Statistics and Machine Learning in Python

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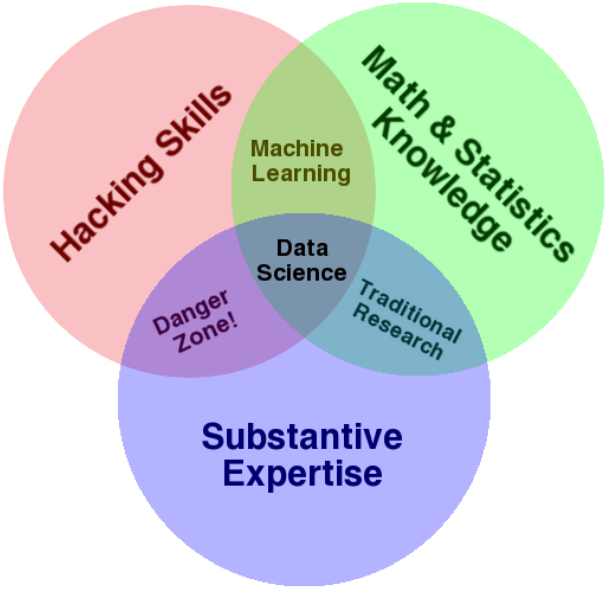
CHAPTER

ONE

INTRODUCTION TO MACHINE LEARNING

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).

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: python library adept at handling sets of structured data: list, tables.

Statistics and applied mathematics

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

Data analysis methodology

1. **Formalize customer's needs into a learning problem:**
    - **A target variable: supervised problem.**
        - Target is qualitative: classification.
        - Target is qualitative: 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/exlusion criteria. The conditions that define the acquisition of the dataset.
    - For retrospective study formalize the experimental design: inclusion/exlusion 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. (a) 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

Source Kevin Markham https://github.com/justmarkham/python-reference

Set up your programming environment using Anaconda

1. Download anaconda http://continuum.io/downloads
2. Install it, on Linux:

Python 2.7:

```
bash Anaconda2-2.4.0-Linux-x86_64.sh
```

Python 3:

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

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

Python 2.7:

```
export PATH="${HOME}/anaconda2/bin:$PATH"
```

Python 3:

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

4. Optional: install additionnal packages:

Using `conda`:

```
conda install seaborn
```

Using `pip`:

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

Optional:

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

5. Python editor `spyder`:
    - Consoles/Open IPython console.

- Left panel text editor
- Right panel ipython console
- F9 run selection or curent line (in recent version of spyder)

6. Python interpreter: one can use either `python` or `ipython`, with later being an interpretive shell within python that provides additional features: https://docs.python.org/3/tutorial/ & http://ipython.readthedocs.io/en/stable/interactive/tutorial.html.

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)
```

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('')     # empty string
```

```
bool([])     # empty list
bool({})     # empty dictionary

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

```
True
```

Math

```
# basic operations
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

# force '/' in Python 2.x to perform 'true division' (unnecessary in Python 3.x)
from __future__ import division
10 / 4           # true division (returns 2.5)
10 // 4          # floor division (returns 2)
```

```
2
```

Comparisons and 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
```

```
True
```

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'
```

```
positive
positive
positive
positive
```

```
'positive'
```

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

```
# 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)
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)

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

```
['a', 'a', 'b', 'b', 'b']
```

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
```

Strings

A sequence of characters, they are iterable, immutable

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

# 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'

# normal strings versus raw strings
print('first line\nsecond line')     # normal strings allow for escaped characters
print(r'first line\nfirst line')     # raw strings treat backslashes as literal␣
↪characters
```

```
first line
second line
first linenfirst line
```

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)
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'
```

```
Error 'grandma'
```

```
'youngest child is maggie'
```

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
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]
```

```
Error 'c'
```

```
[0, 1, 2, 9]
```

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):
    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
```

```
this is text
3
3
```

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'
```

```
APPLE
BANANA
CHERRY
APPLE
BANANA
CHERRY
mom marge
dad homer
size 6
0 apple
1 banana
2 cherry
Found the banana!
This will print 5 times
This will print 5 times
This will print 5 times
This will print 5 times
This will print 5 times
```

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}
```

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)
```

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

Basic operating system interfaces (os)

```
import os
import tempfile

tmpdir = tempfile.gettempdir()

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

# Change the current working directory to path.
os.chdir(tmpdir)

# Get current working directory.
print('Working dir:', os.getcwd())

# Join paths
mytmpdir = os.path.join(tmpdir, "foobar")

# Create a directory
if not os.path.exists(mytmpdir):
    os.mkdir(mytmpdir)

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()

## 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]
```

```
Working dir: /tmp
/tmp/foobar/myfile.txt
```

```
---------------------------------------------------------------------------

TypeError                                 Traceback (most recent call last)

<ipython-input-15-6c4c2de1560a> in <module>()
     27
     28 ## write line by line
---> 29 fd = open(filename, "w")
     30 fd.write(lines[0] + "\n")
     31 fd.write(lines[1]+ "\n")


TypeError: an integer is required (got type str)
```

Object Oriented Programing (OOP)

Sources

- http://python-textbok.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

# 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")
```

Exercises

Exercise 1: functions

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

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]`

Exercise 3: File I/O

Copy/past the bsd 4 clause license into a text file. Read, the file (assuming this file could be huge) and count the occurrences of each word within the file. Words are separated by whitespace or new line characters.

Exercise 4: OOP

1. Create a class `Employee` with 2 attributes provided in the constructor: `name`, `years_of_service`. With one method `salary` with is obtained by `1500 + 100 * years_of_service`.
2. Create a subclass `Manager` which redefine `salary` method `2500 + 120 * 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

CHAPTER

THREE

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

```
from __future__ import print_function
import numpy as np
```

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

# 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)

# 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)
```

Reshaping

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

# Add an axis
a = np.array([0, 1])
a_col = a[:, np.newaxis]
# array([[0],
#        [1]])

# Transpose
a_col.T
#array([[0, 1]])
```

Stack arrays

Stack flat arrays in columns

Selection

Single item

```
arr1[0]          # 0th element (slices like a list)
arr2[0, 3]       # row 0, column 3: returns 4
arr2[0][3]       # alternative syntax
```

Slicing

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

Views and copies

```
arr = np.arange(10)
arr[5:8]                    # returns [5, 6, 7]
arr[5:8] = 12               # all three values are overwritten (would give error on a␣
↪list)
arr_view = arr[5:8]         # creates a "view" on arr, not a copy
arr_view[:] = 13            # modifies arr_view AND arr
arr_copy = arr[5:8].copy()  # makes a copy instead
arr_copy[:] = 14            # only modifies arr_copy
```

using boolean arrays

```
arr[arr > 5]
```

Boolean selection return a view which authorizes the modification of the original array

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


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
```

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)
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

# reshape, transpose, flatten
nums = np.arange(32).reshape(8, 4) # creates 8x4 array
nums.T                          # transpose
nums.flatten()                  # flatten

# 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
```

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])
a + b
```

```
array([[ 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
```

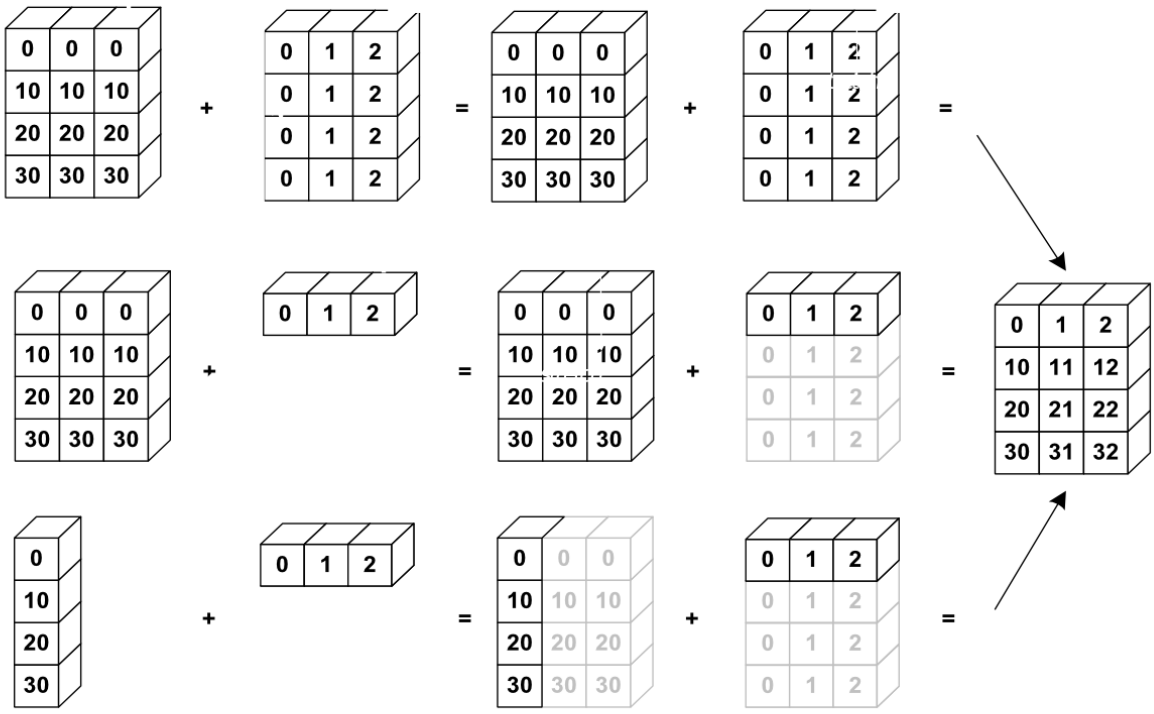


Fig. 3.1: Broadcasting (http://www.scipy-lectures.org)

```
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
```

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).

CHAPTER

FOUR

PANDAS: DATA MANIPULATION

It is often said that 80% of data analysis is spent on the cleaning and preparing data. To get a handle on the problem, this chapter focuses on a 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
```

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']))
```

Concatenate DataFrame

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

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

Join DataFrame

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

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

# Use intersection of keys from both frames
merge_inter = pd.merge(users, user4, on="name")

print(merge_inter)

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

# Use union of keys from both frames
users = pd.merge(users, user4, on="name", how='outer')
print(users)

#   age gender         job   name  height
#0   19      F     student  alice     165
#1   26      M     student   john     180
#2   22      M     student   eric     175
#3   58      F     manager   paul     NaN
#4   33      M    engineer  peter     NaN
#5   44      F   scientist  julie     171
```

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
users.describe()         # summarize all numeric columns
#             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

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)

# summarize all columns (new in pandas 0.15.0)
users.describe(include='all')        # describe all Series
#              age gender      job   name      height
#count    6.000000      6        6      6    4.000000
#unique        NaN      2        4      6         NaN
#top           NaN      M  student  alice         NaN
#freq          NaN      3        3      1         NaN
#mean    33.666667    NaN      NaN    NaN  172.750000
#std     14.895189    NaN      NaN    NaN    6.344289
#min     19.000000    NaN      NaN    NaN  165.000000
#25%     23.000000    NaN      NaN    NaN  169.500000
#50%     29.500000    NaN      NaN    NaN  173.000000
#75%     41.250000    NaN      NaN    NaN  176.250000
#max     58.000000    NaN      NaN    NaN  180.000000

users.describe(include=['object'])  # limit to one (or more) types
#       gender      job   name
#count       6        6      6
#unique      2        4      6
#top         M  student  alice
#freq        3        3      1
```

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
```

Rows selection

```
# 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

# 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
```

Rows selction / 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...
users[young_bool]             # ...and use that Series to filter rows
users[users.age < 20].job     # select one column from the filtered results

# 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
```

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
```

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)

#     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
#             ...
#11  julie   gender          F
#12  alice      job    student
#             ...
#17  julie      job  scientist
#18  alice   height        165
#             ...
#23  julie   height        171

# "pivots" a DataFrame from long (stacked) format to wide format,
print(staked.pivot(index='name', columns='variable', values='value'))

#variable age gender height        job
#name
#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
```

Quality control: 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
```

Quality control: 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
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

# Strategy2: fill in missing values
df.height.mean()
df = users.copy()

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

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
```

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) https://fr.wikipedia.org/wiki/Loi_normale#/media/File:Boxplot_vs_PDF.svg

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

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

```
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())
```

Groupby

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

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/data/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')
```

Exercises

Data Frame

1. Read the iris dataset at 'https://raw.github.com/neurospin/pystatsml/master/data/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.

CHAPTER

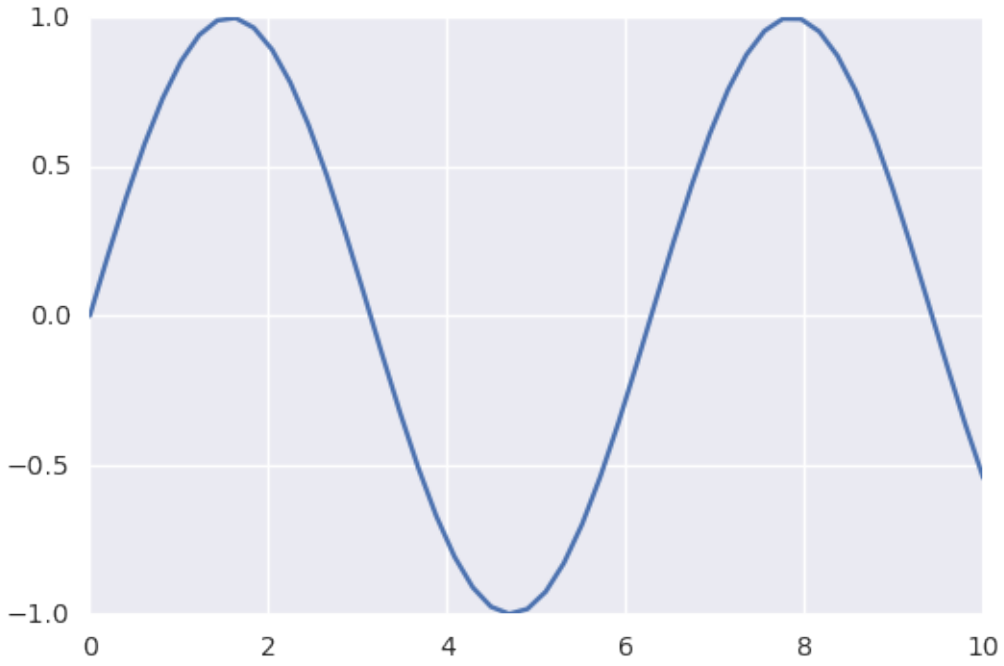
FIVE

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

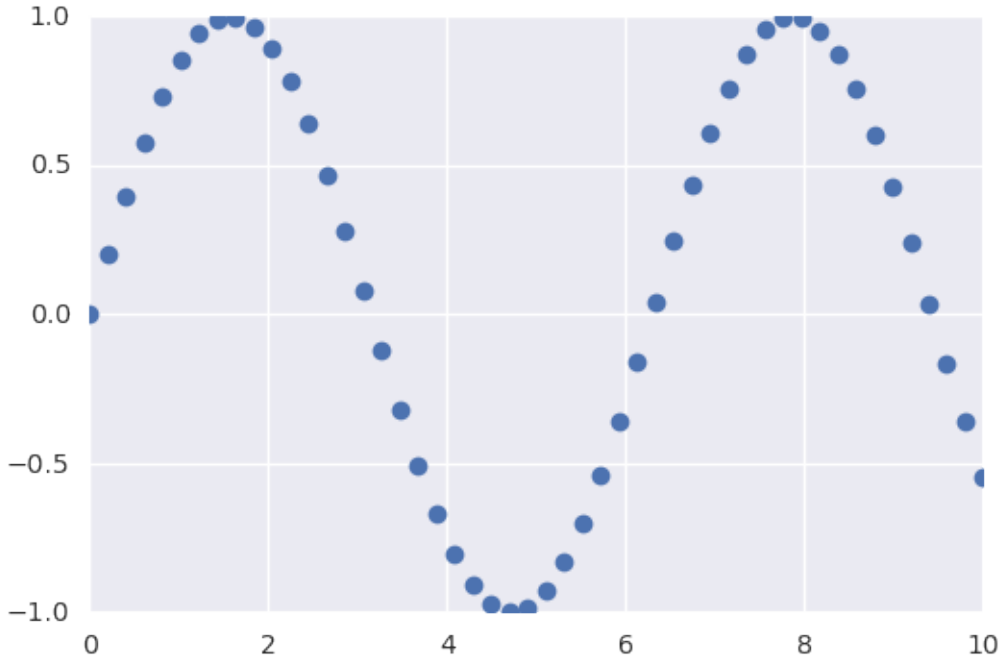
Basic plots

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

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

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

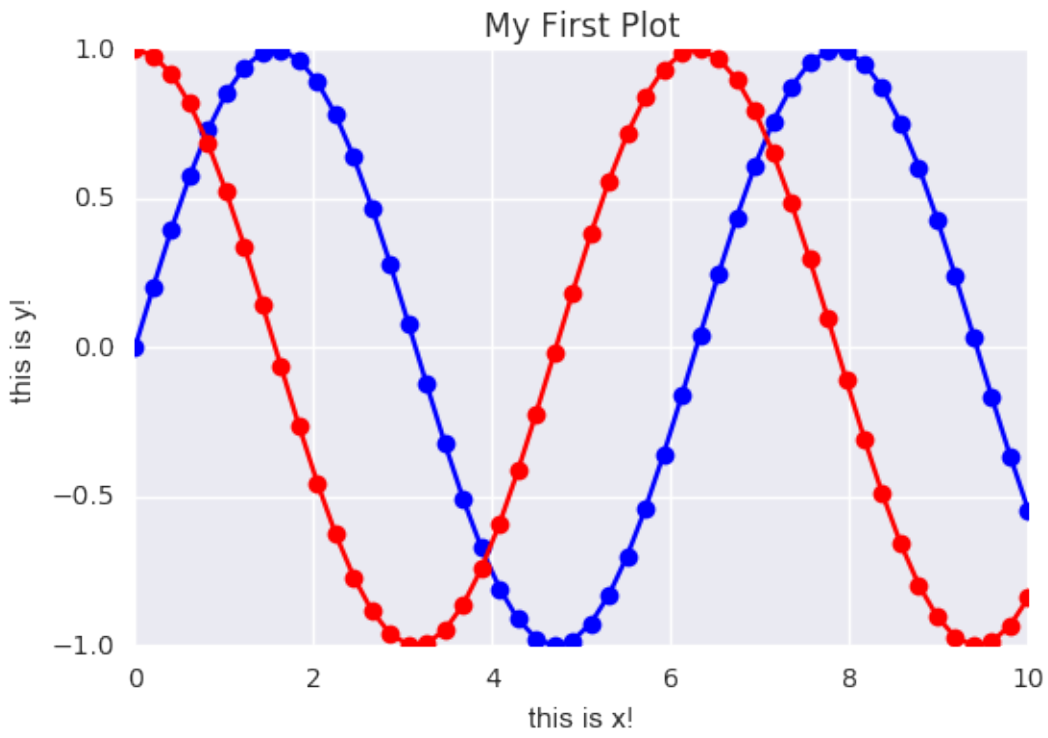



```
plt.plot(x, sinus, "o")
plt.show()
```

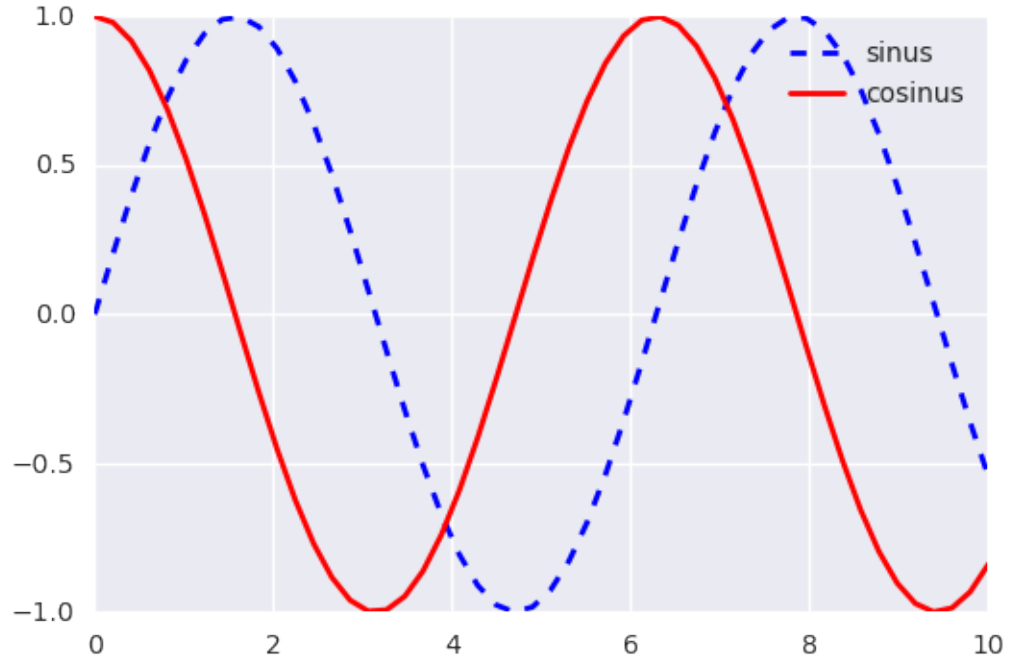
```
# use plt.plot to get color / marker abbreviations
```




```
# 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()
```



Scatter (2D) plots

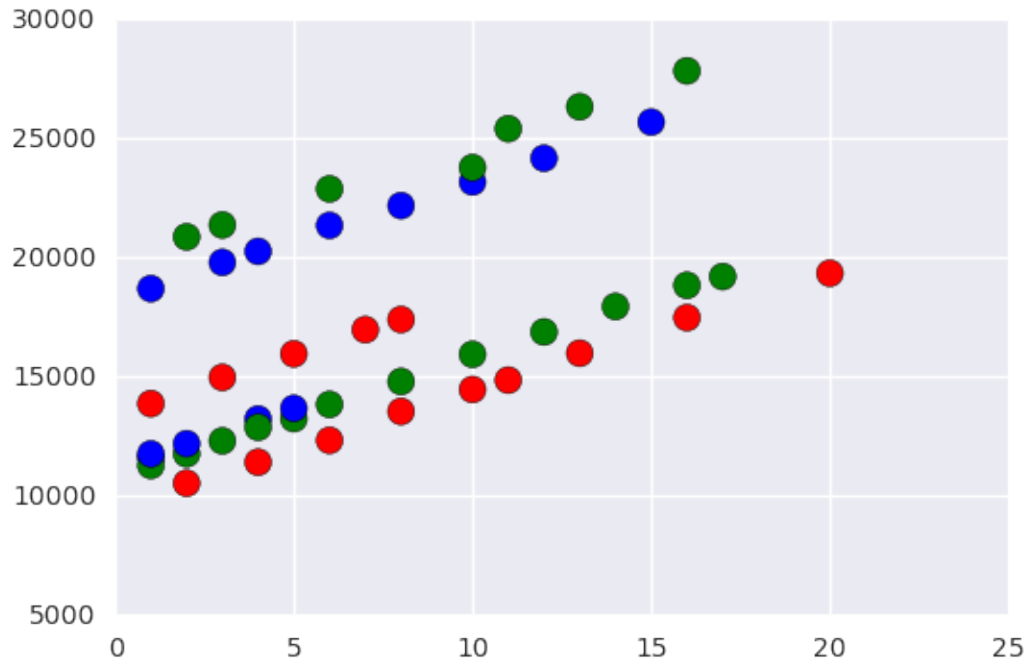
Load dataset

```
import pandas as pd
try:
    salary = pd.read_csv("../data/salary_table.csv")
except:
    url = 'https://raw.github.com/duchesnay/pylearn-doc/master/data/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)
```

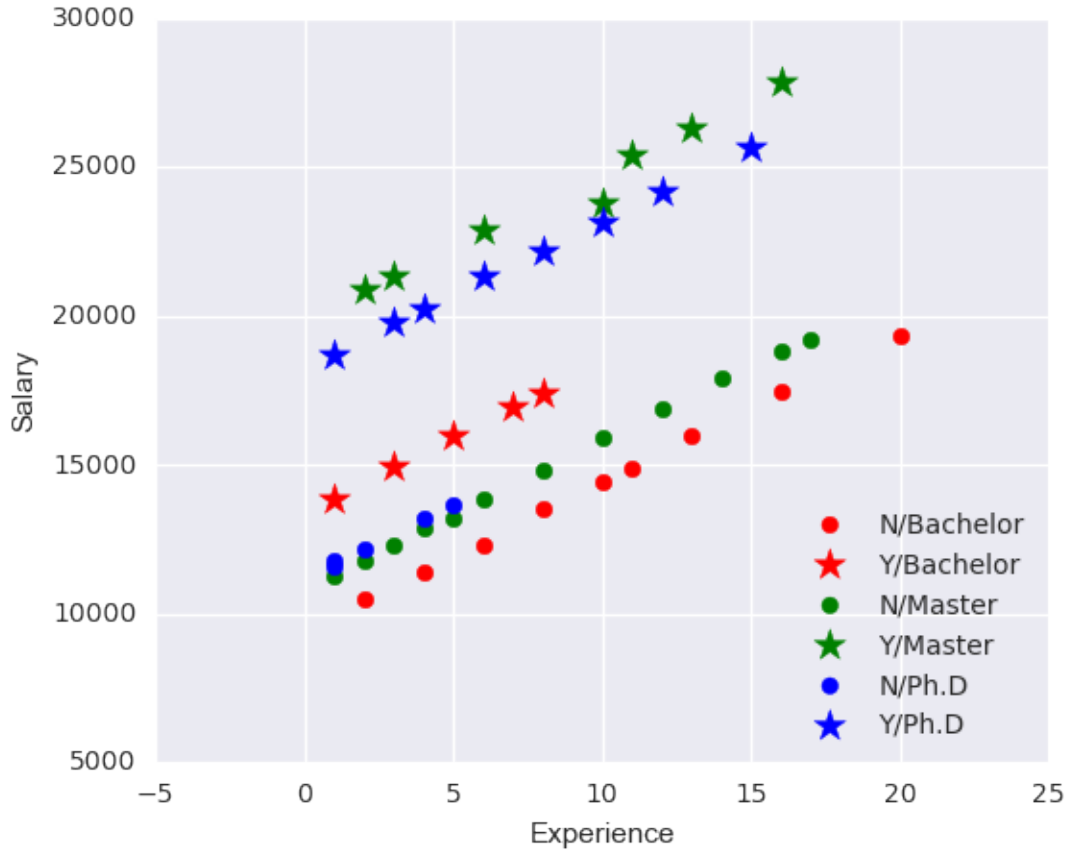
```
<matplotlib.collections.PathCollection at 0x7f78c2ab25f8>
```



Scatter plot with colors and symbols

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

## Define colors / sumbols 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()
```



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()
```

Exploring data (with seaborn)

Sources: http://stanford.edu/~mwaskom/software/seaborn

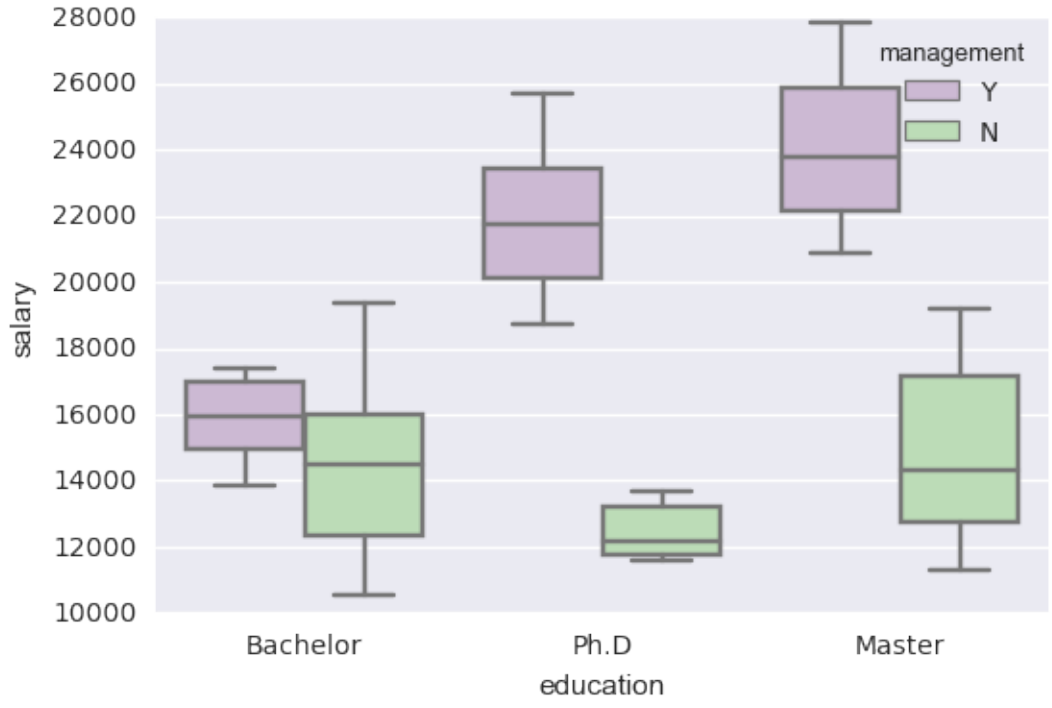
Install using: `pip install -U --user seaborn`

Boxplot

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

```
import seaborn as sns

sns.boxplot(x="education", y="salary", hue="management", data=salary, palette="PRGn")
```

```
<matplotlib.axes._subplots.AxesSubplot at 0x7f78c2ab44a8>
```




```
sns.boxplot(x="management", y="salary", hue="education", data=salary, palette="PRGn")
```

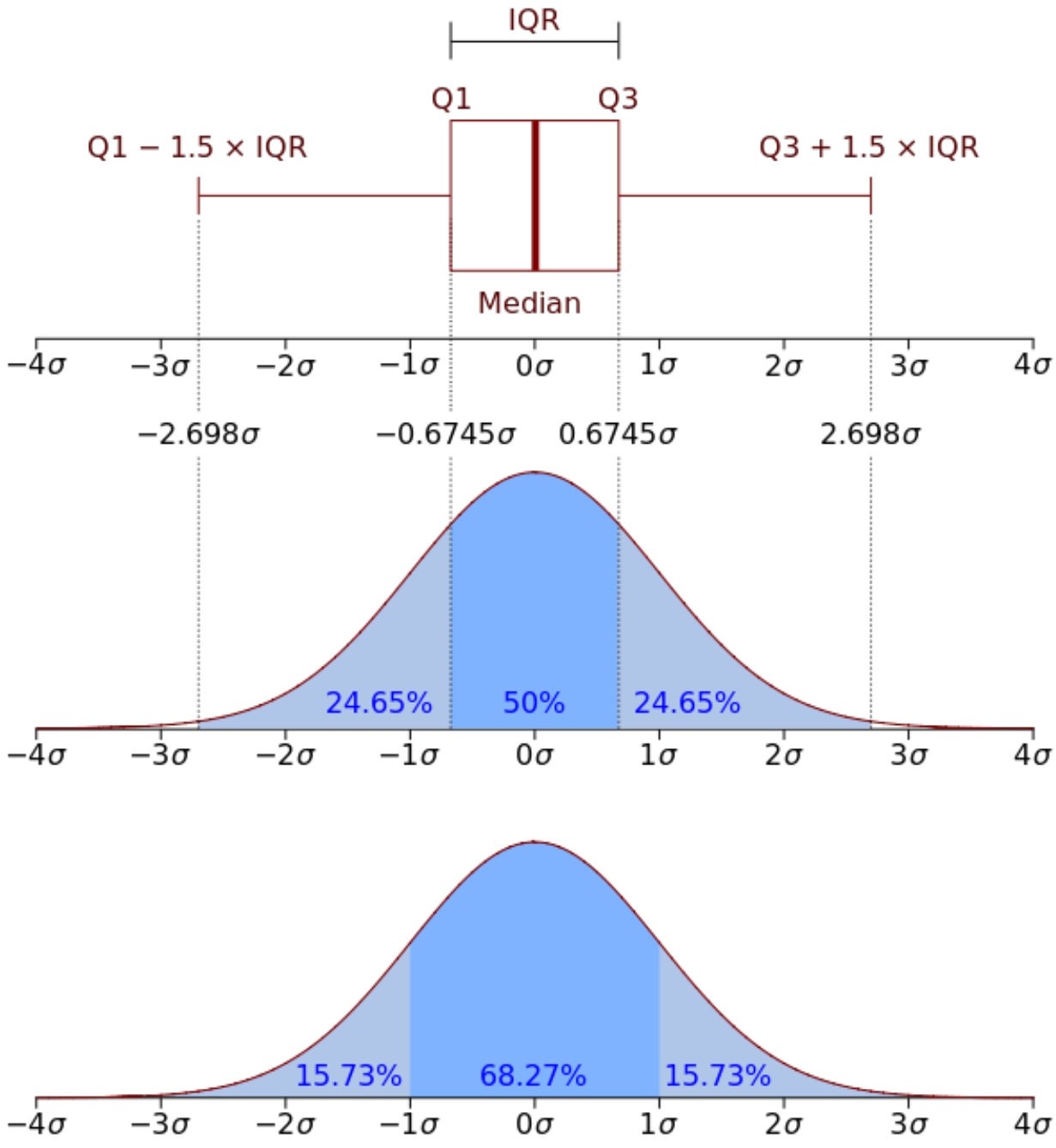
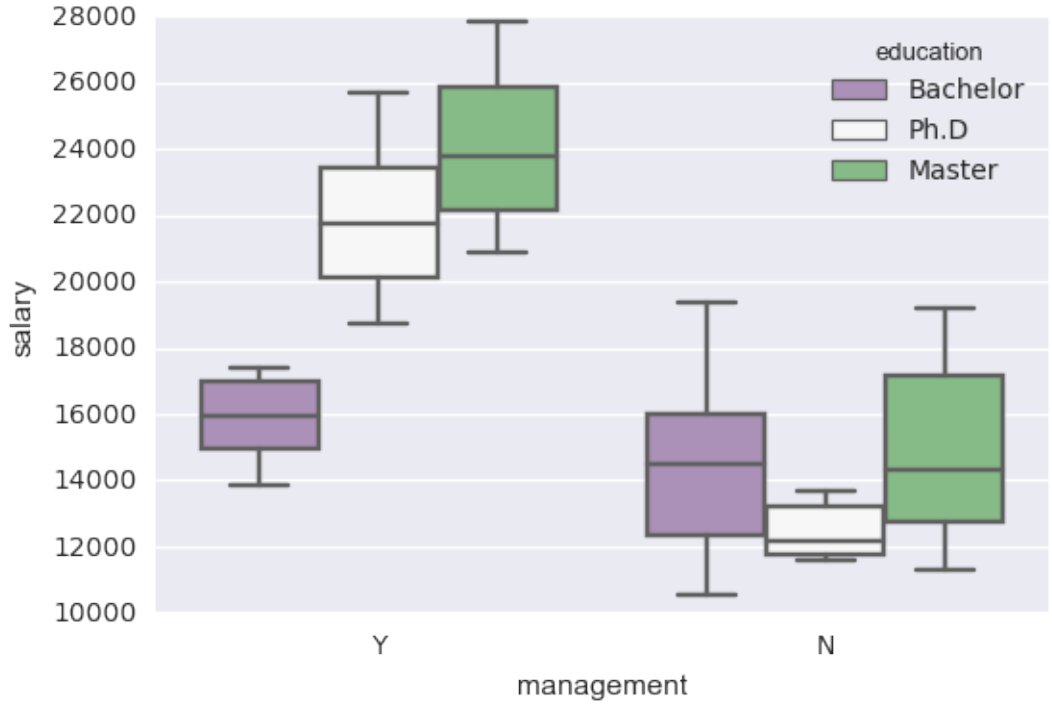

IQR
Q1
Q3
Q1 − 1.5 × IQR
Q3 + 1.5 × IQR
Median
−4σ
−3σ
−2σ
−1σ
0σ
1σ
2σ
3σ
4σ
−2.698σ
−0.6745σ
0.6745σ
2.698σ
24.65%
50%
24.65%
15.73%
68.27%
15.73%

Fig. 5.1: title

```
<matplotlib.axes._subplots.AxesSubplot at 0x7f78c27d9358>
```



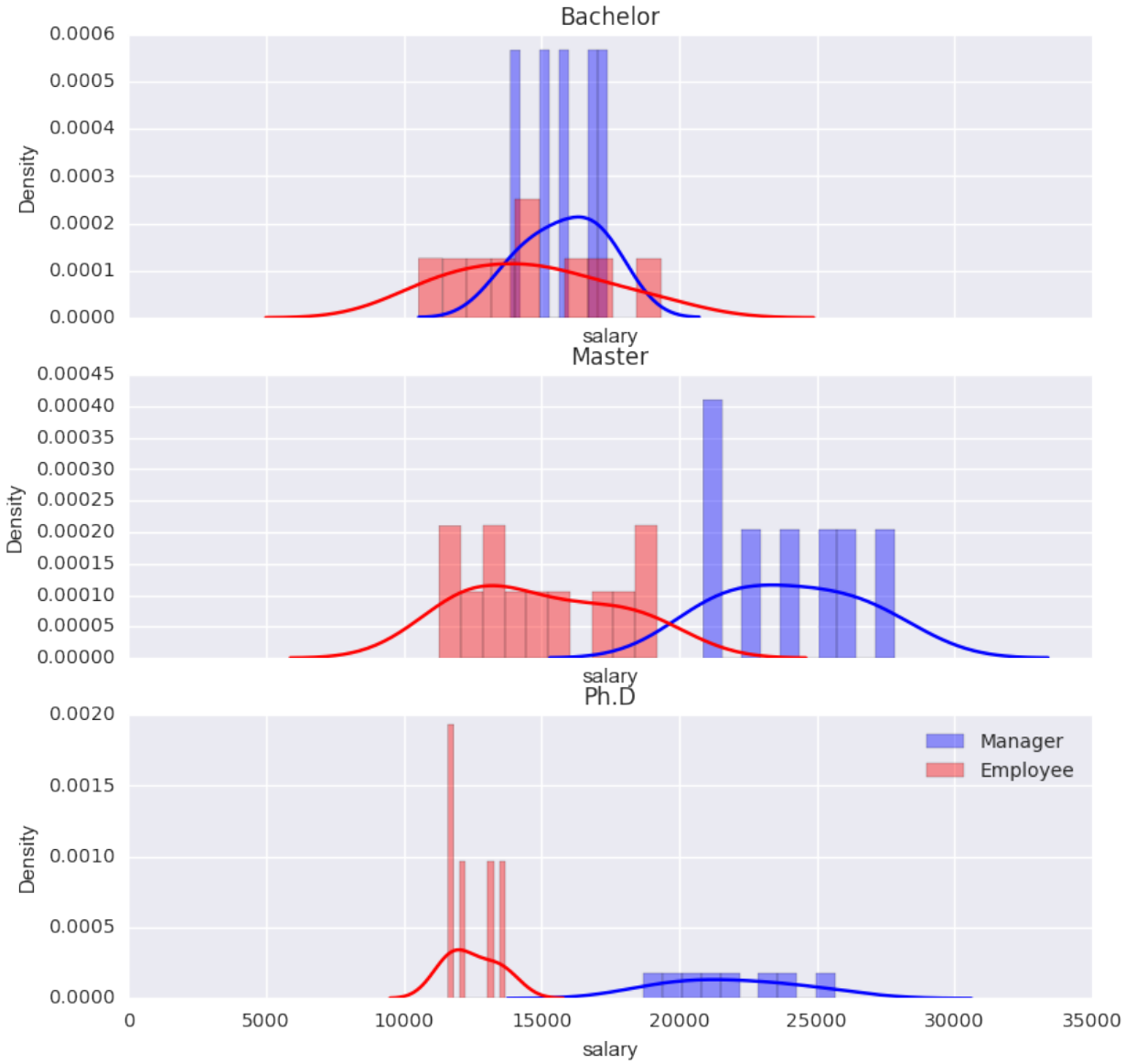
Density plot with one figure containing multiple axis

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
plt.legend()
```

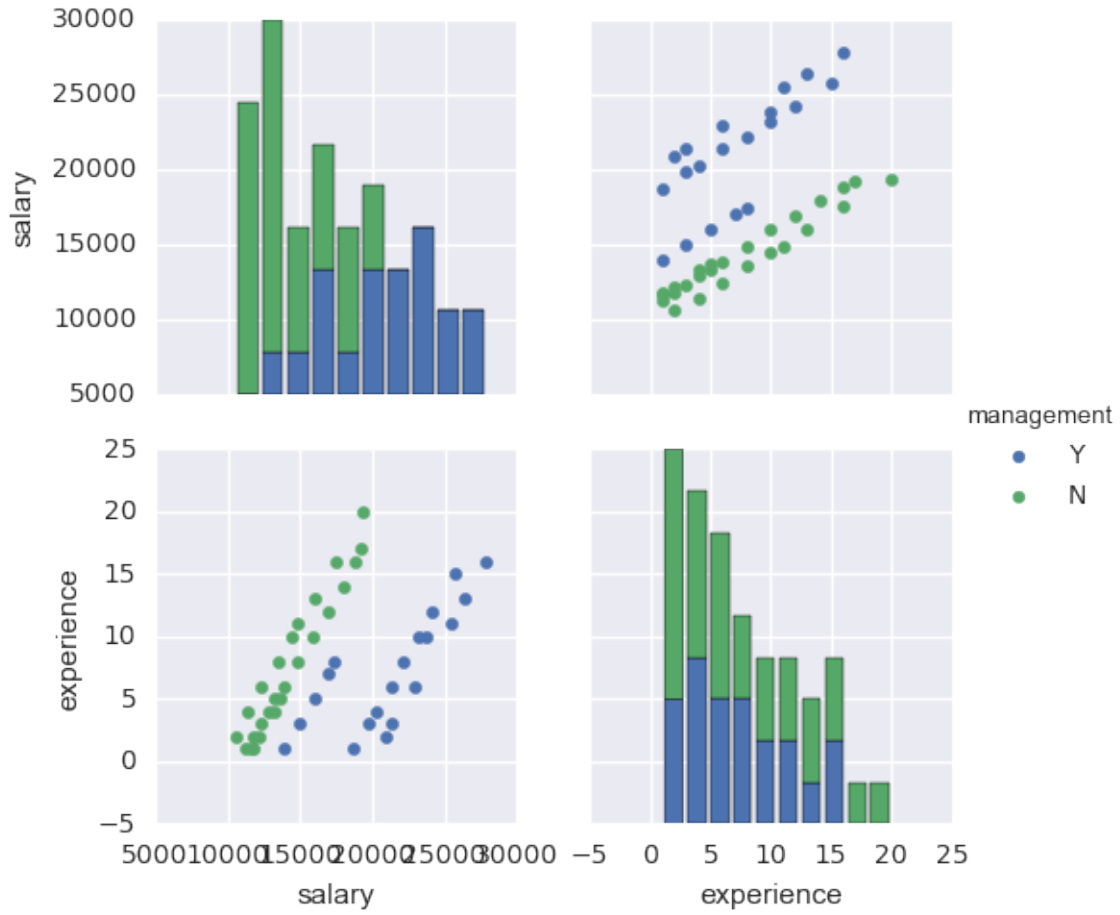
```
/usr/local/anaconda3/lib/python3.5/site-packages/statsmodels/nonparametric/kdetools.
 ↪py:20: VisibleDeprecationWarning: using a non-integer number instead of an integer␣
 ↪will result in an error in the future
  y = X[:m/2+1] + np.r_[0,X[m/2+1:],0]*1j
```

```
<matplotlib.legend.Legend at 0x7f78c32ca9b0>
```




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

```
<seaborn.axisgrid.PairGrid at 0x7f78c2994dd8>
```


salary
experience
management
Y
N
30000
25000
20000
15000
10000
5000
25
20
15
10
5
0
−5
5000
10000
15000
20000
25000
30000
−5
0
5
10
15
20
25

CHAPTER

SIX

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 multivariate 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.

Estimators of the main statistical measures

Mean

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

$$E(X + c) = E(X) + c \tag{6.1}$$
$$E(X + Y) = E(X) + E(Y) \tag{6.2}$$
$$E(aX) = aE(X) \tag{6.3}$$

The estimator $\bar{x}$ on a sample of size n: $x = x_1, ..., x_n$ 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:

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

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 $SE(\bar{x}) = \sigma_x/\sqrt{n}$.

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`, `xycov`) 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.

Main distributions

Normal distribution

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

The Chi-Square distribution

The chi-square or χ^2_n 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 $Z^2 \sim \chi^2_1$ (one df).
- **The distribution of sum of squares** of n normal random variables: $\sum_i^n Z_i^2 \sim \chi^2_n$

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

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

The Fisher's F-distribution

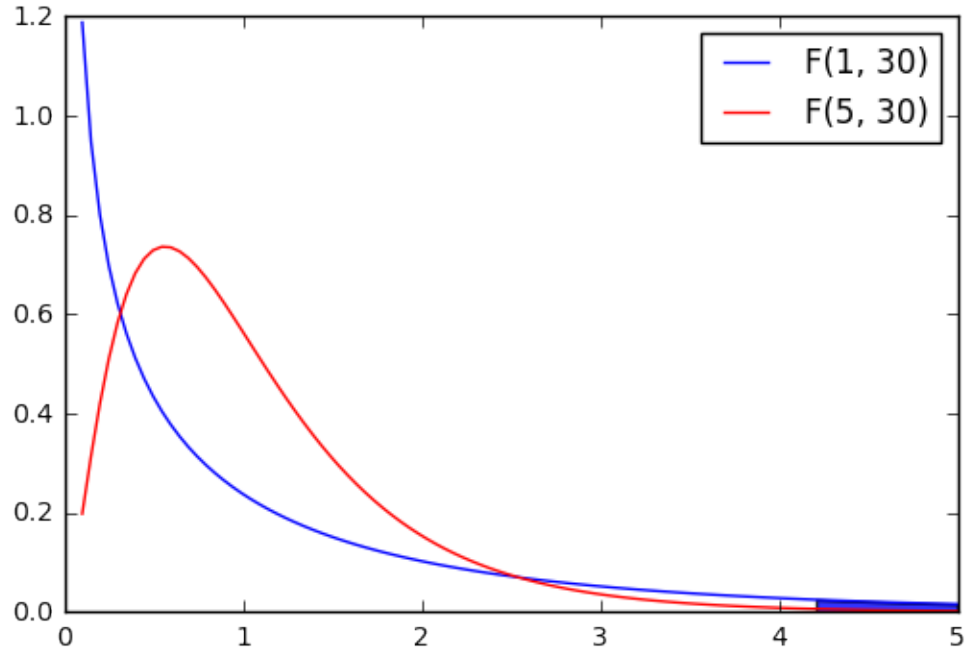
The F-distribution, $F_{n,p}$, with n and p degrees of freedom is the ratio of two independent χ^2 variables. Let $X \sim \chi^2_n$ and $Y \sim \chi^2_p$ then:

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

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 $V \sim \chi^2_n$. 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?**

Testing pairwise associations

Mass univariate statistical analysis: explore association betweens pairs of variable.

- 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 possibles 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/

Pearson correlation test (quantitative ~ quantitative)

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

```
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)
```

One sample t-test (quantitative ~ constant)

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: $X \sim \mathcal{N}(\mu, \sigma)$.

2. Fit: estimate the model parameters

$\bar{x}, \sigma_x$ are the estimators of μ, σ.

3. Test

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

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

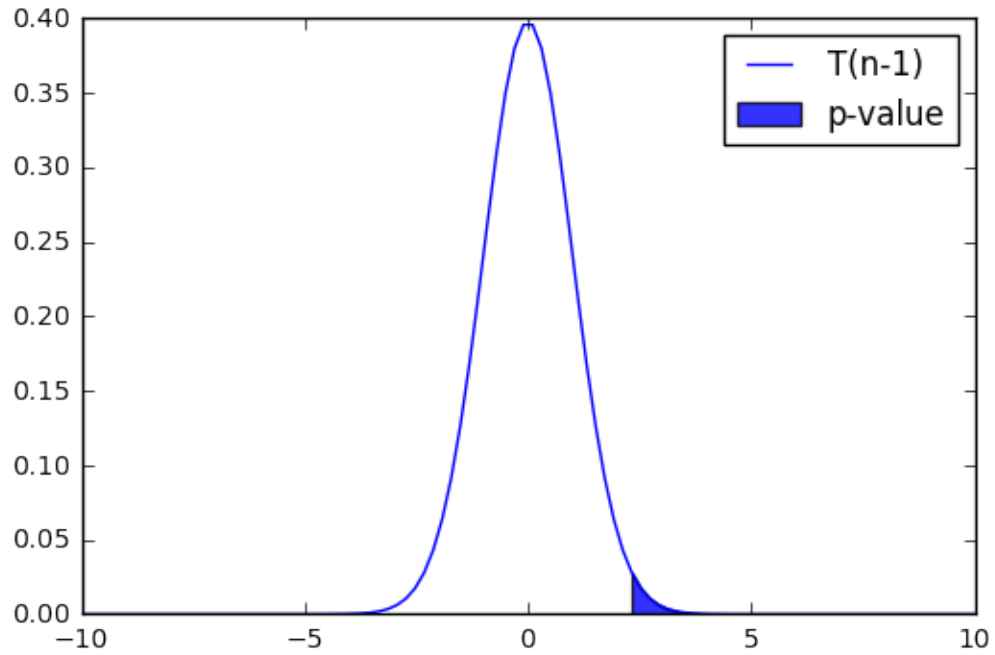
Although the parent population does not need to be normally distributed, the distribution of the population of sample means, $\overline{x}$, is assumed to be normal. By the central limit theorem, if the sampling of the parent population is independent then the sample means will be approximately normal.

Exercise

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
import scipy.stats as stats
import matplotlib.pyplot as plt
np.random.seed(seed=42)  # make example reproducible
n = 100
x = np.random.normal(loc=1.78, scale=.1, size=n)  # the sample is here

# Compute everything with scipy
tval, pval = stats.ttest_1samp(x, 1.75)

#tval = 2.1598800019529265 # 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 > tval]
plt.fill_between(upper_tval_tvalues, 0, stats.t.pdf(upper_tval_tvalues, n-1), alpha=.
↪8, label="p-value")
_ = plt.legend()
```



- Compute the t-value (`tval`) (using only numpy, not scipy).
- Compute the p-value: `P(T(n-1)>tval)`.
- The p-value is one-sided: a two-sided test would test `P(T(n-1) > tval)` and `P(T(n-1) < -tval)`. What would the two-sided p-value be?
- Compare the two-sided p-value with the one obtained by `stats.ttest_1samp` using `assert np.allclose(arr1,arr2)`.

Two sample t-test (quantitative ~ categorial (2 levels))

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: $x \sim \mathcal{N}(\mu_x, \sigma_x), y \sim \mathcal{N}(\mu_y, \sigma_y)$.

2. Fit: estimate the model parameters

Estimate means and variances: $\bar{x}, \sigma_x, \bar{y}, \sigma_y$.

3. t-test

Generally t-tests form the ratio between the amount of information explained by the model (i.e. the effect size) with the square root of the unexplained variance.

In testing the null hypothesis that the two population means are equal, one uses the t-statistic of unpaired two samples t-test:

$$t = \frac{\text{effect size}}{\sqrt{\text{unexplained variance}}}$$

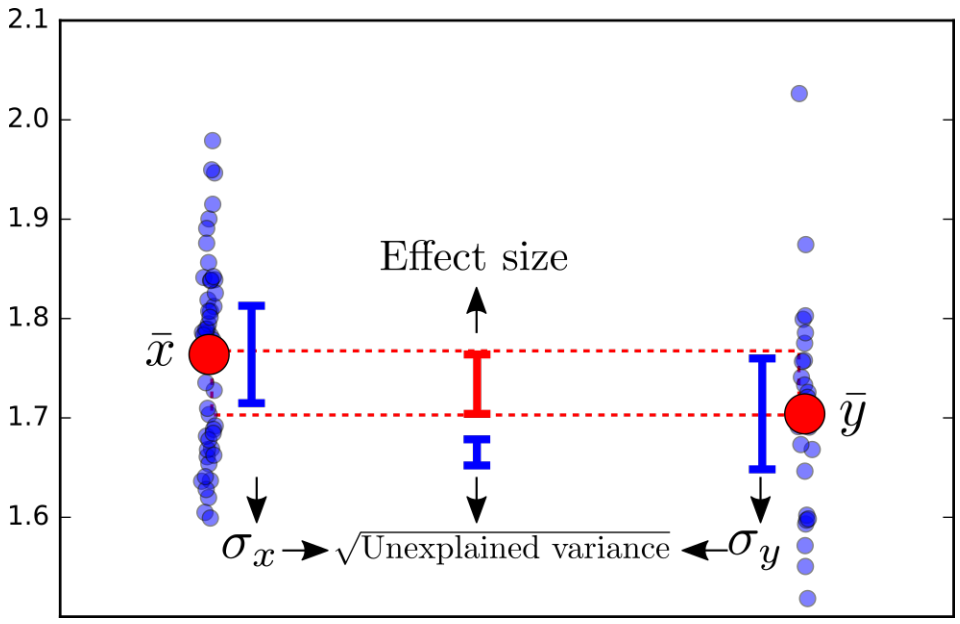


Fig. 6.1: title

Equal or unequal sample sizes, equal variance

This test is used only when it can be assumed that the two distributions have the same variance. The t statistic, that is used to test whether the means are different is:

$$t = \frac{\bar{x} - \bar{y}}{\sigma \cdot \sqrt{\frac{1}{n_x} + \frac{1}{n_y}}},$$

where

$$\sigma = \sqrt{\frac{\sigma_x^2(n_x - 1) + \sigma_y^2(n_y - 1)}{n_x + n_y - 2}}$$

is an estimator of the common standard deviation of the two samples: it is defined in this way so that its square is an unbiased estimator of the common variance whether or not the population means are the same.

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

Welch's t-test defines the t statistic as

$$t = \frac{\bar{x} - \bar{y}}{\sqrt{\frac{\sigma_x^2}{n_x} + \frac{\sigma_y^2}{n_y}}}.$$

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

$$\nu \approx \frac{\left(\frac{\sigma_x^2}{n_x} + \frac{\sigma_y^2}{n_y}\right)^2}{\frac{\sigma_x^4}{n_x^2(n_x-1)} + \frac{\sigma_y^4}{n_y^2(n_y-1)}}.$$

Exercise

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

```
import scipy.stats as stats
nx, ny = 50, 25
x = np.random.normal(loc=1.76, scale=0.1, size=nx)
y = np.random.normal(loc=1.70, scale=0.12, size=ny)

# Compute with scipy
tval, pval = stats.ttest_ind(x, y, equal_var=True)
```

- Compute the t-value.
- 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)`.

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.

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: $\bar{y}_i, \sigma_i, \quad \forall i \in \{1, 2, 3\}$.

3. F-test

Source: https://en.wikipedia.org/wiki/F-test

The ANOVA F-test can be used to assess whether any of the strategies is on average superior, or inferior, to the others versus the null hypothesis that all four strategies yield the same mean response (increase of business volume). This is an example of an "omnibus" test, meaning that a single test is performed to detect any of several possible differences. Alternatively, we could carry out pair-wise tests among the strategies. 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.

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

$$F = \frac{\text{explained variance}}{\text{unexplained variance}},$$

or

$$F = \frac{\text{between-group variability}}{\text{within-group variability}}.$$

The "explained variance", or "between-group variability" is

$$\sum_i n_i(\bar{Y}_{i\cdot} - \bar{Y})^2/(K-1),$$

where $\bar{Y}_{i\cdot}$ denotes the sample mean in the ith group, n_i is the number of observations in the ith 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

$$\sum_{ij}(Y_{ij} - \bar{Y}_{i\cdot})^2/(N-K),$$

where Y_{ij} is the jth observation in the ith 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.

Exercise

Perform an ANOVA on the following dataset

- 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])
```

Chi-square, χ^2 (categorial ~ categorial)

Computes the chi-square, χ^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: 15 patients with cancer, two observed categorial variables: canalar tumor (Y/N) and metastasis (Y/N). χ^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 with canalar tumor, 5 last without
canalar_tumor = np.array([1] * 10 + [0] * 5)
# 8 first with metastasis, 6 without, the last with.
meta = np.array([1] * 8 + [0] * 6 + [1])

crosstab = pd.crosstab(canalar_tumor, meta, rownames=['canalar_tumor'], colnames=[
↪'meta'])
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:
---------------
meta           0  1
canalar_tumor
0              4  1
1              2  8
Statistics:
-----------
Chi2 = 2.812500, pval = 0.093533
Expected table:
---------------
[[ 2.  3.]
 [ 4.  6.]]
```

Computing expected cross-table

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

canalar_tumor_marg = crosstab.sum(axis=1)
canalar_tumor_freq = canalar_tumor_marg / canalar_tumor_marg.sum()

print('Canalar tumor frequency? Yes: %.2f' % canalar_tumor_freq[0], 'No: %.2f' %␣
↪canalar_tumor_freq[1])
print('Metastasis frequency? Yes: %.2f' % meta_freq[0], 'No: %.2f' % meta_freq[1])

print('Expected frequencies:')
print(np.outer(canalar_tumor_freq, meta_freq))

print('Expected cross-table (frequencies * N): ')
print(np.outer(canalar_tumor_freq, meta_freq) * len(canalar_tumor))
```

```
Canalar tumor frequency? Yes: 0.33 No: 0.67
Metastasis frequency? Yes: 0.40 No: 0.60
Expected frequencies:
[[ 0.13333333  0.2       ]
 [ 0.26666667  0.4       ]]
Expected cross-table (frequencies * N):
[[ 2.  3.]
 [ 4.  6.]]
```

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.

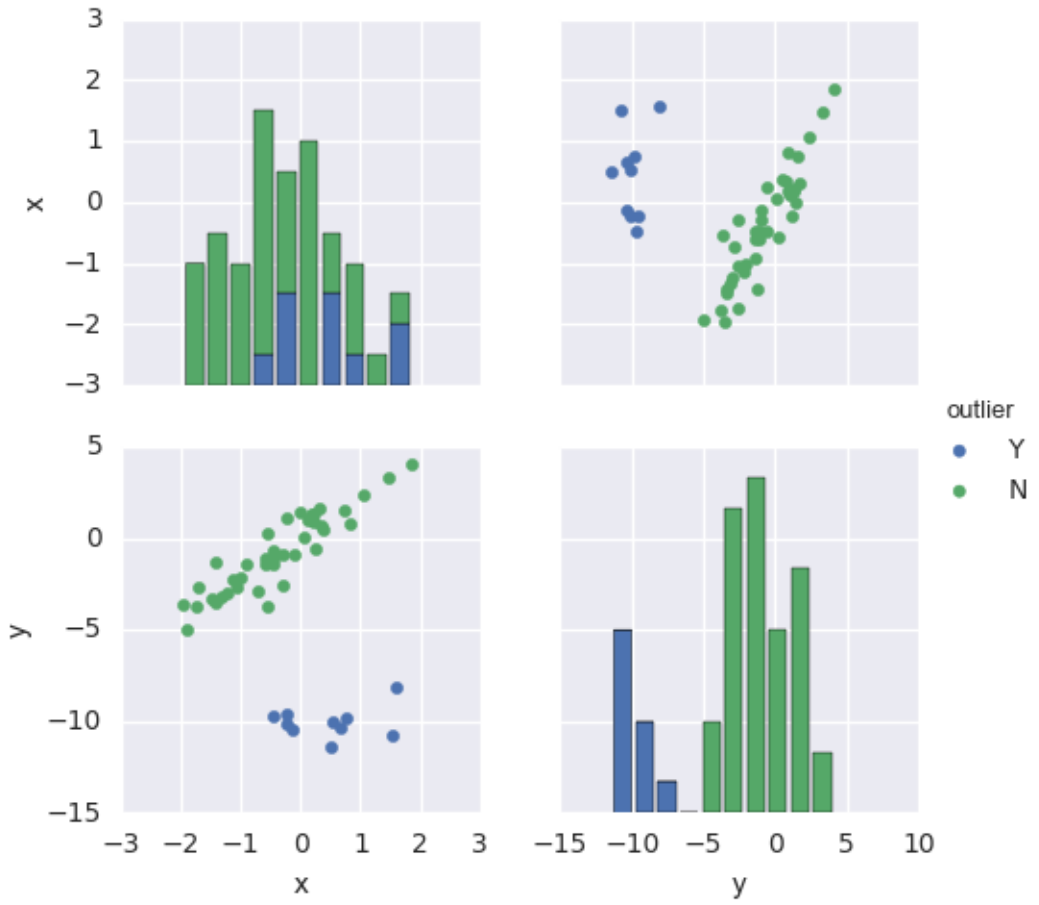
When to use it? Observe the data distribution: - presence of **outliers** - the distribution of the residuals is not Gaussian.

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 pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns

np.random.seed(seed=42)  # make example reproducible

n = 50
noutliers = 10
x = np.random.normal(size=n)
y = 2 * x + np.random.normal(size=n)
y[:noutliers] = np.random.normal(loc=-10, size=noutliers)  # Add 40 outliers
outlier = np.array(["N"] * n)
outlier[:noutliers] = "Y"

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

# Plot distribution + pairwise scatter plot
df = pd.DataFrame(dict(x=x, y=y, outlier=outlier))
g = sns.PairGrid(df, hue="outlier")
g.map_diag(plt.hist)
g.map_offdiag(plt.scatter)
g = g.add_legend()

# Compute the parametric Pearsonw 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: 0.2996, pval: 0.0345
Parametric Pearson cor test: cor: 0.0426, pval: 0.7687
```



Wilcoxon signed-rank test (quantitative ~ cte)

Source: 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
print(stats.ttest_rel(bv0, bv1))

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

```
Ttest_relResult(statistic=0.82290246738044537, pvalue=0.42077212061718194)
WilcoxonResult(statistic=43.0, pvalue=0.020633435105949553)
```

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=0.62748520384004158, pvalue=0.53409388734462837)
MannwhitneyuResult(statistic=43.0, pvalue=1.1512354940556314e-05)
```

Linear model

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

$$y_i = \beta_0 + \beta_1 x_i^1 + \cdots + \beta_p x_i^p + \varepsilon_i \qquad i = 1, \ldots, n$$

- **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 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 linear regression (one continuous independent variable (IV))

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.github.com/neurospin/pystatsml/master/data/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

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

- β: the slope or coefficient or parameter of the model,
- β_0: the **intercept** or **bias** is the second parameter of the model,
- ϵ_i: is the ith error, or residual with $\epsilon \sim \mathcal{N}(0, \sigma^2)$.

This model is similar to a correlation.

2. Fit: estimate the model parameters

The goal it so estimate β, β_0 and σ^2.

Minimizes the **mean squared error (MSE)** or the **Sum squared error (SSE)**. The so-called **Ordinary Least Squares (OLS)** finds β, β_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 β_0:

$$\sum_i x_i(y_i - \beta\, x_i - \bar{y} + \beta\bar{x}) = 0$$

$$\sum_i x_i y_i - \bar{y}\sum_i x_i = \beta \sum_i (x_i - \bar{x})$$

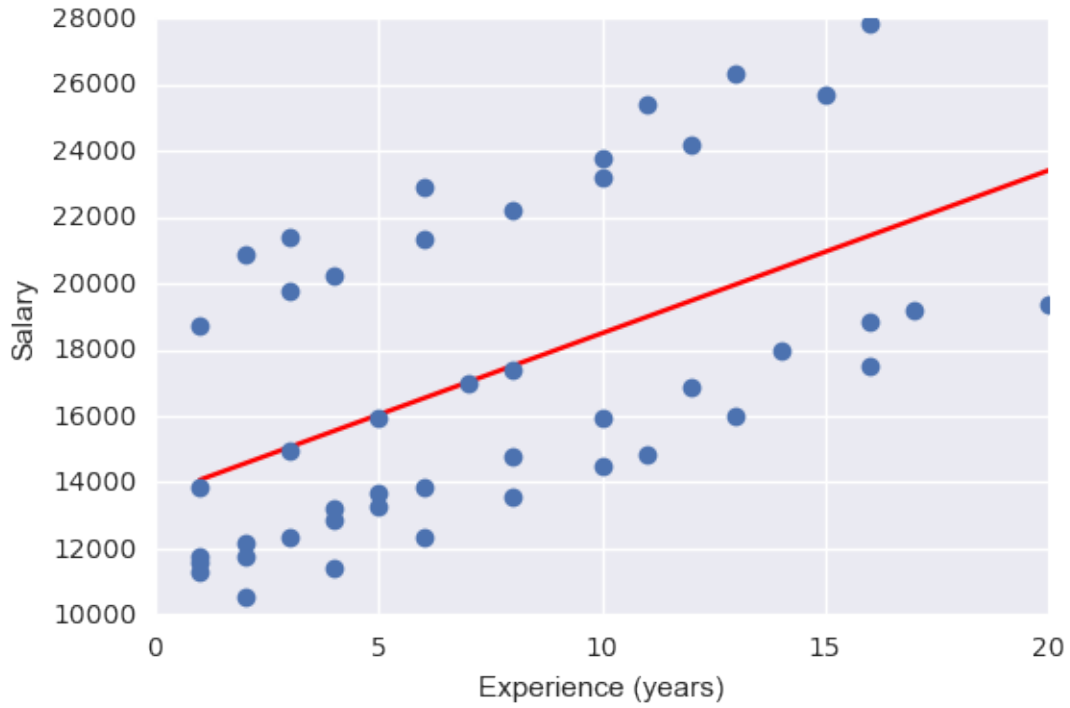
Divide both sides by n:

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

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

```
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))
# plotting the line
yhat = beta * x  +  beta0 # regression line
plt.plot(x, yhat, 'r-', x, y,'o')
plt.xlabel('Experience (years)')
plt.ylabel('Salary')
plt.show()
```

```
y = 491.486913 x + 13584.043803,  r: 0.538886, r-squared: 0.290398,
p-value: 0.000112, std_err: 115.823381
```



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

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

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.

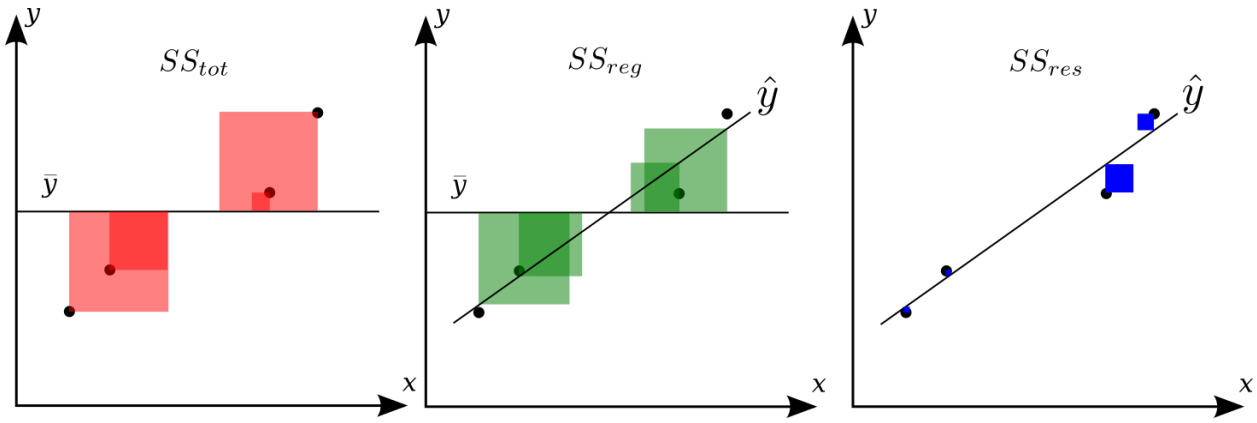


Fig. 6.2: title

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.

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

3.2 Test

Let $\hat{\sigma}^2 = SS_{\text{res}}/(n-2)$ be an estimator of the variance of ϵ. 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 $(1 - \text{Cumulative Distribution Function})$ at x of the given F-distribution.

Multiple regression

Theory

Muliple Linear Regression is the most basic supervised learning algorithm.

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

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

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

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 $X = [x_0^T, ..., x_N^T]$ be a $N \times P + 1$ matrix of N samples of P input features with one column of one and let be $y = [y_1, ..., y_N]$ 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 β that minimises the MSE can be found by:

$$\nabla_\beta \left(\frac{1}{N} ||y - X\beta||_2^2 \right) = 0 \tag{6.4}$$

$$\frac{1}{N} \nabla_\beta (y - X\beta)^T (y - X\beta) = 0 \tag{6.5}$$

$$\frac{1}{N} \nabla_\beta (y^T y - 2\beta^T X^T y + \beta X^T X \beta) = 0 \tag{6.6}$$

$$-2X^T y + 2X^T X\beta = 0 \tag{6.7}$$

$$X^T X\beta = X^T y \tag{6.8}$$

$$\beta = (X^T X)^{-1} X^T y, \tag{6.9}$$

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

Fit with `numpy`

```
import numpy as np
import scipy
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 = scipy.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]
```

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:                Sun, 15 Oct 2017   Prob (F-statistic):           0.000106
Time:                        23:14:05   Log-Likelihood:                -71.271
No. Observations:                  50   AIC:                             150.5
Df Residuals:                      46   BIC:                             158.2
Df Model:                           3
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [95.0% Conf. Int.]
------------------------------------------------------------------------------
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
```

```
==============================================================================
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
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is 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 ~ x1 + x2`.

```
import statsmodels.formula.api as smfrmla

df = pd.DataFrame(np.column_stack([X, y]), columns=['inter', 'x1','x2', 'x3', 'y'])

# Build a model excluding the intercept, it is implicit
model = smfrmla.ols("y ~ x1 + x2 + x3", df).fit()
print(model.summary())
```

```
                            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:                Sun, 15 Oct 2017   Prob (F-statistic):           0.000106
Time:                        23:14:05   Log-Likelihood:                -71.271
No. Observations:                  50   AIC:                             150.5
Df Residuals:                      46   BIC:                             158.2
Df Model:                           3
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [95.0% Conf. Int.]
------------------------------------------------------------------------------
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
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
==============================================================================
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
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is 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("../data/salary_table.csv")
except:
    url = 'https://raw.github.com/neurospin/pystatsml/master/data/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
==============================================================================
Dep. Variable:                 salary   R-squared:                       0.865
Model:                            OLS   Adj. R-squared:                  0.859
Method:                 Least Squares   F-statistic:                     138.2
Date:                Sun, 15 Oct 2017   Prob (F-statistic):           1.90e-19
Time:                        23:14:05   Log-Likelihood:                -407.76
No. Observations:                  46   AIC:                             821.5
Df Residuals:                      43   BIC:                             827.0
Df Model:                           2
Covariance Type:            nonrobust
================================================================================
                   coef    std err          t      P>|t|      [95.0% Conf. Int.]
--------------------------------------------------------------------------------
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
==============================================================================
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
==============================================================================

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:                Sun, 15 Oct 2017   Prob (F-statistic):           2.23e-27
Time:                        23:14:05   Log-Likelihood:                -381.63
No. Observations:                  46   AIC:                             773.3
Df Residuals:                      41   BIC:                             782.4
Df Model:                           4
Covariance Type:            nonrobust
================================================================================================
                           coef    std err          t      P>|t|      [95.0% Conf. Int.
↪]
------------------------------------------------------------------------------------------------
↪-
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
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
==============================================================================
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
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is 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
```

```
(43.351589459181056, 7.6724495704954452e-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.]]
```

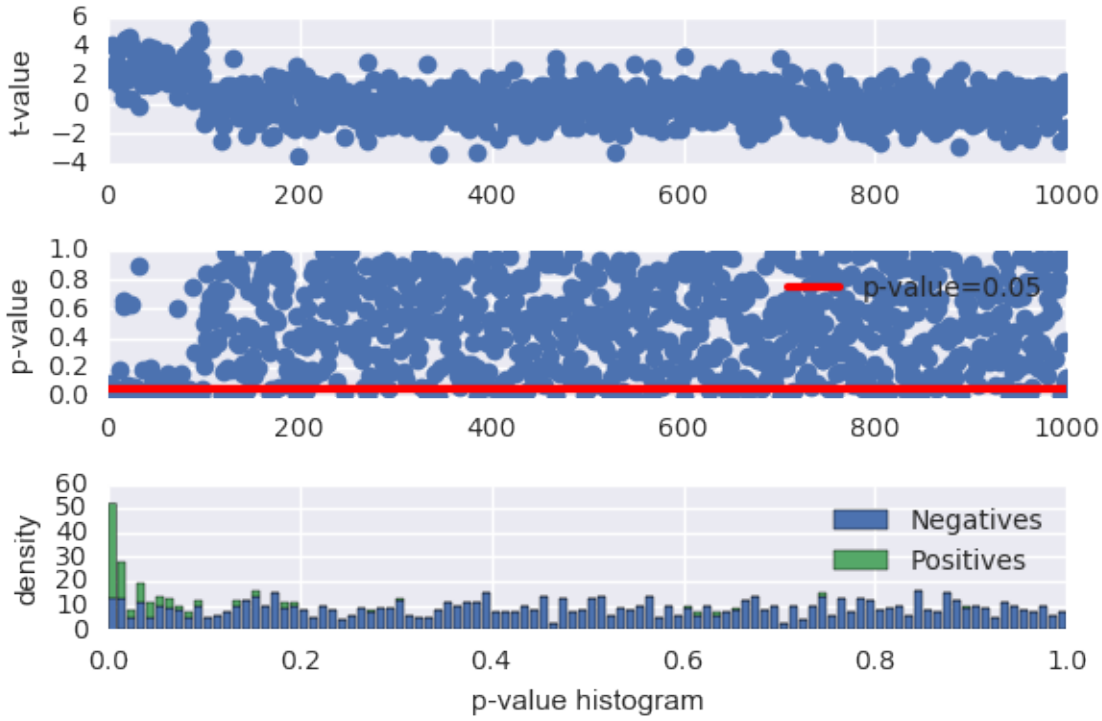
Contrasts and post-hoc tests

```
# 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|      [95.0% Conf. Int.]
------------------------------------------------------------------------------
c0           546.1840     30.519     17.896      0.000       484.549   607.819
==============================================================================
                            Test for Constraints
==============================================================================
                 coef    std err          t      P>|t|      [95.0% Conf. Int.]
------------------------------------------------------------------------------
c0           147.8249    387.659      0.381      0.705      -635.069   930.719
==============================================================================
```

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')
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
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 α (usually 0.05), then the Bonferroni correction would test each individual hypothesis at a significance level of α/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
```

Exercise

Parametric univariate testing

Write a function `univar_stat(df,target,variables)` that computes the parametric statistics and p-values between the `target` variable (provided as as 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/data/salary_table.csv, with target being `S`: salaries for IT staff in a corporation.

Simple linear regression

Considering the salary and the experience of the salary table.

Compute:

- $\bar{y}$: `y_mu`
- SS_{tot}: `ss_tot`
- SS_{reg}: `ss_reg`
- SS_{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 to fit the linear regression with numpy:

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

Multiple comparisons

This exercise has 2 goals: apply you 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.

CHAPTER

SEVEN

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** $[\mathbf{x}_1, \ldots, \mathbf{x}_i, \ldots, \mathbf{x}_N]$ of length P

$$\mathbf{X} = \begin{bmatrix} -\mathbf{x}_1^T- \\ \vdots \\ -\mathbf{x}_i^T- \\ \vdots \\ -\mathbf{x}_P^T- \end{bmatrix} = \begin{bmatrix} x_{11} & \cdots & x_{1j} & \cdots & x_{1P} \\ \vdots & & \vdots & & \vdots \\ x_{i1} & \cdots & x_{ij} & \cdots & x_{iP} \\ \vdots & & \vdots & & \vdots \\ x_{N1} & \cdots & x_{Nj} & \cdots & x_{NP} \end{bmatrix} = \begin{bmatrix} x_{11} & \ldots & x_{1P} \\ \vdots & & \vdots \\ & \mathbf{X} & \\ \vdots & & \vdots \\ x_{N1} & \ldots & x_{NP} \end{bmatrix}_{N \times P}.$$

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 ‘‘$\cdot$‘‘ of two P-dimensional vectors $\mathbf{a} = [a_1, a_2, ..., a_P]$ and $\mathbf{a} = [b_1, b_2, ..., b_P]$ is defined as

$$\mathbf{a} \cdot \mathbf{b} = \mathbf{a}^T\mathbf{b} = \sum_i a_i b_i = \begin{bmatrix} a_1 & \ldots & \mathbf{a}^T & \ldots & a_P \end{bmatrix} \begin{bmatrix} b_1 \\ \vdots \\ \mathbf{b} \\ \vdots \\ b_P \end{bmatrix}.$$

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 θ 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° and

$$\mathbf{a} \cdot \mathbf{b} = 0.$$

At the other extreme, if they are codirectional, then the angle between them is 0° 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 θ is the angle between $\mathbf{a}$ and $\mathbf{b}$.

In terms of the geometric definition of the dot product, this can be rewritten

$$a_b = \frac{\mathbf{a} \cdot \mathbf{b}}{\|\mathbf{b}\|_2},$$

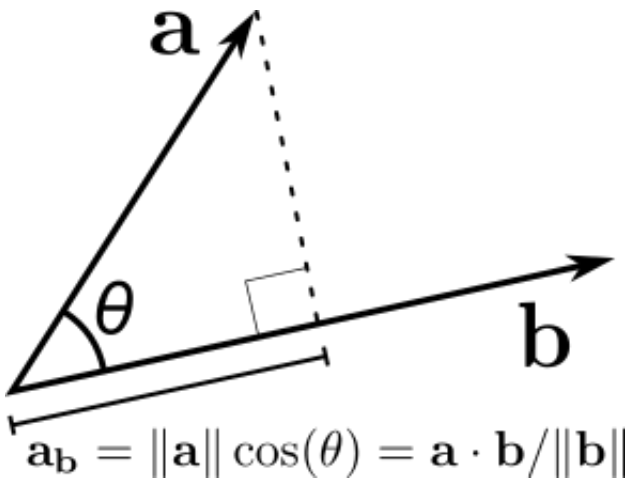


Fig. 7.1: Projection.

```
import numpy as np
np.random.seed(42)

a = np.random.randn(10)
b = np.random.randn(10)

np.dot(a, b)
```

```
-4.0857885326599241
```

Mean vector

The mean $(P \times 1)$ column-vector μ whose estimator is

$$\bar{\mathbf{x}} = \frac{1}{N}\sum_{i=1}^{N}\mathbf{x_i} = \frac{1}{N}\sum_{i=1}^{N}\begin{bmatrix} x_{i1} \\ \vdots \\ x_{ij} \\ \vdots \\ x_{iP} \end{bmatrix} = \begin{bmatrix} \bar{x}_1 \\ \vdots \\ \bar{x}_j \\ \vdots \\ \bar{x}_P \end{bmatrix}.$$

Covariance matrix

- The covariance matrix $\mathbf{\Sigma_{XX}}$ 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:

$$\mathbf{\Sigma_{XX}} = E(\mathbf{X} - E(\mathbf{X}))^T E(\mathbf{X} - E(\mathbf{X})),$$

whose estimator $\mathbf{S_{XX}}$ is a $P \times P$ matrix given by

$$\mathbf{S_{XX}} = \frac{1}{N-1}(\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}^T)^T(\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}^T).$$

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

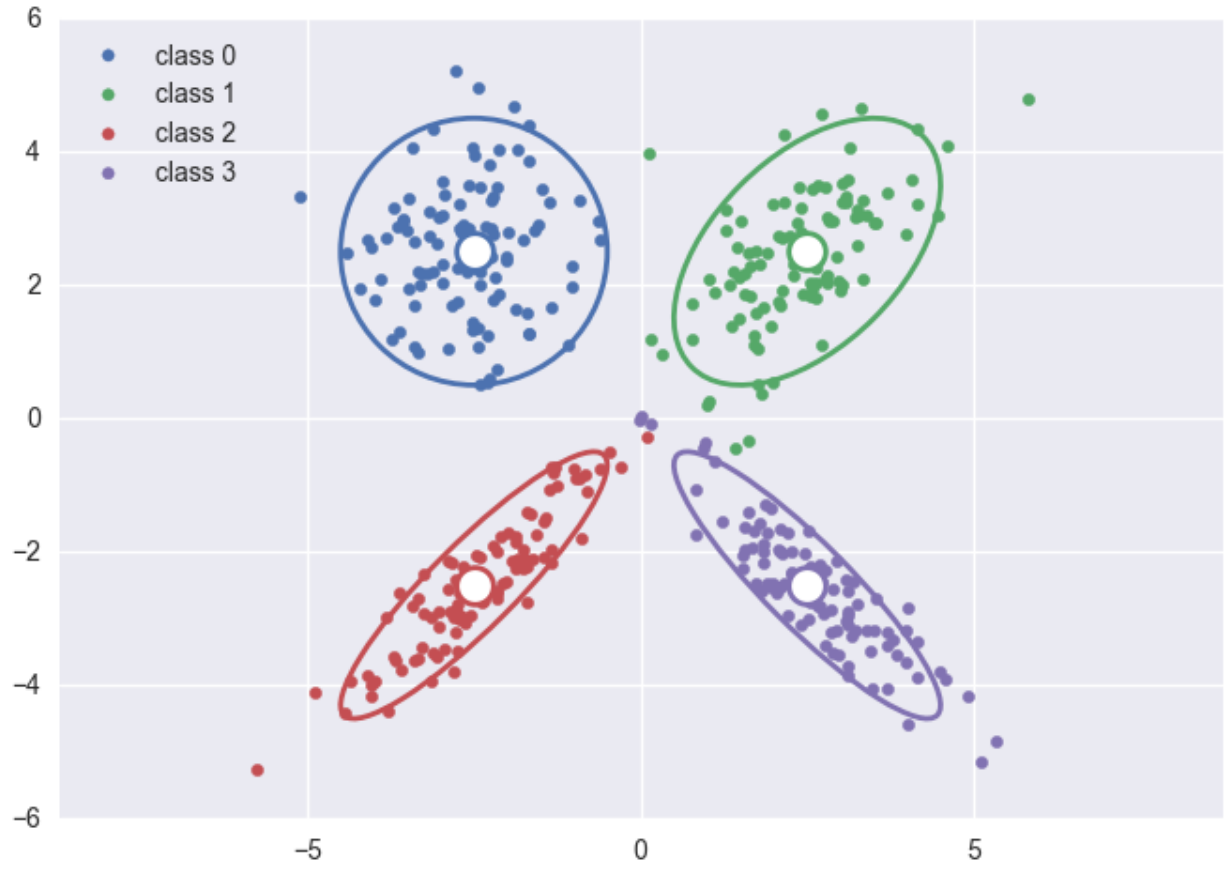
$$\mathbf{S_{XX}} = \frac{1}{N-1}\mathbf{X}^T\mathbf{X} = \frac{1}{N-1}\begin{bmatrix} x_{11} & \cdots & x_{N1} \\ x_{1j} & \cdots & x_{Nj} \\ \vdots & & \vdots \\ x_{1P} & \cdots & x_{NP} \end{bmatrix}\begin{bmatrix} x_{11} & \cdots & x_{1k} & x_{1P} \\ \vdots & & \vdots & \vdots \\ x_{N1} & \cdots & x_{Nk} & x_{NP} \end{bmatrix} = \begin{bmatrix} s_1 & \cdots & s_{1k} & s_{1P} \\ & \ddots & s_{jk} & \vdots \\ & & s_k & s_{kP} \\ & & & s_P \end{bmatrix},$$

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, facecolors='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')
```



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.    0.   -4.74  5.26  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]]
```

Mahalanobis distance

- The Mahalanobis distance is a measure of the distance between two points $\mathbf{x}$ and μ 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

$$D_M(\mathbf{x}, \mu) = \sqrt{(\mathbf{x} - \mu)^T \mathbf{\Sigma}^{-1} (\mathbf{x} - \mu)}.$$

Intuitions

- Distances along the principal directions of dispersion are contracted since they correspond to likely dispersion of points.
- Distances othogonal to the principal directions of dispersion are dilated since they correspond to unlikely dispersion of points.

For example

$$D_M(\mathbf{1}) = \sqrt{\mathbf{1}^T \mathbf{\Sigma}^{-1} \mathbf{1}}.$$

```
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))
```

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 $\mathbf{x}$ and a distribution $\mathcal{N}(\mathbf{x}|\mu, \mathbf{\Sigma})$. It is a multi-dimensional generalization of the idea of measuring how many standard deviations away $\mathbf{x}$ is from the mean. This distance is zero if $\mathbf{x}$ is at the mean, and grows as $\mathbf{x}$ moves away from the mean: along each principal component axis, it measures the number of standard deviations from $\mathbf{x}$ to the mean of the distribution.

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 $\mathbf{x} = [x_1, x_2, \ldots, x_P]^T$ is

$$\mathcal{N}(\mathbf{x}|\mu, \mathbf{\Sigma}) = \frac{1}{(2\pi)^{P/2}|\mathbf{\Sigma}|^{1/2}} \exp\{-\frac{1}{2}(\mathbf{x}-\mu)^T\mathbf{\Sigma}^{-1}(\mathbf{x}-\mu)\}.$$

```
import numpy as np
import matplotlib.pyplot as plt
import scipy.stats
from scipy.stats import multivariate_normal
from mpl_toolkits.mplot3d import Axes3D


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_scpy = multivariate_normal(mu, sigma).pdf(np.stack((x, y), axis=2))
assert np.allclose(norm, norm_scpy)
```

```
# 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.zaxis.set_major_locator(plt.LinearLocator(10))
ax.zaxis.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()
```

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, $\mathbf{x}$.
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 $\mathcal{N}(\mu, \mathbf{\Sigma})$ where $\mu = [1, 1]^T$ and $\mathbf{\Sigma} = \begin{bmatrix} 1 & 0.8 \\ 0.8, 1 \end{bmatrix}$.
2. Compute the mean vector $\bar{\mathbf{x}}$ and center $\mathbf{X}$. Compare the estimated mean $\bar{\mathbf{x}}$ to the true mean, μ.
3. Compute the empirical covariance matrix $\mathbf{S}$. Compare the estimated covariance matrix $\mathbf{S}$ to the true covariance matrix, $\mathbf{\Sigma}$.
4. Compute $\mathbf{S}^{-1}$ (`Sinv`) 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 $\mathbf{x}$ to the mean, $\bar{\mathbf{x}}$.
6. Compute the Mahalanobis and Euclidean distances of each sample $\mathbf{x}_i$ to the mean $\bar{\mathbf{x}}$. Store the results in a 100×2 dataframe.

CHAPTER

EIGHT

DIMENSION REDUCTION AND FEATURE EXTRACTION

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 $\mathbf{\Sigma_{XX}}$ between the input features.

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 $\mathbf{V}_{P \times K}$.

$$\mathbf{X} = \mathbf{U}\mathbf{V}^T,$$

If we consider only a subset of components $K < rank(\mathbf{X}) < \min(P, N-1)$, $\mathbf{X}$ is approximated by a matrix $\hat{\mathbf{X}}$:

$$\mathbf{X} \approx \hat{\mathbf{X}} = \mathbf{U}\mathbf{V}^T,$$

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.).

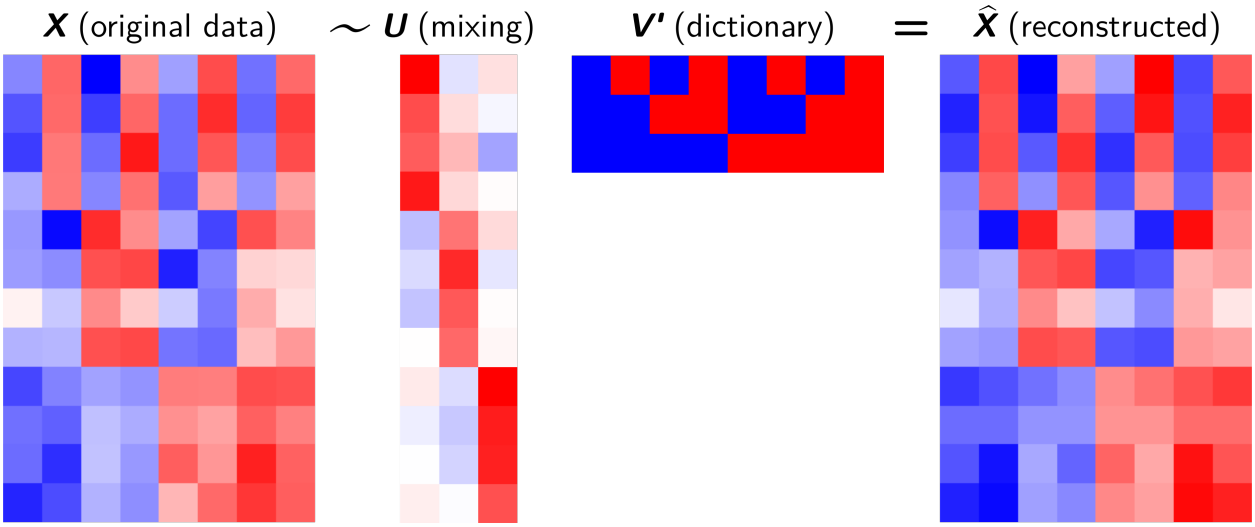


Fig. 8.1: Matrix factorization

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

$$\begin{bmatrix} x_{11} & & x_{1P} \\ & \mathbf{X} & \\ x_{N1} & & x_{NP} \end{bmatrix} = \begin{bmatrix} u_{11} & & u_{1K} \\ & \mathbf{U} & \\ u_{N1} & & u_{NK} \end{bmatrix} \begin{bmatrix} d_1 & & 0 \\ & \mathbf{D} & \\ 0 & & d_K \end{bmatrix} \begin{bmatrix} v_{11} & & v_{1P} \\ & \mathbf{V}^T & \\ v_{K1} & & v_{KP} \end{bmatrix}.$$

U: **right-singular**

- $\mathbf{V} = [\mathbf{v}_1, \cdots, \mathbf{v}_K]$ 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.
- $\mathbf{V}$ perfoms 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 $d_1 \geq d_2 \geq \cdots \geq d_K \geq 0$.
- $\mathbf{D}$ scale the projection along the coordinate axes by $d_1, d_2, \cdots, d_K$.
- Singular values are the square roots of the eigenvalues of $\mathbf{X}^T\mathbf{X}$.

V: **left-singular vectors**

- $\mathbf{U} = [\mathbf{u}_1, \cdots, \mathbf{u}_K]$ 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

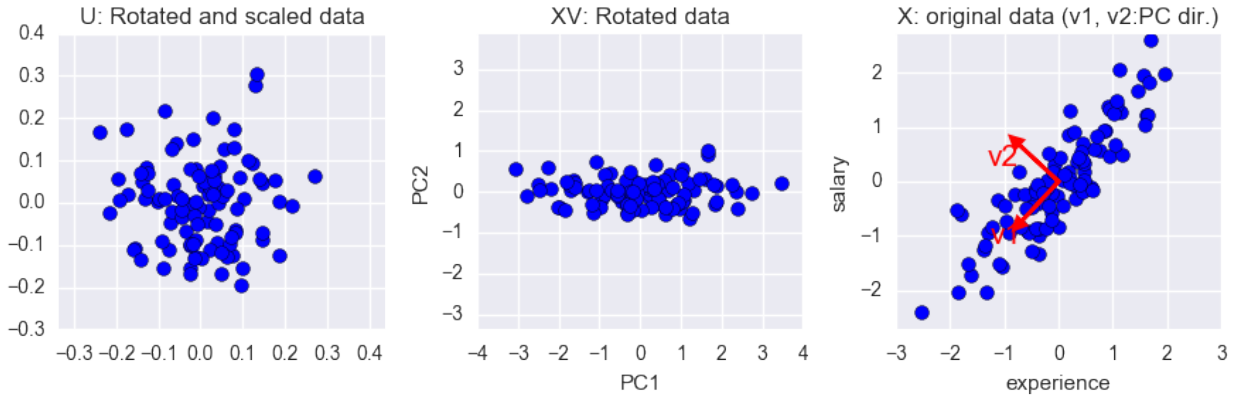
$\mathbf{V}$ transforms correlated variables ($\mathbf{X}$) into a set of uncorrelated ones ($\mathbf{UD}$) that better expose the various relationships among the original data items.

$$\mathbf{X} = \mathbf{UDV}^T, \tag{8.1}$$
$$\mathbf{XV} = \mathbf{UDV}^T\mathbf{V}, \tag{8.2}$$
$$\mathbf{XV} = \mathbf{UDI}, \tag{8.3}$$
$$\mathbf{XV} = \mathbf{UD} \tag{8.4}$$

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.

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()
```



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 save 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 mains 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

$$\mathbf{v} = \arg\max_{\|\mathbf{v}\|=1} \frac{1}{N}\sum_i \left(\mathbf{x}_i^T\mathbf{v}\right)^2.$$

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 estiamte 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 $\|\mathbf{v}_2\| \to \infty$. 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 λ, 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, λ. 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, $\mathbf{v_1}, \ldots, \mathbf{v_K}$, of the data covariance matrix $\mathbf{S}_{\mathbf{XX}}$ that corresponds to the K largest eigenvalues, $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_K$.

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

$$\begin{aligned}
\mathbf{X}^T\mathbf{X} &= (\mathbf{U}\mathbf{D}\mathbf{V}^T)^T(\mathbf{U}\mathbf{D}\mathbf{V}^T) \\
&= \mathbf{V}\mathbf{D}^T\mathbf{U}^T\mathbf{U}\mathbf{D}\mathbf{V}^T \\
&= \mathbf{V}\mathbf{D}^2\mathbf{V}^T \\
\mathbf{V}^T\mathbf{X}^T\mathbf{X}\mathbf{V} &= \mathbf{D}^2 \\
\frac{1}{N-1}\mathbf{V}^T\mathbf{X}^T\mathbf{X}\mathbf{V} &= \frac{1}{N-1}\mathbf{D}^2 \\
\mathbf{V}^T\mathbf{S}_{\mathbf{XX}}\mathbf{V} &= \frac{1}{N-1}\mathbf{D}^2
\end{aligned}$$

.

Considering only the k^{th} right-singular vectors $\mathbf{v}_k$ associated to the singular value d_k

$$\mathbf{v_k}^T \mathbf{S_{XX}} \mathbf{v_k} = \frac{1}{N-1} d_k^2,$$

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 $\mathbf{S_{XX}}$ are equivalent to the right singular vectors, $\mathbf{V}$, of $\mathbf{X}$. - The eigenvalues, λ_k, of $\mathbf{S_{XX}}$, 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 $\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^T$ and $\mathbf{V}$ is orthogonal ($\mathbf{V}^T\mathbf{V} = \mathbf{I}$):

$$\mathbf{C}_{N\times K} = \mathbf{U}\mathbf{D}\mathbf{V}^T_{N\times P}\mathbf{V}_{P\times K} \tag{8.5}$$
$$\mathbf{C}_{N\times K} = \mathbf{U}\mathbf{D}^T_{N\times K}\mathbf{I}_{K\times K} \tag{8.6}$$
$$\mathbf{C}_{N\times K} = \mathbf{U}\mathbf{D}^T_{N\times K} \tag{8.7}$$
$$\tag{8.8}$$

Thus $\mathbf{c}_j = \mathbf{X}\mathbf{v}_j = \mathbf{u}_j d_j$, for $j = 1, \ldots K$. 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.

$$\mathbf{c}_1 = \begin{bmatrix} x_{1,1}v_{1,1} + \ldots + x_{1,P}v_{1,P} \\ x_{2,1}v_{1,1} + \ldots + x_{2,P}v_{1,P} \\ \vdots \\ x_{N,1}v_{1,1} + \ldots + x_{N,P}v_{1,P} \end{bmatrix}$$

3. The **variance** of each component is given by the eigen values $\lambda_k, k = 1, \ldots K$. It can be obtained from the singular values:

$$var(\mathbf{c}_k) = \frac{1}{N-1}(\mathbf{X}\mathbf{v}_k)^2 \tag{8.9}$$
$$= \frac{1}{N-1}(\mathbf{u}_k d_k)^2 \tag{8.10}$$
$$= \frac{1}{N-1} d_k^2 \tag{8.11}$$

Determining the number of PCs

We must choose $K^* \in [1, \ldots, K]$, 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 projeted 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:

$$\mathbf{c} = \mathbf{X}\mathbf{v} \tag{8.12}$$

$$\mathbf{X}^T\mathbf{c} = \mathbf{X}^T\mathbf{X}\mathbf{v} \tag{8.13}$$

$$(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{c} = \mathbf{v} \tag{8.14}$$

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 $j = 1, \ldots, P$. For the k^{th} PC, compute and plot the correlations with all original variables

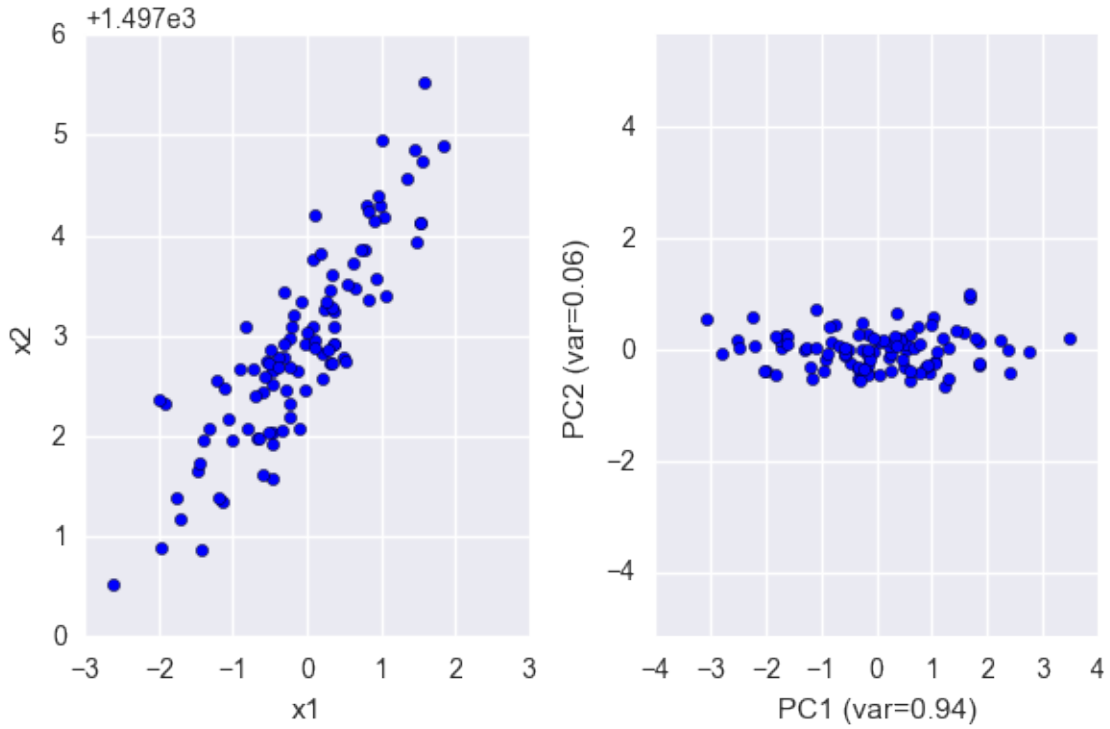
$$cor(\mathbf{c}_k, \mathbf{x}_j), j = 1 \ldots K, j = 1 \ldots K.$$

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]
```



Multi-dimensional Scaling (MDS)

Resources:

- http://www.stat.pitt.edu/sungkyu/course/2221Fall13/lec8_mds_combined.pdf
- 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 $\mathbf{x}_1, \ldots, \mathbf{x}_N \in \mathbb{R}^K$, 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**

$$\text{stress}(\mathbf{X}) = \sum_{i \neq j} \left(d_{ij} - \|\mathbf{x}_i - \mathbf{x}_j\|\right)^2 .$$

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

$$\text{stress}_{\text{classical}}(\mathbf{X}) = \sum_{i \neq j} \left(b_{ij} - \langle \mathbf{x}_i, \mathbf{x}_j \rangle\right)^2.$$

- 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` datset 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 = '../data/eurodist.csv'
    df = pd.read_csv(url)
except:
    url = 'https://raw.github.com/neurospin/pystatsml/master/data/eurodist.csv'
    df = pd.read_csv(url)

print(df.ix[:5, :5])

city = df["city"]
D = np.array(df.ix[:, 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
```

```
2   Brussels     2963        1318          0      204
3     Calais     3175        1326        204        0
4  Cherbourg     3339        1294        583      460
5    Cologne     2762        1498        206      409
```

Recover coordinates of the cities in Euclidean referential whose orientation is arbitrary:

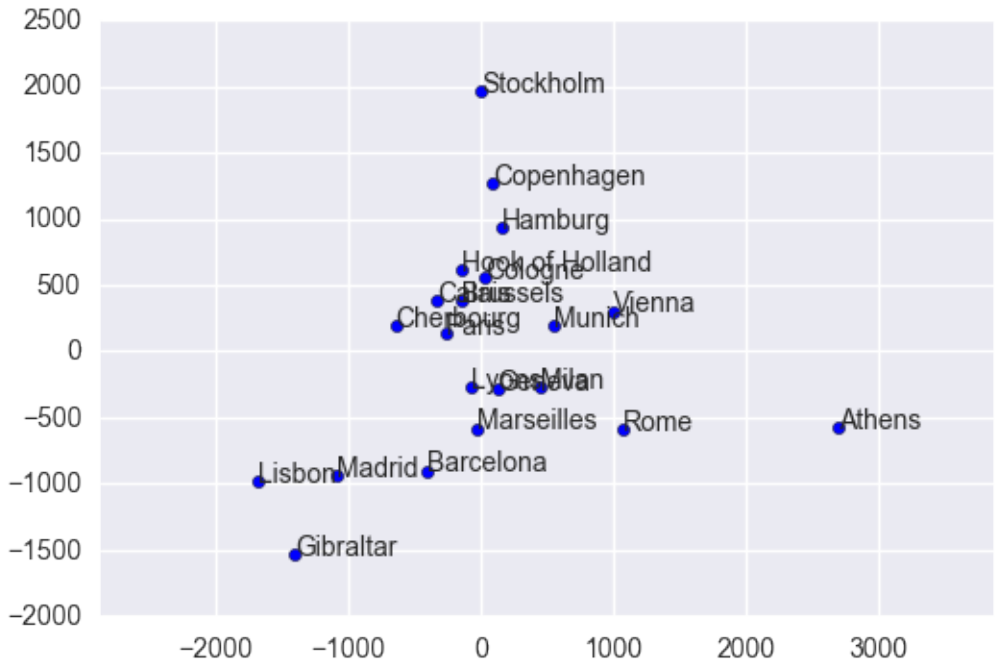
```
from sklearn import metrics
Deuclidean = metrics.pairwise.pairwise_distances(X, metric='euclidean')
print(np.round(Deuclidean[:5, :5]))
```

```
[[    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')
```

```
(-2000.0, 3000.0, -2000.0, 2500.0)
```



Determining the number of components

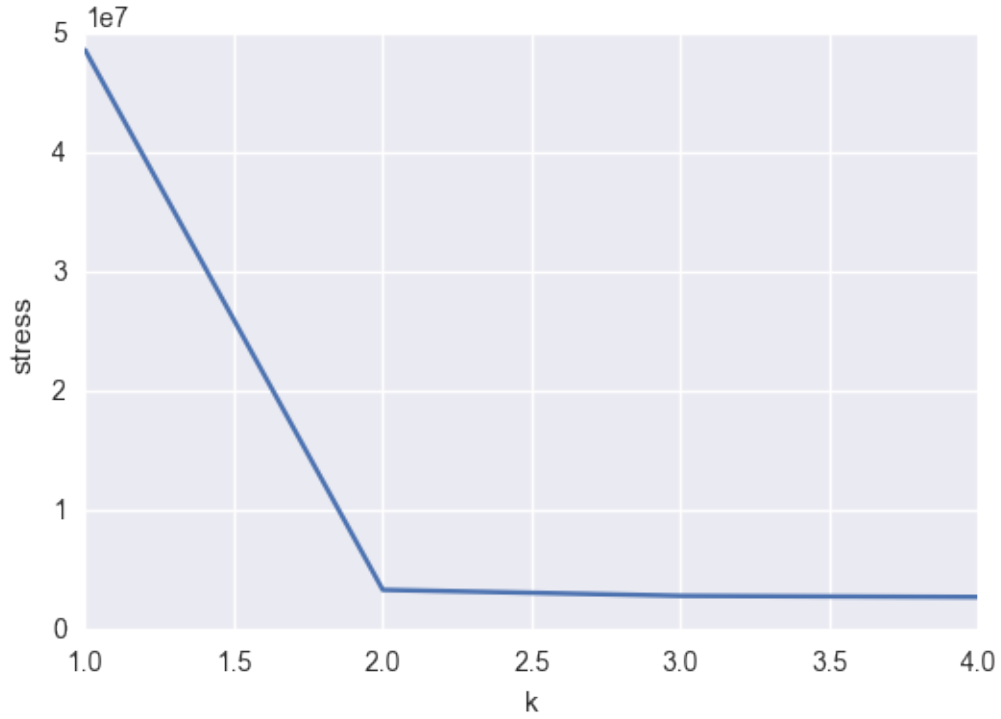
We must choose $K^* \in \{1, \ldots, K\}$ the number of required components. Plotting the values of the stress function, obtained using $k \leq N - 1$ components. In general, start with $1, \ldots K \leq 4$. Choose K^* where you can clearly distinguish an *elbow* in the stress curve.

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")
```

```
[48644495.285714284, 3356497.3657523869, 2858455.4958879612, 2756310.6376280105]
```

```
<matplotlib.text.Text at 0x7fefc49a2518>
```



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.

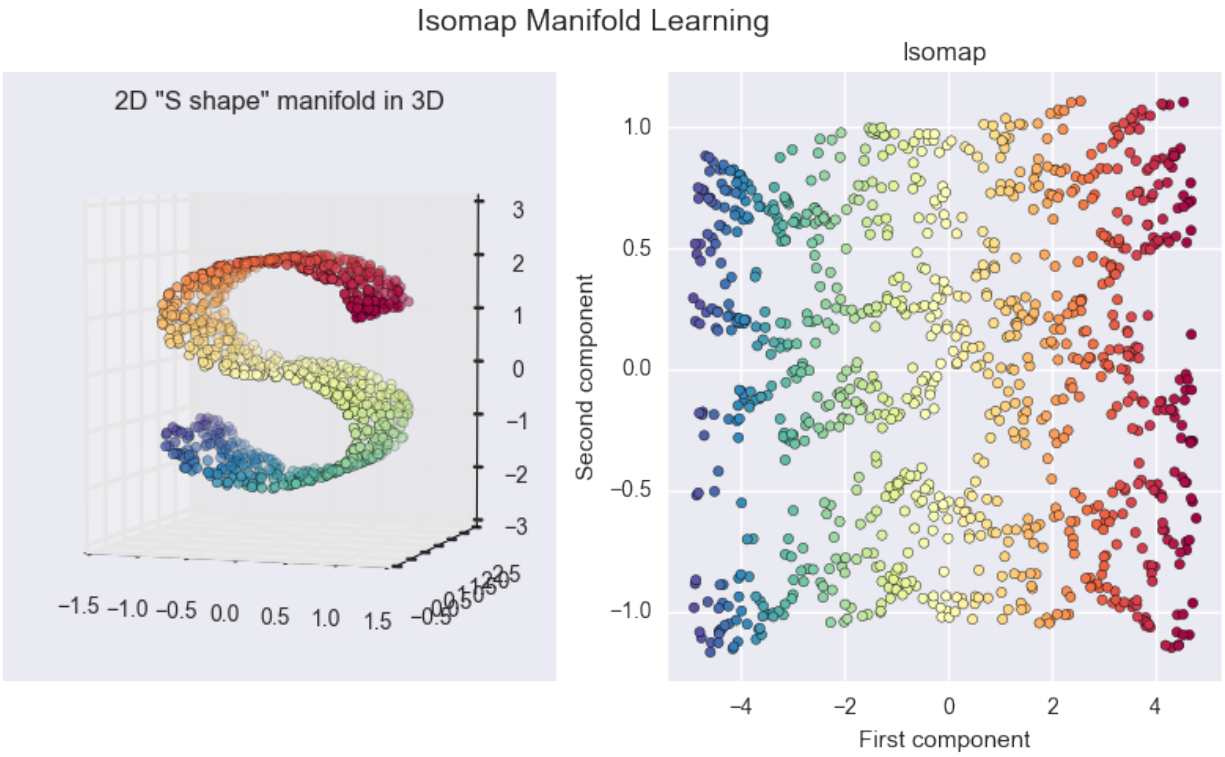
Isomap

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

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')
```

```
(-5.4131242078919239,
 5.2729984345096854,
 -1.2877687637642998,
 1.2316524684384262)
```



Exercises

PCA

Write a basic PCA class

Write a class `BasicPCA` with two methods:

- `fit(X)` that estimates the data mean, principal components directions $\mathbf{V}$ 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/data/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/data/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.

CHAPTER

NINE

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 task 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

K-means clustering

Source: C. M. Bishop *Pattern Recognition and Machine Learning*, Springer, 2006

Suppose we have a data set $X = \{x_1, \cdots, x_N\}$ 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 μ_k, where $k = 1, \ldots, K$, in which μ_k is a **prototype** associated with the k^{th} cluster. As we shall see shortly, we can think of the μ_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 μ_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 $k = 1, \ldots, K$, 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 μ_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 μ_k . First we choose some initial values for the μ_k. Then in the first phase we minimize J with respect to the r_{ik}, keeping the μ_k fixed. In the second phase we minimize J with respect to the μ_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 μ_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 in 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 ith data point to the closest cluster centre. More formally, this can be expressed as

$$r_{ik} = \begin{cases} 1, & \text{if } k = \arg\min_j ||x_i - \mu_j||^2. \\ 0, & \text{otherwise.} \end{cases} \tag{9.1}$$

Now consider the optimization of the μ_k with the r_{ik} held fixed. The objective function J is a quadratic function of μ_k, and it can be minimized by setting its derivative with respect to μ_k to zero giving

$$2 \sum_i r_{ik}(x_i - \mu_k) = 0$$

which we can easily solve for μ_k to give

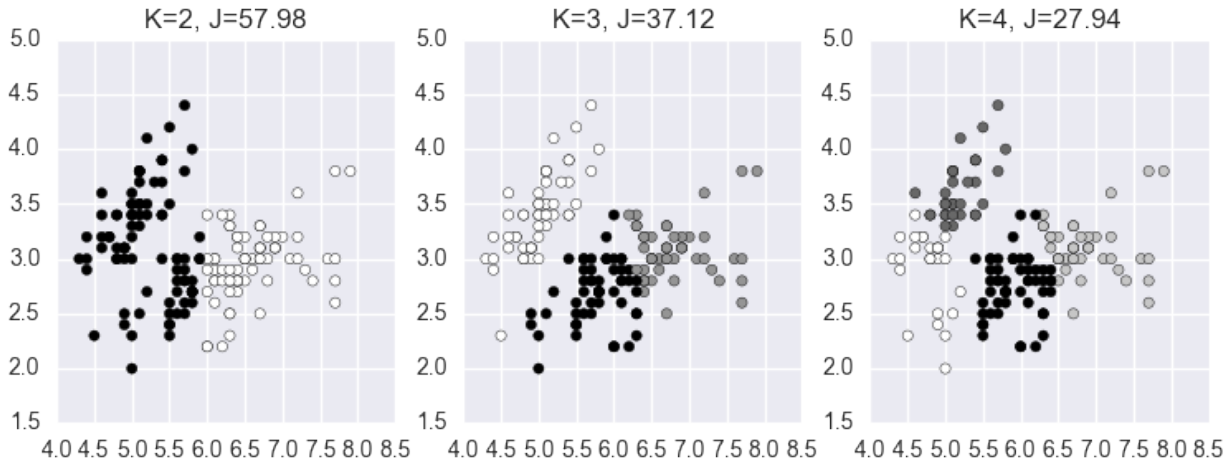
$$\mu_k = \frac{\sum_i r_{ik} x_i}{\sum_i r_{ik}}.$$

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 μ_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_)
```

```
<matplotlib.text.Text at 0x7fe4ad47b710>
```



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

2. Re-implement the K-means clustering algorithm (homework)

Write a function `kmeans(X,K)` that return an integer vector of the samples' labels.

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

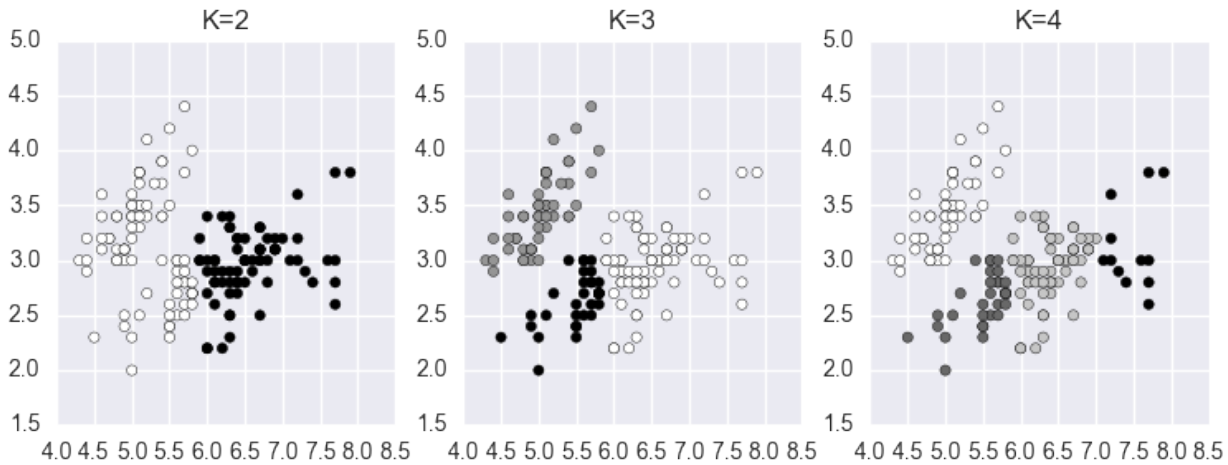
Ward clustering belongs to the family of agglomerative hierarchical clustering algorithms. This means that they are based on a "bottoms up" approach: each sample starts in its own cluster, and pairs of clusters are merged as one moves up the hierarchy.

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")
```

```
<matplotlib.text.Text at 0x7fe4ace5cfd0>
```



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:

$$p(x) = \sum_{k=1}^{K} \mathcal{N}(x \mid \mu_k, \Sigma_k) p(k),$$

where:

- $\mathcal{N}(x \mid \mu_k, \Sigma_k)$ is the multivariate Gaussian distribution defined over a P-dimensional vector x of continuous variables.
- The $p(k)$ are the mixing coefficients also know as the class probability of class k, and they sum to one: $\sum_{k=1}^{K} p(k) = 1$.
- $\mathcal{N}(x \mid \mu_k, \Sigma_k) = p(x \mid k)$ is the conditional distribution of x given a particular class k.

The goal is to maximize the log-likelihood of the GMM:

$$\ln \prod_{i=1}^{N} \left\{ \sum_{k=1}^{K} \mathcal{N}(x \mid \mu_k, \Sigma_k) p(k) \right\} = \sum_{i=1}^{N} \ln \left\{ \sum_{k=1}^{K} \mathcal{N}(x \mid \mu_k, \Sigma_k) p(k) \right\}.$$

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: $p(k \mid x_i)$ such that for each point its contribution to all classes sum to one $\sum_k p(k \mid x_i) = 1$. This contribution is the conditional probability of class k given x: $p(k \mid x)$ (sometimes called the posterior). It can be computed using Bayes' rule:

$$p(k \mid x) = \frac{p(x \mid k) p(k)}{p(x)} \tag{9.2}$$

$$= \frac{\mathcal{N}(x \mid \mu_k, \Sigma_k) p(k)}{\sum_{k=1}^{K} \mathcal{N}(x \mid \mu_k, \Sigma_k) p(k)} \tag{9.3}$$

Since the class parameters, $p(k)$, μ_k and Σ_k, depend on the responsibilities $p(k \mid x)$ 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 μ_k, covariances Σ_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

$$p(k \mid x_i) = \frac{\mathcal{N}(x_i \mid \mu_k, \Sigma_k)p(k)}{\sum_{k=1}^{K} \mathcal{N}(x_i \mid \mu_k, \Sigma_k)p(k)}$$

2. **M step**. For each class, re-estimate the parameters using the current responsibilities

$$\mu_k^{\text{new}} = \frac{1}{N_k} \sum_{i=1}^{N} p(k \mid x_i) x_i \tag{9.4}$$

$$\Sigma_k^{\text{new}} = \frac{1}{N_k} \sum_{i=1}^{N} p(k \mid x_i)(x_i - \mu_k^{\text{new}})(x_i - \mu_k^{\text{new}})^T \tag{9.5}$$

$$p^{\text{new}}(k) = \frac{N_k}{N} \tag{9.6}$$

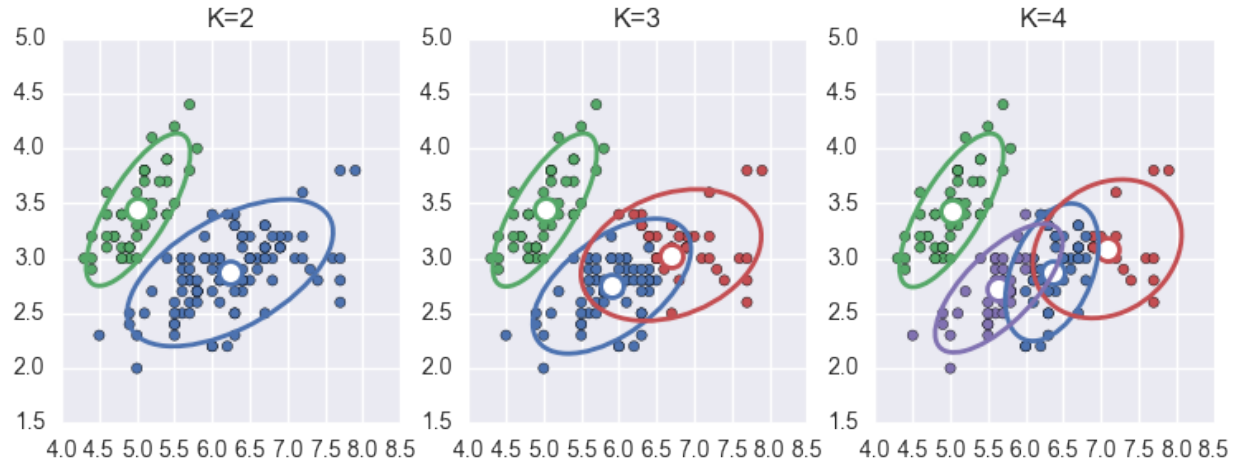
3. Evaluate the log-likelihood

$$\sum_{i=1}^{N} \ln \left\{ \sum_{k=1}^{K} \mathcal{N}(x|\mu_k, \Sigma_k)p(k) \right\},$$

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)
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")
```



Model selection

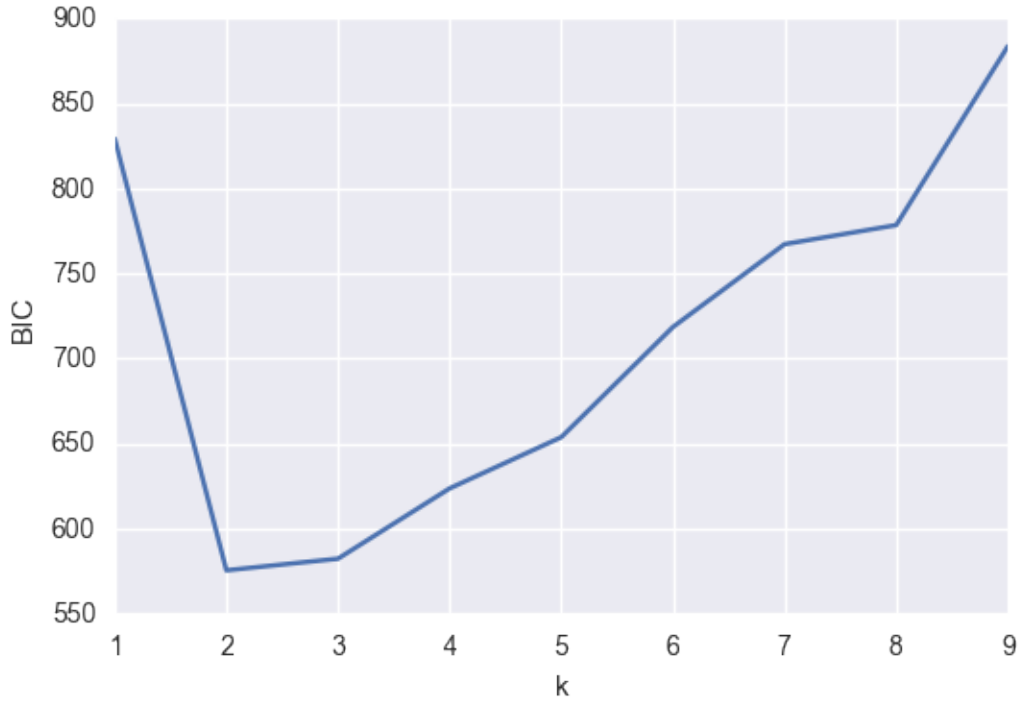
Bayesian information criterion

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")

print("Choose k=", k_chosen)
```

```
Choose k= 2
```



CHAPTER

TEN

LINEAR METHODS FOR REGRESSION

Ordinary least squares

Linear regression models the **output**, or **target** variable $y \in \mathrm{R}$ as a linear combination of the $(P-1)$-dimensional input $x \in \mathrm{R}^{(P-1)}$. 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 $\mathbf{y}$ given $\mathbf{X}$ using the **parameter vector**, or **weight vector** $\boldsymbol{\beta} \in \mathrm{R}^P$ according to

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon},$$

where $\boldsymbol{\varepsilon} \in \mathrm{R}^N$ are the **residuals**, or the errors of the prediction. The $\boldsymbol{\beta}$ is found by minimizing an **objective function**, which is the **loss function**, $\mathcal{L}(\boldsymbol{\beta})$, 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.

$$\begin{aligned}
\mathrm{OLS}(\boldsymbol{\beta}) &= \mathcal{L}(\boldsymbol{\beta}) && (10.1)\\
&= \mathrm{SSE}(\boldsymbol{\beta}) && (10.2)\\
&= \sum_{i}^{N} (y_i - \mathbf{x}_i^T \boldsymbol{\beta})^2 && (10.3)\\
&= (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) && (10.4)\\
&= \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2, && (10.5)
\end{aligned}$$

which is a simple **ordinary least squares (OLS)** minimization.

Linear regression with scikit-learn

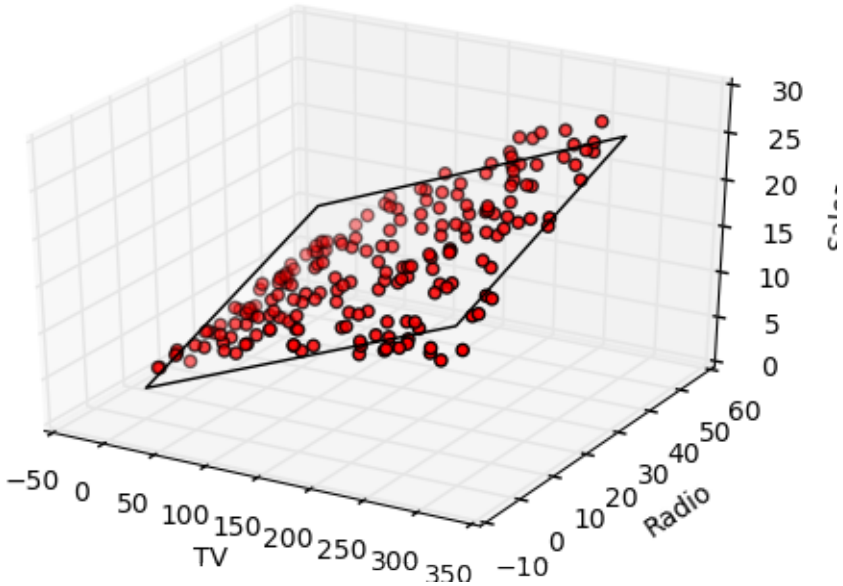
Scikit learn offer many models for supervised learning, and they all follow the same application programming interface (API), namely:

```
model = Estimator()
model.fit(X, y)
predictions = model.predict(X)
```

```
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('http://www-bcf.usc.edu/~gareth/ISL/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),
    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')
```

```
R-squared = 0.897194261083
Coefficients = [ 0.04575482  0.18799423]
```



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

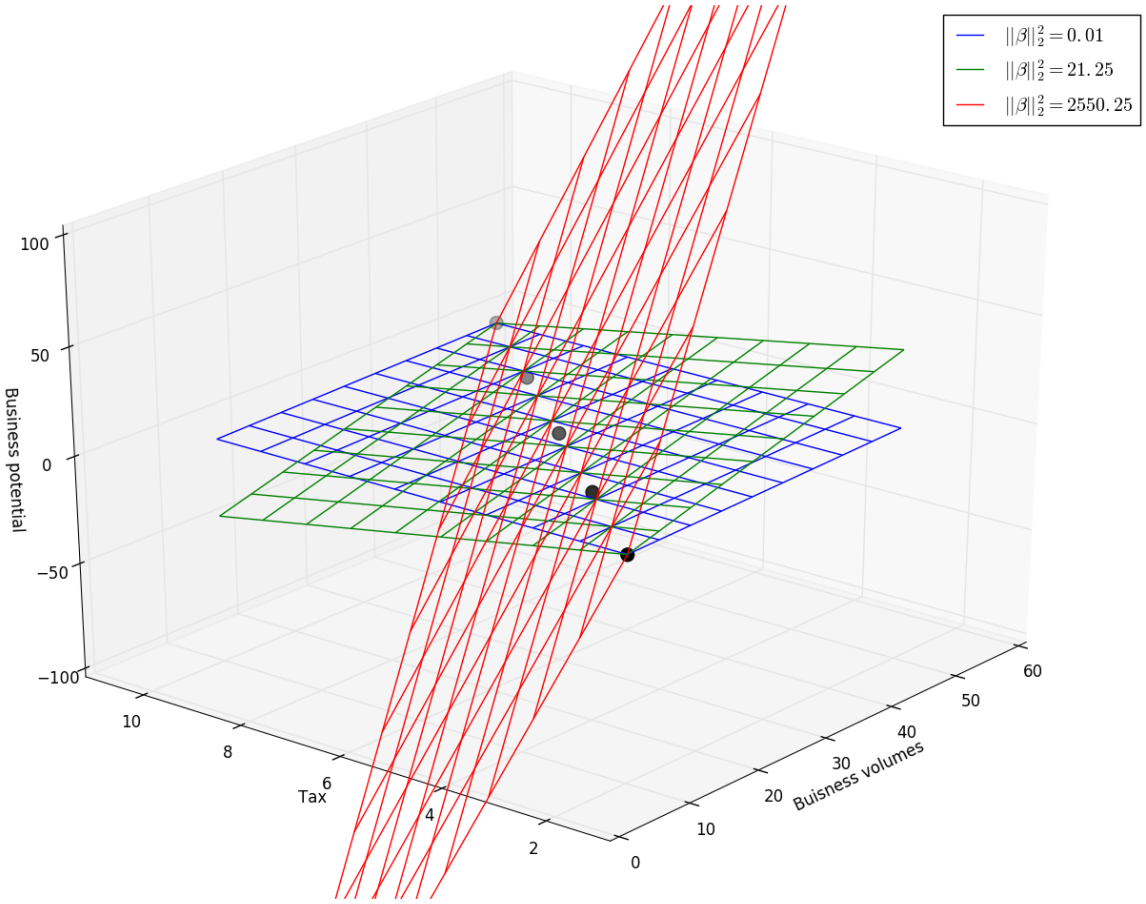
Predictors are highly correlated, meaning that one can be linearly predicted from the others. In this situation the coefficient estimates of the multiple regression may change erratically in response to small changes in the model or the data. Multicollinearity does not reduce the predictive power or 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 $\mathbf{y} = \mathbf{X}\boldsymbol{\beta}+\boldsymbol{\varepsilon}$, the ordinary least-squares estimator, $\boldsymbol{\beta}_{OLS} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$, 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. ℓ_2 shrinkage: Introduce a bias in the solution by making $(X^T X)^{-1}$ non-singular. See ℓ_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 ℓ_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.

- Remenber 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

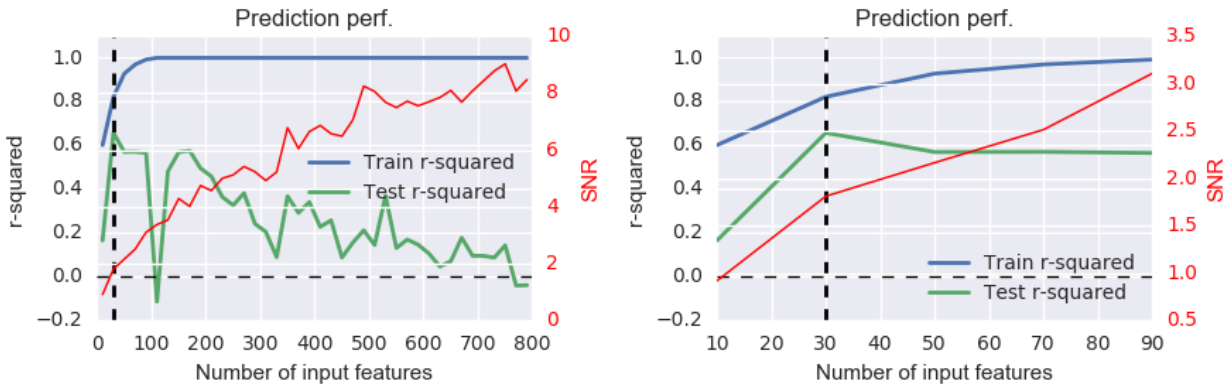
$$d(P, N) = \left(1 - \frac{1}{2}^N\right)^{1/P}.$$

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)

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_ylim(-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()
```



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?

Ridge regression (ℓ_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** $\mathcal{L}(\boldsymbol{\beta})$ (generally the SSE) is combined with a **penalty function** $\Omega(\boldsymbol{\beta})$ leading to the general form:

$$\text{Penalized}(\boldsymbol{\beta}) = \mathcal{L}(\boldsymbol{\beta}) + \lambda\Omega(\boldsymbol{\beta})$$

The respective contribution of the loss and the penalty is controlled by the **regularization parameter** λ.

Ridge regression impose a ℓ_2 penalty on the coefficients, i.e. it penalizes with the Euclidean norm of the coefficients while minimizing SSE. The objective function becomes:

$$\text{Ridge}(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 + \lambda\|\boldsymbol{\beta}\|_2^2.$$

The $\boldsymbol{\beta}$ that minimises $F_{Ridge}(\boldsymbol{\beta})$ can be found by the following derivation:

$$\nabla_{\boldsymbol{\beta}}\text{Ridge}(\boldsymbol{\beta}) = 0 \tag{10.6}$$

$$\nabla_{\boldsymbol{\beta}}\big((\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) + \lambda\boldsymbol{\beta}^T\boldsymbol{\beta}\big) = 0 \tag{10.7}$$

$$\nabla_{\boldsymbol{\beta}}\big((\mathbf{y}^T\mathbf{y} - 2\boldsymbol{\beta}^T\mathbf{X}^T\mathbf{y} + \boldsymbol{\beta}^T\mathbf{X}^T\mathbf{X}\boldsymbol{\beta} + \lambda\boldsymbol{\beta}^T\boldsymbol{\beta})\big) = 0 \tag{10.8}$$

$$-2\mathbf{X}^T\mathbf{y} + 2\mathbf{X}^T\mathbf{X}\boldsymbol{\beta} + 2\lambda\boldsymbol{\beta} = 0 \tag{10.9}$$

$$-\mathbf{X}^T\mathbf{y} + (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})\boldsymbol{\beta} = 0 \tag{10.10}$$

$$(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})\boldsymbol{\beta} = \mathbf{X}^T\mathbf{y} \tag{10.11}$$

$$\boldsymbol{\beta} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y} \tag{10.12}$$

- The solution adds a positive constant to the diagonal of $\mathbf{X}^T\mathbf{X}$ before inversion. This makes the problem non-singular, even if $\mathbf{X}^T\mathbf{X}$ is not of full rank, and was the main motivation behind ridge regression.
- Increasing λ shrinks the $\boldsymbol{\beta}$ 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 ℓ_1 and ℓ_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.

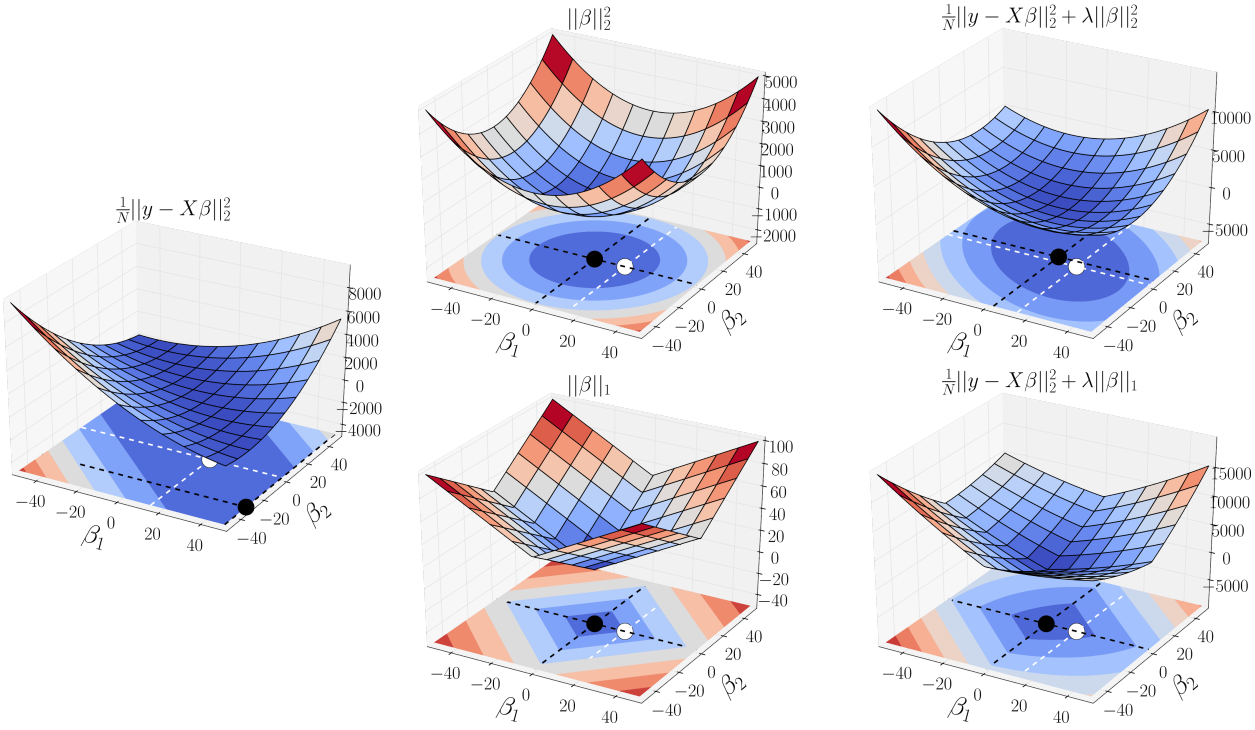
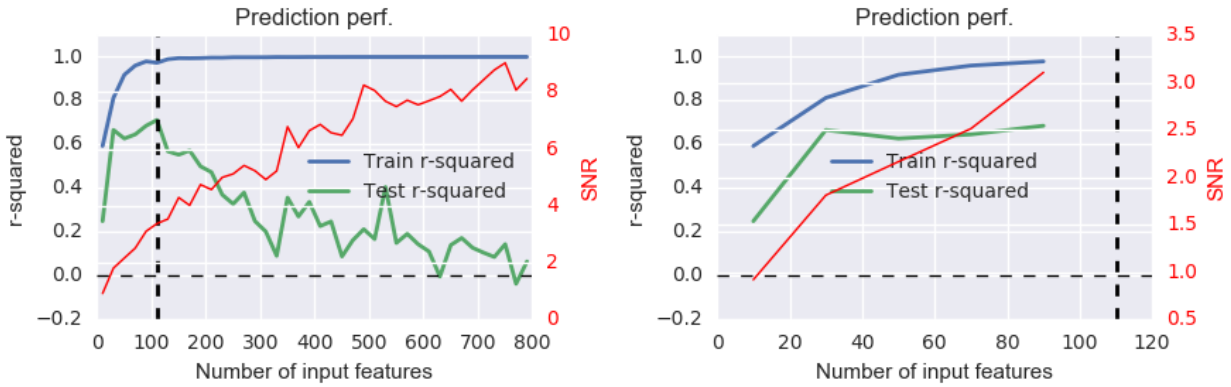


Fig. 10.1: ℓ_1 and ℓ_2 shrinkages

```
import matplotlib.pyplot as plt
import numpy as np
import sklearn.linear_model as lm

# 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 ℓ_2 regularization?

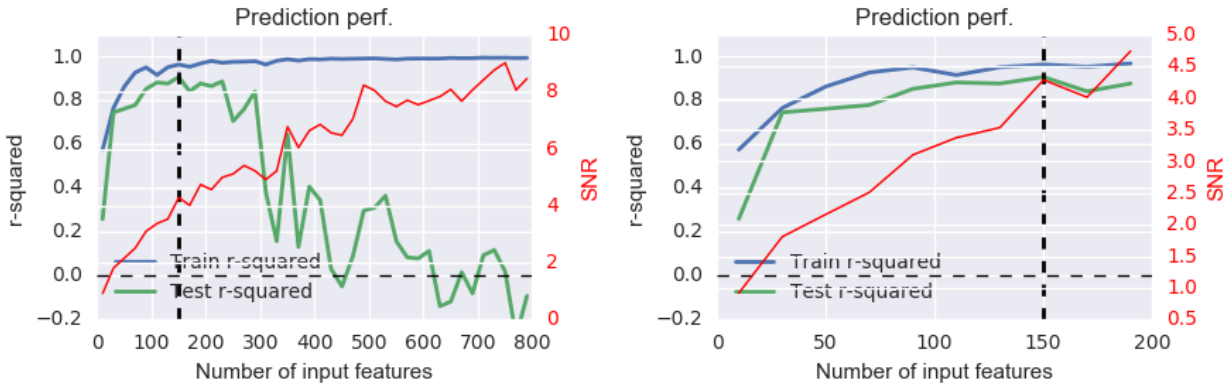
Lasso regression (ℓ_1-regularization)

Lasso regression penalizes the coefficients by the ℓ_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:

$$\text{Lasso}(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 + \lambda\|\boldsymbol{\beta}\|_1. \tag{10.13}$$

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 ℓ_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 ℓ_2 ($\|\boldsymbol{\beta}\|_2$) or ℓ_1 ($\|\boldsymbol{\beta}\|_1$) norm of $\boldsymbol{\beta}$, i.e. ℓ_2 or ℓ_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 ℓ_1 penalty

The penalty based on the ℓ_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 bellow illustrates the OLS loss under a constraint acting on the ℓ_1 norm of the coefficient vector. I.e., it illustrates the following optimization problem:

$$\underset{\boldsymbol{\beta}}{\text{minimize}} \ \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2$$

$$\text{subject to } \|\boldsymbol{\beta}\|_1 \leq 1.$$

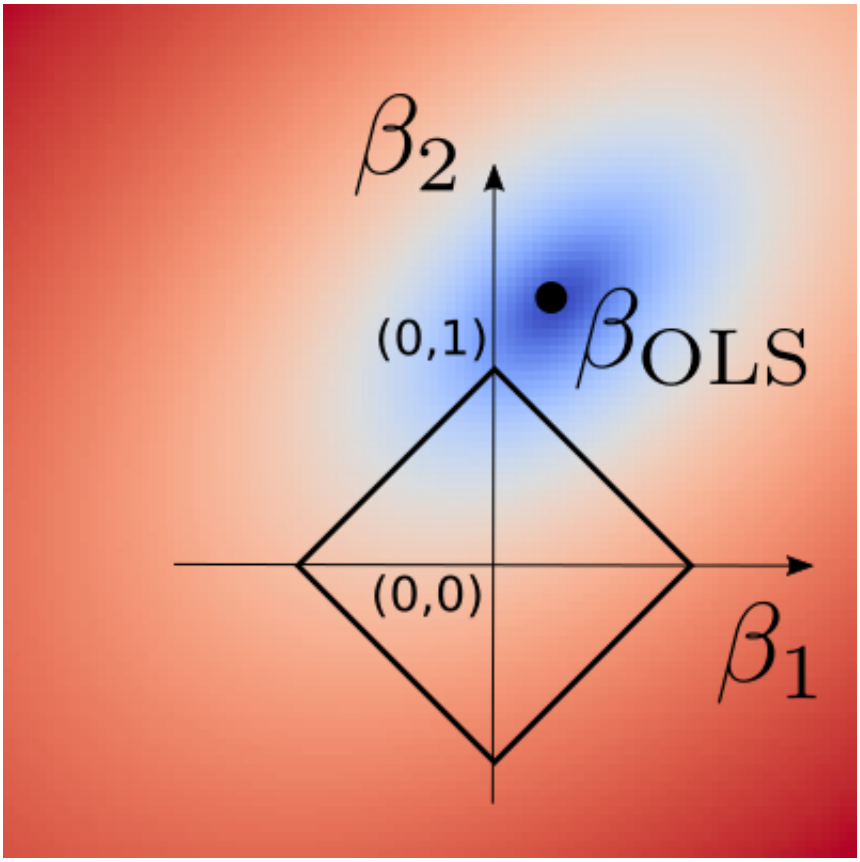


Fig. 10.2: Sparsity of L1 norm

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.

Elastic-net regression (ℓ_2-ℓ_1-regularization)

The Elastic-net estimator combines the ℓ_1 and ℓ_2 penalties, and results in the problem to

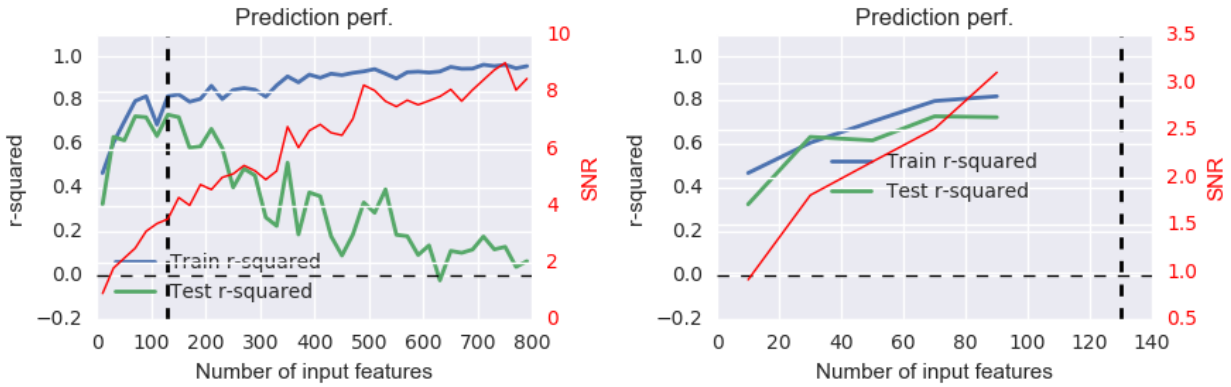
$$\text{Enet}(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X}^T\boldsymbol{\beta}\|_2^2 + \alpha\left(\rho\|\boldsymbol{\beta}\|_1 + (1-\rho)\|\boldsymbol{\beta}\|_2^2\right), \tag{10.14}$$

where α acts as a global penalty and ρ as an ℓ_1/ℓ_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()
```


Prediction perf.
r-squared
SNR
Train r-squared
Test r-squared
Number of input features
Prediction perf.
r-squared
SNR
Train r-squared
Test r-squared
Number of input features

CHAPTER

ELEVEN

LINEAR CLASSIFICATION

A linear classifier achieves its classification decision of $\hat{y}_i$ based on the value of a linear combination of the input features of a given sample $\boldsymbol{x_i}$, such that

$$\hat{y}_i = f(\boldsymbol{w} \cdot \boldsymbol{x_i}),$$

where $\boldsymbol{w} \cdot \boldsymbol{x_i} := \boldsymbol{w}^T \boldsymbol{x_i}$ is the dot product between $\boldsymbol{w}$ and $\boldsymbol{x_i}$.

Linear classifiers looks for a weight vector, $\boldsymbol{w}$, that minimizes a given loss function,

$$\mathcal{L}(y_i, \hat{y}_i),$$

and some penalties on the weights vector.

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 $\boldsymbol{\mu_0}$ and $\boldsymbol{\mu_1}$ and the same total within-class scatter ("covariance") matrix,

$$\boldsymbol{S_W} = \sum_{i \in C_0} (\boldsymbol{x_i} - \boldsymbol{\mu_0})(\boldsymbol{x_i} - \boldsymbol{\mu_0})^T + \sum_{j \in C_1} (\boldsymbol{x_j} - \boldsymbol{\mu_1})(\boldsymbol{x_j} - \boldsymbol{\mu_1})^T \tag{11.1}$$

$$= \boldsymbol{X_c}^T \boldsymbol{X_c}, \tag{11.2}$$

where $\boldsymbol{X_c}$ is the $(N \times P)$ matrix of data centered on their respective means:

$$\boldsymbol{X_c} = \begin{bmatrix} \boldsymbol{X_0} - \boldsymbol{\mu_0} \\ \boldsymbol{X_1} - \boldsymbol{\mu_1} \end{bmatrix},$$

where $\boldsymbol{X_0}$ and $\boldsymbol{X_1}$ are the $(N_0 \times P)$ and $(N_1 \times P)$ matrices of samples of classes C_0 and C_1.

Let $\boldsymbol{S_B}$ being the scatter "between-class" matrix, given by

$$\boldsymbol{S_B} = (\boldsymbol{\mu_1} - \boldsymbol{\mu_0})(\boldsymbol{\mu_1} - \boldsymbol{\mu_0})^T.$$

The linear combination of features $\boldsymbol{w}^T x$ have means $\boldsymbol{w}^T \mu_i$ for $i = 0, 1$, and variance $\boldsymbol{w}^T \boldsymbol{X_c^T} \boldsymbol{X_c} \boldsymbol{w}$. Fisher defined the separation between these two distributions to be the ratio of the variance between the classes to the variance within

the classes:

$$F_{\text{Fisher}}(\boldsymbol{w}) = \frac{\sigma^2_{\text{between}}}{\sigma^2_{\text{within}}} \tag{11.3}$$

$$= \frac{(\boldsymbol{w}^T\boldsymbol{\mu_1} - \boldsymbol{w}^T\boldsymbol{\mu_0})^2}{\boldsymbol{w}^T X_c^T \boldsymbol{X_c}\boldsymbol{w}} \tag{11.4}$$

$$= \frac{(\boldsymbol{w}^T(\boldsymbol{\mu_1} - \boldsymbol{\mu_0}))^2}{\boldsymbol{w}^T X_c^T \boldsymbol{X_c}\boldsymbol{w}} \tag{11.5}$$

$$= \frac{\boldsymbol{w}^T(\boldsymbol{\mu_1} - \boldsymbol{\mu_0})(\boldsymbol{\mu_1} - \boldsymbol{\mu_0})^T w}{\boldsymbol{w}^T X_c^T \boldsymbol{X_c}\boldsymbol{w}} \tag{11.6}$$

$$= \frac{\boldsymbol{w}^T \boldsymbol{S_B} w}{\boldsymbol{w}^T \boldsymbol{S_W}\boldsymbol{w}}. \tag{11.7}$$

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 ${\boldsymbol{S_B}}^{-1}$, so that

$$\boldsymbol{w} \propto {\boldsymbol{S_W}}^{-1}(\boldsymbol{\mu_1} - \boldsymbol{\mu_0}).$$

Demonstration

Differentiating $F_{\text{Fisher}}(w)$ with respect to w gives

$$\begin{aligned}
\nabla_{\boldsymbol{w}} F_{\text{Fisher}}(\boldsymbol{w}) &= 0 \\
\nabla_{\boldsymbol{w}} \left(\frac{\boldsymbol{w}^T \boldsymbol{S_B} w}{\boldsymbol{w}^T \boldsymbol{S_W}\boldsymbol{w}} \right) &= 0 \\
(\boldsymbol{w}^T \boldsymbol{S_W}\boldsymbol{w})(2\boldsymbol{S_B}\boldsymbol{w}) - (\boldsymbol{w}^T \boldsymbol{S_B}\boldsymbol{w})(2\boldsymbol{S_W}\boldsymbol{w}) &= 0 \\
(\boldsymbol{w}^T \boldsymbol{S_W}\boldsymbol{w})(\boldsymbol{S_B}\boldsymbol{w}) &= (\boldsymbol{w}^T \boldsymbol{S_B}\boldsymbol{w})(\boldsymbol{S_W}\boldsymbol{w}) \\
\boldsymbol{S_B}\boldsymbol{w} &= \frac{\boldsymbol{w}^T \boldsymbol{S_B}\boldsymbol{w}}{\boldsymbol{w}^T \boldsymbol{S_W}\boldsymbol{w}}(\boldsymbol{S_W}\boldsymbol{w}) \\
\boldsymbol{S_B}\boldsymbol{w} &= \lambda(\boldsymbol{S_W}\boldsymbol{w}) \\
{\boldsymbol{S_W}}^{-1}\boldsymbol{S_B}\boldsymbol{w} &= \lambda\boldsymbol{w}.
\end{aligned}$$

Since we do not care about the magnitude of w, only its direction, we replaced the scalar factor $(\boldsymbol{w}^T \boldsymbol{S_B}\boldsymbol{w})/(\boldsymbol{w}^T \boldsymbol{S_W}\boldsymbol{w})$ by λ.

In the multiple-class case, the solutions w are determined by the eigenvectors of ${\boldsymbol{S_W}}^{-1}\boldsymbol{S_B}$ that correspond to the $K-1$ largest eigenvalues.

However, in the two-class case (in which $\boldsymbol{S_B} = (\boldsymbol{\mu_1} - \boldsymbol{\mu_0})(\boldsymbol{\mu_1} - \boldsymbol{\mu_0})^T$) it is easy to show that $w = {\boldsymbol{S_W}}^{-1}(\boldsymbol{\mu_1} - \boldsymbol{\mu_0})$ is the unique eigenvector of ${\boldsymbol{S_W}}^{-1}\boldsymbol{S_B}$:

$$\begin{aligned}
{\boldsymbol{S_W}}^{-1}(\boldsymbol{\mu_1} - \boldsymbol{\mu_0})(\boldsymbol{\mu_1} - \boldsymbol{\mu_0})^T\boldsymbol{w} &= \lambda\boldsymbol{w} \\
{\boldsymbol{S_W}}^{-1}(\boldsymbol{\mu_1} - \boldsymbol{\mu_0})(\boldsymbol{\mu_1} - \boldsymbol{\mu_0})^T{\boldsymbol{S_W}}^{-1}(\boldsymbol{\mu_1} - \boldsymbol{\mu_0}) &= \lambda{\boldsymbol{S_W}}^{-1}(\boldsymbol{\mu_1} - \boldsymbol{\mu_0}),
\end{aligned}$$

where here $\lambda = (\boldsymbol{\mu_1} - \boldsymbol{\mu_0})^T{\boldsymbol{S_W}}^{-1}(\boldsymbol{\mu_1} - \boldsymbol{\mu_0})$. Which leads to the result

$$\boldsymbol{w} \propto {\boldsymbol{S_W}}^{-1}(\boldsymbol{\mu_1} - \boldsymbol{\mu_0}).$$

The separating hyperplane

The separating hyperplane is a $P-1$-dimensional hyper surface, orthogonal to the projection vector, w. There is no single best way to find the origin of the plane along 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

$$T = \boldsymbol{w} \cdot \frac{1}{2}(\boldsymbol{\mu_1} - \boldsymbol{\mu_0}).$$

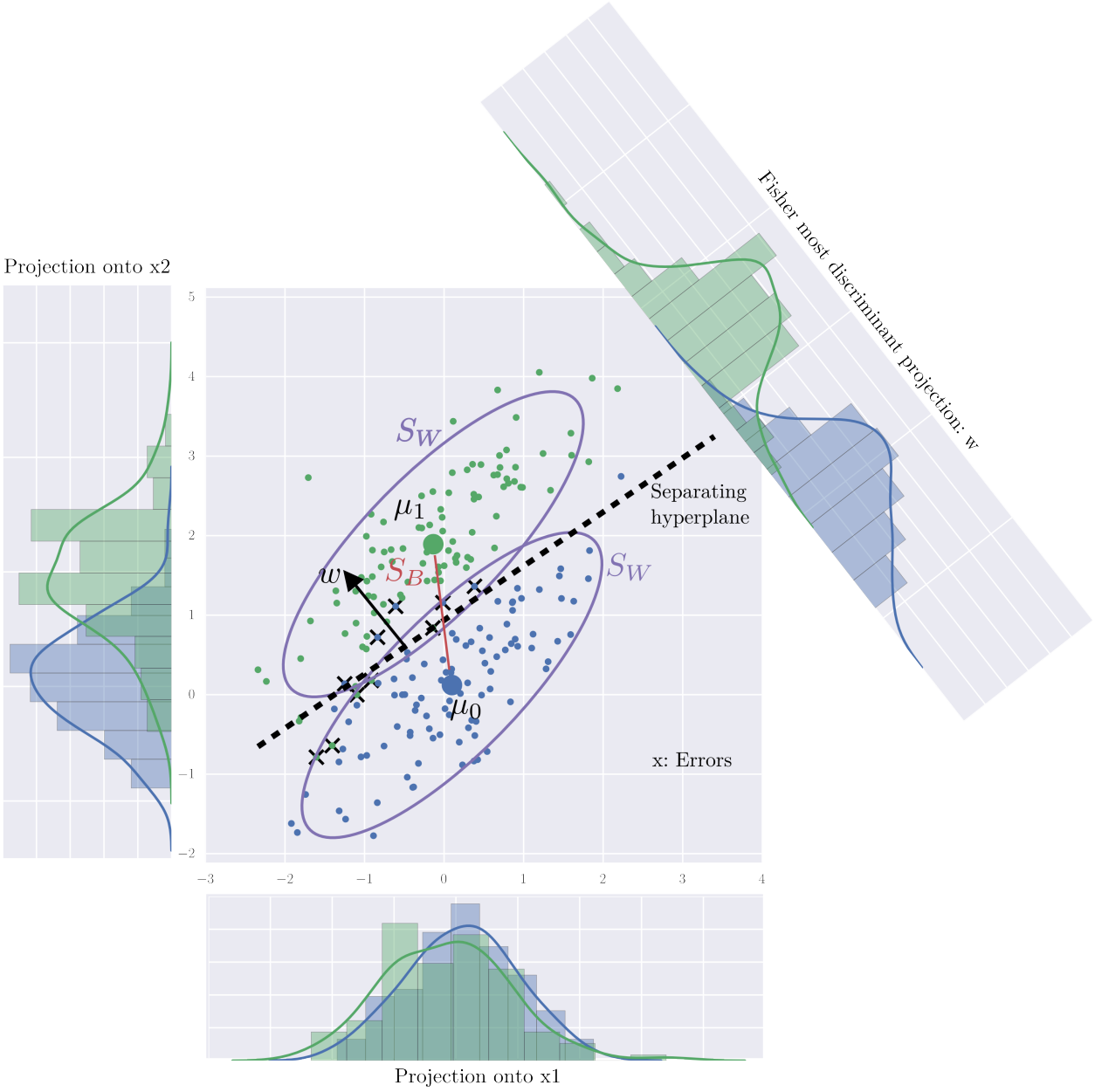


Fig. 11.1: The Fisher most discriminant projection

Exercise

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.

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.

1. First compute the The class-**conditional distributions** of $\boldsymbol{x}$ given class C_k: $p(x|C_k) = \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu_k}, \boldsymbol{S_W})$. Where $\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu_k}, \boldsymbol{S_W})$ is the multivariate Gaussian distribution defined over a P-dimensional vector x of continuous variables, which is given by

$$\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu_k}, \boldsymbol{S_W}) = \frac{1}{(2\pi)^{P/2}|\boldsymbol{S_W}|^{1/2}} \exp\{-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu_k})^T \boldsymbol{S_W}^{-1}(x - \boldsymbol{\mu_k})\}$$

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:

$$p(C_k|\boldsymbol{x}) = \frac{p(C_k)p(\boldsymbol{x}|C_k)}{p(\boldsymbol{x})}$$

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

$$p(x) = \sum_k p(\boldsymbol{x}|C_k)p(C_k)$$

4. Classify $\boldsymbol{x}$ using the Maximum-a-Posteriori probability: $C_k = \arg\max_{C_k} p(C_k|\boldsymbol{x})$

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 ?

```
%matplotlib inline

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)))
```

```
Nb errors=10, error rate=0.05
```

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:

$$p(C_k|w, \boldsymbol{x_i}) = \frac{1}{1 + \exp(-\boldsymbol{w} \cdot \boldsymbol{x_i})}$$

Logistic regression seeks to minimizes the likelihood L as **Loss function** $\mathcal{L}$:

$$\min L(\boldsymbol{w}) = \Pi_i^N p(C_k|\boldsymbol{w}, \boldsymbol{x_i})$$

Partically, the Loss function $\mathcal{L}$ is the log-likelihood:

$$\min \mathcal{L}(\boldsymbol{w}) = \log L(\boldsymbol{w}) = \sum_i^N \log p(C_k|\boldsymbol{w}, \boldsymbol{x_i})$$

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 $p(C_0|\boldsymbol{w}, \boldsymbol{x_i}) = 1 - p(C_1|\boldsymbol{w}, \boldsymbol{x_i})$, the log-likelihood can be re-witten:

$$\log L(\boldsymbol{w}) = \sum_i^N \{y_i \log p(C_1|\boldsymbol{w}, \boldsymbol{x_i}) + (1 - y_i) \log(1 - p(C_1|\boldsymbol{w}, \boldsymbol{x_i}))\} \tag{11.8}$$

$$\log L(\boldsymbol{w}) = \sum_i^N \{y_i \, \boldsymbol{w} \cdot \boldsymbol{x_i} - \log(1 + \exp^{\boldsymbol{w} \cdot \boldsymbol{x_i}})\} \tag{11.9}$$

$$\tag{11.10}$$

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.

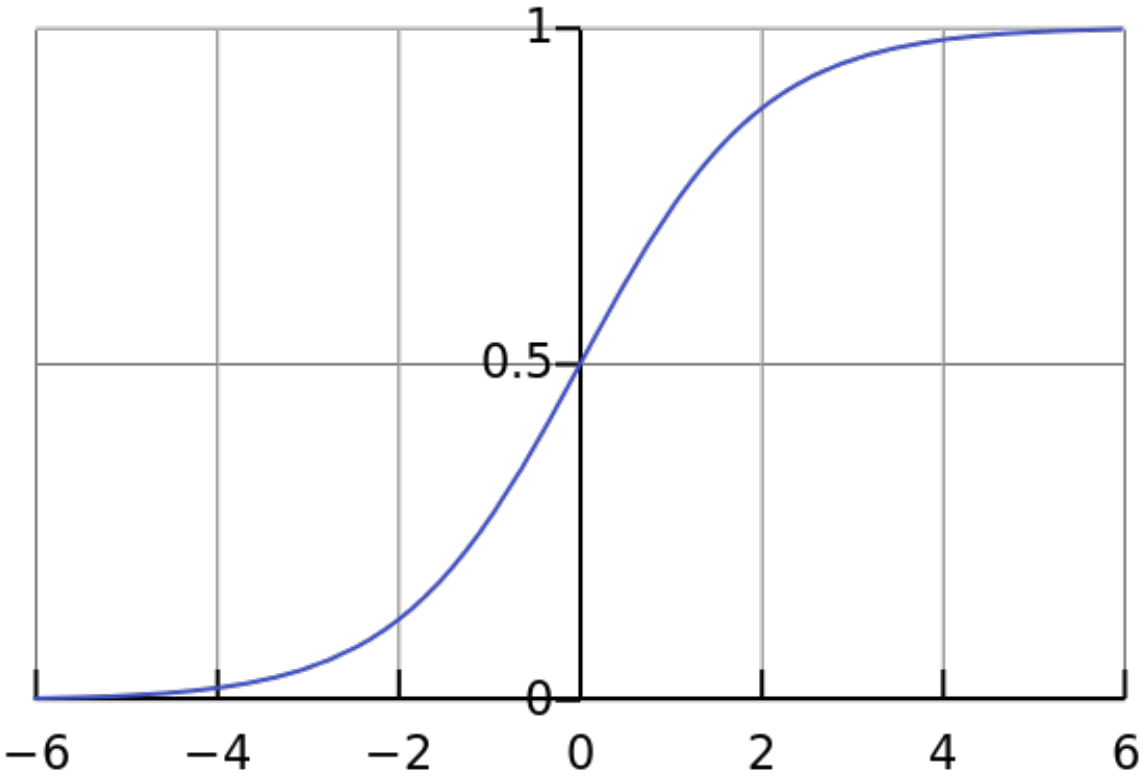


Fig. 11.2: logistic sigmoid function

```
from sklearn import linear_model
logreg = linear_model.LogisticRegression(C=1e8)
# 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
[[-5.15162649  5.57299286]]
```

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 $p(C_1) = p(C_0)$.

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.

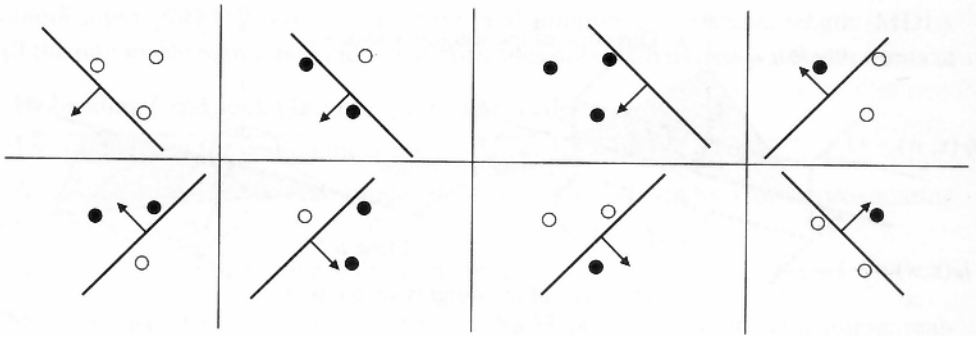


Fig. 11.3: In 2D we can shatter any three non-collinear points

Ridge Fisher's linear classification (L2-regularization)

When the matrix $\boldsymbol{S_W}$ 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 $\boldsymbol{S_W}$:

$$\boldsymbol{S_W}^{Ridge} = \boldsymbol{S_W} + \lambda \boldsymbol{I}$$

where I is the $P \times P$ identity matrix. This leads to the regularized (ridge) estimator of the Fisher's linear discriminant analysis:

$$\boldsymbol{w}^{Ridge} \propto (\boldsymbol{S_W} + \lambda \boldsymbol{I})^{-1}(\boldsymbol{\mu_1} - \boldsymbol{\mu_0})$$

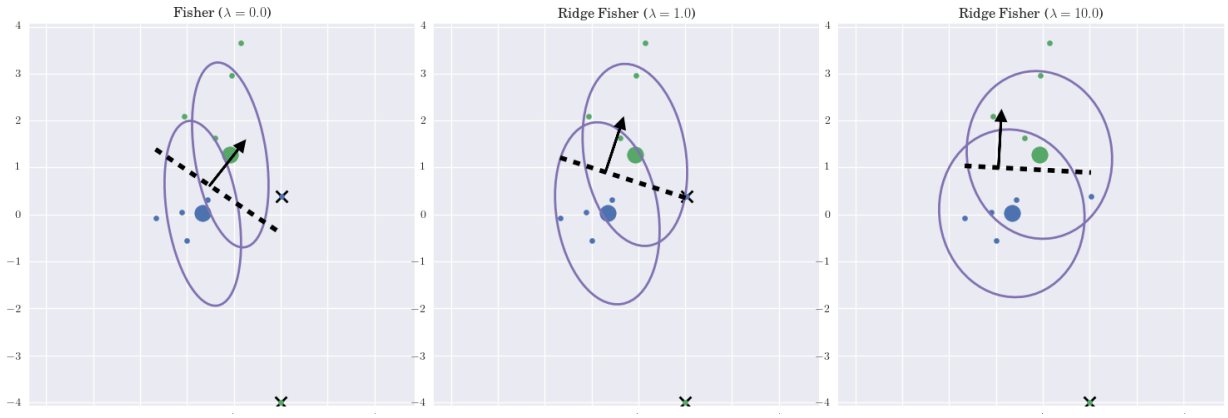


Fig. 11.4: The Ridge Fisher most discriminant projection

Increasing λ will:

- Shrinks the coefficients toward zero.
- The covariance will converge toward the diagonal matrix, reducing the contribution of the pairwise covariances.

Ridge logistic regression (L2-regularization)

The **objective function** to be minimized is now the combination of the logistic loss $\log L(\boldsymbol{w})$ with a penalty of the L2 norm of the weights vector. In the two-class case, using the 0/1 coding we obtain:

$$\min \text{ Logistic ridge}(\boldsymbol{w}) = \log L(\boldsymbol{w}) + \lambda \|\boldsymbol{w}\|^2 \tag{11.11}$$

$$= \sum_i^N \{y_i \boldsymbol{w}^T \boldsymbol{x_i} - \log(1 + \exp^{\boldsymbol{w}^T \boldsymbol{x_i}})\} + \lambda \|\boldsymbol{w}\|^2 \tag{11.12}$$

$$\tag{11.13}$$

```
# 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)
```

```
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]]
```

Lasso logistic regression (L1-regularization)

The **objective function** to be minimized is now the combination of the logistic loss $\log L(\boldsymbol{w})$ with a penalty of the L1 norm of the weights vector. In the two-class case, using the 0/1 coding we obtain:

$$\min \text{ Logistic Lasso}(w) = \log L(\boldsymbol{w}) + \lambda \|\boldsymbol{w}\|_1 \tag{11.14}$$

$$= \sum_i^N \{y_i \, \boldsymbol{w} \cdot \boldsymbol{x_i} - \log(1 + \exp^{\boldsymbol{w} \cdot \boldsymbol{x_i}})\} + \lambda \|\boldsymbol{w}\|_1 \tag{11.15}$$

```
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
[[-0.11335795  0.68150965  0.          0.          0.19754476  0.36480308
```

```
  0.0805774   0.06205936  0.76017405  0.         -0.10810091  0.          0.
  0.33749265  0.          0.          0.07903044  0.20159231  0.48383422
  0.        ]]
```

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 ± 1 coding (ie.: y_i $\{-1, +1\}$). In the next figure the legend aply to samples of "dot" class.

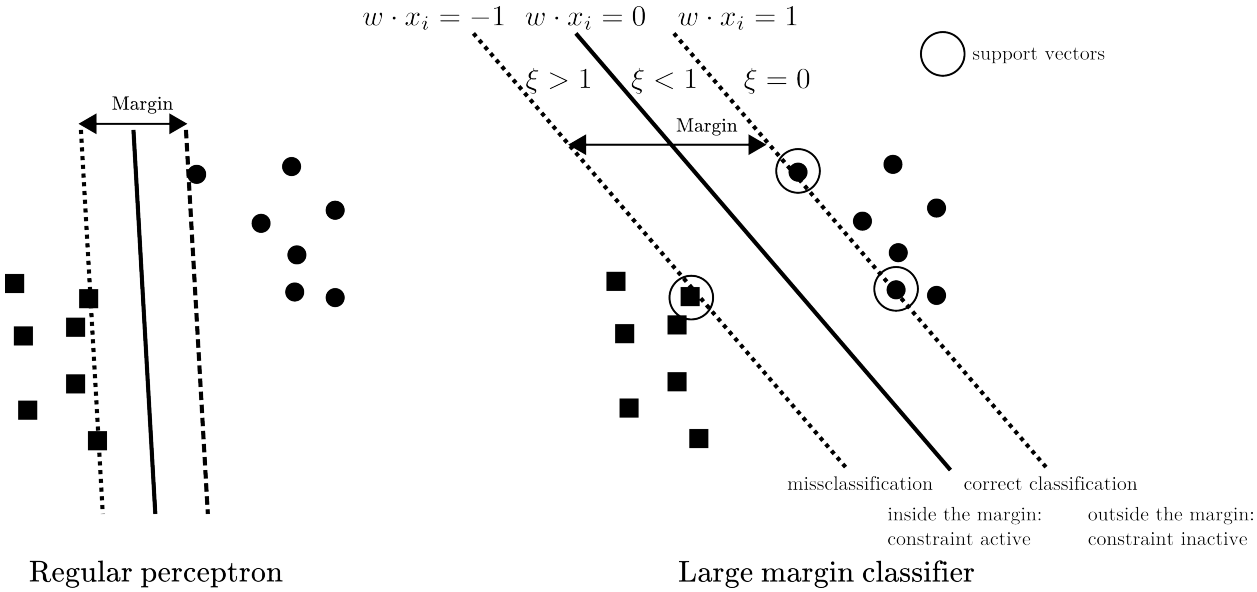


Fig. 11.5: Linear lar margin classifiers

Linear SVM for classification (also called SVM-C or SVC) minimizes:

$$\begin{array}{lll} \min & \text{Linear SVM}(\boldsymbol{w}) & = \text{penalty}(w) + C\ \text{Hinge loss}(w) \\ & & = \|w\|_2 + C\ \sum_i^N \xi_i \\ \text{with} & \forall i & y_i(w \cdot \boldsymbol{x_i}) \geq 1 - \xi_i \end{array}$$

Here we introduced the slack variables: ξ_i, with $\xi_i = 0$ for points that are on or inside the correct margin boundary and $\xi_i = |y_i - (w\ cdot \cdot \boldsymbol{x_i})|$ for other points. Thus:

1. If $y_i(w \cdot \boldsymbol{x_i}) \geq 1$ 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 $1 > y_i(w \cdot \boldsymbol{x_i}) \geq 0$ 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 $0 < y_i(w \cdot \boldsymbol{x_i}))$ 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:

$$\max(0, 1 - y_i\ (w \cdot \boldsymbol{x_i}))$$

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)
y_pred_svmlin = svmlin.predict(X)

errors =  y_pred_svmlin != y
print("Nb errors=%i, error rate=%.2f" % (errors.sum(), errors.sum() / len(y_pred_
↪svmlin)))
print(svmlin.coef_)
```

```
Nb errors=26, error rate=0.26
[[-0.05611026  0.31189817  0.00272904 -0.05149528  0.0994013   0.17726815
   0.06520128  0.08921178  0.35339409  0.00601206 -0.06200898 -0.00741242
  -0.02156839  0.1827221  -0.02163261 -0.04060274  0.07204827  0.13083533
   0.23722076  0.00823331]]
```

Lasso linear Support Vector Machine (L1-regularization)

Linear SVM for classification (also called SVM-C or SVC) with l1-regularization

$$\begin{array}{ll} \min & F_{\text{Lasso linear SVM}}(w) = \lambda\,||w||_1 + C\,\sum_i^N \xi_i \\ \text{with} & \forall i \qquad\qquad\quad y_i(w \cdot \boldsymbol{x_i}) \geq 1 - \xi_i \end{array}$$

```
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=%.2f" % (errors.sum(), errors.sum() / len(y_pred_
↪svmlinl1)))
print(svmlinl1.coef_)
```

```
Nb errors=26, error rate=0.26
[[-0.05333774  0.29934019  0.         -0.03541597  0.09261431  0.16763056
   0.05807924  0.07587815  0.34065253  0.         -0.05559017 -0.00194111
  -0.01312278  0.16866252 -0.01450365 -0.02500341  0.06073941  0.11739257
   0.22485376  0.00473435]]
```

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 their 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.

Elastic-net classification (L2-L1-regularization)

The **objective function** to be minimized is now the combination of the logistic loss $\log L(\boldsymbol{w})$ or the hinge loss with combination of L1 and L2 penalties. In the two-class case, using the 0/1 coding we obtain:

$$\min \text{ Logistic enet}(\boldsymbol{w}) = \log L(\boldsymbol{w}) + \alpha \left(\rho \|\boldsymbol{w}\|_1 + (1-\rho) \|\boldsymbol{w}\|_2^2\right) \tag{11.16}$$

$$\min \text{ Hinge enet}(\boldsymbol{w}) = \text{Hinge loss}(\boldsymbol{w}) + \alpha \left(\rho \|\boldsymbol{w}\|_1 + (1-\rho) \|\boldsymbol{w}\|_2^2\right) \tag{11.17}$$

```
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)
```

```
SGDClassifier(alpha=0.0001, average=False, class_weight='balanced',
       epsilon=0.1, eta0=0.0, fit_intercept=True, l1_ratio=0.15,
       learning_rate='optimal', loss='hinge', n_iter=5, n_jobs=1,
       penalty='elasticnet', power_t=0.5, random_state=None, shuffle=True,
       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.

Metrics of classification performance evaluation

Metrics for binary classification

source: 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):

  ACC = (TP + TN) / (TP + FP + FN + TN)
- **Sensitivity** (SEN) or **recall** of the positive class or true positive rate (TPR) or hit rate:

  SEN = TP / P = TP / (TP+FN)
- **Specificity** (SPC) or **recall** of the negative class or true negative rate:

  SPC = TN / N = TN / (TN+FP)
- **Precision** or positive predictive value (PPV):

  PPV = TP / (TP + 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 usefull to deal with imballaced datasets

The four outcomes can be formulated in a 2×2 contingency table or confusion matrix https://en.wikipedia.org/wiki/Sensitivity_and_specificity

For more precision see: 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 an 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 an recall on each individual class
p, r, f, s = metrics.precision_recall_fscore_support(y_true, y_pred)
```

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.

```
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 0]
Recalls: [ 1.  0.]
AUC: 1.0
```

```
/usr/local/anaconda3/lib/python3.5/site-packages/sklearn/metrics/classification.py:
↪1113: 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)
```

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 `clas\boldsymbol{S_W}eight` 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.rint(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, clas\boldsymbol{S_W}eight=
↪"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')
```

```
  File "<ipython-input-34-2de881c6d3f4>", line 43
    lr_inter_reweight = linear_model.LogisticRegression(C=1, clas\boldsymbol{S_W}
↪eight="balanced")
                                                                                ␣
↪             ^
SyntaxError: unexpected character after line continuation character
```

CHAPTER

TWELVE

NON LINEAR LEARNING ALGORITHMS

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 α_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.

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:

$$K(x_i, x_j) = \exp\left(-\frac{\|x_i - x_j\|^2}{2\sigma^2}\right) \tag{12.1}$$

$$= \exp\left(-\gamma \, \|x_i - x_j\|^2\right) \tag{12.2}$$

Where σ (or γ) 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.

```
import numpy as np
from sklearn.svm import SVC
from sklearn import datasets
```

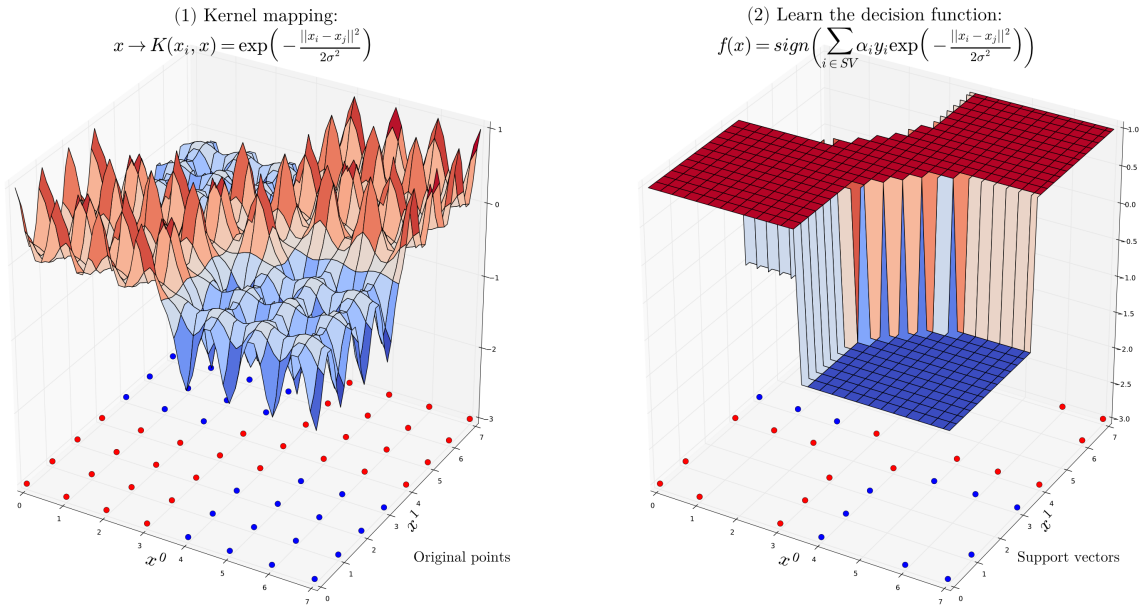


Fig. 12.1: Support Vector Machines.

```
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)

# Usefull internals:
# Array of support vectors
clf.support_vectors_

# indices of support vectors within original X
np.all(X[clf.support_,:] == clf.support_vectors_)
```

```
#Errors: 0
```

```
True
```

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.

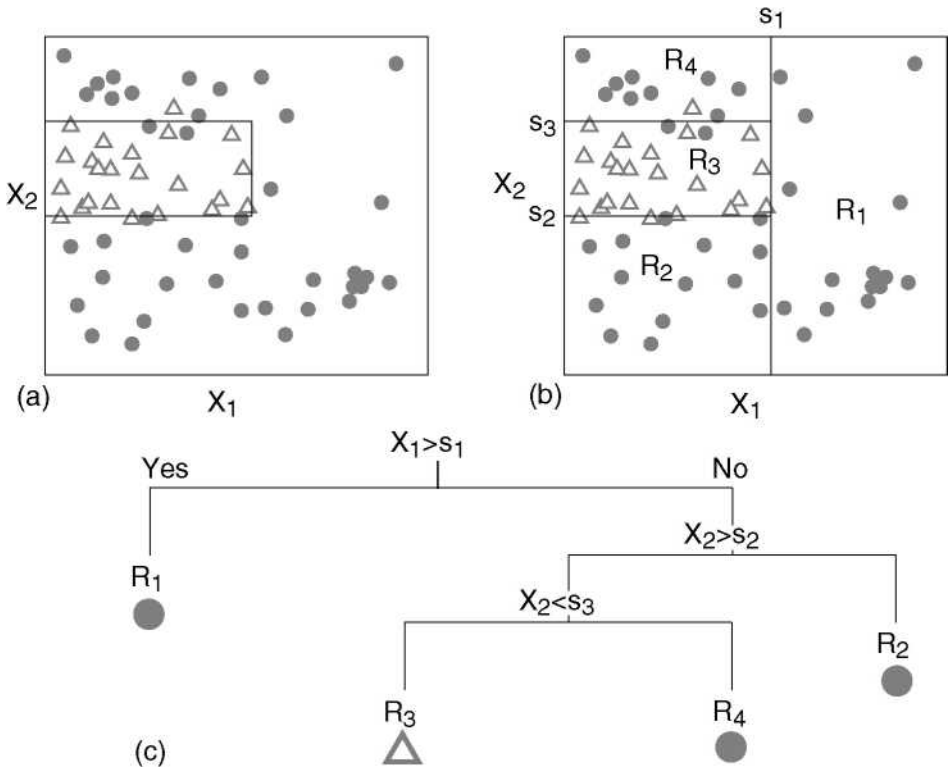


Fig. 12.2: Classification tree.

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)

print("#Errors: %i" % np.sum(y != forest.predict(X)))
```

CHAPTER

THIRTEEN

RESAMPLING METHODS

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.

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: $(f(X_{-K}, y_{-K}))$.

The mean error measure (generally a loss function) is evaluated of the on the observations in the held-out fold. For each sample i we consider the model estimated on the data set that did not contain it, 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 $(f(X_{-K(i)}) = \hat{y_i})$ with true value y_i using a Error function $L()$. Then the cross validation estimate of prediction error is

$$CV(f) = \frac{1}{N} \sum_{i}^{N} L\left(y_i, f(X_{-K(i)})\right).$$

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 $L()$ is the r-squared score. 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.cross_validation 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(len(y), n_folds=5, random_state=42)
y_test_pred = np.zeros(len(y))
y_train_pred = np.zeros(len(y))

for train, test in cv:
    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))
```

```
Train r2:0.99
Test  r2:0.72
```

Scikit-learn provides user-friendly function to perform CV:

```
from sklearn.cross_validation 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
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` with 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.cross_validation import StratifiedKFold

X, y = datasets.make_classification(n_samples=100, n_features=100,
                                n_informative=10, random_state=42)
```

```
model = lm.LogisticRegression(C=1)

cv = StratifiedKFold(y, n_folds=5)
y_test_pred = np.zeros(len(y))
y_train_pred = np.zeros(len(y))

for train, test in cv:
    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:0.80; SEN:0.82
Test  ACC:0.81
```

Scikit-learn provides user-friendly function to perform CV:

```
from sklearn.cross_validation 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):
    '''
    Balanced acuracy scorer
    '''
    return metrics.recall_score(y, estimator.predict(X), average=None).mean()

scores = cross_val_score(estimator=model, X=X, y=y, cv=cv, scoring=balanced_acc)
print("Test  ACC:%.2f" % scores.mean())
```

```
Test  ACC:0.81
```

Note that with Scikit-learn user-friendly function we average the scores' average obtained on individual folds which may provide slightly different results that the overall average presented earlier.

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 α_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 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.grid_search import GridSearchCV
import sklearn.metrics as metrics
from sklearn.cross_validation 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]}


# Warp
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(len(y), n_folds=5, random_state=42)
y_test_pred = np.zeros(len(y))
y_train_pred = np.zeros(len(y))
alphas = list()

for train, test in cv:
    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.cross_validation import cross_val_score
scores = cross_val_score(estimator=model, X=X, y=y, cv=cv)
print("Test  r2:%.2f" % scores.mean())
```

```
SNR: 2.63584694464
Train r2:0.96
{'l1_ratio': 0.9, 'alpha': 1.0}
Train r2:1.00
Test  r2:0.62
Selected alphas: [{'l1_ratio': 0.9, '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}]
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.cross_validation 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()
# 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)
# 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())

print("== ElasticNet (L1 penalty) ==")
model = lm.ElasticNetCV(l1_ratio=[.1, .5, .9], n_jobs=-1)
# 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  r2:0.23
== Lasso (L1 penalty) ==
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.cross_validation import cross_val_score

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):
    '''
    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)
# 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) ==
Test  ACC:0.77
```

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}.

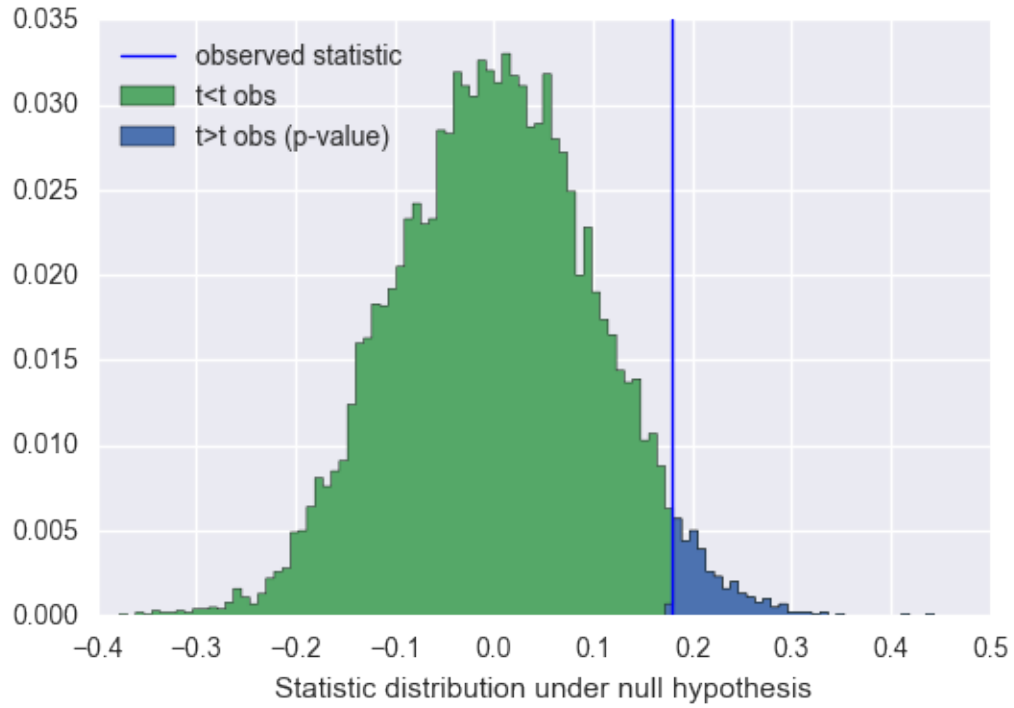
Example with a correlation

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, pval_test))
```

```
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.

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 using the 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, 0.01])

print("r-squared: Mean=%.2f, SE=%.2f, CI=(%.2f %.2f)" %\
      tuple(scores_stat.ix[["mean", "std", "5%", "95%"], "r2"]))

coefs_boot = pd.DataFrame(coefs_boot)
coefs_stat = coefs_boot.describe(percentiles=[.99, .95, .5, .1, .05, 0.01])
print("Coefficients distribution")
print(coefs_stat)
```

```
Coefficients on all data:
[ 0.98143428  0.84248041  0.12029217  0.09319979  0.08717254]
r-squared: Mean=0.57, SE=0.09, CI=(0.39 0.70)
Coefficients distribution
                0           1           2           3           4
count  100.000000  100.000000  100.000000  100.000000  100.000000
mean     0.975189    0.831922    0.116888    0.099109    0.085516
std      0.106367    0.096548    0.108676    0.090312    0.091446
min      0.745082    0.593736   -0.112740   -0.126522   -0.141713
1%       0.770362    0.640142   -0.088238   -0.094403   -0.113375
5%       0.787463    0.657473   -0.045593   -0.046201   -0.090458
10%      0.829129    0.706492   -0.037838   -0.020650   -0.044990
50%      0.980603    0.835724    0.133070    0.093240    0.088968
95%      1.127518    0.999604    0.278735    0.251137    0.221887
99%      1.144834    1.036715    0.292784    0.291197    0.287006
max      1.146670    1.077265    0.324374    0.298135    0.289569
```

CHAPTER

FOURTEEN

SCIKIT-LEARN PROCESSING PIPELINES

Data preprocessing

Sources: http://www.faqs.org/faqs/ai-faq/neural-nets/part2/section-16.html

Encoding categorical features

To be done

```
import pandas as pd

pd.get_dummies(['A', 'B', 'C', 'A', 'B', 'D'])
```

Standardization of input features

Sources:

- http://scikit-learn.org/stable/modules/preprocessing.html
- http://stats.stackexchange.com/questions/111017/question-about-standardizing-in-ridge-regression

"Standardizing" or mean removal and variance scaling, is not systematic. For example multiple linear regression does not require it. However it is a good practice in many cases:

- The **variable combination method is sensitive scales**. If the input variables are combined via a distance function (such as Euclidean distance) in an RBF network, standardizing inputs can be crucial. The contribution of an input will depend heavily on its variability relative to other inputs. If one input has a range of 0 to 1, while another input has a range of 0 to 1,000,000, then the contribution of the first input to the distance will be swamped by the second input.
- **Regularized learning algorithm**. Lasso or Ridge regression regularize the linear regression by imposing a penalty on the size of coefficients. Thus the coefficients are shrunk toward zero and toward each other. But when this happens and if the independent variables does not have the same scale, the shrinking is not fair. Two independent variables with different scales will have different contributions to the penalized terms, because the penalized term is norm (a sum of squares, or absolute values) of all the coefficients. To avoid such kind of problems, very often, the independent variables are centered and scaled in order to have variance 1.

```
import numpy as np

# dataset
np.random.seed(42)
n_samples, n_features, n_features_info = 100, 5, 3
```

```
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

X[:, 0] *= 1e6  # inflate the first feature
X[:, 1] += 1e6  # bias the second feature
y = 100 * y + 1000  # bias and scale the output

import sklearn.linear_model as lm
from sklearn import preprocessing
from sklearn.cross_validation import cross_val_score

print("== Linear regression: scaling is not required ==")
model =lm.LinearRegression()
model.fit(X, y)
print("Coefficients:", model.coef_, model.intercept_)
print("Test R2:%.2f" % cross_val_score(estimator=model, X=X, y=y, cv=5).mean())

print("== Lasso without scaling ==")
model = lm.LassoCV()
model.fit(X, y)
print("Coefficients:", model.coef_, model.intercept_)
print("Test R2:%.2f" % cross_val_score(estimator=model, X=X, y=y, cv=5).mean())

print("== Lasso with scaling ==")
model = lm.LassoCV()
scaler = preprocessing.StandardScaler()
Xc = scaler.fit(X).transform(X)
model.fit(Xc, y)
print("Coefficients:", model.coef_, model.intercept_)
print("Test R2:%.2f" % cross_val_score(estimator=model, X=Xc, y=y, cv=5).mean())
```

```
== Linear regression: scaling is not required ==
Coefficients: [  1.05421281e-04   1.13551103e+02   9.78705905e+01   1.60747221e+01
  -7.23145329e-01] -113550117.827
Test R2:0.77
== Lasso without scaling ==
Coefficients: [  8.61125764e-05   0.00000000e+00   0.00000000e+00   0.00000000e+00
   0.00000000e+00] 986.15608907
Test R2:0.09
== Lasso with scaling ==
Coefficients: [  87.46834069  105.13635448   91.22718731    9.22953206   -0.        ]␣
↪982.302793647
Test R2:0.77
```

Scikit-learn pipelines

Sources: http://scikit-learn.org/stable/modules/pipeline.html

Note that statistics such as the mean and standard deviation are computed from the training data, not from the validation or test data. The validation and test data must be standardized using the statistics computed from the training data. Thus Standardization should be merged together with the learner using a `Pipeline`.

Pipeline chain multiple estimators into one. All estimators in a pipeline, except the last one, must have the `fit()` and `transform()` methods. The last must implement the `fit()` and `predict()` methods.

Standardization of input features

```
from sklearn import preprocessing
import sklearn.linear_model as lm

from sklearn.pipeline import make_pipeline
model = make_pipeline(preprocessing.StandardScaler(), lm.LassoCV())

# or
from sklearn.pipeline import Pipeline
model = Pipeline([('standardscaler', preprocessing.StandardScaler()),
                  ('lassocv', lm.LassoCV())])

scores = cross_val_score(estimator=model, X=X, y=y, cv=5)
print("Test  r2:%.2f" % scores.mean())
```

```
Test  r2:0.77
```

Features selection

An alternative to features selection based on ℓ_1 penalty is to use a preprocessing stp of univariate feature selection.

Such methods, called **filters**, are a simple, widely used method for supervised dimension reduction [26]. Filters are univariate methods that rank features according to their ability to predict the target, independently of other features. This ranking may be based on parametric (e.g., t-tests) or nonparametric (e.g., Wilcoxon tests) statistical methods. Filters are computationally efficient and more robust to overfitting than multivariate methods. However, they are blind to feature interrelations, a problem that can be addressed only with multivariate selection such as learning with ℓ_1 penalty.

```
import numpy as np
import sklearn.linear_model as lm
from sklearn import preprocessing
from sklearn.cross_validation import cross_val_score
from sklearn.feature_selection import SelectKBest
from sklearn.feature_selection import f_regression
from sklearn.pipeline import Pipeline

np.random.seed(42)
n_samples, n_features, n_features_info = 100, 100, 3
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

X[:, 0] *= 1e6  # inflate the first feature
X[:, 1] += 1e6  # bias the second feature
y = 100 * y + 1000  # bias and scale the output

model = Pipeline([('anova', SelectKBest(f_regression, k=3)),
                  ('lm', lm.LinearRegression())])
```

```
scores = cross_val_score(estimator=model, X=X, y=y, cv=5)
print("Anova filter + linear regression, test  r2:%.2f" % scores.mean())

from sklearn.pipeline import Pipeline
model = Pipeline([('standardscaler', preprocessing.StandardScaler()),
                  ('lassocv', lm.LassoCV())])
scores = cross_val_score(estimator=model, X=X, y=y, cv=5)
print("Standardize + Lasso, test  r2:%.2f" % scores.mean())
```

```
Anova filter + linear regression, test  r2:0.72
Standardize + Lasso, test  r2:0.66
```

Regression pipelines with CV for parameters selection

Now we combine standardization of input features, feature selection and learner with hyper-parameter within a pipeline which is warped in a grid search procedure to select the best hyperparameters based on a (inner)CV. The overall is plugged in an outer CV.

```
import numpy as np
from sklearn import datasets
import sklearn.linear_model as lm
from sklearn import preprocessing
from sklearn.cross_validation import cross_val_score
from sklearn.feature_selection import SelectKBest
from sklearn.feature_selection import f_regression
from sklearn.pipeline import Pipeline
from sklearn.grid_search import GridSearchCV
import sklearn.metrics as metrics

# Datasets
n_samples, n_features, noise_sd = 100, 100, 20
X, y, coef = datasets.make_regression(n_samples=n_samples, n_features=n_features,
                                      noise=noise_sd, n_informative=5,
                                      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)

print("================================")
print("== Basic linear regression ==")
print("================================")

scores = cross_val_score(estimator=lm.LinearRegression(), X=X, y=y, cv=5)
print("Test  r2:%.2f" % scores.mean())

print("================================================")
print("== Scaler + anova filter + ridge regression ==")
print("================================================")

anova_ridge = Pipeline([
    ('standardscaler', preprocessing.StandardScaler()),
    ('selectkbest', SelectKBest(f_regression)),
    ('ridge', lm.Ridge())
])
param_grid = {'selectkbest__k':np.arange(10, 110, 10),
```

```
              'ridge__alpha':[.001, .01, .1, 1, 10, 100] }

# Expect execution in ipython, for python remove the %time
print("----------------------------")
print("-- Parallelize inner loop --")
print("----------------------------")

anova_ridge_cv = GridSearchCV(anova_ridge, cv=5,  param_grid=param_grid, n_jobs=-1)
%time scores = cross_val_score(estimator=anova_ridge_cv, X=X, y=y, cv=5)
print("Test r2:%.2f" % scores.mean())

print("----------------------------")
print("-- Parallelize outer loop --")
print("----------------------------")

anova_ridge_cv = GridSearchCV(anova_ridge, cv=5,  param_grid=param_grid)
%time scores = cross_val_score(estimator=anova_ridge_cv, X=X, y=y, cv=5, n_jobs=-1)
print("Test r2:%.2f" % scores.mean())


print("====================================")
print("== Scaler + Elastic-net regression ==")
print("====================================")

alphas = [.0001, .001, .01, .1, 1, 10, 100, 1000]
l1_ratio = [.1, .5, .9]

print("----------------------------")
print("-- Parallelize outer loop --")
print("----------------------------")

enet = Pipeline([
    ('standardscaler', preprocessing.StandardScaler()),
    ('enet', lm.ElasticNet(max_iter=10000)),
])
param_grid = {'enet__alpha':alphas ,
              'enet__l1_ratio':l1_ratio}
enet_cv = GridSearchCV(enet, cv=5,  param_grid=param_grid)
%time scores = cross_val_score(estimator=enet_cv, X=X, y=y, cv=5, n_jobs=-1)
print("Test r2:%.2f" % scores.mean())

print("-----------------------------------------------")
print("-- Parallelize outer loop + built-in CV      --")
print("-- Remark: scaler is only done on outer loop --")
print("-----------------------------------------------")

enet_cv = Pipeline([
    ('standardscaler', preprocessing.StandardScaler()),
    ('enet', lm.ElasticNetCV(max_iter=10000, l1_ratio=l1_ratio, alphas=alphas)),
])

%time scores = cross_val_score(estimator=enet_cv, X=X, y=y, cv=5)
print("Test r2:%.2f" % scores.mean())
```

```
SNR: 3.28668201676
============================
== Basic linear regression ==
============================
```

```
Test  r2:0.29
============================================
== Scaler + anova filter + ridge regression ==
============================================
----------------------------
-- Parallelize inner loop --
----------------------------
CPU times: user 6.06 s, sys: 836 ms, total: 6.9 s
Wall time: 7.97 s
Test r2:0.86
----------------------------
-- Parallelize outer loop --
----------------------------
CPU times: user 270 ms, sys: 129 ms, total: 399 ms
Wall time: 3.51 s
Test r2:0.86
====================================
== Scaler + Elastic-net regression ==
====================================
----------------------------
-- Parallelize outer loop --
----------------------------
CPU times: user 44.4 ms, sys: 80.5 ms, total: 125 ms
Wall time: 1.43 s
Test r2:0.82
------------------------------------------------
-- Parallelize outer loop + built-in CV      --
-- Remark: scaler is only done on outer loop --
------------------------------------------------
CPU times: user 227 ms, sys: 0 ns, total: 227 ms
Wall time: 225 ms
Test r2:0.82
```

Classification pipelines with CV for parameters selection

Now we combine standardization of input features, feature selection and learner with hyper-parameter within a pipeline which is warped in a grid search procedure to select the best hyperparameters based on a (inner)CV. The overall is plugged in an outer CV.

```
import numpy as np
from sklearn import datasets
import sklearn.linear_model as lm
from sklearn import preprocessing
from sklearn.cross_validation import cross_val_score
from sklearn.feature_selection import SelectKBest
from sklearn.feature_selection import f_classif
from sklearn.pipeline import Pipeline
from sklearn.grid_search import GridSearchCV
import sklearn.metrics as metrics

# Datasets
n_samples, n_features, noise_sd = 100, 100, 20
X, y = datasets.make_classification(n_samples=n_samples, n_features=n_features,
                           n_informative=5, random_state=42)
```

```
def balanced_acc(estimator, X, y):
    '''
    Balanced acuracy scorer
    '''
    return metrics.recall_score(y, estimator.predict(X), average=None).mean()

print("============================")
print("== Basic logistic regression ==")
print("============================")

scores = cross_val_score(estimator=lm.LogisticRegression(C=1e8, class_weight='balanced
↪'),
                         X=X, y=y, cv=5, scoring=balanced_acc)
print("Test  bACC:%.2f" % scores.mean())

print("=========================================================")
print("== Scaler + anova filter + ridge logistic regression ==")
print("=========================================================")

anova_ridge = Pipeline([
    ('standardscaler', preprocessing.StandardScaler()),
    ('selectkbest', SelectKBest(f_classif)),
    ('ridge', lm.LogisticRegression(penalty='l2', class_weight='balanced'))
])
param_grid = {'selectkbest__k':np.arange(10, 110, 10),
              'ridge__C':[.0001, .001, .01, .1, 1, 10, 100, 1000, 10000]}


# Expect execution in ipython, for python remove the %time
print("----------------------------")
print("-- Parallelize inner loop --")
print("----------------------------")

anova_ridge_cv = GridSearchCV(anova_ridge, cv=5,  param_grid=param_grid,
                              scoring=balanced_acc, n_jobs=-1)
%time scores = cross_val_score(estimator=anova_ridge_cv, X=X, y=y, cv=5,\
                               scoring=balanced_acc)
print("Test bACC:%.2f" % scores.mean())

print("----------------------------")
print("-- Parallelize outer loop --")
print("----------------------------")

anova_ridge_cv = GridSearchCV(anova_ridge, cv=5,  param_grid=param_grid,
                              scoring=balanced_acc)
%time scores = cross_val_score(estimator=anova_ridge_cv, X=X, y=y, cv=5,\
                               scoring=balanced_acc, n_jobs=-1)
print("Test bACC:%.2f" % scores.mean())


print("========================================")
print("== Scaler + lasso logistic regression ==")
print("========================================")

Cs = np.array([.0001, .001, .01, .1, 1, 10, 100, 1000, 10000])
alphas = 1 / Cs
l1_ratio = [.1, .5, .9]
```

```
print("----------------------------")
print("-- Parallelize outer loop --")
print("----------------------------")

lasso = Pipeline([
    ('standardscaler', preprocessing.StandardScaler()),
    ('lasso', lm.LogisticRegression(penalty='l1', class_weight='balanced')),
])
param_grid = {'lasso__C':Cs}
enet_cv = GridSearchCV(lasso, cv=5,  param_grid=param_grid, scoring=balanced_acc)
%time scores = cross_val_score(estimator=enet_cv, X=X, y=y, cv=5,\
                               scoring=balanced_acc, n_jobs=-1)
print("Test bACC:%.2f" % scores.mean())


print("-----------------------------------------------")
print("-- Parallelize outer loop + built-in CV      --")
print("-- Remark: scaler is only done on outer loop --")
print("-----------------------------------------------")

lasso_cv = Pipeline([
    ('standardscaler', preprocessing.StandardScaler()),
    ('lasso', lm.LogisticRegressionCV(Cs=Cs, scoring=balanced_acc)),
])

%time scores = cross_val_score(estimator=lasso_cv, X=X, y=y, cv=5)
print("Test bACC:%.2f" % scores.mean())


print("=============================================")
print("== Scaler + Elasticnet logistic regression ==")
print("=============================================")

print("----------------------------")
print("-- Parallelize outer loop --")
print("----------------------------")

enet = Pipeline([
    ('standardscaler', preprocessing.StandardScaler()),
    ('enet', lm.SGDClassifier(loss="log", penalty="elasticnet",
                              alpha=0.0001, l1_ratio=0.15, class_weight='balanced')),
])

param_grid = {'enet__alpha':alphas,
              'enet__l1_ratio':l1_ratio}

enet_cv = GridSearchCV(enet, cv=5,  param_grid=param_grid, scoring=balanced_acc)
%time scores = cross_val_score(estimator=enet_cv, X=X, y=y, cv=5,\
    scoring=balanced_acc, n_jobs=-1)
print("Test bACC:%.2f" % scores.mean())
```

```
============================
== Basic logistic regression ==
============================
Test  bACC:0.52
=====================================================
== Scaler + anova filter + ridge logistic regression ==
```

```
=====================================================
----------------------------
-- Parallelize inner loop --
----------------------------
CPU times: user 3.02 s, sys: 562 ms, total: 3.58 s
Wall time: 4.43 s
Test bACC:0.67
----------------------------
-- Parallelize outer loop --
----------------------------
CPU times: user 59.3 ms, sys: 114 ms, total: 174 ms
Wall time: 1.88 s
Test bACC:0.67
=======================================
== Scaler + lasso logistic regression ==
=======================================
----------------------------
-- Parallelize outer loop --
----------------------------
CPU times: user 81 ms, sys: 96.7 ms, total: 178 ms
Wall time: 484 ms
Test bACC:0.57
-----------------------------------------------
-- Parallelize outer loop + built-in CV      --
-- Remark: scaler is only done on outer loop --
-----------------------------------------------
CPU times: user 575 ms, sys: 3.01 ms, total: 578 ms
Wall time: 327 ms
Test bACC:0.60
=============================================
== Scaler + Elasticnet logistic regression ==
=============================================
----------------------------
-- Parallelize outer loop --
----------------------------
CPU times: user 429 ms, sys: 100 ms, total: 530 ms
Wall time: 979 ms
Test bACC:0.61
```

CHAPTER

FIFTEEN

CASE STUDIES OF ML

Default of credit card clients Data Set

Sources:

http://archive.ics.uci.edu/ml/datasets/default+of+credit+card+clients Yeh, I. C., & Lien, C. H. (2009). The comparisons of data mining techniques for the predictive accuracy of probability of default of credit card clients. Expert Systems with Applications, 36(2), 2473-2480.

Data Set Information:

This research aimed at the case of customers default payments in Taiwan.

Attribute Information:

This research employed a binary variable, default payment (Yes = 1, No = 0), as the response variable. This study reviewed the literature and used the following 23 variables as explanatory variables:

- X1: Amount of the given credit (NT dollar): it includes both the individual consumer credit and his/her family (supplementary) credit.
- X2: Gender (1 = male; 2 = female).
- X3: Education (1 = graduate school; 2 = university; 3 = high school; 4 = others).
- X4: Marital status (1 = married; 2 = single; 3 = others).
- X5: Age (year).
- X6 - X11: History of past payment. We tracked the past monthly payment records (from April to September, 2005) as follows: X6 = the repayment status in September, 2005; X7 = the repayment status in August, 2005;...;X11 = the repayment status in April, 2005. The measurement scale for the repayment status is: -1 = pay duly; 1 = payment delay for one month; 2 = payment delay for two months;...; 8 = payment delay for eight months; 9 = payment delay for nine months and above.
- X12-X17: Amount of bill statement (NT dollar). X12 = amount of bill statement in September, 2005; X13 = amount of bill statement in August, 2005;...; X17 = amount of bill statement in April, 2005.
- X18-X23: Amount of previous payment (NT dollar). X18 = amount paid in September, 2005; X19 = amount paid in August, 2005;...;X23 = amount paid in April, 2005.

Read dataset

```
from __future__ import print_function

import pandas as pd
import numpy as np

url = 'https://raw.github.com/neurospin/pystatsml/master/data/default%20of%20credit
↪%20card%20clients.xls'
data = pd.read_excel(url, skiprows=1, sheetname='Data')

df = data.copy()
target = 'default payment next month'
print(df.columns)

#Index(['ID', 'LIMIT_BAL', 'SEX', 'EDUCATION', 'MARRIAGE', 'AGE', 'PAY_0',
#       'PAY_2', 'PAY_3', 'PAY_4', 'PAY_5', 'PAY_6', 'BILL_AMT1', 'BILL_AMT2',
#       'BILL_AMT3', 'BILL_AMT4', 'BILL_AMT5', 'BILL_AMT6', 'PAY_AMT1',
#       'PAY_AMT2', 'PAY_AMT3', 'PAY_AMT4', 'PAY_AMT5', 'PAY_AMT6',
#       'default payment next month'],
#      dtype='object')
```

Data recoding of categorial factors

- Categorial factors with 2 levels are kept
- Categorial that are ordinal are kept
- Undocumented values are replaced with NaN

Missing data

```
print(df.isnull().sum())
#ID                             0
#LIMIT_BAL                      0
#SEX                            0
#EDUCATION                    468
#MARRIAGE                     377
#AGE                            0
#PAY_0                          0
#PAY_2                          0
#PAY_3                          0
#PAY_4                          0
#PAY_5                          0
#PAY_6                          0
#BILL_AMT1                      0
#BILL_AMT2                      0
#BILL_AMT3                      0
#BILL_AMT4                      0
#BILL_AMT5                      0
#BILL_AMT6                      0
#PAY_AMT1                       0
#PAY_AMT2                       0
#PAY_AMT3                       0
#PAY_AMT4                       0
```

```
#PAY_AMT5                          0
#PAY_AMT6                          0
#default payment next month        0
#dtype: int64

df.ix[df["EDUCATION"].isnull(), "EDUCATION"] = df["EDUCATION"].mean()
df.ix[df["MARRIAGE"].isnull(), "MARRIAGE"] = df["MARRIAGE"].mean()
print(df.isnull().sum().sum())
# 0

describe_factor(df[target])
{0: 23364, 1: 6636}
```

Prepare Data set

```
predictors = df.columns.drop(['ID', target])
X = np.asarray(df[predictors])
y = np.asarray(df[target])
```

Univariate analysis

Machine Learning with SVM

On this large dataset, we can afford to set aside some test samples. This will also save computation time. However we will have to do some manual work.

```
import numpy as np
from sklearn import datasets
import sklearn.svm as svm
from sklearn import preprocessing
from sklearn.cross_validation import cross_val_score, train_test_split
from sklearn.cross_validation import StratifiedKFold
from sklearn.feature_selection import SelectKBest
from sklearn.feature_selection import f_classif
from sklearn.pipeline import Pipeline
from sklearn.grid_search import GridSearchCV
import sklearn.metrics as metrics

def balanced_acc(estimator, X, y):
    return metrics.recall_score(y, estimator.predict(X), average=None).mean()

print("================================================")
print("== Put aside half of the samples as test set ==")
print("================================================")

Xtr, Xte, ytr, yte = train_test_split(X, y, test_size=0.5, random_state=0, stratify=y)

print("================================")
print("== Scale trainin and test data ==")
print("================================")

scaler = preprocessing.StandardScaler()
Xtrs = scaler.fit(Xtr).transform(Xtr)
Xtes = scaler.transform(Xte)
```

```
print("=========")
print("== SVM ==")
print("=========")

svc = svm.LinearSVC(class_weight='balanced', dual=False)
%time scores = cross_val_score(estimator=svc,\
                           X=Xtrs, y=ytr, cv=2, scoring=balanced_acc)
print("Validation bACC:%.2f" % scores.mean())
#CPU times: user 1.01 s, sys: 39.7 ms, total: 1.05 s
#Wall time: 112 ms
#Validation  bACC:0.67

svc_rbf = svm.SVC(kernel='rbf', class_weight='balanced')
%time scores = cross_val_score(estimator=svc_rbf,\
                           X=Xtrs, y=ytr, cv=2, scoring=balanced_acc)
print("Validation bACC:%.2f" % scores.mean())
#CPU times: user 10.2 s, sys: 136 ms, total: 10.3 s
#Wall time: 10.3 s
#Test  bACC:0.71

svc_lasso = svm.LinearSVC(class_weight='balanced', penalty='l1', dual=False)
%time scores = cross_val_score(estimator=svc_lasso,\
                           X=Xtrs, y=ytr, cv=2, scoring=balanced_acc)
print("Validation bACC:%.2f" % scores.mean())
#CPU times: user 4.51 s, sys: 168 ms, total: 4.68 s
#Wall time: 544 ms
#Test  bACC:0.67

print("========================")
print("== SVM CV Grid search ==")
print("========================")
Cs = [0.001, .01, .1, 1, 10, 100, 1000]
param_grid = {'C':Cs}

print("-------------------")
print("-- SVM Linear L2 --")
print("-------------------")

svc_cv = GridSearchCV(svc, cv=3,  param_grid=param_grid, scoring=balanced_acc,
                      n_jobs=-1)
# What are the best parameters ?
%time svc_cv.fit(Xtrs, ytr).best_params_
#CPU times: user 211 ms, sys: 209 ms, total: 421 ms
#Wall time: 1.07 s
#{'C': 0.01}
scores = cross_val_score(estimator=svc_cv,\
                           X=Xtrs, y=ytr, cv=2, scoring=balanced_acc)
print("Validation bACC:%.2f" % scores.mean())
#Validation bACC:0.67

print("-------------")
print("-- SVM RBF --")
print("-------------")

svc_rbf_cv = GridSearchCV(svc_rbf, cv=3,  param_grid=param_grid,
                          scoring=balanced_acc, n_jobs=-1)
# What are the best parameters ?
```

```
%time svc_rbf_cv.fit(Xtrs, ytr).best_params_
#Wall time: 1min 10s
#Out[6]: {'C': 1}

# reduce the grid search
svc_rbf_cv.param_grid={'C': [0.1, 1, 10]}
scores = cross_val_score(estimator=svc_rbf_cv,\
                         X=Xtrs, y=ytr, cv=2, scoring=balanced_acc)
print("Validation bACC:%.2f" % scores.mean())
#Validation bACC:0.71

print("--------------------")
print("-- SVM Linear L1 --")
print("--------------------")

svc_lasso_cv = GridSearchCV(svc_lasso, cv=3,  param_grid=param_grid,
                            scoring=balanced_acc, n_jobs=-1)
# What are the best parameters ?
%time svc_lasso_cv.fit(Xtrs, ytr).best_params_
#CPU times: user 514 ms, sys: 181 ms, total: 695 ms
#Wall time: 2.07 s
#Out[10]: {'C': 0.1}

# reduce the grid search
svc_lasso_cv.param_grid={'C': [0.1, 1, 10]}

scores = cross_val_score(estimator=svc_lasso_cv,\
                         X=Xtrs, y=ytr, cv=2, scoring=balanced_acc)
print("Validation bACC:%.2f" % scores.mean())
#Validation bACC:0.67



print("SVM-RBF, test bACC:%.2f" % balanced_acc(svc_rbf_cv, Xtes, yte))
# SVM-RBF, test bACC:0.70

print("SVM-Lasso, test bACC:%.2f" % balanced_acc(svc_lasso_cv, Xtes, yte))
# SVM-Lasso, test bACC:0.67
```

CHAPTER

SIXTEEN

INDICES AND TABLES

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