the two-class case, the maximum separation occurs by a projection on the  $(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)$  using the Mahalanobis metric  $S_W^{-1}$ , so that

$$\mathbf{w} \propto S_W^{-1} (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0).$$

### Demonstration

Differentiating  $F_{\text{Fisher}}(w)$  with respect to  $w$  gives

$$\begin{aligned}
 \nabla_{\mathbf{w}} F_{\text{Fisher}}(\mathbf{w}) &= 0 \\
 \nabla_{\mathbf{w}} \left( \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}} \right) &= 0 \\
 (\mathbf{w}^T \mathbf{S}_W \mathbf{w})(2\mathbf{S}_B \mathbf{w}) - (\mathbf{w}^T \mathbf{S}_B \mathbf{w})(2\mathbf{S}_W \mathbf{w}) &= 0 \\
 (\mathbf{w}^T \mathbf{S}_W \mathbf{w})(\mathbf{S}_B \mathbf{w}) &= (\mathbf{w}^T \mathbf{S}_B \mathbf{w})(\mathbf{S}_W \mathbf{w}) \\
 \mathbf{S}_B \mathbf{w} &= \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}} (\mathbf{S}_W \mathbf{w}) \\
 \mathbf{S}_B \mathbf{w} &= \lambda (\mathbf{S}_W \mathbf{w}) \\
 \mathbf{S}_W^{-1} \mathbf{S}_B \mathbf{w} &= \lambda \mathbf{w}.
 \end{aligned}$$

Since we do not care about the magnitude of  $\mathbf{w}$ , only its direction, we replaced the scalar factor  $(\mathbf{w}^T \mathbf{S}_B \mathbf{w}) / (\mathbf{w}^T \mathbf{S}_W \mathbf{w})$  by  $\lambda$ .

In the multiple-class case, the solutions  $\mathbf{w}$  are determined by the eigenvectors of  $\mathbf{S}_W^{-1} \mathbf{S}_B$  that correspond to the  $K - 1$  largest eigenvalues.

However, in the two-class case (in which  $\mathbf{S}_B = (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^T$ ) it is easy to show that  $\mathbf{w} = \mathbf{S}_W^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)$  is the unique eigenvector of  $\mathbf{S}_W^{-1} \mathbf{S}_B$ :

$$\begin{aligned}
 \mathbf{S}_W^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^T \mathbf{w} &= \lambda \mathbf{w} \\
 \mathbf{S}_W^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^T \mathbf{S}_W^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0) &= \lambda \mathbf{S}_W^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0),
 \end{aligned}$$

where here  $\lambda = (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^T \mathbf{S}_W^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)$ . Which leads to the result

$$\mathbf{w} \propto \mathbf{S}_W^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0).$$

### The separating hyperplane

The separating hyperplane is a  $P - 1$ -dimensional hyper surface, orthogonal to the projection vector,  $\mathbf{w}$ . There is no single best way to find the origin of the plane along  $\mathbf{w}$ , or equivalently the classification threshold that determines whether a point should be classified as belonging to  $C_0$  or to  $C_1$ . However, if the projected points have roughly the same distribution, then the threshold can be chosen as the hyperplane exactly between the projections of the two means, i.e. as

$$T = \mathbf{w} \cdot \frac{1}{2}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0).$$

```
%matplotlib inline
import warnings
warnings.filterwarnings('once')
```

### 5.4.2 Linear discriminant analysis (LDA)

Linear discriminant analysis (LDA) is a probabilistic generalization of Fisher's linear discriminant. It uses Bayes' rule to fix the threshold based on prior probabilities of classes.

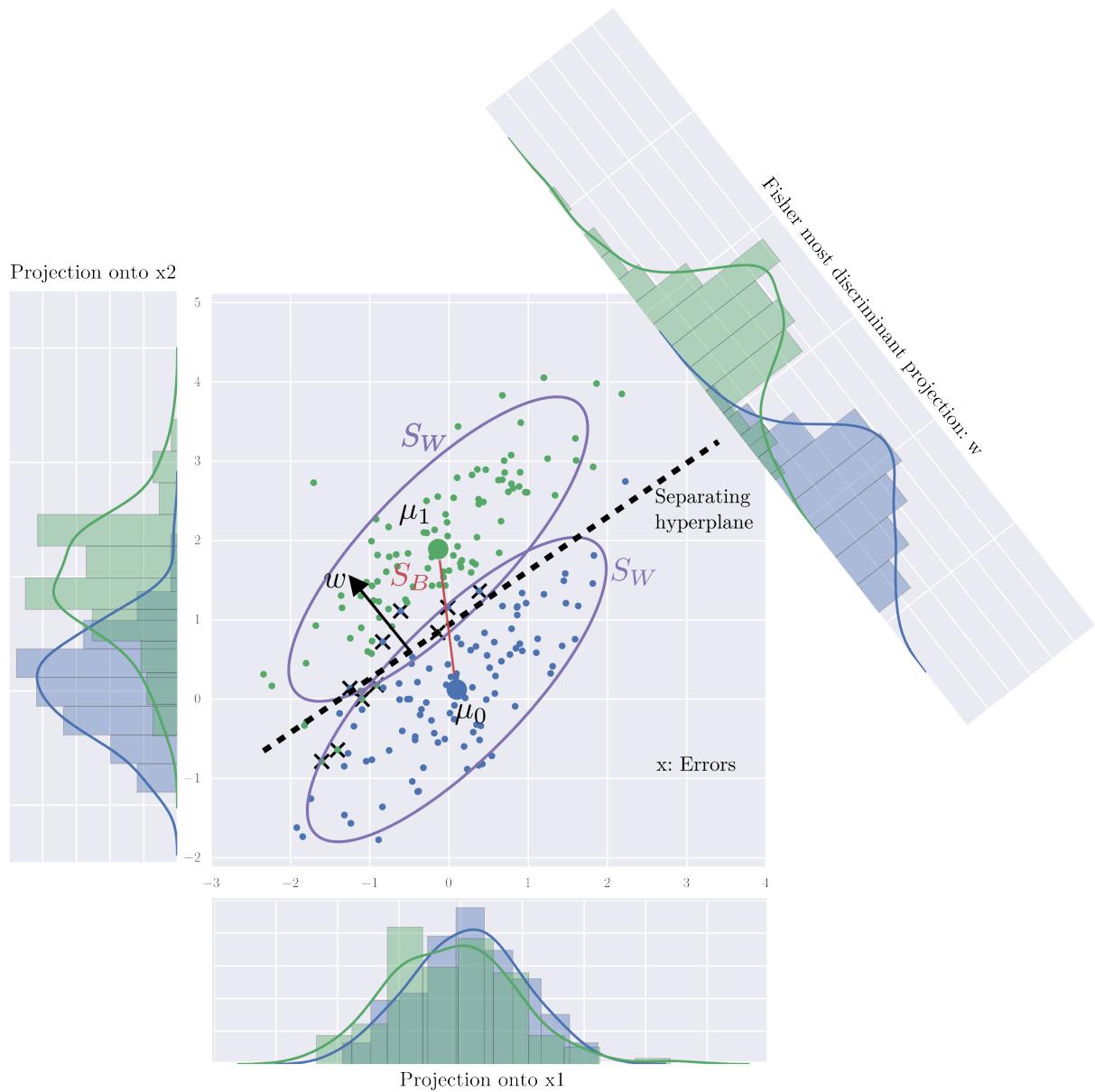


Fig. 4: The Fisher most discriminant projection

1. First compute the **class-conditional distributions** of  $x$  given class  $C_k$ :  $p(x|C_k) = \mathcal{N}(x|\mu_k, S_W)$ . Where  $\mathcal{N}(x|\mu_k, S_W)$  is the multivariate Gaussian distribution defined over a P-dimensional vector  $x$  of continuous variables, which is given by

$$\mathcal{N}(x|\mu_k, S_W) = \frac{1}{(2\pi)^{P/2}|S_W|^{1/2}} \exp\left\{-\frac{1}{2}(x - \mu_k)^T S_W^{-1}(x - \mu_k)\right\}$$

2. Estimate the **prior probabilities** of class  $k$ ,  $p(C_k) = N_k/N$ .
3. Compute **posterior probabilities** (ie. the probability of a each class given a sample) combining conditional with priors using Bayes' rule:

$$p(C_k|x) = \frac{p(C_k)p(x|C_k)}{p(x)}$$

Where  $p(x)$  is the marginal distribution obtained by suming of classes: As usual, the denominator in Bayes' theorem can be found in terms of the quantities appearing in the numerator, because

$$p(x) = \sum_k p(x|C_k)p(C_k)$$

4. Classify  $x$  using the Maximum-a-Posteriori probability:  $C_k = \arg \max_{C_k} p(C_k|x)$

LDA is a **generative model** since the class-conditional distributions cal be used to generate samples of each classes.

LDA is useful to deal with imbalanced group sizes (eg.:  $N_1 \gg N_0$ ) since priors probabilities can be used to explicitly re-balance the classification by setting  $p(C_0) = p(C_1) = 1/2$  or whatever seems relevant.

LDA can be generalised to the multiclass case with  $K > 2$ .

With  $N_1 = N_0$ , LDA lead to the same solution than Fisher's linear discriminant.

## Exercise

How many parameters are required to estimate to perform a LDA ?

```
import numpy as np
from sklearn.discriminant_analysis import LinearDiscriminantAnalysis as LDA

# Dataset
n_samples, n_features = 100, 2
mean0, mean1 = np.array([0, 0]), np.array([0, 2])
Cov = np.array([[1, .8], [.8, 1]])
np.random.seed(42)
X0 = np.random.multivariate_normal(mean0, Cov, n_samples)
X1 = np.random.multivariate_normal(mean1, Cov, n_samples)
X = np.vstack([X0, X1])
y = np.array([0] * X0.shape[0] + [1] * X1.shape[0])

# LDA with scikit-learn
lda = LDA()
proj = lda.fit(X, y).transform(X)
y_pred_lda = lda.predict(X)

errors = y_pred_lda != y
print("Nb errors=%i, error rate=%.2f" % (errors.sum(), errors.sum() / len(y_pred_lda)))
```

```
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
→ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
→got 216 from PyObject
    return f(*args, **kwds)
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
→ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
→got 216 from PyObject
    return f(*args, **kwds)
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
→ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
→got 216 from PyObject
    return f(*args, **kwds)
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
→ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
→got 216 from PyObject
    return f(*args, **kwds)
```

Nb errors=10, error rate=0.05

```
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
→ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
→got 216 from PyObject
    return f(*args, **kwds)
```

### 5.4.3 Logistic regression

Logistic regression is called a generalized linear models. ie.: it is a linear model with a link function that maps the output of linear multiple regression to the posterior probability of each class  $p(C_k|x) \in [0, 1]$  using the logistic sigmoid function:

$$p(C_k|\mathbf{w}, \mathbf{x}_i) = \frac{1}{1 + \exp(-\mathbf{w} \cdot \mathbf{x}_i)}$$

Logistic regression seeks to minimizes the likelihood  $L$  as **Loss function**  $\mathcal{L}$ :

$$\min L(\mathbf{w}) = \prod_i^N p(C_k|\mathbf{w}, \mathbf{x}_i)$$

Partically, the Loss function  $\mathcal{L}$  is the log-likelihood:

$$\min \mathcal{L}(\mathbf{w}) = \log L(\mathbf{w}) = \sum_i^N \log p(C_k|\mathbf{w}, \mathbf{x}_i)$$

In the two-class case the algorithms simplify considerably by coding the two-classes ( $C_0$  and  $C_1$ ) via a 0/1 response  $y_i$ . Indeed, since  $p(C_0|\mathbf{w}, \mathbf{x}_i) = 1 - p(C_1|\mathbf{w}, \mathbf{x}_i)$ , the log-likelihood can be re-written:

$$\log L(\mathbf{w}) = \sum_i^N \{y_i \log p(C_1|\mathbf{w}, \mathbf{x}_i) + (1 - y_i) \log(1 - p(C_1|\mathbf{w}, \mathbf{x}_i))\} \quad (5.42)$$

$$\log L(\mathbf{w}) = \sum_i^N \{y_i \mathbf{w} \cdot \mathbf{x}_i - \log(1 + \exp^{\mathbf{w} \cdot \mathbf{x}_i})\} \quad (5.43)$$

$$(5.44)$$

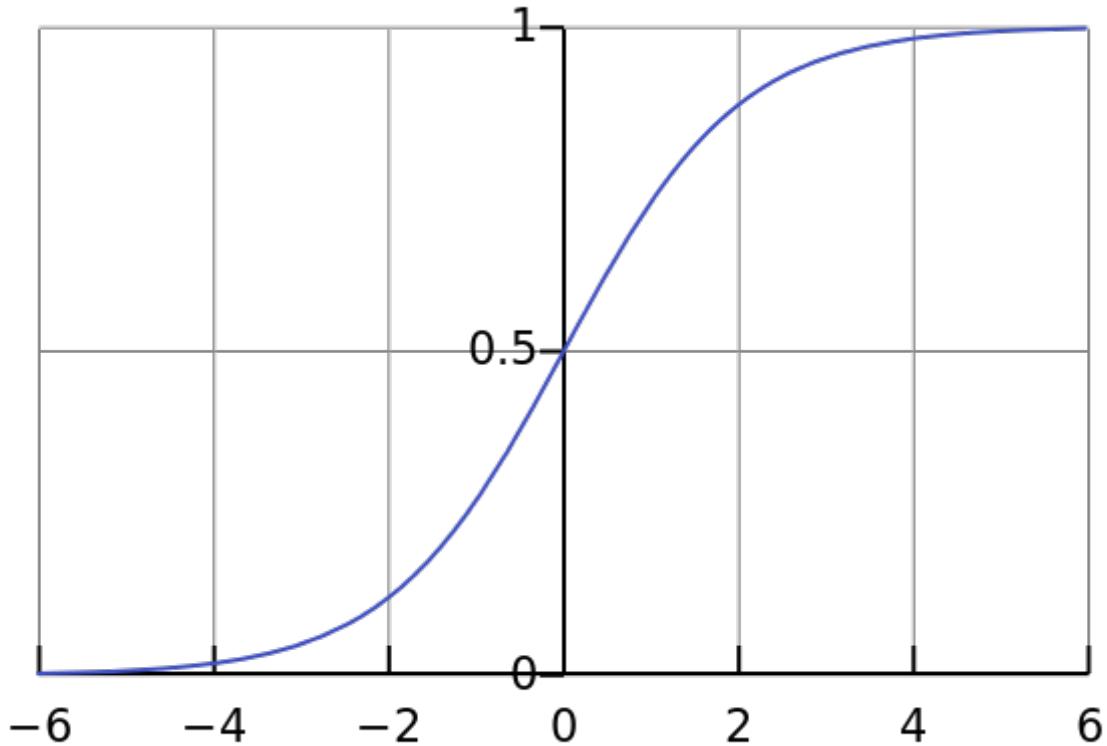


Fig. 5: logistic sigmoid function

Logistic regression is a **discriminative model** since it focuses only on the posterior probability of each class  $p(C_k|x)$ . It only requires to estimate the  $P$  weight of the  $w$  vector. Thus it should be favoured over LDA with many input features. In small dimension and balanced situations it would provide similar predictions than LDA.

However imbalanced group sizes cannot be explicitly controlled. It can be managed using a reweighting of the input samples.

```
from sklearn import linear_model
logreg = linear_model.LogisticRegression(C=1e8, solver='lbfgs')
# This class implements regularized logistic regression. C is the Inverse of
# regularization strength.
# Large value => no regularization.

logreg.fit(X, y)
y_pred_logreg = logreg.predict(X)

errors = y_pred_logreg != y
print("Nb errors=%i, error rate=%.2f" % (errors.sum(), errors.sum() / len(y_pred_logreg)))
print(logreg.coef_)
```

```
Nb errors=10, error rate=0.05
[[-5.1516729  5.57303883]]
```

## Exercise

Explore the Logistic Regression parameters and proposes a solution in cases of highly imbalanced training dataset  $N_1 \gg N_0$  when we know that in reality both classes have the same probability  $p(C_1) = p(C_0)$ .

### 5.4.4 Overfitting

VC dimension (for Vapnik–Chervonenkis dimension) is a measure of the **capacity** (complexity, expressive power, richness, or flexibility) of a statistical classification algorithm, defined as the cardinality of the largest set of points that the algorithm can shatter.

Theorem: Linear classifier in  $R^P$  have VC dimension of  $P + 1$ . Hence in dimension two ( $P = 2$ ) any random partition of 3 points can be learned.

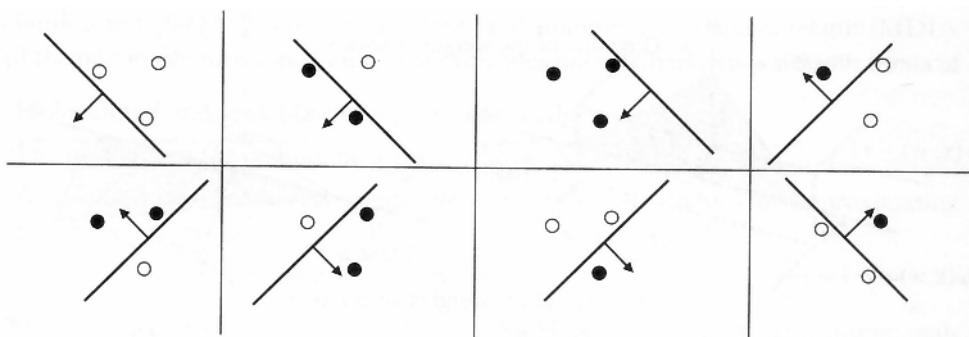


Fig. 6: In 2D we can shatter any three non-collinear points

### 5.4.5 Ridge Fisher's linear classification (L2-regularization)

When the matrix  $S_W$  is not full rank or  $P \gg N$ , the The Fisher most discriminant projection estimate of the is not unique. This can be solved using a biased version of  $S_W$ :

$$S_W^{Ridge} = S_W + \lambda I$$

where  $I$  is the  $P \times P$  identity matrix. This leads to the regularized (ridge) estimator of the Fisher's linear discriminant analysis:

$$\mathbf{w}^{Ridge} \propto (S_W + \lambda I)^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)$$

Increasing  $\lambda$  will:

- Shrinks the coefficients toward zero.
- The covariance will converge toward the diagonal matrix, reducing the contribution of the pairwise covariances.

### 5.4.6 Ridge logistic regression (L2-regularization)

The **objective function** to be minimized is now the combination of the logistic loss  $\log L(\mathbf{w})$  with a penalty of the L2 norm of the weights vector. In the two-class case, using the 0/1 coding we obtain:

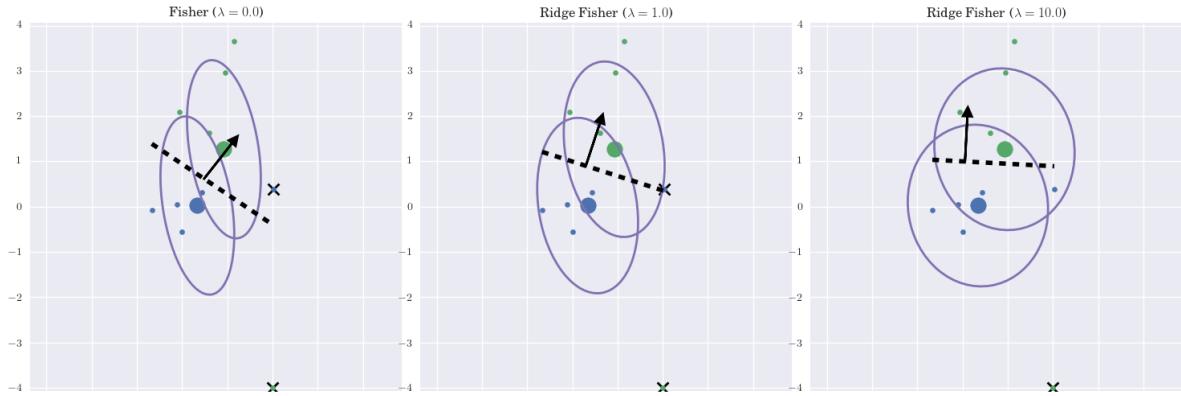


Fig. 7: The Ridge Fisher most discriminant projection

$$\min \text{ Logistic ridge}(\mathbf{w}) = \log L(\mathbf{w}) + \lambda \|\mathbf{w}\|^2 \quad (5.45)$$

$$= \sum_i^N \{y_i \mathbf{w}^T \mathbf{x}_i - \log(1 + \exp^{\mathbf{w}^T \mathbf{x}_i})\} + \lambda \|\mathbf{w}\|^2 \quad (5.46)$$

(5.47)

```
# Dataset
# Build a classification task using 3 informative features
from sklearn import datasets

X, y = datasets.make_classification(n_samples=100,
                                    n_features=20,
                                    n_informative=3,
                                    n_redundant=0,
                                    n_repeated=0,
                                    n_classes=2,
                                    random_state=0,
                                    shuffle=False)
```

```
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
  ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,
  got 216 from PyObject
  return f(*args, **kwds)
```

```
from sklearn import linear_model
lr = linear_model.LogisticRegression(C=1)
# This class implements regularized logistic regression. C is the Inverse of
# regularization strength.
# Large value => no regularization.

lr.fit(X, y)
y_pred_lr = lr.predict(X)

errors = y_pred_lr != y
print("Nb errors=%i, error rate=%.2f" % (errors.sum(), errors.sum() / len(y)))
print(lr.coef_)
```

```
Nb errors=26, error rate=0.26
[[-0.12061092  0.7357655 -0.01842318 -0.10835785  0.25328562  0.4221318
 0.15152184  0.16522461  0.84404799  0.01962765 -0.15995078 -0.01925974
 -0.02807379  0.42939869 -0.06368702 -0.07922044  0.15529371  0.29963205
 0.54633137  0.03866807]]
```

```
/home/edouard/anaconda3/lib/python3.7/site-packages/sklearn/linear_model/logistic.py:433:_
FutureWarning: Default solver will be changed to 'lbfgs' in 0.22. Specify a solver to_
silence this warning.
FutureWarning)
```

### 5.4.7 Lasso logistic regression (L1-regularization)

The **objective function** to be minimized is now the combination of the logistic loss  $\log L(\mathbf{w})$  with a penalty of the L1 norm of the weights vector. In the two-class case, using the 0/1 coding we obtain:

$$\min \text{ Logistic Lasso}(\mathbf{w}) = \log L(\mathbf{w}) + \lambda \|\mathbf{w}\|_1 \quad (5.48)$$

$$= \sum_i^N \{y_i \mathbf{w} \cdot \mathbf{x}_i - \log(1 + \exp^{\mathbf{w} \cdot \mathbf{x}_i})\} + \lambda \|\mathbf{w}\|_1 \quad (5.49)$$

```
from sklearn import linear_model
lrl1 = linear_model.LogisticRegression(penalty='l1')
# This class implements regularized logistic regression. C is the Inverse of_
# regularization strength.
# Large value => no regularization.

lrl1.fit(X, y)
y_pred_lrl1 = lrl1.predict(X)

errors = y_pred_lrl1 != y
print("Nb errors=%i, error rate=%.2f" % (errors.sum(), errors.sum() / len(y_pred_lrl1)))
print(lrl1.coef_)
```

```
Nb errors=27, error rate=0.27
[[-0.11337193  0.68158741  0.          0.          0.19755791  0.36483513
 0.08057281  0.06205131  0.76016935  0.          -0.10808194  0.
 0.          0.33749287  0.          0.          0.0790326   0.20158542
 0.48384386  0.          ]]
```

```
/home/edouard/anaconda3/lib/python3.7/site-packages/sklearn/linear_model/logistic.py:433:_
FutureWarning: Default solver will be changed to 'lbfgs' in 0.22. Specify a solver to_
silence this warning.
FutureWarning)
```

### 5.4.8 Ridge linear Support Vector Machine (L2-regularization)

Support Vector Machine seek for separating hyperplane with maximum margin to enforce robustness against noise. Like logistic regression it is a **discriminative method** that only focuses of predictions.

Here we present the non separable case of Maximum Margin Classifiers with  $\pm 1$  coding (ie.:  $y_i \in \{-1, +1\}$ ). In the next figure the legend apply to samples of “dot” class.

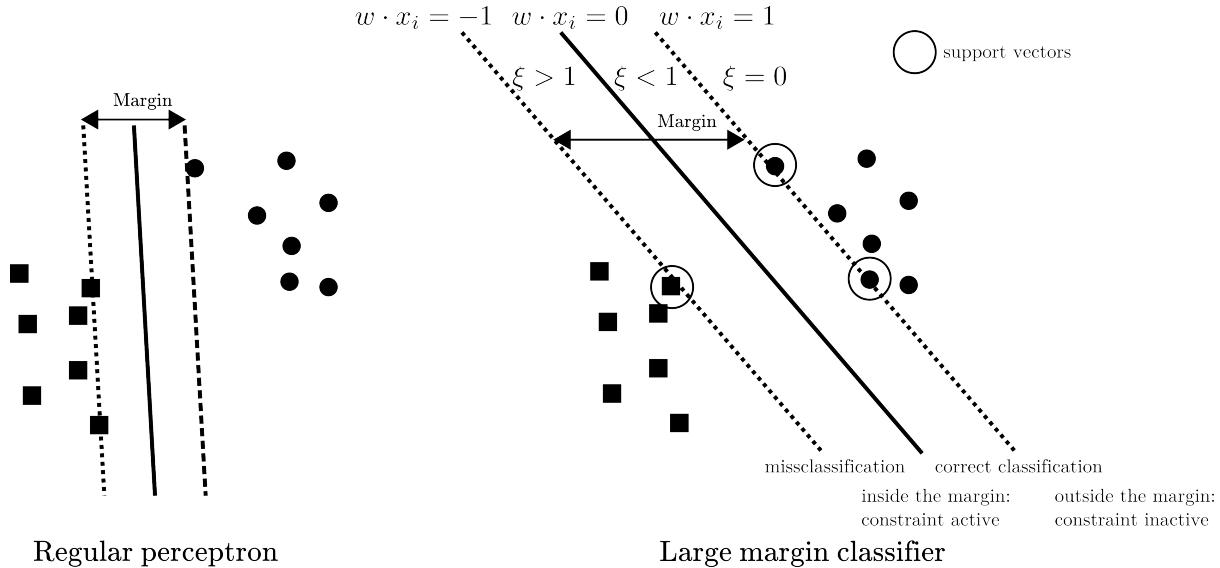


Fig. 8: Linear margin classifiers

Linear SVM for classification (also called SVM-C or SVC) minimizes:

$$\begin{aligned} \min \quad & \text{Linear SVM}(\mathbf{w}) = \text{penalty}(\mathbf{w}) + C \text{ Hinge loss}(\mathbf{w}) \\ &= \|\mathbf{w}\|_2 + C \sum_i^N \xi_i \\ \text{with } & \forall i \quad y_i(w \cdot \mathbf{x}_i) \geq 1 - \xi_i \end{aligned}$$

Here we introduced the slack variables:  $\xi_i$ , with  $\xi_i = 0$  for points that are on or inside the correct margin boundary and  $\xi_i = |y_i - (w \cdot \mathbf{x}_i)|$  for other points. Thus:

1. If  $y_i(w \cdot \mathbf{x}_i) \geq 1$  then the point lies outside the margin but on the correct side of the decision boundary. In this case  $\xi_i = 0$ . The constraint is thus not active for this point. It does not contribute to the prediction.
2. If  $1 > y_i(w \cdot \mathbf{x}_i) \geq 0$  then the point lies inside the margin and on the correct side of the decision boundary. In this case  $0 < \xi_i \leq 1$ . The constraint is active for this point. It does contribute to the prediction as a support vector.
3. If  $0 < y_i(w \cdot \mathbf{x}_i)$  then the point is on the wrong side of the decision boundary (missclassification). In this case  $0 < \xi_i > 1$ . The constraint is active for this point. It does contribute to the prediction as a support vector.

This loss is called the hinge loss, defined as:

$$\max(0, 1 - y_i(w \cdot \mathbf{x}_i))$$

So linear SVM is closed to Ridge logistic regression, using the hinge loss instead of the logistic loss. Both will provide very similar predictions.

```
from sklearn import svm

svmlin = svm.LinearSVC()
# Remark: by default LinearSVC uses squared_hinge as loss
svmlin.fit(X, y)
```

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```
y_pred_svmlin = svmlin.predict(X)

errors = y_pred_svmlin != y
print("Nb errors=%i, error rate=%f" % (errors.sum(), errors.sum() / len(y_pred_svmlin)))
print(svmlin.coef_)
```

```
Nb errors=26, error rate=0.26
[[-0.05604866  0.31187658  0.00275339 -0.05153703  0.09938239  0.17724479
 0.06520118  0.08921076  0.35336289  0.00599675 -0.06201396 -0.00742017
 -0.02159905  0.18271488 -0.02164397 -0.04061358  0.0720389   0.13085078
 0.23720691  0.00826935]]
```

```
/home/edouard/anaconda3/lib/python3.7/site-packages/sklearn/svm/base.py:931:_
←ConvergenceWarning: Liblinear failed to converge, increase the number of iterations.
 "the number of iterations.", ConvergenceWarning)
```

### 5.4.9 Lasso linear Support Vector Machine (L1-regularization)

Linear SVM for classification (also called SVM-C or SVC) with l1-regularization

$$\begin{aligned} \min_{\mathbf{w}} \quad & F_{\text{Lasso linear SVM}}(\mathbf{w}) = \lambda \|\mathbf{w}\|_1 + C \sum_i^N \xi_i \\ \text{with} \quad & \forall i \quad y_i(\mathbf{w} \cdot \mathbf{x}_i) \geq 1 - \xi_i \end{aligned}$$

```
from sklearn import svm

svmlinl1 = svm.LinearSVC(penalty='l1', dual=False)
# Remark: by default LinearSVC uses squared_hinge as loss

svmlinl1.fit(X, y)
y_pred_svmlinl1 = svmlinl1.predict(X)

errors = y_pred_svmlinl1 != y
print("Nb errors=%i, error rate=%f" % (errors.sum(), errors.sum() / len(y_pred_
←svmlinl1)))
print(svmlinl1.coef_)
```

```
Nb errors=26, error rate=0.26
[[-0.05334026  0.29934473  0.          -0.03541313  0.09261404  0.16763294
 0.05808033  0.07587505  0.34065177  0.          -0.05558916 -0.00194123
 -0.01312461  0.1686629   -0.01450446 -0.02500537  0.06074148  0.11738861
 0.22485536  0.00473342]]
```

## Exercise

Compare predictions of Logistic regression (LR) and their SVM counterparts, ie.: L2 LR vs L2 SVM and L1 LR vs L1 SVM

- Compute the correlation between pairs of weights vectors.
- Compare the predictions of two classifiers using their decision function:
  - Give the equation of the decision function for a linear classifier, assuming that there is no intercept.

- Compute the correlation decision function.
- Plot the pairwise decision function of the classifiers.
- Conclude on the differences between Linear SVM and logistic regression.

#### 5.4.10 Elastic-net classification (L2-L1-regularization)

The **objective function** to be minimized is now the combination of the logistic loss  $\log L(\mathbf{w})$  or the hinge loss with combination of L1 and L2 penalties. In the two-class case, using the 0/1 coding we obtain:

$$\min \text{ Logistic enet}(\mathbf{w}) = \log L(\mathbf{w}) + \alpha (\rho \|\mathbf{w}\|_1 + (1 - \rho) \|\mathbf{w}\|_2^2) \quad (5.50)$$

$$\min \text{ Hinge enet}(\mathbf{w}) = \text{Hinge loss}(\mathbf{w}) + \alpha (\rho \|\mathbf{w}\|_1 + (1 - \rho) \|\mathbf{w}\|_2^2) \quad (5.51)$$

```
from sklearn import datasets
from sklearn import linear_model as lm
import matplotlib.pyplot as plt

X, y = datasets.make_classification(n_samples=100,
                                    n_features=20,
                                    n_informative=3,
                                    n_redundant=0,
                                    n_repeated=0,
                                    n_classes=2,
                                    random_state=0,
                                    shuffle=False)

enetloglike = lm.SGDClassifier(loss="log", penalty="elasticnet",
                                alpha=0.0001, l1_ratio=0.15, class_weight='balanced')
enetloglike.fit(X, y)

enethinge = lm.SGDClassifier(loss="hinge", penalty="elasticnet",
                             alpha=0.0001, l1_ratio=0.15, class_weight='balanced')
enethinge.fit(X, y)
```

```
/home/edouard/anaconda3/lib/python3.7/site-packages/sklearn/linear_model/stochastic_
↪gradient.py:166: FutureWarning: max_iter and tol parameters have been added in
↪SGDClassifier in 0.19. If both are left unset, they default to max_iter=5 and tol=None. ↴
↪If tol is not None, max_iter defaults to max_iter=1000. From 0.21, default max_iter
↪will be 1000, and default tol will be 1e-3.
FutureWarning)
/home/edouard/anaconda3/lib/python3.7/site-packages/sklearn/linear_model/stochastic_
↪gradient.py:166: FutureWarning: max_iter and tol parameters have been added in
↪SGDClassifier in 0.19. If both are left unset, they default to max_iter=5 and tol=None. ↴
↪If tol is not None, max_iter defaults to max_iter=1000. From 0.21, default max_iter
↪will be 1000, and default tol will be 1e-3.
FutureWarning)
```

```
SGDClassifier(alpha=0.0001, average=False, class_weight='balanced',
              early_stopping=False, epsilon=0.1, eta0=0.0, fit_intercept=True,
              l1_ratio=0.15, learning_rate='optimal', loss='hinge', max_iter=None,
```

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```
n_iter=None, n_iter_no_change=5, n_jobs=None, penalty='elasticnet',
power_t=0.5, random_state=None, shuffle=True, tol=None,
validation_fraction=0.1, verbose=0, warm_start=False)
```

## Exercise

Compare predictions of Elastic-net Logistic regression (LR) and Hinge-loss Elastic-net

- Compute the correlation between pairs of weights vectors.
- Compare the predictions of two classifiers using their decision function:
  - Compute the correlation decision function.
  - Plot the pairwise decision function of the classifiers.
- Conclude on the differences between the two losses.

### 5.4.11 Metrics of classification performance evaluation

#### Metrics for binary classification

source: [https://en.wikipedia.org/wiki/Sensitivity\\_and\\_specificity](https://en.wikipedia.org/wiki/Sensitivity_and_specificity)

Imagine a study evaluating a new test that screens people for a disease. Each person taking the test either has or does not have the disease. The test outcome can be positive (classifying the person as having the disease) or negative (classifying the person as not having the disease). The test results for each subject may or may not match the subject's actual status. In that setting:

- True positive (TP): Sick people correctly identified as sick
- False positive (FP): Healthy people incorrectly identified as sick
- True negative (TN): Healthy people correctly identified as healthy
- False negative (FN): Sick people incorrectly identified as healthy
- **Accuracy (ACC):**

$$\text{ACC} = (\text{TP} + \text{TN}) / (\text{TP} + \text{FP} + \text{FN} + \text{TN})$$

- **Sensitivity (SEN)** or **recall** of the positive class or true positive rate (TPR) or hit rate:

$$\text{SEN} = \text{TP} / \text{P} = \text{TP} / (\text{TP} + \text{FN})$$

- **Specificity (SPC)** or **recall** of the negative class or true negative rate:

$$\text{SPC} = \text{TN} / \text{N} = \text{TN} / (\text{TN} + \text{FP})$$

- **Precision** or positive predictive value (PPV):

$$\text{PPV} = \text{TP} / (\text{TP} + \text{FP})$$

- **Balanced accuracy (bACC):** is a useful performance measure is the balanced accuracy which avoids inflated performance estimates on imbalanced datasets (Brodersen, et al. (2010). “The balanced accuracy and its posterior distribution”). It is defined as the arithmetic mean of sensitivity and specificity, or the average accuracy obtained on either class:

$$bACC = 1/2 * (SEN + SPC)$$

- F1 Score (or F-score) which is a weighted average of precision and recall are useful to deal with imbalanced datasets

The four outcomes can be formulated in a  $2 \times 2$  contingency table or confusion matrix [https://en.wikipedia.org/wiki/Sensitivity\\_and\\_specificity](https://en.wikipedia.org/wiki/Sensitivity_and_specificity)

For more precision see: [http://scikit-learn.org/stable/modules/model\\_evaluation.html](http://scikit-learn.org/stable/modules/model_evaluation.html)

```
from sklearn import metrics
y_pred = [0, 1, 0, 0]
y_true = [0, 1, 0, 1]

metrics.accuracy_score(y_true, y_pred)

# The overall precision and recall
metrics.precision_score(y_true, y_pred)
metrics.recall_score(y_true, y_pred)

# Recalls on individual classes: SEN & SPC
recalls = metrics.recall_score(y_true, y_pred, average=None)
recalls[0] # is the recall of class 0: specificity
recalls[1] # is the recall of class 1: sensitivity

# Balanced accuracy
b_acc = recalls.mean()

# The overall precision and recall on each individual class
p, r, f, s = metrics.precision_recall_fscore_support(y_true, y_pred)
```

## Significance of classification rate

P-value associated to classification rate. Compared the number of correct classifications ( $=\text{accuracy} \times N$ ) to the null hypothesis of Binomial distribution of parameters  $p$  (typically 50% of chance level) and  $N$  (Number of observations).

Is 60% of accuracy a significant prediction rate among 62 observations?

Since this is an exact, **two-sided** test of the null hypothesis, the p-value can be divided by 2 since we test that the accuracy is superior to the chance level.

```
import scipy.stats

acc, N = 0.62, 62
pval = scipy.stats.binom_test(x=int(acc * N), n=N, p=0.5) / 2
print(pval)
```

0.04897722025975367

### Area Under Curve (AUC) of Receiver operating characteristic (ROC)

Some classifier may have found a good discriminative projection  $w$ . However if the threshold to decide the final predicted class is poorly adjusted, the performances will highlight an high specificity and a low sensitivity or the contrary.

In this case it is recommended to use the AUC of a ROC analysis which basically provide a measure of overlap of the two classes when points are projected on the discriminative axis. For more detail on ROC and AUC see:[https://en.wikipedia.org/wiki/Receiver\\_operating\\_characteristic](https://en.wikipedia.org/wiki/Receiver_operating_characteristic).

```
from sklearn import metrics
score_pred = np.array([.1, .2, .3, .4, .5, .6, .7, .8])
y_true = np.array([0, 0, 0, 0, 1, 1, 1, 1])
thres = .9
y_pred = (score_pred > thres).astype(int)

print("Predictions:", y_pred)
metrics.accuracy_score(y_true, y_pred)

# The overall precision an recall on each individual class
p, r, f, s = metrics.precision_recall_fscore_support(y_true, y_pred)
print("Recalls:", r)
# 100% of specificity, 0% of sensitivity

# However AUC=1 indicating a perfect separation of the two classes
auc = metrics.roc_auc_score(y_true, score_pred)
print("AUC:", auc)
```

```
Predictions: [0 0 0 0 0 0 0]
Recalls: [1. 0.]
AUC: 1.0
```

```
/home/edouard/anaconda3/lib/python3.7/site-packages/sklearn/metrics/classification.
→py:1143: UndefinedMetricWarning: Precision and F-score are ill-defined and being set to
→0.0 in labels with no predicted samples.
'precision', 'predicted', average, warn_for)
```

### 5.4.12 Imbalanced classes

Learning with discriminative (logistic regression, SVM) methods is generally based on minimizing the misclassification of training samples, which may be unsuitable for imbalanced datasets where the recognition might be biased in favor of the most numerous class. This problem can be addressed with a generative approach, which typically requires more parameters to be determined leading to reduced performances in high dimension.

Dealing with imbalanced class may be addressed by three main ways (see Japkowicz and Stephen (2002) for a review), resampling, reweighting and one class learning.

In **sampling strategies**, either the minority class is oversampled or majority class is undersampled or some combination of the two is deployed. Undersampling (Zhang and Mani, 2003) the majority class would lead to a poor usage of the left-out samples. Sometime one cannot afford such strategy since we are also facing a small sample size problem even for the majority class. Informed oversampling, which goes beyond a trivial duplication of minority class samples, requires the estimation of class conditional distributions in order to generate synthetic samples. Here generative models are required. An alternative, proposed in (Chawla et al., 2002) generate samples along the line segments joining any/all of the k minority class nearest neighbors. Such procedure blindly generalizes the minority area without regard to the majority class, which may be particularly problematic with high-dimensional and potentially skewed class distribution.

**Reweighting**, also called cost-sensitive learning, works at an algorithmic level by adjusting

the costs of the various classes to counter the class imbalance. Such reweighting can be implemented within SVM (Chang and Lin, 2001) or logistic regression (Friedman et al., 2010) classifiers. Most classifiers of Scikit learn offer such reweighting possibilities.

The `class_weight` parameter can be positioned into the "balanced" mode which uses the values of `y` to automatically adjust weights inversely proportional to class frequencies in the input data as  $N/(2N_k)$ .

```
import numpy as np
from sklearn import linear_model
from sklearn import datasets
from sklearn import metrics
import matplotlib.pyplot as plt

# dataset
X, y = datasets.make_classification(n_samples=500,
                                    n_features=5,
                                    n_informative=2,
                                    n_redundant=0,
                                    n_repeated=0,
                                    n_classes=2,
                                    random_state=1,
                                    shuffle=False)

print(*["#samples of class %i = %i;" % (lev, np.sum(y == lev)) for lev in np.unique(y)])

print('# No Reweighting balanced dataset')
lr_inter = linear_model.LogisticRegression(C=1)
lr_inter.fit(X, y)
p, r, f, s = metrics.precision_recall_fscore_support(y, lr_inter.predict(X))
print("SPC: %.3f; SEN: %.3f" % tuple(r))
print('# => The predictions are balanced in sensitivity and specificity\n')

# Create imbalanced dataset, by subsampling sample of class 0: keep only 10% of
# class 0's samples and all class 1's samples.
n0 = int(np.floor(np.sum(y == 0) / 20))
subsample_idx = np.concatenate((np.where(y == 0)[0][:n0], np.where(y == 1)[0]))
Ximb = X[subsample_idx, :]
yimb = y[subsample_idx]
print(*["#samples of class %i = %i;" % (lev, np.sum(yimb == lev)) for lev in
       np.unique(yimb)])

print('# No Reweighting on imbalanced dataset')
lr_inter = linear_model.LogisticRegression(C=1)
lr_inter.fit(Ximb, yimb)
p, r, f, s = metrics.precision_recall_fscore_support(yimb, lr_inter.predict(Ximb))
print("SPC: %.3f; SEN: %.3f" % tuple(r))
print('# => Sensitivity >> specificity\n')

print('# Reweighting on imbalanced dataset')
lr_inter_reweight = linear_model.LogisticRegression(C=1, class_weight="balanced")
lr_inter_reweight.fit(Ximb, yimb)
p, r, f, s = metrics.precision_recall_fscore_support(yimb,
                                                       lr_inter_reweight.predict(Ximb))
print("SPC: %.3f; SEN: %.3f" % tuple(r))
print('# => The predictions are balanced in sensitivity and specificity\n')
```

```
#samples of class 0 = 250; #samples of class 1 = 250;
# No Reweighting balanced dataset
SPC: 0.940; SEN: 0.928
# => The predictions are balanced in sensitivity and specificity

#samples of class 0 = 12; #samples of class 1 = 250;
# No Reweighting on imbalanced dataset
SPC: 0.750; SEN: 0.992
# => Sensitivity >> specificity

# Reweighting on imbalanced dataset
SPC: 1.000; SEN: 0.972
# => The predictions are balanced in sensitivity and specificity
```

```
/home/edouard/anaconda3/lib/python3.7/site-packages/sklearn/linear_model/logistic.py:433:_
  ↪FutureWarning: Default solver will be changed to 'lbfgs' in 0.22. Specify a solver to_
  ↪silence this warning.
  FutureWarning)
/home/edouard/anaconda3/lib/python3.7/site-packages/sklearn/linear_model/logistic.py:433:_
  ↪FutureWarning: Default solver will be changed to 'lbfgs' in 0.22. Specify a solver to_
  ↪silence this warning.
  FutureWarning)
/home/edouard/anaconda3/lib/python3.7/site-packages/sklearn/linear_model/logistic.py:433:_
  ↪FutureWarning: Default solver will be changed to 'lbfgs' in 0.22. Specify a solver to_
  ↪silence this warning.
  FutureWarning)
```

### 5.4.13 Exercise

#### Fisher linear discriminant rule

Write a class `FisherLinearDiscriminant` that implements the Fisher's linear discriminant analysis. This class must be compliant with the scikit-learn API by providing two methods: - `fit(X, y)` which fits the model and returns the object itself; - `predict(X)` which returns a vector of the predicted values. Apply the object on the dataset presented for the LDA.

## 5.5 Non linear learning algorithms

### 5.5.1 Support Vector Machines (SVM)

SVM are based kernel methods require only a user-specified kernel function  $K(x_i, x_j)$ , i.e., a **similarity function** over pairs of data points  $(x_i, x_j)$  into kernel (dual) space on which learning algorithms operate linearly, i.e. every operation on points is a linear combination of  $K(x_i, x_j)$ .

Outline of the SVM algorithm:

1. Map points  $x$  into kernel space using a kernel function:  $x \rightarrow K(x, .)$ .
2. Learning algorithms operate linearly by dot product into high-kernel space  $K(., x_i) \cdot K(., x_j)$ .
  - Using the kernel trick (Mercer's Theorem) replace dot product in hgh dimensional space by a simpler operation such that  $K(., x_i) \cdot K(., x_j) = K(x_i, x_j)$ . Thus we only

need to compute a similarity measure for each pairs of point and store in a  $N \times N$  Gram matrix.

- Finally, The learning process consist of estimating the  $\alpha_i$  of the decision function that maximises the hinge loss (of  $f(x)$ ) plus some penalty when applied on all training points.

$$f(x) = \text{sign} \left( \sum_i^N \alpha_i y_i K(x_i, x) \right).$$

3. Predict a new point  $x$  using the decision function.

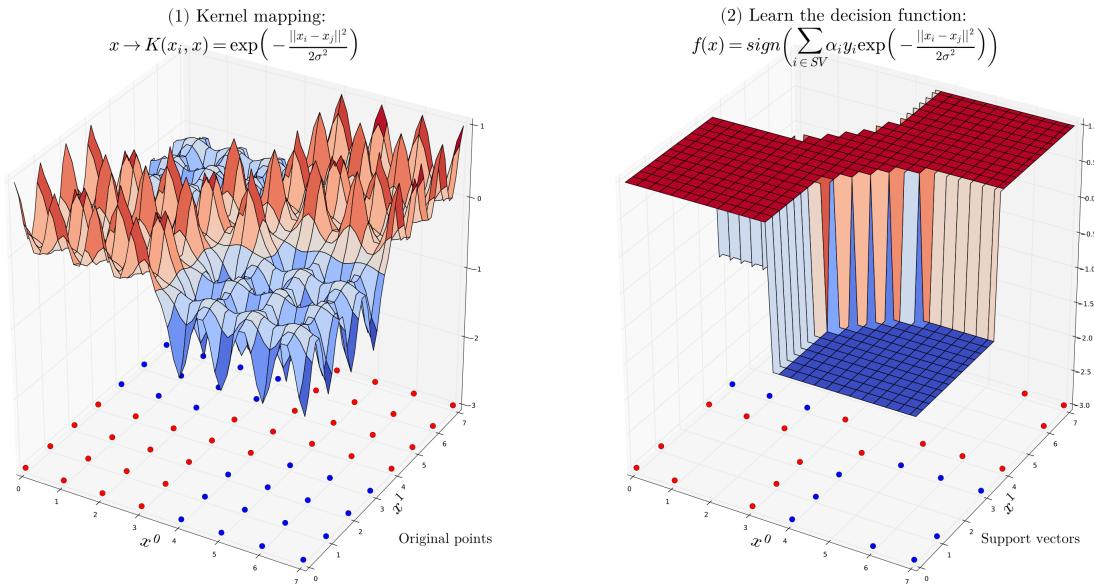


Fig. 9: Support Vector Machines.

#### Gaussian kernel (RBF, Radial Basis Function):

One of the most commonly used kernel is the Radial Basis Function (RBF) Kernel. For a pair of points  $x_i, x_j$  the RBF kernel is defined as:

$$K(x_i, x_j) = \exp \left( -\frac{\|x_i - x_j\|^2}{2\sigma^2} \right) \quad (5.52)$$

$$= \exp(-\gamma \|x_i - x_j\|^2) \quad (5.53)$$

Where  $\sigma$  (or  $\gamma$ ) defines the kernel width parameter. Basically, we consider a Gaussian function centered on each training sample  $x_i$ . it has a ready interpretation as a similarity measure as it decreases with squared Euclidean distance between the two feature vectors.

Non linear SVM also exists for regression problems.

```
%matplotlib inline
import warnings
warnings.filterwarnings('once')
```

```

import numpy as np
from sklearn.svm import SVC
from sklearn import datasets
import matplotlib.pyplot as plt

# dataset
X, y = datasets.make_classification(n_samples=10, n_features=2, n_redundant=0,
                                    n_classes=2,
                                    random_state=1,
                                    shuffle=False)

clf = SVC(kernel='rbf')#, gamma=1)
clf.fit(X, y)
print("#Errors: %i" % np.sum(y != clf.predict(X)))

clf.decision_function(X)

# Useful internals:
# Array of support vectors
clf.support_vectors_

# indices of support vectors within original X
np.all(X[clf.support_,:] == clf.support_vectors_)

```

```

/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
    ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
    got 216 from PyObject
    return f(*args, **kwds)
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
    ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
    got 216 from PyObject
    return f(*args, **kwds)
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
    ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
    got 216 from PyObject
    return f(*args, **kwds)
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
    ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
    got 216 from PyObject
    return f(*args, **kwds)

```

```
#Errors: 0
```

```

/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
    ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
    got 216 from PyObject
    return f(*args, **kwds)
/home/edouard/anaconda3/lib/python3.7/site-packages/sklearn/svm/base.py:196:_
    FutureWarning: The default value of gamma will change from 'auto' to 'scale' in version
    0.22 to account better for unscaled features. Set gamma explicitly to 'auto' or 'scale'
    to avoid this warning.
    "avoid this warning.", FutureWarning)

```

```
True
```

## 5.5.2 Random forest

A random forest is a meta estimator that fits a number of **decision tree learners** on various sub-samples of the dataset and use averaging to improve the predictive accuracy and control over-fitting.

```
### Decision tree learner
```

A tree can be “learned” by splitting the training dataset into subsets based on an features value test.

Each internal node represents a “test” on an feature resulting on the split of the current sample. At each step the algorithm selects the feature and a cutoff value that maximises a given metric. Different metrics exist for regression tree (target is continuous) or classification tree (the target is qualitative).

This process is repeated on each derived subset in a recursive manner called recursive partitioning. The recursion is completed when the subset at a node has all the same value of the target variable, or when splitting no longer adds value to the predictions. This general principle is implemented by many recursive partitioning tree algorithms.

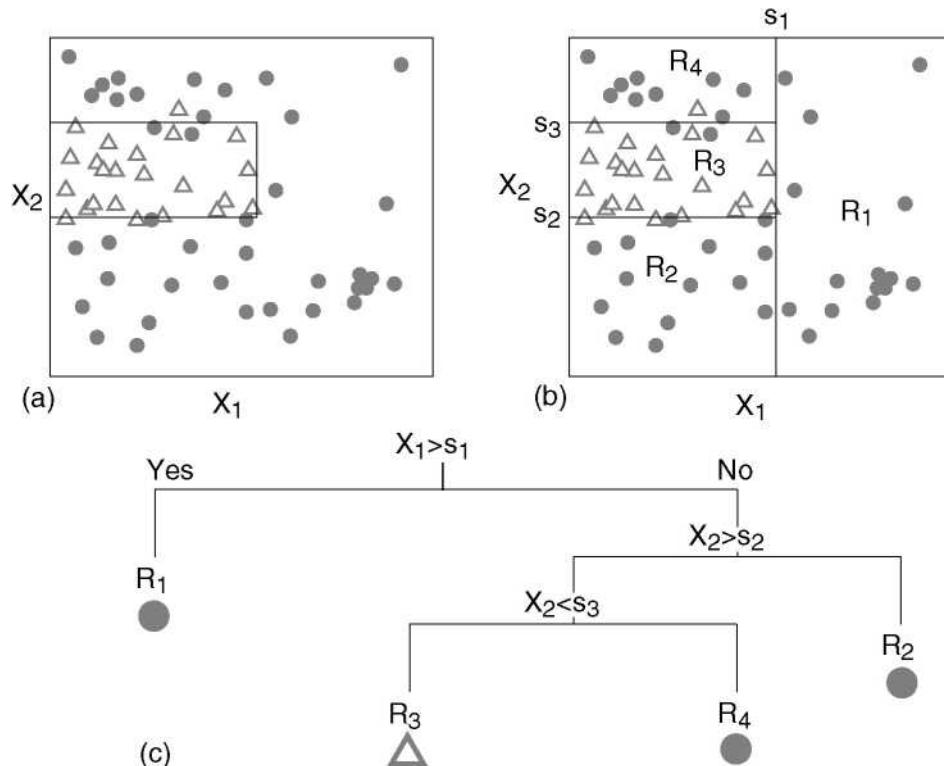


Fig. 10: Classification tree.

Decision trees are simple to understand and interpret however they tend to overfit the data. However decision trees tend to overfit the training set. Leo Breiman propose random forest to deal with this issue.

```
from sklearn.ensemble import RandomForestClassifier
forest = RandomForestClassifier(n_estimators = 100)
forest.fit(X, y)
```

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```
print("#Errors: %i" % np.sum(y != forest.predict(X)))
```

```
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
  ↪ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
  ↪got 216 from PyObject
    return f(*args, **kwds)
```

```
#Errors: 0
```

## 5.6 Resampling Methods

### 5.6.1 Left out samples validation

The **training error** can be easily calculated by applying the statistical learning method to the observations used in its training. But because of overfitting, the training error rate can dramatically underestimate the error that would be obtained on new samples.

The **test error** is the average error that results from a learning method to predict the response on a new samples that is, on samples that were not used in training the method. Given a data set, the use of a particular learning method is warranted if it results in a low test error. The test error can be easily calculated if a designated test set is available. Unfortunately, this is usually not the case.

Thus the original dataset is generally split in a training and a test (or validation) data sets. Large training set (80%) small test set (20%) might provide a poor estimation of the predictive performances. On the contrary, large test set and small training set might produce a poorly estimated learner. This is why, on situation where we cannot afford such split, it recommended to use cross-validation scheme to estimate the predictive power of a learning algorithm.

### 5.6.2 Cross-Validation (CV)

Cross-Validation scheme randomly divides the set of observations into  $K$  groups, or **folds**, of approximately equal size. The first fold is treated as a validation set, and the method  $f()$  is fitted on the remaining union of  $K - 1$  folds:  $(f(\mathbf{X}_{-K}, \mathbf{y}_{-K}))$ .

The measure of performance (the score function  $\mathcal{S}$ ), either a error measure or an correct prediction measure is an average of a loss error or correct prediction measure, noted  $\mathcal{L}$ , between a true target value and the predicted target value. The score function is evaluated of the on the observations in the held-out fold. For each sample  $i$  we consider the model estimated  $f(\mathbf{X}_{-k(i)}, \mathbf{y}_{-k(i)})$  on the data set without the group  $k$  that contains  $i$  noted  $-k(i)$ . This procedure is repeated  $K$  times; each time, a different group of observations is treated as a test set. Then we compare the predicted value ( $f_{-k(i)}(\mathbf{x}_i) = \hat{y}_i$ ) with true value  $y_i$  using a Error or Loss function  $\mathcal{L}(y, \hat{y})$ . We can the compute a score  $\mathcal{S}$  averaging over all samples:

$$\mathcal{S}(f) = \frac{1}{N} \sum_i^N \mathcal{L} \left( y_i, f(\mathbf{x}_{-k(i)}, \mathbf{y}_{-k(i)}) \right).$$

Similarly we can compute a score  $\mathcal{S}$  on each each fold  $k$  and average accross folds:

$$\begin{aligned}\mathcal{S}(f) &= \frac{1}{K} \sum_k^K \mathcal{S}_k(f). \\ \mathcal{S}(f) &= \frac{1}{K} \sum_k^K \frac{1}{N_k} \sum_{i \in k} \mathcal{L} \left( y_i, f(\mathbf{x}_{-k(i)}, \mathbf{y}_{-k(i)}) \right).\end{aligned}$$

these two measures (an average of average vs. a global average) are generally similar. They may differ slightly if folds are of different sizes.

This validation scheme is known as the **K-Fold CV**. Typical choices of  $K$  are 5 or 10, [Kohavi 1995]. The extreme case where  $K = N$  is known as **leave-one-out cross-validation, LOO-CV**.

## CV for regression

Usually the error function  $\mathcal{L}()$  is the r-squared score. However other function could be used.

```
%matplotlib inline
import warnings
warnings.filterwarnings(action='once')

import numpy as np
from sklearn import datasets
import sklearn.linear_model as lm
import sklearn.metrics as metrics
from sklearn.model_selection import KFold

X, y = datasets.make_regression(n_samples=100, n_features=100,
                                n_informative=10, random_state=42)
model = lm.Ridge(alpha=10)

cv = KFold(n_splits=5, random_state=42)
y_test_pred = np.zeros(len(y))
y_train_pred = np.zeros(len(y))

for train, test in cv.split(X):
    X_train, X_test, y_train, y_test = X[train, :], X[test, :], y[train], y[test]
    model.fit(X_train, y_train)
    y_test_pred[test] = model.predict(X_test)
    y_train_pred[train] = model.predict(X_train)

print("Train r2:%.2f" % metrics.r2_score(y, y_train_pred))
print("Test r2:%.2f" % metrics.r2_score(y, y_test_pred))
```

```
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
˓→ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
˓→got 216 from PyObject
    return f(*args, **kwds)
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
˓→ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
˓→got 216 from PyObject
    return f(*args, **kwds)
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
˓→ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
˓→got 216 from PyObject
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```

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```
return f(*args, **kwds)
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
    ↵ufunc size changed, may indicate binary incompatibility. Expected 192 from C header, ↵
    ↵got 216 from PyObject
return f(*args, **kwds)
```

```
Train r2:0.99
Test  r2:0.72
```

```
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
    ↵ufunc size changed, may indicate binary incompatibility. Expected 192 from C header, ↵
    ↵got 216 from PyObject
return f(*args, **kwds)
```

Scikit-learn provides user-friendly function to perform CV:

```
from sklearn.model_selection import cross_val_score

scores = cross_val_score(estimator=model, X=X, y=y, cv=5)
print("Test  r2:%.2f" % scores.mean())

# provide a cv
cv = KFold(n_splits=5, random_state=42)
scores = cross_val_score(estimator=model, X=X, y=y, cv=cv)
print("Test  r2:%.2f" % scores.mean())
```

```
Test  r2:0.73
Test  r2:0.73
```

## CV for classification

With classification problems it is essential to sample folds where each set contains approximately the same percentage of samples of each target class as the complete set. This is called **stratification**. In this case, we will use `StratifiedKFold` which is a variation of k-fold which returns stratified folds.

Usually the error function  $L()$  are, at least, the sensitivity and the specificity. However other function could be used.

```
import numpy as np
from sklearn import datasets
import sklearn.linear_model as lm
import sklearn.metrics as metrics
from sklearn.model_selection import StratifiedKFold

X, y = datasets.make_classification(n_samples=100, n_features=100,
                                    n_informative=10, random_state=42)

model = lm.LogisticRegression(C=1, solver='lbfgs')

cv = StratifiedKFold(n_splits=5)
y_test_pred = np.zeros(len(y))
```

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```
y_train_pred = np.zeros(len(y))

for train, test in cv.split(X, y):
    X_train, X_test, y_train, y_test = X[train, :], X[test, :], y[train], y[test]
    model.fit(X_train, y_train)
    y_test_pred[test] = model.predict(X_test)
    y_train_pred[train] = model.predict(X_train)

recall_test = metrics.recall_score(y, y_test_pred, average=None)
recall_train = metrics.recall_score(y, y_train_pred, average=None)
acc_test = metrics.accuracy_score(y, y_test_pred)

print("Train SPC:%.2f; SEN:%.2f" % tuple(recall_train))
print("Test SPC:%.2f; SEN:%.2f" % tuple(recall_test))
print("Test ACC:%.2f" % acc_test)
```

```
Train SPC:1.00; SEN:1.00
Test SPC:0.78; SEN:0.82
Test ACC:0.80
```

Scikit-learn provides user-friendly function to perform CV:

```
from sklearn.model_selection import cross_val_score

scores = cross_val_score(estimator=model, X=X, y=y, cv=5)
scores.mean()

# provide CV and score
def balanced_acc(estimator, X, y, **kwargs):
    ...
    Balanced accuracy scorer
    ...
    return metrics.recall_score(y, estimator.predict(X), average=None).mean()

scores = cross_val_score(estimator=model, X=X, y=y, cv=5, scoring=balanced_acc)
print("Test ACC:%.2f" % scores.mean())
```

```
Test ACC:0.80
```

Note that with Scikit-learn user-friendly function we average the scores' average obtained on individual folds which may provide slightly different results than the overall average presented earlier.

### 5.6.3 Parallel computation with joblib

Dataset

```
import numpy as np
from sklearn import datasets
import sklearn.linear_model as lm
import sklearn.metrics as metrics
from sklearn.model_selection import StratifiedKFold
```

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```
X, y = datasets.make_classification(n_samples=20, n_features=100, n_informative=10, random_state=42)
cv = StratifiedKFold(n_splits=5)
```

### Use cross\_validate function

```
from sklearn.model_selection import cross_validate

estimator = lm.LogisticRegression(C=1, solver='lbfgs')
cv_results = cross_validate(estimator, X, y, cv=cv, n_jobs=5)
print(np.mean(cv_results['test_score']), cv_results['test_score'])
```

```
0.65 [0.5 0.25 0.75 0.75 1.]
```

### ## Sequential computation

If we want have full control of the operations performed within each fold (retrieve the models parameters, etc.). We would like to parallelize the folowing sequetial code:

```
estimator = lm.LogisticRegression(C=1, solver='lbfgs')
y_test_pred_seq = np.zeros(len(y)) # Store predictions in the original order
coefs_seq = list()
for train, test in cv.split(X, y):
    X_train, X_test, y_train, y_test = X[train, :], X[test, :], y[train], y[test]
    estimator.fit(X_train, y_train)
    y_test_pred_seq[test] = estimator.predict(X_test)
    coefs_seq.append(estimator.coef_)

test_accs = [metrics.accuracy_score(y[test], y_test_pred_seq[test]) for train, test in cv.split(X, y)]
print(np.mean(test_accs), test_accs)
```

```
0.65 [0.5, 0.25, 0.75, 0.75, 1.0]
```

### Parallel computation with joblib

```
from sklearn.externals.joblib import Parallel, delayed, logger
from sklearn.base import is_classifier, clone

def _split_fit_predict(estimator, X, y, train, test):
    X_train, X_test, y_train, y_test = X[train, :], X[test, :], y[train], y[test]
    estimator.fit(X_train, y_train)
    return [estimator.predict(X_test), estimator.coef_]

estimator = lm.LogisticRegression(C=1, solver='lbfgs')

parallel = Parallel(n_jobs=5)
cv_ret = parallel(
    delayed(_split_fit_predict)(
        clone(estimator), X, y, train, test)
    for train, test in cv.split(X, y))
```

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```
y_test_pred_cv, coefs_cv = zip(*cv_ret)

# Retrieve predictions in the original order
y_test_pred = np.zeros(len(y))
for i, (train, test) in enumerate(cv.split(X, y)):
    y_test_pred[test] = y_test_pred_cv[i]

test_accs = [metrics.accuracy_score(y[test], y_test_pred[test]) for train, test in cv.split(X, y)]
print(np.mean(test_accs), test_accs)
```

```
0.65 [0.5, 0.25, 0.75, 0.75, 1.0]
```

Test same predictions and same coefficients

```
assert np.all(y_test_pred == y_test_pred_seq)
assert np.allclose(np.array(coefs_cv).squeeze(), np.array(coefs_seq).squeeze())
```

#### 5.6.4 CV for model selection: setting the hyper parameters

It is important to note CV may be used for two separate goals:

1. **Model assessment:** having chosen a final model, estimating its prediction error (generalization error) on new data.
2. **Model selection:** estimating the performance of different models in order to choose the best one. One special case of model selection is the selection model's hyper parameters. Indeed remember that most of learning algorithm have a hyper parameters (typically the regularization parameter) that has to be set.

Generally we must address the two problems simultaneously. The usual approach for both problems is to randomly divide the dataset into three parts: a training set, a validation set, and a test set.

- The **training set** (train) is used to fit the models;
- the **validation set** (val) is used to estimate prediction error for model selection or to determine the hyper parameters over a grid of possible values.
- the **test set** (test) is used for assessment of the generalization error of the final chosen model.

### Grid search procedure

Model selection of the best hyper parameters over a grid of possible values

For each possible values of hyper parameters  $\alpha_k$ :

1. Fit the learner on training set:  $f(X_{train}, y_{train}, \alpha_k)$
2. Evaluate the model on the validation set and keep the parameter(s) that minimises the error measure

$$\alpha_* = \arg \min L(f(X_{train}), y_{val}, \alpha_k)$$

3. Refit the learner on all training + validation data using the best hyper parameters:  $f^* \equiv f(X_{train \cup val}, y_{train \cup val}, \alpha_*)$
4. \*\* Model assessment \*\* of  $f^*$  on the test set:  $L(f^*(X_{test}), y_{test})$

## Nested CV for model selection and assessment

Most of time, we cannot afford such three-way split. Thus, again we will use CV, but in this case we need two nested CVs.

One **outer CV loop, for model assessment**. This CV performs  $K$  splits of the dataset into training plus validation  $(X_{-K}, y_{-K})$  set and a test set  $X_K, y_K$

One **inner CV loop, for model selection**. For each run of the outer loop, the inner loop performs  $L$  splits of dataset  $(X_{-K}, y_{-K})$  into training set:  $(X_{-K,-L}, y_{-K,-L})$  and a validation set:  $(X_{-K,L}, y_{-K,L})$ .

## Implementation with scikit-learn

Note that the inner CV loop combined with the learner form a new learner with an automatic model (parameter) selection procedure. This new learner can be easily constructed using Scikit-learn. The learned is wrapped inside a GridSearchCV class.

Then the new learned can be plugged into the classical outer CV loop.

```
import numpy as np
from sklearn import datasets
import sklearn.linear_model as lm
from sklearn.model_selection import GridSearchCV
import sklearn.metrics as metrics
from sklearn.model_selection import KFold

# Dataset
noise_sd = 10
X, y, coef = datasets.make_regression(n_samples=50, n_features=100, noise=noise_sd,
                                       n_informative=2, random_state=42, coef=True)

# Use this to tune the noise parameter such that snr < 5
print("SNR:", np.std(np.dot(X, coef)) / noise_sd)

# param grid over alpha & l1_ratio
param_grid = {'alpha': 10. ** np.arange(-3, 3), 'l1_ratio':[.1, .5, .9]}

# Wrap
model = GridSearchCV(lm.ElasticNet(max_iter=10000), param_grid, cv=5)

# 1) Biased usage: fit on all data, ommit outer CV loop
model.fit(X, y)
print("Train r2:%.2f" % metrics.r2_score(y, model.predict(X)))
print(model.best_params_)

# 2) User made outer CV, useful to extract specific information
cv = KFold(n_splits=5, random_state=42)
y_test_pred = np.zeros(len(y))
```

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```
y_train_pred = np.zeros(len(y))
alphas = list()

for train, test in cv.split(X, y):
    X_train, X_test, y_train, y_test = X[train, :], X[test, :], y[train], y[test]
    model.fit(X_train, y_train)
    y_test_pred[test] = model.predict(X_test)
    y_train_pred[train] = model.predict(X_train)
    alphas.append(model.best_params_)

print("Train r2:%.2f" % metrics.r2_score(y, y_train_pred))
print("Test r2:%.2f" % metrics.r2_score(y, y_test_pred))
print("Selected alphas:", alphas)

# 3.) user-friendly sklearn for outer CV
from sklearn.model_selection import cross_val_score
scores = cross_val_score(estimator=model, X=X, y=y, cv=cv)
print("Test r2:%.2f" % scores.mean())
```

```
SNR: 2.6358469446381614
Train r2:0.96
{'alpha': 1.0, 'l1_ratio': 0.9}
Train r2:1.00
Test r2:0.62
Selected alphas: [{'alpha': 0.001, 'l1_ratio': 0.9}, {'alpha': 0.001, 'l1_ratio': 0.9}, {
    ↪ 'alpha': 0.001, 'l1_ratio': 0.9}, {'alpha': 0.01, 'l1_ratio': 0.9}, {'alpha': 0.001,
    ↪ 'l1_ratio': 0.9}]
Test r2:0.55
```

## Regression models with built-in cross-validation

Sklearn will automatically select a grid of parameters, most of time use the defaults values.

`n_jobs` is the number of CPUs to use during the cross validation. If -1, use all the CPUs.

```
from sklearn import datasets
import sklearn.linear_model as lm
import sklearn.metrics as metrics
from sklearn.model_selection import cross_val_score

# Dataset
X, y, coef = datasets.make_regression(n_samples=50, n_features=100, noise=10,
                                       n_informative=2, random_state=42, coef=True)

print("== Ridge (L2 penalty) ==")
model = lm.RidgeCV(cv=3)
# Let sklearn select a list of alphas with default LOO-CV
scores = cross_val_score(estimator=model, X=X, y=y, cv=5)
print("Test r2:%.2f" % scores.mean())

print("== Lasso (L1 penalty) ==")
model = lm.LassoCV(n_jobs=-1, cv=3)
# Let sklearn select a list of alphas with default 3CV
```

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```
scores = cross_val_score(estimator=model, X=X, y=y, cv=5)
print("Test r2:%.2f" % scores.mean())

print("== ElasticNet (L1 penalty) ==")
model = lm.ElasticNetCV(l1_ratio=[.1, .5, .9], n_jobs=-1, cv=3)
# Let sklearn select a list of alphas with default 3CV
scores = cross_val_score(estimator=model, X=X, y=y, cv=5)
print("Test r2:%.2f" % scores.mean())
```

```
== Ridge (L2 penalty) ==
Test r2:0.16
== Lasso (L1 penalty) ==
```

```
/home/edouard/anaconda3/lib/python3.7/site-packages/sklearn/model_selection/_  
search.py:841: DeprecationWarning: The default of the iid parameter will change  
from True to False in version 0.22 and will be removed in 0.24. This will  
change numeric results when test-set sizes are unequal.  
DeprecationWarning)  
/home/edouard/anaconda3/lib/python3.7/site-packages/sklearn/model_selection/_  
search.py:841: DeprecationWarning: The default of the iid parameter will change  
from True to False in version 0.22 and will be removed in 0.24. This will  
change numeric results when test-set sizes are unequal.  
DeprecationWarning)  
/home/edouard/anaconda3/lib/python3.7/site-packages/sklearn/model_selection/_  
search.py:841: DeprecationWarning: The default of the iid parameter will change  
from True to False in version 0.22 and will be removed in 0.24. This will  
change numeric results when test-set sizes are unequal.  
DeprecationWarning)  
/home/edouard/anaconda3/lib/python3.7/site-packages/sklearn/model_selection/_  
search.py:841: DeprecationWarning: The default of the iid parameter will change  
from True to False in version 0.22 and will be removed in 0.24. This will  
change numeric results when test-set sizes are unequal.  
DeprecationWarning)  
/home/edouard/anaconda3/lib/python3.7/site-packages/sklearn/model_selection/_  
search.py:841: DeprecationWarning: The default of the iid parameter will change  
from True to False in version 0.22 and will be removed in 0.24. This will  
change numeric results when test-set sizes are unequal.  
DeprecationWarning)
```

```
Test r2:0.74
== ElasticNet (L1 penalty) ==
Test r2:0.58
```

## Classification models with built-in cross-validation

```
from sklearn import datasets
import sklearn.linear_model as lm
import sklearn.metrics as metrics
from sklearn.model_selection import cross_val_score
```

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```
X, y = datasets.make_classification(n_samples=100, n_features=100,
                                    n_informative=10, random_state=42)

# provide CV and score
def balanced_acc(estimator, X, y, **kwargs):
    """
    Balanced accuracy scorer
    ...
    return metrics.recall_score(y, estimator.predict(X), average=None).mean()

print("== Logistic Ridge (L2 penalty) ==")
model = lm.LogisticRegressionCV(class_weight='balanced', scoring=balanced_acc, n_jobs=-1, cv=3)
# Let sklearn select a list of alphas with default LOO-CV
scores = cross_val_score(estimator=model, X=X, y=y, cv=5)
print("Test ACC:%.2f" % scores.mean())
```

```
== Logistic Ridge (L2 penalty) ==
```

```
/home/edouard/anaconda3/lib/python3.7/site-packages/sklearn/linear_model/logistic.
→py:1926: ChangedBehaviorWarning: The long-standing behavior to use the accuracy score
→has changed. The scoring parameter is now used. This warning will disappear in version
→0.22.
    ChangedBehaviorWarning)
/home/edouard/anaconda3/lib/python3.7/site-packages/sklearn/linear_model/logistic.
→py:1926: ChangedBehaviorWarning: The long-standing behavior to use the accuracy score
→has changed. The scoring parameter is now used. This warning will disappear in version
→0.22.
    ChangedBehaviorWarning)
/home/edouard/anaconda3/lib/python3.7/site-packages/sklearn/linear_model/logistic.
→py:1926: ChangedBehaviorWarning: The long-standing behavior to use the accuracy score
→has changed. The scoring parameter is now used. This warning will disappear in version
→0.22.
    ChangedBehaviorWarning)
```

```
Test ACC:0.77
```

```
/home/edouard/anaconda3/lib/python3.7/site-packages/sklearn/linear_model/logistic.
→py:1926: ChangedBehaviorWarning: The long-standing behavior to use the accuracy score
→has changed. The scoring parameter is now used. This warning will disappear in version
→0.22.
    ChangedBehaviorWarning)
/home/edouard/anaconda3/lib/python3.7/site-packages/sklearn/linear_model/logistic.
→py:1926: ChangedBehaviorWarning: The long-standing behavior to use the accuracy score
→has changed. The scoring parameter is now used. This warning will disappear in version
→0.22.
    ChangedBehaviorWarning)
```

## 5.6.5 Random Permutations

A permutation test is a type of non-parametric randomization test in which the null distribution of a test statistic is estimated by randomly permuting the observations.

Permutation tests are highly attractive because they make no assumptions other than that the observations are independent and identically distributed under the null hypothesis.

1. Compute a observed statistic  $t_{obs}$  on the data.
2. Use randomization to compute the distribution of  $t$  under the null hypothesis: Perform  $N$  random permutation of the data. For each sample of permuted data,  $i$  the data compute the statistic  $t_i$ . This procedure provides the distribution of  $t$  under the null hypothesis  $H_0$ :  $P(t|H_0)$
3. Compute the p-value =  $P(t > t_{obs}|H_0) |\{t_i > t_{obs}\}|$ , where  $t_i$ 's include  $t_{obs}$ .

### Example with a correlation

The statistic is the correlation.

```
import numpy as np
import scipy.stats as stats
import matplotlib.pyplot as plt
import seaborn as sns
%matplotlib inline
#%matplotlib qt

np.random.seed(42)
x = np.random.normal(loc=10, scale=1, size=100)
y = x + np.random.normal(loc=-3, scale=3, size=100) # snr = 1/2

# Permutation: simulate the null hypothesis
nperm = 10000
perms = np.zeros(nperm + 1)

perms[0] = np.corrcoef(x, y)[0, 1]

for i in range(1, nperm):
    perms[i] = np.corrcoef(np.random.permutation(x), y)[0, 1]

# Plot
# Re-weight to obtain distribution
weights = np.ones(perms.shape[0]) / perms.shape[0]
plt.hist([perms[perms >= perms[0]], perms], histtype='stepfilled',
         bins=100, label=["t>t obs (p-value)", "t<t obs"],
         weights=[weights[perms >= perms[0]], weights])

plt.xlabel("Statistic distribution under null hypothesis")
plt.axvline(x=perms[0], color='blue', linewidth=1, label="observed statistic")
_ = plt.legend(loc="upper left")

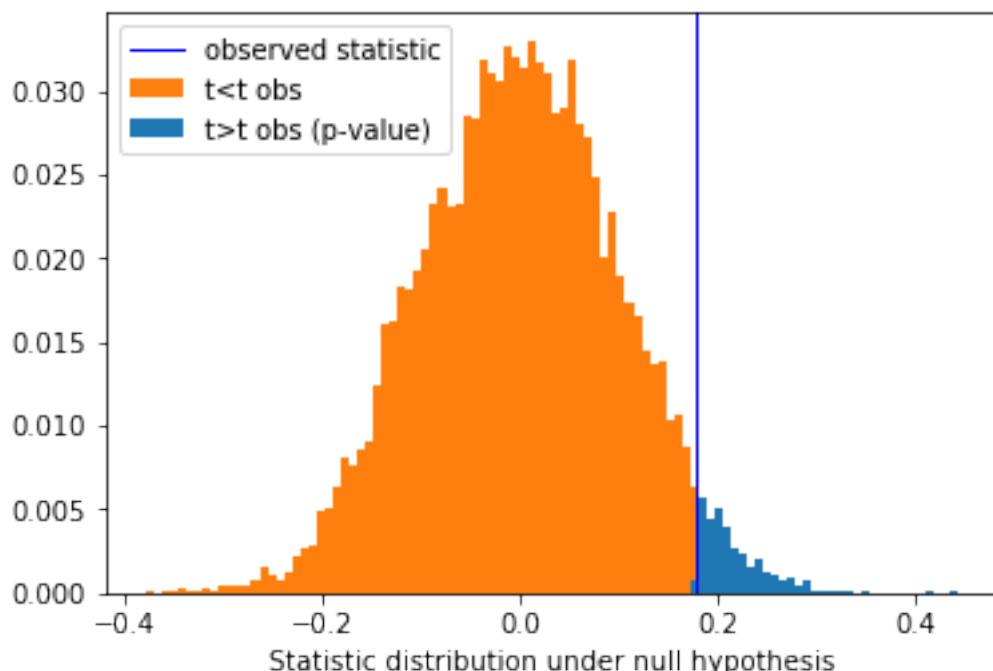
# One-tailed empirical p-value
pval_perm = np.sum(perms >= perms[0]) / perms.shape[0]

# Compare with Pearson's correlation test
_, pval_test = stats.pearsonr(x, y)

print("Permutation two tailed p-value=%5f. Pearson test p-value=%5f" % (2*pval_perm, _
```

```
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
    ↵ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
    ↵got 216 from PyObject
    ↵return f(*args, **kwds)
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
    ↵ufunc size changed, may indicate binary incompatibility. Expected 216, got 192
    ↵return f(*args, **kwds)
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: ImportWarning: can't_
    ↵resolve package from __spec__ or __package__, falling back on __name__ and __path__
    ↵return f(*args, **kwds)
/home/edouard/anaconda3/lib/python3.7/importlib/_bootstrap.py:219: RuntimeWarning: numpy.
    ↵ufunc size changed, may indicate binary incompatibility. Expected 192 from C header,_
    ↵got 216 from PyObject
    ↵return f(*args, **kwds)
```

Permutation two tailed p-value=0.06959. Pearson test p-value=0.07355



## Exercise

Given the logistic regression presented above and its validation given a 5 folds CV.

1. Compute the p-value associated with the prediction accuracy using a permutation test.
2. Compute the p-value associated with the prediction accuracy using a parametric test.

### 5.6.6 Bootstrapping

Bootstrapping is a random sampling with replacement strategy which provides an non-parametric method to assess the variability of performances scores such standard errors or confidence intervals.

A great advantage of bootstrap is its simplicity. It is a straightforward way to derive estimates of standard errors and confidence intervals for complex estimators of complex parameters of the distribution, such as percentile points, proportions, odds ratio, and correlation coefficients.

1. Perform  $B$  sampling, with replacement, of the dataset.
2. For each sample  $i$  fit the model and compute the scores.
3. Assess standard errors and confidence intervals of scores obtained on the  $B$  resampled dataset.

```
import numpy as np
from sklearn import datasets
import sklearn.linear_model as lm
import sklearn.metrics as metrics
import pandas as pd

# Regression dataset
n_features = 5
n_features_info = 2
n_samples = 100
X = np.random.randn(n_samples, n_features)
beta = np.zeros(n_features)
beta[:n_features_info] = 1
Xbeta = np.dot(X, beta)
eps = np.random.randn(n_samples)
y = Xbeta + eps

# Fit model on all data (!! risk of overfit)
model = lm.RidgeCV()
model.fit(X, y)
print("Coefficients on all data:")
print(model.coef_)

# Bootstrap loop
nboot = 100 # !! Should be at least 1000
scores_names = ["r2"]
scores_boot = np.zeros((nboot, len(scores_names)))
coefs_boot = np.zeros((nboot, X.shape[1]))

orig_all = np.arange(X.shape[0])
for boot_i in range(nboot):
    boot_tr = np.random.choice(orig_all, size=len(orig_all), replace=True)
    boot_te = np.setdiff1d(orig_all, boot_tr, assume_unique=False)
    Xtr, ytr = X[boot_tr, :], y[boot_tr]
    Xte, yte = X[boot_te, :], y[boot_te]
    model.fit(Xtr, ytr)
    y_pred = model.predict(Xte).ravel()
    scores_boot[boot_i, :] = metrics.r2_score(yte, y_pred)
    coefs_boot[boot_i, :] = model.coef_

# Compute Mean, SE, CI
scores_boot = pd.DataFrame(scores_boot, columns=scores_names)
scores_stat = scores_boot.describe(percentiles=[.99, .95, .5, .1, .05, .01])

print("r-squared: Mean=% .2f, SE=% .2f, CI=(% .2f % .2f)" %\
      tuple(scores_stat.loc[["mean", "std", "5%", "95%"], "r2"]))
```

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```
coefs_boot = pd.DataFrame(coefs_boot)
coefs_stat = coefs_boot.describe(percentiles=[.99, .95, .5, .1, .05, .01])
print("Coefficients distribution")
print(coefs_stat)
```

```
Coefficients on all data:
[ 1.01094082  0.92410534 -0.07588245  0.13848944  0.19659906]
r-squared: Mean=0.59, SE=0.11, CI=(0.39 0.74)
Coefficients distribution
      0         1         2         3         4
count 100.000000 100.000000 100.000000 100.000000 100.000000
mean   1.007552   0.927999  -0.072079   0.166443   0.188892
std    0.105309   0.118476   0.092189   0.109172   0.089533
min    0.710004   0.676758  -0.331354  -0.059170  -0.043120
1%     0.787546   0.695238  -0.261349  -0.058613  0.001962
5%     0.835648   0.741149  -0.219243  0.009053  0.050575
10%    0.878441   0.775851  -0.202235  0.042002  0.079449
50%    1.013152   0.921445  -0.083346  0.167349  0.190600
95%    1.211640   1.108971  0.052410  0.352416  0.345560
99%    1.254097   1.180027  0.150143  0.383904  0.399238
max    1.290094   1.264742  0.153999  0.511701  0.401858
```

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**CHAPTER  
SIX**

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- modindex
- search