

Homework 1

Pattern Mining and Social Network Analysis

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Classification

Overall

Classification algorithms have categorical responses. In classification we build a function $f(X)$ that takes a vector of input variables X and predicts its class membership, such that Y in C .

Possibilities of models

There are classifiers as logistic regression, Decision tree, Perceptron / Neural networks, K-nearest-neighbors, linear and quadratic logistic regression, Bayes ...

Some indicators

Sensitivity and recall

The sensitivity (also named recall) is the percentage of true defaulters that are identified (True positive tests). For example, probability of predicting disease given true state is disease.

$$sensitivity = recall = \frac{TruePositiveTests}{PositivePopulation}$$

Specificity

The specificity is the percentage of non-defaulters that are correctly identified (True negative tests). 1 - specificity is the Type 1 error, it is the false positive rate. For example, probability of predicting non-disease given true state is non- disease.

$$specificity = \frac{TrueNegativeTests}{NegativePopulation}$$

Precision

The precision is the proportion of true positive tests among the positive tests.

$$precision = \frac{TruePositiveTests}{PositiveTests}$$

F-Mesure

The traditional F measure is calculated as follows:

$$F_{Measure} = \frac{(2 * Precision * Recall)}{(Precision + Recall)}$$

Rand index

The rand index is a mesure of similarity between two partitions from a single set.

Given two partitions π_1 and π_2 in E :

- a, the number of elements in π_1 and π_2
- b, the number of elements in π_1 and not in π_2
- c, the number of elements in π_2 and not in π_1
- d, the number of elements not in both π_1 and π_2

	in π_2	not in π_2
in π_1	a	b
not in π_1	c	d

$$RI(\pi_1, \pi_2) = \frac{a + d}{a + b + c + d}$$

Accuracy of a model

How do we determine which model is best? Various statistics can be used to judge the quality of a model. \ These include Mallows's C_p , Akaike information criterion (AIC), Bayesian information criterion (BIC), and adjusted R^2 .

Mallow's C_p

TO DO

If there are d predictors :

$$C_p = \frac{RSS + 2d\hat{\sigma}^2}{n}$$

AIC : Akaike information criterion

TO DO

$$AIC = \frac{RSS + 2d\hat{\sigma}^2}{n\hat{\sigma}^2}$$

BIC : Bayesian information criterion

TO DO

$$BIC = \frac{RSS + \log(n)d\hat{\sigma}^2}{n}$$

Adjusted R statistic

TO DO

$$Adjusted R^2 = 1 - \frac{\frac{RSS}{n-d-1}}{\frac{TSS}{n-1}}$$

Logistic Regression

How it works

In logistic regression, for covariates (X_1, \dots, X_p) , we want to estimate $p_i = P_r(Y_i = 1|X_1, \dots, X_p)$

$$p_i = \frac{e^{\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \beta_4 x_{i4} + \dots}}{1 + e^{\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \beta_4 x_{i4} + \dots}}$$

To come back to linear regression we define the logistic function as follow.

$$\text{logit}(p_i) = \log\left(\frac{p_i}{1 - p_i}\right) = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \beta_4 x_{i4} + \dots$$

We can define the odds :

$$\frac{\text{odds}(Y_i = 1|X1 = x_{i1} + 1)}{\text{odds}(Y_i = 1|X1 = x_{i1})} = e^{\beta_1}$$

Which indicator for validity ?

We use Maximum Likelihood :

$$L(\beta) = \prod_{i=1}^n p_i^{y_i} * (1 - p_i)^{1-y_i}$$

The goal is to maximise it by adjusting β vector.

Example on the the Wimbledon tennis tournament

We use a dataset from the Wimbledon tennis tournament for Women in 2013. We will predict the result for player 1 (win=1 or loose=0) based on the number of aces won by each player and the number of unforced errors committed by both players. The data set is a subset of a data set from <https://archive.ics.uci.edu/ml/datasets/Tennis+Major+Tournament+Match+Statistics>.

##	Player1	Player2	Result	ACE.1	UFE.1	ACE.2	UFE.2
## 1	M.Koehler	V.Azarenka	0	2	18	3	14
## 2	E.Baltacha	F.Pennetta	0	0	10	4	14
## 3	S-W.Hsieh	T.Maria	1	1	13	2	29
## 4	A.Cornet	V.King	1	4	30	0	45
## 5	Y.Putintseva	K.Flipkens	0	2	28	6	19
## 6	A.Tomljanovic	B.Jovanovski	0	6	42	11	40

On R

```
##          Player1      Player2 Result ACE.1 UFE.1 ACE.2 UFE.2 ACEdiff UFEdiff
## 1      M.Koehler    V.Azarenka     0     2    18     3    14      -1     4
## 2      E.Baltacha    F.Pennetta     0     0    10     4    14      -4    -4
## 3      S-W.Hsieh     T.Maria       1     1    13     2    29      -1   -16
## 4      A.Cornet      V.King        1     4    30     0    45       4   -15
## 5      Y.Putintseva  K.Flipkens     0     2    28     6    19      -4     9
## 6      A.Tomljanovic B.Jovanovski   0     6    42    11    40      -5     2

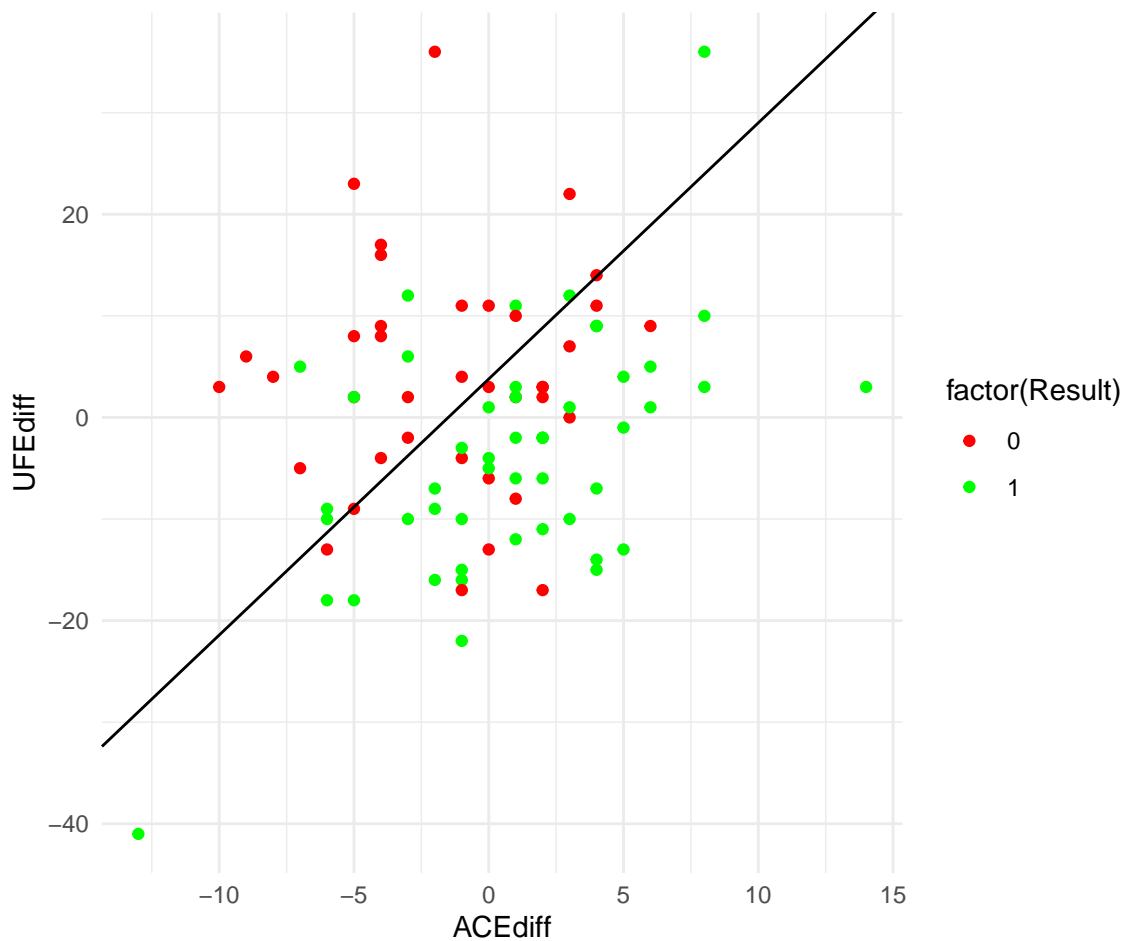
##
## Call:
## glm(formula = Result ~ ACEdiff + UFEdiff, family = "binomial",
##      data = tennisTrain)
##
## Deviance Residuals:
##      Min       1Q   Median       3Q      Max
## -2.1204  -0.9994   0.5662   0.8918   1.8714
##
## Coefficients:
##              Estimate Std. Error z value Pr(>|z|)
## (Intercept)   0.31318    0.24439   1.281  0.20004
## ACEdiff       0.20856    0.06575   3.172  0.00151 **
## UFEdiff      -0.08272    0.02454  -3.371  0.00075 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
```

```
##
## Null deviance: 120.352 on 87 degrees of freedom
## Residual deviance: 99.102 on 85 degrees of freedom
## AIC: 105.1
##
## Number of Fisher Scoring iterations: 4
```

With the model, we can draw the slope which indicates the category of a point.

```
#We calculate the slope
glm.b = -r.tennis2$coefficients[2]/r.tennis2$coefficients[3]
glm.a = -r.tennis2$coefficients[1]/r.tennis2$coefficients[3]

ggplot() + geom_point(aes(ACEdiff, UFEdiff, color = factor(Result)), data = tennisTrain, ) + scale_color_manual(
  geom_abline(slope = glm.b, intercept = glm.a) +
  theme_minimal()
```



We can write :

$$\text{logit}(p_i) = \log\left(\frac{p_i}{1-p_i}\right) = 0,31318 + 0,20856 * ACEDiff - 0,08272 * UFEDiff$$

We can observe $AIC = 105.1$

The confusion matrix is :

```
##
```

```
## glm.Result_pred  0  1
##                  0 15  5
##                  1  2  8
```

The accuracy rate is $\frac{15+8}{30} = 0.7667$.

The sensitivity is the percentage of true output giving Player1-winner among the population of true Player1-winner :

```
## [1] 0.6153846
```

The specificity is the percentage of true output giving Player2-winner (= Player1-looser) among the population of true Player2-winner:

```
## [1] 0.8823529
```

The precision is the percentage of true output giving Player1-winner among all the outputs giving Player1-winner (even if not winner) :

```
## [1] 0.8
```

So the F_Mesure is :

```
## [1] 0.6956522
```

In python with scikit learn

Decision trees and Random Forest

Example on the the Wimbledon tennis tournament

On R

```
## [1] 2
##      MSE      R2      RMSE      MAE
## 1 0.2074194 0.1835982 0.4554331 0.4063749
```

The confusion matrix is :

```
##
## model.Result_pred  0  1
##                  0 10  4
##                  1  7  9
```

The accuracy rate is :

```
## [1] 0.6333333
```

The sensitivity is the percentage of true output giving Player1-winner among the population of true Player1-winner :

```
## [1] 0.6923077
```

The specificity is the percentage of true output giving Player2-winner (= Player1-looser) among the population of true Player2-winner:

```
## [1] 0.5882353
```

The precision is the percentage of true output giving Player1-winner among all the outputs giving Player1-winner (even if not winner) :

```
## [1] 0.5625
```

So the F_Mesure is :

```
## [1] 0.6206897
```

In python with scikit learn TO DO

Regression

Overall

TO DO

Possibilities of models

TO DO

Accuracy of a model

MSE : The Mean Squared error

The MSE measures the mean accuracy of the predicted responses values for given observations. There are two MSE : the train MSE and the test MSE. \ The train MSE is use to fit a model while training. \ The test MSE is use to choose between models already trained. \

Let's define the mean squared error or MSE.

$$MSE = \frac{1}{n} \sum_i (y_i - \hat{f}(x_i))^2$$

Then the expected test MSE refers to the average test MSE that we would obtain if we repeatedly estimated f using a large number of training sets, and tested each at x_0 . So that the expected test MSE is :

$$E(y_0 - \hat{f}(x_0))^2$$

$$E(y_0 - \hat{f}(x_0))^2 = Var(\hat{f}(x_0)) + (f(x_0) - E(\hat{f}(x_0)))^2 + Var(\varepsilon)$$

$Var(\varepsilon)$ represents the irreducible error. This term can not be reduced regardless how well our statistical model fits the data.

$(f(x_0) - E(\hat{f}(x_0)))^2 = [Bias(\hat{f}(x_0))]^2$ is the squared Bias and refers to the error that is introduced by approximating a real-life problem, which may be extremely complicated, by a much simpler model. If the bias is low the model gives a prediction which is close to the true value.

$Var(\hat{f}(x_0))$ is the Variance of the prediction at $\hat{f}(x_0)$ and refers to the amount by which \hat{f} would change if we estimated it using a different training data set. If the variance is high, there is a large uncertainty associated with the prediction.

RMSE

Root Mean Squared Error (RMSE), which measures the average prediction error made by the model in predicting the outcome for an observation. That is, the average difference between the observed known outcome values and the values predicted by the model. The lower the RMSE, the better the model.

RSS : residual sum of squares

We define the residual sum of squares (RSS) as :

$$RSS = \sum (y_i - \hat{y}_i)^2$$

We want to minimize the RSS.

RSE : residual standard error

TO DO

$$RSE = \sqrt{\frac{1}{n-2}RSS}$$

R statistic

TO DO

$$R^2 = 1 - \frac{RSS}{TSS}$$

$$TSS = \sum (y_i - \bar{y})^2$$

is the total sum of squares. TSS measures the total variance in the response Y.

TSS – RSS measures the amount of variability in the response that is explained.

R^2 measures the proportion of variability in Y that can be explained using X.

MAE

Mean Absolute Error (MAE), an alternative to the RMSE that is less sensitive to outliers. It corresponds to the average absolute difference between observed and predicted outcomes. The lower the MAE, the better the model

Simple Linear Regression

Definition

TO DO

DEFINITION

WHICH INDICATORS CAN WE USE

Simple linear regression lives up to its name: it is a very straightforward approach for predicting a quantitative response Y on the basis of a single predictor variable X. It assumes that there is approximately a linear relationship between X and Y. Mathematically, we can write this linear relationship as

$$Y \approx \beta_0 + \beta_1 * X$$

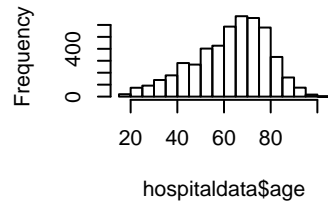
Hospital Costs dataset

The next dataset (source F. E. Harrell, Regression Modeling Strategies) contains the total hospital costs of 9105 patients with certain diseases in American hospitals between 1989 and 1991. The different variables are :

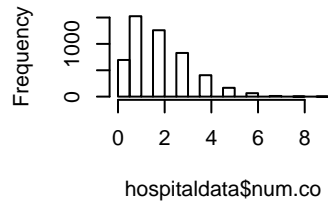
##	age	dzgroup	num.co	edu	income	scoma	totcst	race	meanbp	hrt
## 1	62.85	Lung Cancer	0	11	\$11-\$25k	0	NA	other	97	69
## 2	60.34	Cirrhosis	2	12	\$11-\$25k	44	NA	white	43	112
## 3	52.75	Cirrhosis	2	12	under \$11k	0	NA	white	70	88
## 4	42.38	Lung Cancer	2	11	under \$11k	0	NA	white	75	88
## 5	79.88	ARF/MOSF w/Sepsis	1	NA		26	NA	white	59	112
## 6	93.02	Coma	1	14		55	NA	white	110	101
##	resp	temp	pafi							
## 1	22	36.00	388.00							
## 2	34	34.59	98.00							

```
## 3 28 37.40 231.66
## 4 32 35.00 NA
## 5 20 37.90 173.31
## 6 44 38.40 266.63
```

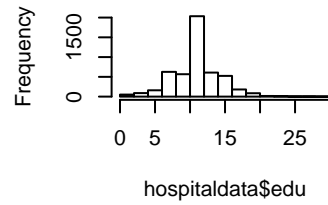
age



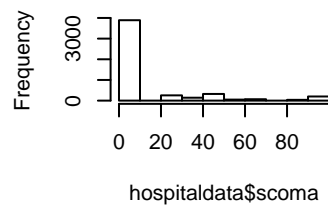
num.co



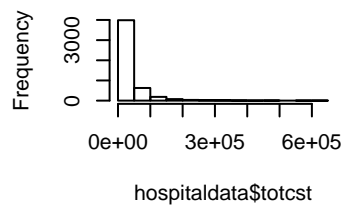
edu



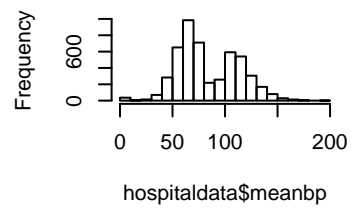
scoma



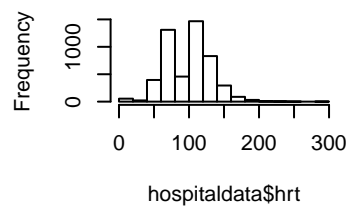
totcst



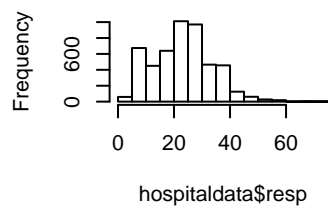
meanbp



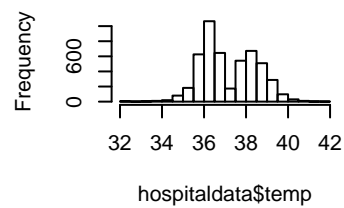
hrt



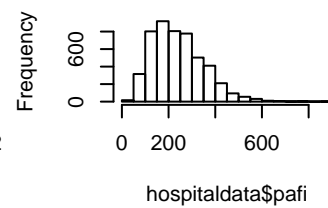
resp

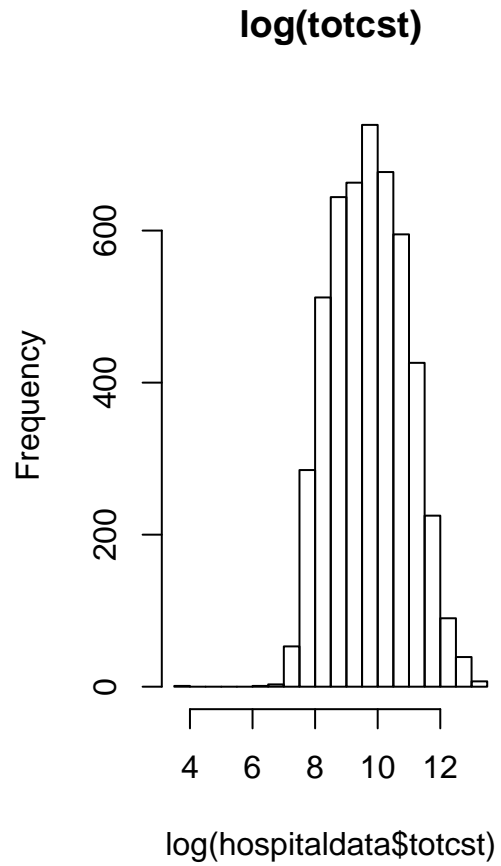
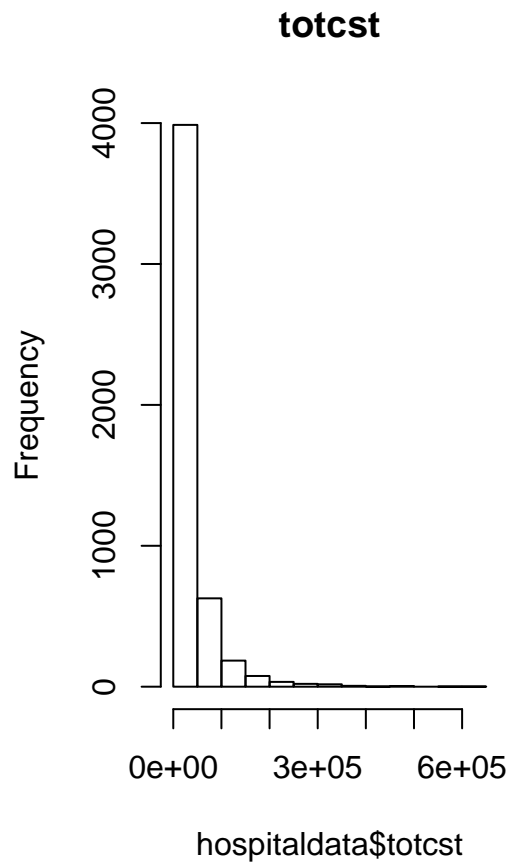


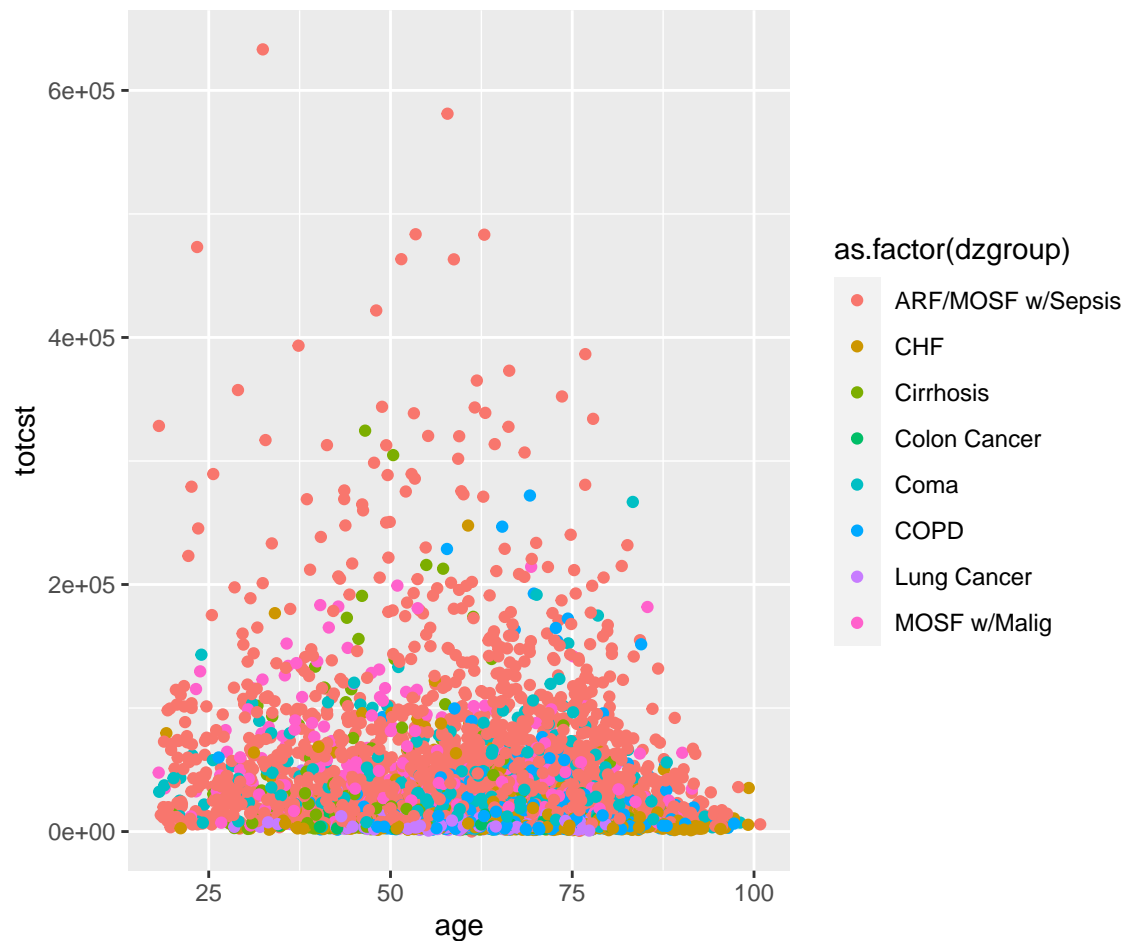
temp



pafi







On R We would like to build models that help us to understand which predictors are mostly driving the total cost.

Looking at the distribution of the cost we see we should apply a log transformation for a better distribution. Moreover it seems that only age and disease have an impact.

```
##
## Call:
## lm(formula = log(totcst) ~ age + temp + edu + resp + num.co +
##     as.factor(dzgroup), data = hospitaldata.train)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -4.0582 -0.6588 -0.0389  0.6184  3.4372
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)    7.848451   0.483978  16.217 < 2e-16 ***
## age           -0.006611   0.001043  -6.341 2.58e-10 ***
## temp           0.075107   0.012571   5.975 2.54e-09 ***
## edu            0.026643   0.004646   5.734 1.06e-08 ***
## resp          -0.004025   0.001541  -2.613 0.009026 **
## num.co        -0.043125   0.012922  -3.337 0.000855 ***
## as.factor(dzgroup)CHF -1.405058   0.052299 -26.866 < 2e-16 ***
```

```
## as.factor(dzgroup)Cirrhosis    -0.923605    0.077611 -11.900 < 2e-16 ***
## as.factor(dzgroup)Colon Cancer -1.458633    0.100672 -14.489 < 2e-16 ***
## as.factor(dzgroup)Coma         -0.452564    0.067303  -6.724 2.06e-11 ***
## as.factor(dzgroup)COPD         -1.242045    0.052407 -23.700 < 2e-16 ***
## as.factor(dzgroup)Lung Cancer  -1.688832    0.064437 -26.209 < 2e-16 ***
## as.factor(dzgroup)MOSF w/Malig -0.256303    0.060087  -4.266 2.05e-05 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.9297 on 3459 degrees of freedom
## Multiple R-squared:  0.3846, Adjusted R-squared:  0.3825
## F-statistic: 180.2 on 12 and 3459 DF, p-value: < 2.2e-16
```

We can that just age and dzgroup seem to have an impact on totcost.

```
##
## Call:
## lm(formula = log(totcost) ~ age + as.factor(dzgroup), data = hospitaldata.train)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -3.9555 -0.6766 -0.0325  0.6116  3.5094
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)    10.885440   0.068097  159.853 < 2e-16 ***
## age           -0.007856   0.001043  -7.529 6.49e-14 ***
## as.factor(dzgroup)CHF      -1.527689   0.048791 -31.311 < 2e-16 ***
## as.factor(dzgroup)Cirrhosis -0.998127   0.076748 -13.005 < 2e-16 ***
## as.factor(dzgroup)Colon Cancer -1.423058   0.101698 -13.993 < 2e-16 ***
## as.factor(dzgroup)Coma      -0.425403   0.067871  -6.268 4.11e-10 ***
## as.factor(dzgroup)COPD      -1.337596   0.051472 -25.987 < 2e-16 ***
## as.factor(dzgroup)Lung Cancer -1.714271   0.065095 -26.335 < 2e-16 ***
## as.factor(dzgroup)MOSF w/Malig -0.241001   0.060559  -3.980 7.04e-05 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.9413 on 3463 degrees of freedom
## Multiple R-squared:  0.3685, Adjusted R-squared:  0.367
## F-statistic: 252.6 on 8 and 3463 DF, p-value: < 2.2e-16
```

We can write :

$$\log(\text{totcost}) = 8.0823597 - 0.0069950 * \text{age} + x_{ij} * \beta_j$$

where x_{ij} is 1 if patient i has disease j and β_j is the coefficient matching the disease in the previous tab.

We can calculate the MSE on the test set to evaluate the simple linear regression model.

```
##           MSE           R2           RMSE           MAE
## 1 0.9017872 0.3660489 0.9496248 0.751934
```

In python with scikit learn

Multiple linear regression

Definition

TO DO

DEFINITION

WHICH INDICATORS ?

Hospital Costs dataset

On R We use the same example than for simple linear regression.

```
##
## Call:
## lm(formula = log(totcst) ~ age * as.factor(dzgroup), data = hospitaldata.train)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -3.9919 -0.6711 -0.0403  0.6162  3.5138
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)    10.737765   0.087214 123.120 < 2e-16 ***
## age           -0.005434   0.001374  -3.955 7.82e-05 ***
## as.factor(dzgroup)CHF -1.223927   0.222589  -5.499 4.11e-08 ***
## as.factor(dzgroup)Cirrhosis -0.581175   0.309688  -1.877  0.06065 .
## as.factor(dzgroup)Colon Cancer -1.264904   0.649568  -1.947  0.05158 .
## as.factor(dzgroup)Coma    0.368400   0.265318   1.389  0.16507
## as.factor(dzgroup)COPD    -1.465964   0.309251  -4.740 2.22e-06 ***
## as.factor(dzgroup)Lung Cancer -2.050794   0.358454  -5.721 1.15e-08 ***
## as.factor(dzgroup)MOSF w/Malig  0.401009   0.240319   1.669  0.09528 .
## age:as.factor(dzgroup)CHF -0.004751   0.003292  -1.443  0.14906
## age:as.factor(dzgroup)Cirrhosis -0.007435   0.005539  -1.342  0.17959
## age:as.factor(dzgroup)Colon Cancer -0.002584   0.009925  -0.260  0.79461
## age:as.factor(dzgroup)Coma    -0.012590   0.004055  -3.104  0.00192 **
## age:as.factor(dzgroup)COPD    0.001504   0.004393   0.342  0.73212
## age:as.factor(dzgroup)Lung Cancer  0.005387   0.005691   0.947  0.34389
## age:as.factor(dzgroup)MOSF w/Malig -0.010661   0.003868  -2.756  0.00589 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.9396 on 3456 degrees of freedom
## Multiple R-squared:  0.372, Adjusted R-squared:  0.3693
## F-statistic: 136.5 on 15 and 3456 DF, p-value: < 2.2e-16
```

We can calculate the MSE on the test set to evaluate the multiple linear regression model.

```
##           MSE           R2          RMSE          MAE
## 1 0.8979065 0.3687867 0.9475793 0.7486429
```

The MSE-test for multiple linear regression is worst than for simple linear regression.

Simple linear regression is the best model so far for this problem.

In python with scikit learn

Validation techniques

Sampling

This consists in dividing the dataset into a training set and a test set.

Cross validation

R2, RMSE and MAE are used to measure the regression model performance during cross-validation.

Validation set approach

TO DO

Example on R

```
##
## Call:
## lm(formula = log(totcst) ~ age + as.factor(dzgroup), data = hospitaldata.train2)
##
## Coefficients:
##              (Intercept)                  age
##              10.912390                 -0.008337
##      as.factor(dzgroup)CHF      as.factor(dzgroup)Cirrhosis
##              -1.530006                 -0.968137
## as.factor(dzgroup)Colon Cancer      as.factor(dzgroup)Coma
##              -1.492058                 -0.397401
##      as.factor(dzgroup)COPD      as.factor(dzgroup)Lung Cancer
##              -1.340868                 -1.735200
## as.factor(dzgroup)MOSF w/Malig
##              -0.272309

##              MSE              R2              RMSE              MAE
## 1 0.9157621 0.3497368 0.9569546 0.7521536
```

Leave One out cross-validation

TO DO

This method works as follow:

Leave out one data point and build the model on the rest of the data set Test the model against the data point that is left out at step 1 and record the test error associated with the prediction Repeat the process for all data points Compute the overall prediction error by taking the average of all these test error estimates recorded at step 2.

Example on R

```
## Linear Regression
##
## 4960 samples
##    2 predictor
##
## No pre-processing
## Resampling: Leave-One-Out Cross-Validation
## Summary of sample sizes: 4959, 4959, 4959, 4959, 4959, 4959, ...
## Resampling results:
```



```
##
##      RMSE      Rsquared    MAE
##    0.944522  0.3656192  0.7552076
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

k-Fold Cross-Validation

TO DO

We divide the set of data in k equals part and we use k-1 parts to train the model and 1 to test. We do do that k times in order to use each part as a test part.

Here are the steps :

1.Split the dataset into k equal partitions (or “folds”)

2.For each fold

One fold is used as the testing set and the union of the other folds as the training set

Calculate testing accuracy for this fold :

$$\hat{f}_i = \frac{1}{K} \sum_{j \in N_0} (y_j)$$

$$MSE = \frac{k}{n} \sum_i I(y_i \neq \hat{y}_i)$$

3.Use the average testing accuracy as the estimate of out-of-sample accuracy :

We would use the cross-validation error :

$$CV_k = \frac{1}{k} \sum_i MSE_i$$

with $I(y_i \neq \hat{y}_i) = 1$ if $y_i \neq \hat{y}_i$, 0 else. So that we calculate the average of wrong predicted values.

Example on R

```
## Linear Regression
##
## 4960 samples
##    2 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 4464, 4464, 4464, 4464, 4464, 4464, ...
## Resampling results:
##
##      RMSE      Rsquared    MAE
##    0.9442358  0.3678628  0.7551859
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

Comparison between R and scikit-learn in python

On classification

Logistic Regression

TO DO : comparison between R and python

	R	Scikit-learn
sensitivity	0.6153846	
specificity	0.8823529	
precision	0.8	
f mesure	0.6956522	
AIC	105.1	

Decision trees

TO DO : comparison between R and python

either knn, or decision trees, or linear discriminant analysis or quadratic discriminant analysis

	R	Scikit-learn
sensitivity	0.6923077	
specificity	0.5882353	
precision	0.5625	
f mesure	0.6206897	
AIC		

On Regression

Simple Linear Regression

	R	Scikit-learn
RMSE	0.9496248	
Rsquared	0.3660489	
MAE	0.751934	

Multiple Linear Regression

	R	Scikit-learn
RMSE	0.9475793	
Rsquared	0.3687867	
MAE	0.7486429	

On Cross Validation

Validation set approach

	R	Scikit-learn
RMSE	0.956954	
Rsquared	0.3497368	
MAE	0.7521536	

Leave One out cross-validation

	R	Scikit-learn
RMSE	0.944522	
Rsquared	0.3656192	
MAE	0.7552076	

k-fold Cross Validation

	R	Scikit-learn
RMSE	0.9442358	
Rsquared	0.3678628	
MAE	0.7551859	