Manon Gnaedig
Pierre-Louis Pécheux

Machine Learning – Project

1. Our dataset

1. Presentation

At the beginning we wanted to find a dataset linked with our IE² project but we didn't find something really useful. So we stay in the health field and we chose the breast cancer dataset.

The dataset had been made to analyse cell characteristics. They took cells from breast, there are cancer cells and normal cells. Our dataset has 699 instances and 10 attributes.
The phenotypes for characterisation are:

- Sample ID (code number)
- Clump thickness
- Uniformity of cell size
- Uniformity of cell shape
- Marginal adhesion
- Single epithelial cell size
- Number of bare nuclei
- Bland chromatin
- Number of normal nuclei
- Mitosis
- Classes, i.e. diagnosis benign or malignant

It is a dataset for classification, our goal to predict if the cell is benign or malignant with our data. Benign and malignant cells have different morphological and functional characteristics.

We do not have the real measures, every predictor value is a score between 1 and 10. So we do not have numeric value. We do not know the signification of the value, we also do not know if the score is linear or not. That is why we do not know if a uniformity of cell size of 3 is 3 times less uniform that a cell with an uniformity of 1 or if it is another scale and the cell with 1 can be 5 or 6 time more uniform. There are 16 missing value. They all are for the predictor *bare nuclei*.

2. Cleaning

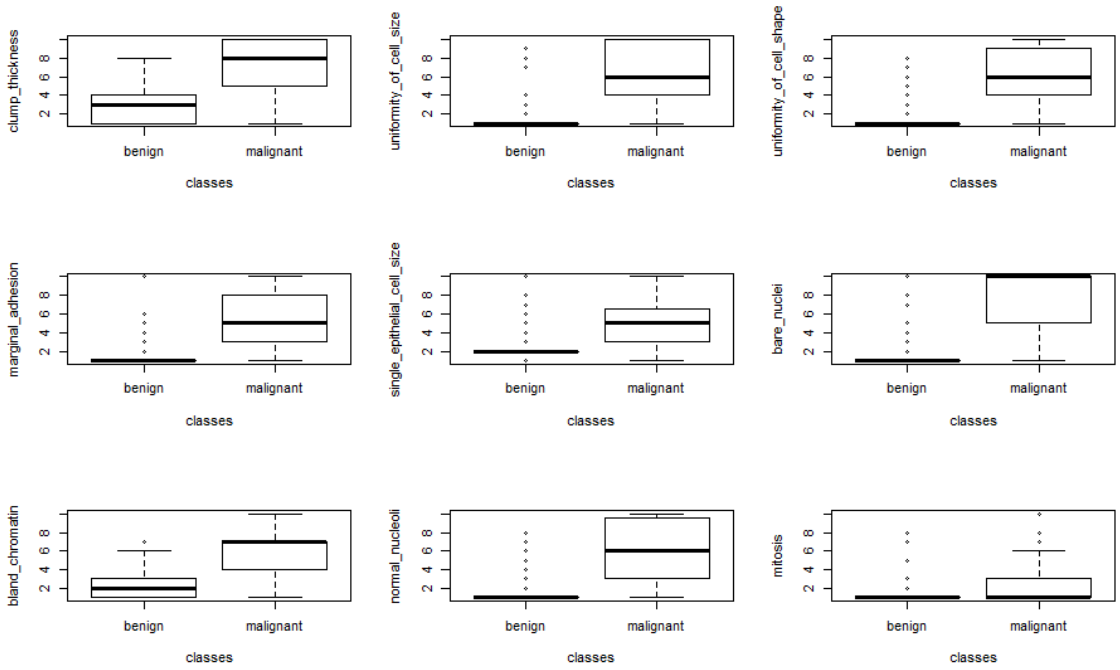
The dataset has no header, so we add the column names in order to have an easier manipulation of the data. We also want to change the name for the response variable. It was 2 for benign and 4 for malignant, we change 2 in 0 and 4 in 1. We also add a column *classes*, with benign or malignant. Thus it is easier to understand when we look quickly to the values. With the function *head()* we can the our 6 first rows.

We have 16 missing data that are all in the *bare_nuclei* column. As the number of observation with missing data is low compared to the total number of observation, we could just ignore these 16 observations for the rest of the study and loose small amount of data. However, we could also replace the missing values by the mean of the column. It does not change the global mean but reduces the variance. We can also try to apply some algorithm that will guess the value with the MICE library. We could also use the library Amelia but we have to make the assumption that all variables follow a multivariate law.

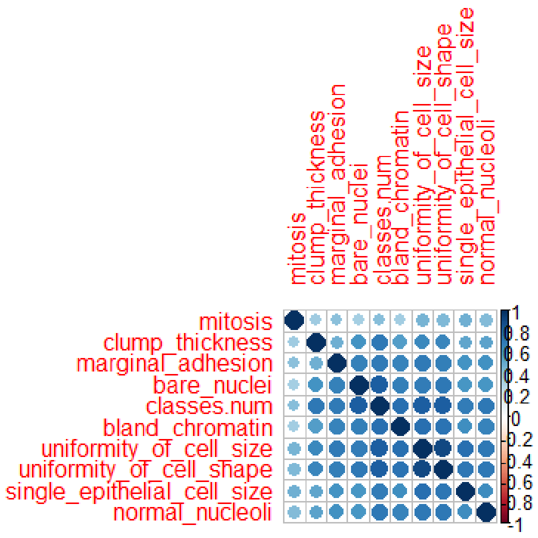
We choose to remove rows with missing data because we do not want to add bias our dataset. We will try later to perform the same study by predicting the missing values using the knn regression and the linear regression and then add the 16 new rows.

3. Visualization

We begin to visualise our data with the plot function. But the most relevant plot is box plot because it is better to display binary variables.



We can see that for almost all predictors, the mean of the observation of malignant cells are different to benign cells.



We can also see the correlation between variables. Therefore, we plot the correlation matrix and we can see that all variables are to some extend correlated.

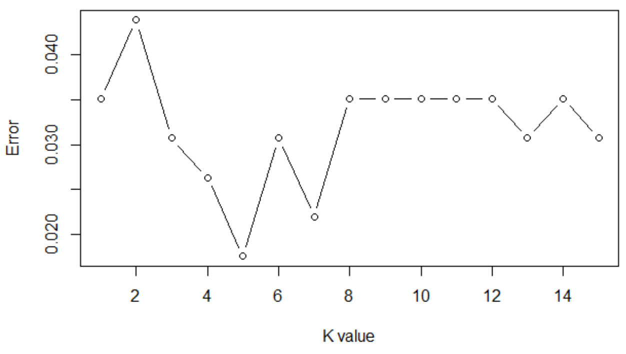
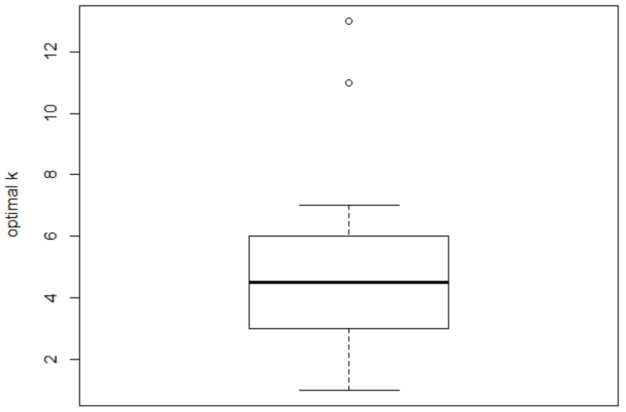
2. Classifiers test

1. K-nearest-neighbour

K-nearest neighbour algorithm is based on the fact that half of the information provided by the training set is contained in the nearest neighbour (asymptotically). However, the KNN classifier breaks down for big dimension of datasets. We have 10 predictors and that is already a lot for KNN.

	Prediction	
	Benign	Malignant
Benign	145	3
Malignant	6	74

We used the knn function in R for K between 1 and 15.

So we compute the Error rate of the classifier for k from 1 to 15. This time the optimal k would have been 5.	But we repeated the process in order to have the mean of the optimal ks by using a loop.
	

On this graph we can see that the best value is 5. Thus we apply the knn function for k=5. We obtain the following matrix of confusion.

We have a really good result. We only have 3 false negative and one false positive.

2. Linear Discriminant Analysis (LDA)

LDA is a generative model and uses the full likelihood based on the joint distribution of X and Y. LDA assumes that all classes share the same covariance matrix.

	Prediction	
	Benign	Malignant
Benign	145	3
Malignant	1	79

We obtain the following confusion matrix:

LDA is usually much more stable than QDA. This method is recommended when n is small.

3. Quadratic Discriminant Analysis

QDA works like LDA but it do not assumes that all classes share the same covariance matrix.

	Prediction	
	Benign	Malignant
Benign	137	11
Malignant	2	78

Results are less good than with LDA for the detection of benign cells. But it is better than LDA for detection of malignant cells. To choose if we want to use LDA or QDA for this case, it depend on our goal. If we really do not want to miss some malignant cell, which mean disease case we should choose QDA. But if we do not want to fear people or give inappropriate treatment we should choose LDA. However, detect all disease cases seems to be the best choice.

4. Naïve Bayes

For Naive Bayes classifier, we set the covariance matrix to diagonal matrix. This assumption means that the predictors are conditionally independent given the class variable Y.

They usually outperform other methods when p is very large.

	Prediction	
	Benign	**Malignant**
Benign	143	10
Malignant	1	78

5. Logistic regression

Logistic regression is a discriminative model and uses the conditional likelihood based on the conditional probabilities $P_k(x)$.

logReg models fit by maximizing the conditional likelihood.

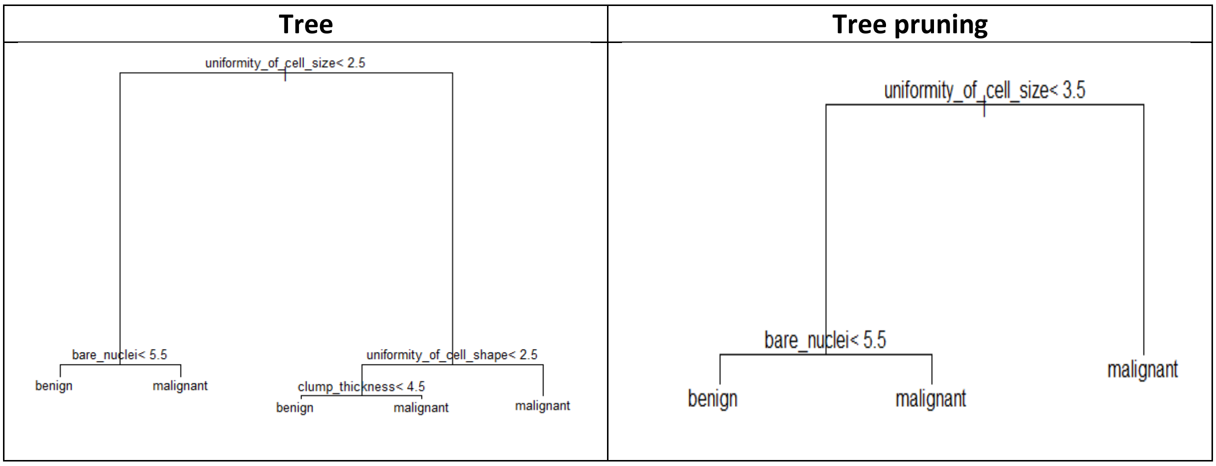
We use the binomial logistic regression because we have only two classes.

	Prediction	
	Benign	**Malignant**
Benign	144	4
Malignant	3	77

3. Tree classifiers

Trees can easily handle qualitative predictors without the need to create dummy variables. But the algorithm of partitioning tends to favor predictor with many levels: they should be avoided. In our case this is not a problem because every predictor has the same number of level.

We used the function *rpart* with *xval = 10*, it is the number of cross validation. *minbucket* is the minimum number of observations in any leaf, we choose 5. *cp* is complexity parameter, any split that does not decrease the overall lack of fit by a factor of cp is not attempted. In order to get the optimal tree size adaptively chosen from the data we use the *prune* algorithm for cp=0.039.



Tree

Tree pruning

	Prediction	
	Benign	**Malignant**
Benign	140	8
Malignant	1	79

Used predictors: uniformity of cell size and shape, bare nuclei and clump thickness

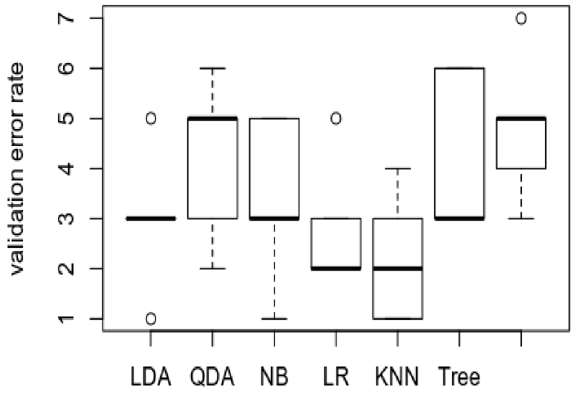
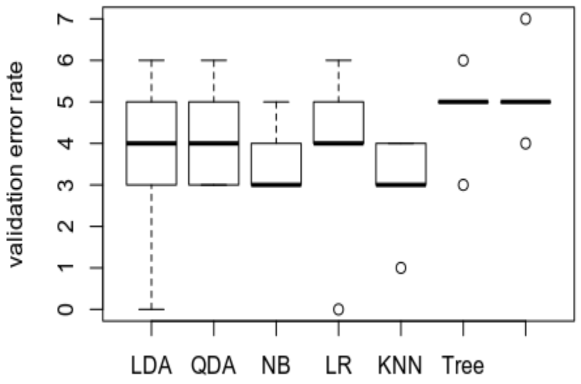
	Prediction	
	Benign	**Malignant**
Benign	140	8
Malignant	1	79

Used predictors : uniformity of size and bare nuclei

4. Comparison

1. Cross Validation

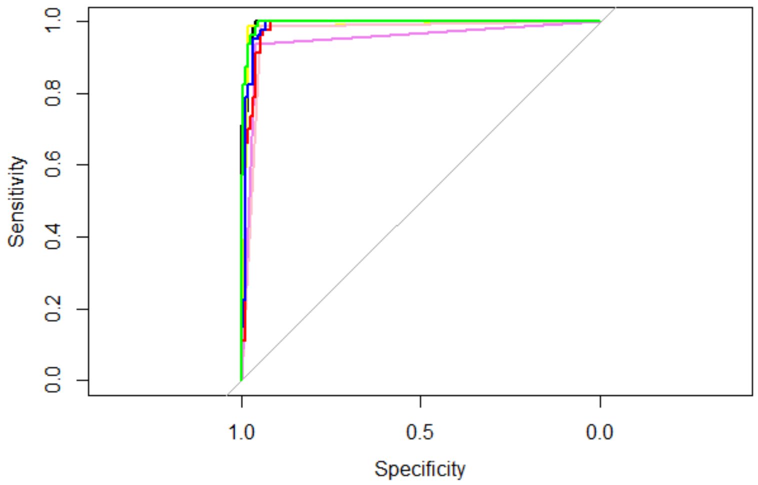
We have chosen the 5 fold cross validation method in order to estimate the error rate of each model without seeing the test set. The idea is to randomly divide the data into 5 equal-sized parts. We live out part k and we fit the model to the other parts combined and then obtain the prediction for the left -out kth part. We do this for k from 1 to 5 and we combine the results.

We can compare our different models that uses as training data only the rows that include no 'NA' :	By using linear regression model to predict the 'NA' of the training set, we were able to add 16 more rows, hoping to improve the quality of the classification:
	

Even by repeating the process, we cannot say that by estimating the missing values with linear regression we improve significantly the quality of the classification. Unfortunately, we did not succeed to do the same comparison by replacing the missing values with the KNN regression.

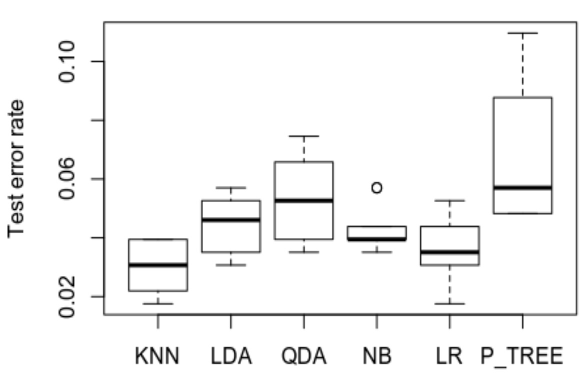
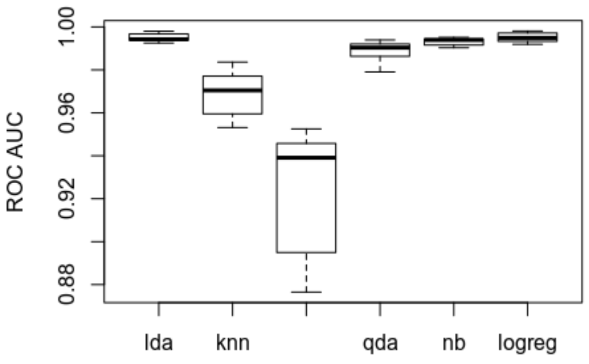
2. Comparison with ROC curve

As we are in a problem of classification with two classes, we can choose a model also by dealing with the false positive and true negative error rates. Therefore it is interesting to plot the ROC curve.



Green=Logistic Regression
Blue=Naïve Bayes
Red=QDA
Purple=Pruning Tree
Pink=Tree
Yellow=KNN
Black=LDA
For this plot, the best ROC is for LDA

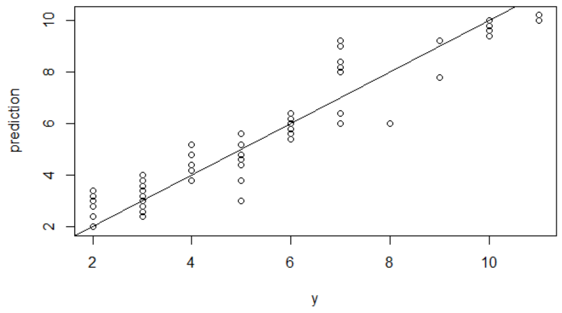
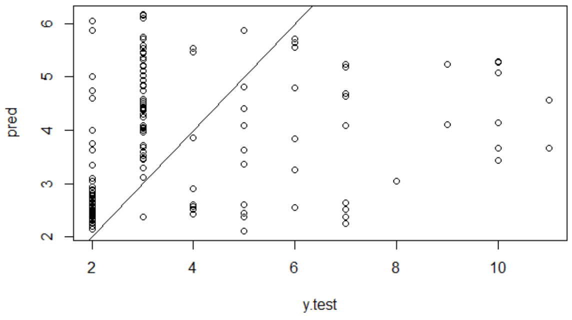
We can repeat the process using different random test sets among the dataset to compute the indicators.

We can compare the model's test error rates	And we can also compute the Area Under the Curve of the ROC
	

It is interesting to see that althrougth knn classifier offers better performances on test error rate compared to the logistic regression model, the LogReg model offers definitly better with the AUC.

5. Regression

We try to do a regression in order to have the missing data of the predictor bare_nuclei. Indeed, we hope that by estimating a value for the missing values will allow us to add the missing rows to the dataset and improve the classification models. At first we tested linear regression and knn regression on our dataset without the row with missing data.

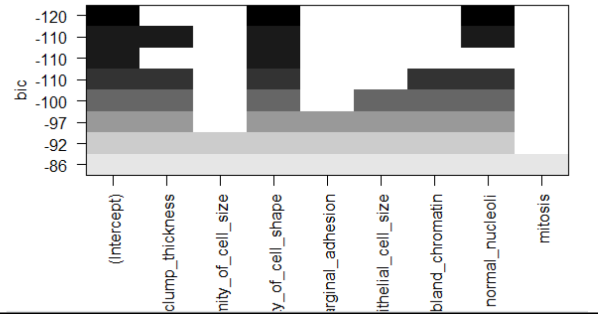
KNN Regression	**Linear Regression**
	

Error : 0.2219298	Error : 3.48129263

KNN regression provide better result than linear regression.

We used model selection in order to know which predictor are more useful to predict our missing data. We used the function regsubsets and obtain the following results.

<table>
<tr><th>BIC</th><th>Adjusted R²</th></tr>
<tr><td>



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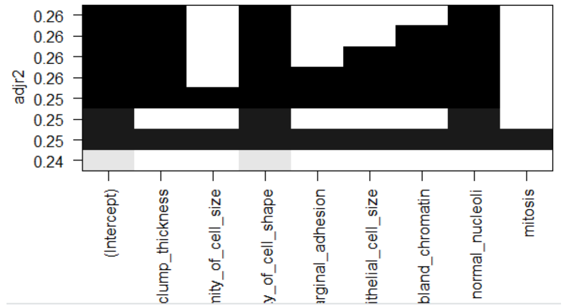
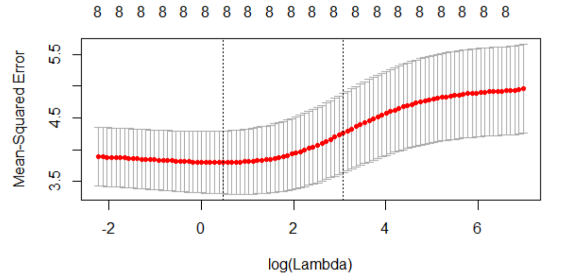


</td></tr>
<tr><td>MSE = 3.543749</td><td>MSE = 3.514410</td></tr>
<tr><td>Best predictors : Uniformity of cell shape, norma l nucleoli</td><td>Best predictors : clump thickness, uniformity of shape, normal nucleoli</td></tr>
</table>

Our results for BIC and adjusted R² are similar. We also used backward selection and optimal selection, they both provide same results than forward regression.

Then, we used Ridge and Lasso regression.

<table>
<tr><th>Ridge Regression</th><th>Lasso Regression</th></tr>
<tr><td>



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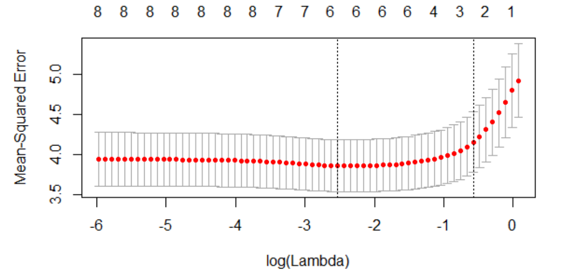

</td></tr>
<tr><td>MSE = 3.437183</td><td>MSE = 3.453140</td></tr>
<tr><td>Best results : With 8 predictors</td><td>Best results : with 6 predictors</td></tr>
</table>

Ridge and Lasso regression allow to delete a lower amount of predictors than BIC and adjusted R².