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 $E(\cdot)$ 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:

$$Cov(X, X) = Var(X)$$

$$Cov(X, Y) = Cov(Y, X)$$

$$Cov(cX, Y) = c Cov(X, Y)$$

$$Cov(X + c, Y) = Cov(X, Y)$$

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

- The squared standard $Z^2 \sim \chi_1^2$ (one df).
- The distribution of sum of squares of n normal random variables: $\sum_{i=1}^{n} Z_i^2 \sim \chi_n^2$

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

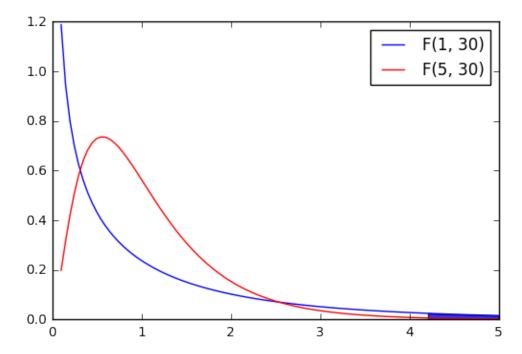
The F-distribution, $F_{n,p}$, with n and p degrees of freedom is the ratio of two independent χ^2 variables. Let $X \sim \chi_n^2$ and $Y \sim \chi_p^2$ then:

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

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

```
import numpy as np
from scipy.stats import f
import matplotlib.pyplot as plt
%matplotlib inline
fvalues = np.linspace(.1, 5, 100)
# pdf(x, df1, df2): Probability density function at x of F.
plt.plot(fvalues, f.pdf(fvalues, 1, 30), 'b-', label="F(1, 30)")
plt.plot(fvalues, f.pdf(fvalues, 5, 30), 'r-', label="F(5, 30)")
plt.legend()
# cdf(x, df1, df2): Cumulative distribution function of F.
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
```

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The Student's t-distribution

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

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

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

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}, σ_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:

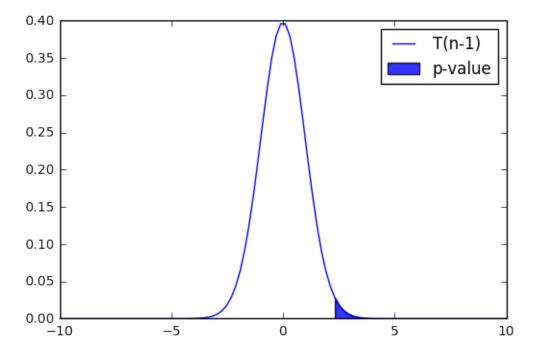
$$t = \frac{\bar{x} - \mu_0}{\sigma_x / \sqrt{n}}$$

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.



- 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 \sim 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:

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

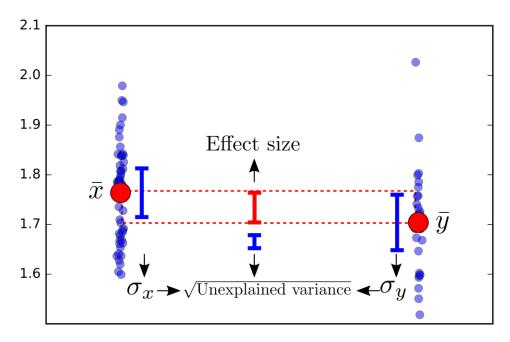


Fig. 6.1: title

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

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

The "unexplained variance", or "within-group variability" is

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

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)
```

Computing expected cross-table

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.

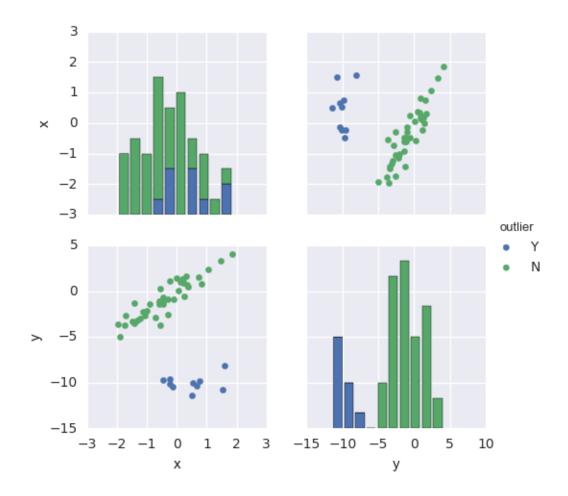
When to use it? Observe the data distribution: - presence of outliers - the distribution of the residuals is not Gaussian.

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

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

• 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.

salary_i =
$$\beta$$
 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 *i*th 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:

$$\frac{\partial SSE}{\partial \beta_0} = \sum_{i} (y_i - \beta x_i - \beta_0) = 0$$
$$\sum_{i} y_i = \beta \sum_{i} x_i + n \beta_0$$
$$n \bar{y} = n \beta \bar{x} + n \beta_0$$
$$\beta_0 = \bar{y} - \beta \bar{x}$$

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To find the regression coefficient, we perform the steps:

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

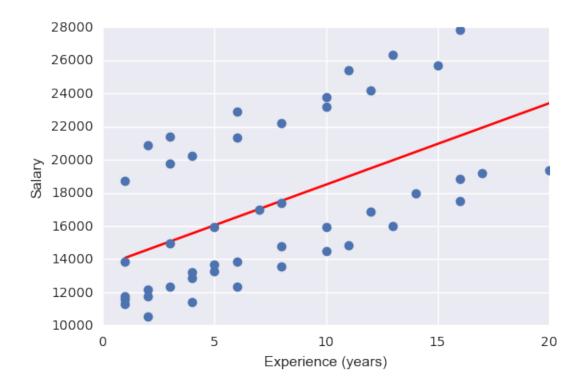
Plug in β_0 :

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

Divide both sides by n:

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

```
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 .

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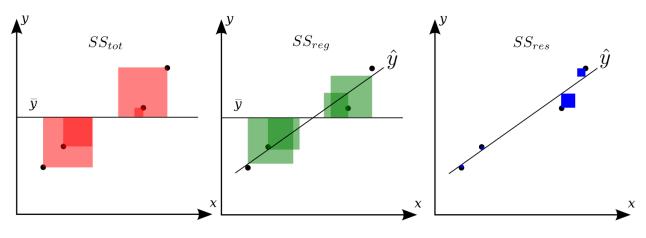


Fig. 6.2: title

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: $\frac{SS_{\mathrm{res}}}{\hat{\sigma}^2} \sim \chi^2_{n-2}$
- Explained variance: $\frac{SS_{\text{reg}}}{\hat{\sigma}^2} \sim \chi_1^2$. The single degree of freedom comes from the difference between $\frac{SS_{\text{test}}}{\hat{\sigma}^2} (\sim \chi_{n-1}^2)$ and $\frac{SS_{\text{res}}}{\hat{\sigma}^2} (\sim \chi_{n-2}^2)$, i.e. (n-1)-(n-2) degree of freedom.

The Fisher statistics of the ratio of two variances:

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

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

Multiple regression

Theory

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.

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

or, simplified

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

Extending each sample with an intercept, $x_i := [1, x_i] \in \mathbb{R}^{P+1}$ 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:

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

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

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

$$-2X^Ty + 2X^TX\beta = 0 ag{6.7}$$

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

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

where $(X^TX)^{-1}X^T$ 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)
```

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```
y = np.dot(X, betastar) + e

# Estimate the parameters

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

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
                              OLS Adj. R-squared:
Model:
                                                                    0.322
                Least Squares F-statistic:
                                                                    8.748
Method:
                  Sun, 15 Oct 2017 Prob (F-statistic):
                                                                0.000106
Date:
                    23:14:05 Log-Likelihood:
Time:
                                                                   -71.271
No. Observations:
                                50 AIC:
                                                                     150.5
                                 46
Df Residuals:
                                    BIC:
                                                                     158.2
Df Model:
Covariance Type:
                         nonrobust
_____
                                      t P>|t| [95.0% Conf. Int.]
               coef std err

    10.1474
    0.150
    67.520
    0.000
    9.845
    10.450

    0.5794
    0.160
    3.623
    0.001
    0.258
    0.901

    0.5165
    0.151
    3.425
    0.001
    0.213
    0.820

    0.1786
    0.144
    1.240
    0.221
    -0.111
    0.469

x1
x2.
x3
```

```
_____
                   2.493 Durbin-Watson:
Omnibus:
Prob(Omnibus):
                                           1.544
                   0.288 Jarque-Bera (JB):
                                           0.462
                  0.330 Prob(JB):
Skew:
                  3.554 Cond. No.
                                            1.27
Kurtosis:
______
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: $y_i = \beta^0 + x_i^1 \beta^1 + x_i^2 \beta^2 + \epsilon_i \equiv y \sim x1 + x2$.

```
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 K	egres:	sion Re: ======	su⊥∟S ========		
Dep. Variable	e:		У	R-squ	ared:		0.363
Model:		OLS		Adj. R-squared:			0.322
		Least Squ	ares	F-stat	tistic:	8.748	
Date: Sun, 15 Oct 2017		Prob (F-statistic):		0.000106			
Time:	23:14:05		4:05	Log-Likelihood:		-71.271	
No. Observations:		50		AIC:		150.5	
Df Residuals:		46		BIC:			158.2
Df Model:			3				
Covariance Ty	pe:	nonro	bust				
	coef	std err		t	P> t	[95.0% Con	f. Int.]
Intercept	10.1474	0.150	6'	7.520	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
х3	0.1786	0.144		1.240	0.221	-0.111	0.469
Omnibus:		2	.493	===== Durbiı	 n-Watson:		 2.369
Prob(Omnibus): 0.288		Jarque-Bera (JB):			1.544		
Skew:				_			0.462
Kurtosis:		3	3.554 Cond. No.				1.27

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
Method:
Date:

Sun, 15 Oct 2017 Prob (F-statistic):

Time:

No. Observations:

Df Residuals:

Df Model:

Cover in the same of 
                                                                                                                                                                                                                                                                                            0.865
                                                                                                                                                                                                                                                                                          0.859
                                                                                                                                                                                                                                                                                            138.2
                                                                                                                                                                                                                                                                        1.90e-19
                                                                                                                                                                                                                                                                                              827.0
   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
   _____
                                                                                                                        11.437 Durbin-Watson:
   Omnibus:
                                                                                                                        2.193
   Prob(Omnibus):
                                                                                                                     -1.131 Prob(JB):
   Kurtosis:
                                                                                                                             3.872 Cond. No.
   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:
Model:
Method:
Date:
                      OLS Adj. R-squared:
                                                   0.953
              Least Squares F-statistic:
                                                    226.8
             Sun, 15 Oct 2017 Prob (F-statistic): 23:14:05 Log-Likelihood:
                                                 2.23e-27
                                                  -381.63
                        46 AIC:
No. Observations:
                                                    773.3
Df Residuals:
                        41 BIC:
                                                    782.4
Df Model:
Covariance Type:
              nonrobust
______
                                t P>|t| [95.0% Conf. Int.
                  coef std err
\hookrightarrow
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.
\hookrightarrow 503
              546.1840 30.519 17.896 0.000
                                                 484.549 607.
experience
→819
______
                      2.293 Durbin-Watson:
Prob(Omnibus):
                      0.318 Jarque-Bera (JB):
                                                   1.362
                     -0.077 Prob(JB):
                                                   0.506
Skew:
                      2.171 Cond. No.
Kurtosis:
Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly...
⇔specified.
                        F PR(>F)
            sum_sq df
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.  1.  0.  0.  1.]

[ 1.  1.  0.  1.  2.]

[ 1.  1.  0.  0.  2.]

[ 1.  0.  1.  0.  2.]

[ 1.  0.  1.  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)

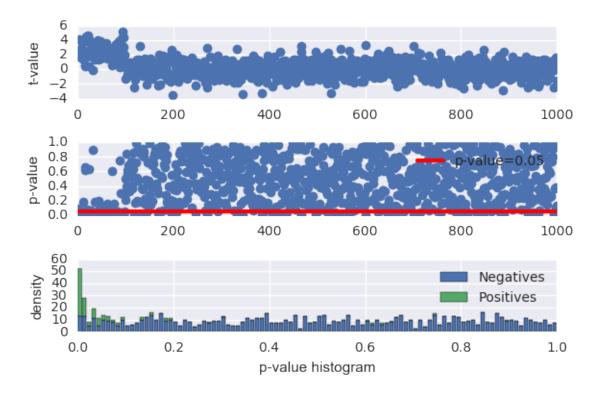
# Alternatively, you can specify the hypothesis tests using a string
twoway.t_test('experience')

# 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							
		std err	t	1 - 1				
c0	546.1840	30.519	17.896	0.000	484.549 607.819			
		Test f	or Constrai	nts				
	coef	std err	t	P> t				
c0	147.8249		0.381		-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))</pre>
```

```
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 $\alpha=0.05/8=0.00625$.

```
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.

```
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

6.8. Exercise 75