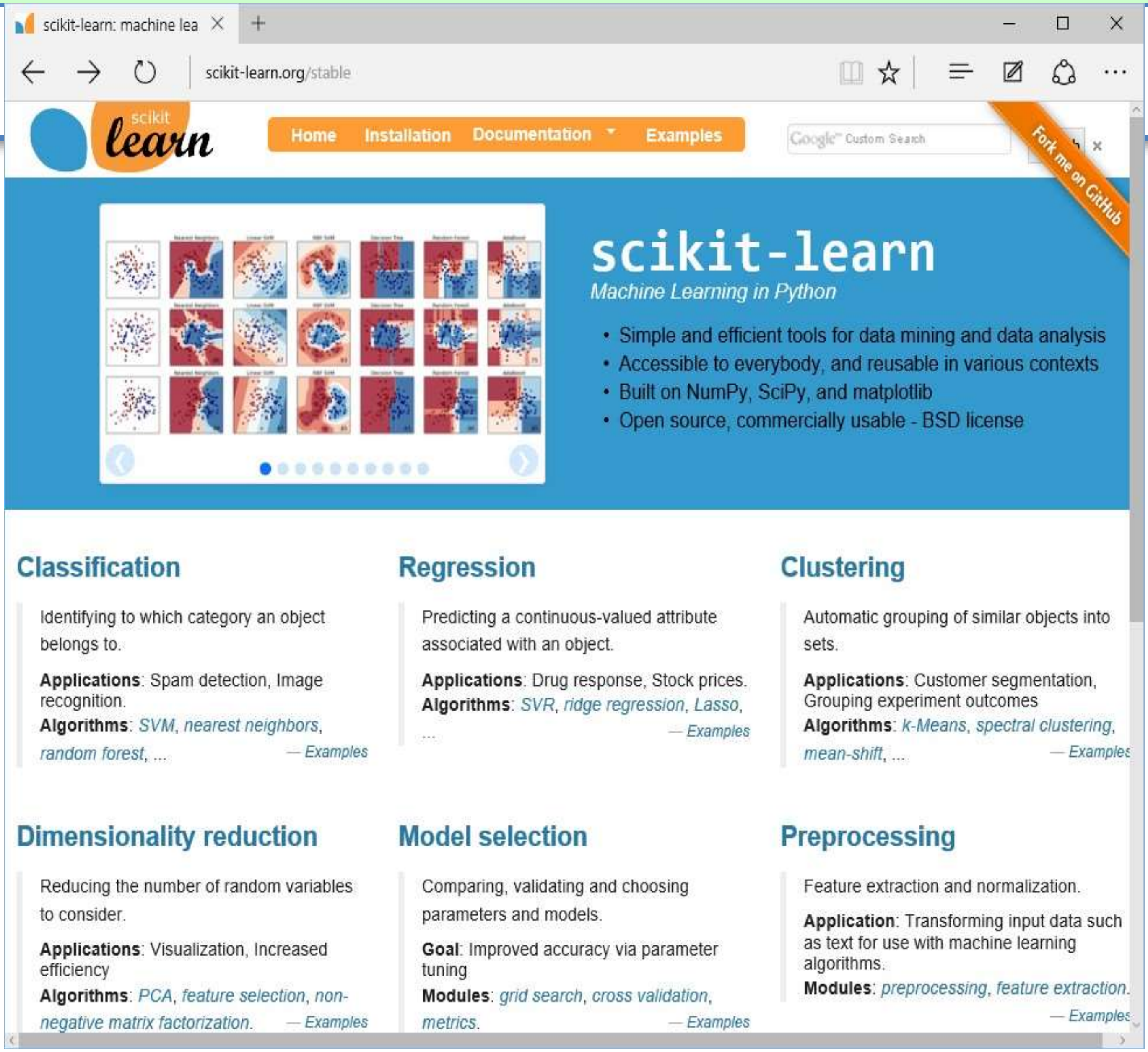
# COSC 3337 : Data Science I

N. Rizk

College of Natural and Applied Sciences

Department of Computer Science

University of Houston




Machine learning explores the study and construction of algorithms that can learn from and make predictions on data. Such algorithms operate by building a model from example inputs in order to make data-driven predictions or decisions…. Machine learning is closely related to computational statistics; a discipline that aims at the design of algorithms for implementing statistical methods on computers (Wikipedia).

# Classification problem

1. A typical classification process
2. Cross-validation evaluation for small dataset
3. Scoring process – Gains chart
4. Search for optimal parameters for algorithms
5. Feature selection

# Dataset – PIMA INDIAN DIABETES

UCI Machine Learning R

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## Pima Indians Diabetes Data Set

*Download*: Data Folder, Data Set Description

**Abstract**: From National Institute of Diabetes and Digestive and Kidney Diseases; Includes cost data (donated by Peter Turney)

| | | | | | |
|---|---|---|---|---|---|
| **Data Set Characteristics:** | Multivariate | **Number of Instances:** | 768 | **Area:** | Life |
| **Attribute Characteristics:** | Integer, Real | **Number of Attributes:** | 8 | **Date Donated** | 1990-05-09 |
| **Associated Tasks:** | Classification | **Missing Values?** | Yes | **Number of Web Hits:** | 154720 |

**Source:**

Original Owners:

National Institute of Diabetes and Digestive and Kidney Diseases

Donor of database:

Vincent Sigillito (vgs '@' aplcen.apl.jhu.edu)
Research Center, RMI Group Leader
Applied Physics Laboratory
The Johns Hopkins University
Johns Hopkins Road
Laurel, MD 20707
(301) 953-6231

<u>Goal:</u> Predict / explain the occurrence of diabetes (target variable) from the characteristics of individuals (age, BMI, etc.) (descriptors). The « pima.txt » data file is in the TSV (tab-separated values) text format (first row = attributes name).

pima.txt

| pregnant | diastolic | triceps | bodymass | pedigree | age | plasma | serum | diabete |
|---|---|---|---|---|---|---|---|---|
| 6 | 72 | 35 | 33.6 | 0.627 | 50 | 148 | 0 | positive |
| 1 | 66 | 29 | 26.6 | 0.351 | 31 | 85 | 0 | negative |
| 8 | 64 | 0 | 23.3 | 0.672 | 32 | 183 | 0 | positive |
| 1 | 66 | 23 | 28.1 | 0.167 | 21 | 89 | 94 | negative |
| 0 | 40 | 35 | 43.1 | 2.288 | 33 | 137 | 168 | positive |
| 5 | 74 | 0 | 25.6 | 0.201 | 30 | 116 | 0 | negative |
| 3 | 50 | 32 | 31 | 0.248 | 26 | 78 | 88 | positive |
| 10 | 0 | 0 | 35.3 | 0.134 | 29 | 115 | 0 | negative |
| 2 | 70 | 45 | 30.5 | 0.158 | 53 | 197 | 543 | positive |
| 8 | 96 | 0 | 0 | 0.232 | 54 | 125 | 0 | positive |
| 4 | 92 | 0 | 37.6 | 0.191 | 30 | 110 | 0 | negative |
| 10 | 74 | 0 | 38 | 0.537 | 34 | 168 | 0 | positive |
| 10 | 80 | 0 | 27.1 | 1.441 | 57 | 139 | 0 | negative |
| 1 | 60 | 23 | 30.1 | 0.398 | 59 | 189 | 846 | positive |
| 5 | 72 | 19 | 25.8 | 0.587 | 51 | 166 | 175 | positive |
| 7 | 0 | 0 | 30 | 0.484 | 32 | 100 | 0 | positive |
| 0 | 84 | 47 | 45.8 | 0.551 | 31 | 118 | 230 | positive |
| 7 | 74 | 0 | 29.6 | 0.254 | 31 | 107 | 0 | positive |
| 1 | 30 | 38 | 43.3 | 0.183 | 33 | 103 | 83 | negative |
| 1 | 70 | 30 | 34.6 | 0.529 | 32 | 115 | 96 | positive |
| 3 | 88 | 41 | 39.3 | 0.704 | 27 | 126 | 235 | negative |
| 8 | 84 | 0 | 35.4 | 0.388 | 50 | 99 | 0 | negative |

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A typical classification process

# CLASSIFICATION PROCESS

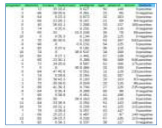
Y : target attribute (diabete)

X1, X2, … : predictive attributes

f(.) the underlying concept with Y = f(X1, X2, …)

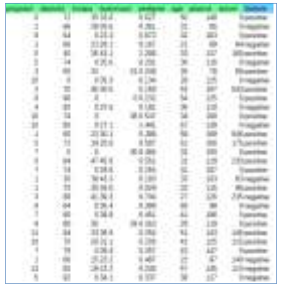
f(.) must be “as accurate as possible” …

Training set



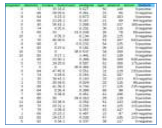
Learning the function f(.) (the parameters of the function) from the training set

$Y = f(X1,X2,\dots) + \varepsilon$



Dataset

Classification of the test set i.e. the model is applied on the test set to obtain the predicted values



Test set

$(Y, \hat{Y})$

Measuring the accuracy of the prediction by comparing Y and Y^: confusion matrix and evaluation measurements

Y : observed class values

Y^ : predicted class values from f(.)

# Reading data file

Pandas: Python Data Analysis Library. The package Pandas provides useful tools for handling, among others, flat data file.

```
#import the Pandas library
import pandas
pima = pandas.read_table("pima.txt",sep="\t",header=0)
```

header = 0, the first row (n°0) correspond to the columns name

```
#number of rows and columns
print(pima.shape) # (768, 9)
```

768 rows (instances) and 9 columns (attributes)

```
#columns name
print(pima.columns) # Index(['pregnant', 'diastolic', 'triceps', 'bodymass', 'pedigree', 'age','plasma', 'serum', 'diabete'], dtype='object')
```

```
#data type for each column
print(pima.dtypes)
```

```
pregnant     int64
diastolic    int64
triceps      int64
bodymass     float64
pedigree     float64
age          int64
plasma       int64
serum        int64
diabete      object
dtype: object (string for our dataset)
```

# Split data into training and test sets

```
#transform the data into a NumPy matrix
data = pima.as_matrix()

#X matrix for the descriptors (input attributes)
X = data[:,0:8]

#y vector for the target attribute
y = data[:,8]

#using the model_selection module of scikit-learn (sklearn)
from sklearn import model_selection

#test set size = 300 ; training set size = 768 – test set = 468
X_app,X_test,y_app,y_test = model_selection.train_test_split(X,y,test_size = 300,random_state=0)
print(X_app.shape,X_test.shape,y_app.shape,y_test.shape)
```

(468,8) (300,8) (468,) (300,)

# Learning the classifier on the training set

```
#from the linear_model module of sklearn
#import the LogisticRegression class
from sklearn.linear_model import LogisticRegression

#lr is an object from the LogisticRegression class
lr = LogisticRegression()

#fitting the model to the labelled training set
#X_app: input data, y_app: target attribute (labels)
modele = lr.fit(X_app,y_app)

#the outputs are lacking
#the coefficients and the intercept
print(modele.coef_,modele.intercept_)
```

We use the logistic regression. Many supervised learning methods are available in scikit-learn.

There are not the usual outputs for logistic regression (tests of significance, standard error of the coefficients, etc.)

```
[[ 8.75111754e-02 -1.59515113e-02   1.70447729e-03   5.18540256e-02
   5.34746050e-01   1.24326526e-02   2.40105095e-02 -2.91593120e-04]] [-5.13484535]
```

# Note about the results of the logistic regression of scikit-learn

<u>Note:</u> The logistic regression of scikit-learn is based on other algorithm than the state-of-art ones (e.g. SAS proc logistic or R glm algorithms)

**Coefficients of SAS**

| Variable | Coefficient |
|---|---|
| Intercept | 8.4047 |
| pregnant | -0.1232 |
| diastolic | 0.0133 |
| triceps | -0.0006 |
| bodymass | -0.0897 |
| pedigree | -0.9452 |
| age | -0.0149 |
| plasma | -0.0352 |
| serum | 0.0012 |

**Coefficients of scikit-learn**

| Variable | Coefficient |
|---|---|
| Intercept | 5.8844 |
| pregnant | -0.1171 |
| diastolic | 0.0169 |
| triceps | -0.0008 |
| bodymass | -0.0597 |
| pedigree | -0.6776 |
| age | -0.0072 |
| plasma | -0.0284 |
| serum | 0.0006 |

The coefficients are similar but different. It does not mean that the model is less efficient in prediction.

**sklearn.linear_model.LogisticRegression**

*class* sklearn.linear_model.**LogisticRegression**(*penalty='l2', dual=False, tol=0.0001, C=1.0, fit_intercept=True, intercept_scaling=1, class_weight=None, random_state=None, solver='liblinear', max_iter=100, multi_class='ovr', verbose=0*) [source]

Logistic Regression (aka logit, MaxEnt) classifier.

In the multiclass case, the training algorithm uses the one-vs-rest (OvR) scheme if the 'multi_class' option is set to 'ovr' and uses the cross-entropy loss, if the 'multi_class' option is set to 'multinomial'. (Currently the 'multinomial' option is supported only by the 'lbfgs' and 'newton-cg' solvers.)

This class implements regularized logistic regression using the liblinear library, newton-cg and lbfgs solvers. It can handle both dense and sparse input. Use C-ordered arrays or CSR matrices containing 64-bit floats for optimal performance; any other input format will be converted (and copied).

The newton-cg and lbfgs solvers support only L2 regularization with primal formulation. The liblinear solver supports both L1 and L2 regularization, with a dual formulation only for the L2 penalty.

Prediction and evaluation on the test set

```
#prediction on the test sample
y_pred = modele.predict(X_test)

#metrics – quantifying the quality of the prediction
from sklearn import metrics

#confusion matrix
#comparison of the observed target values and the prediction
cm = metrics.confusion_matrix(y_test,y_pred)
print(cm)

#accuracy rate
acc = metrics.accuracy_score(y_test,y_pred)
print(acc) # 0.793 = (184 + 54)/ (184 + 17 + 45 + 54)

#error rate
err = 1.0 - acc
print(err) # 0.206 = 1.0 – 0.793

#recall (sensibility)
se = metrics.recall_score(y_test,y_pred,pos_label='positive')
print(se) # 0.545 = 54 / (45+ 54)
```

**Confusion matrix**
Row: observed
Column: prediction

```
[[184  17]
 [ 45  54]]
```

## Create our own performance metric (e.g. specificity)

```
#a function for computing specificity
def specificity(y,y_hat):
    #confusion matrix – a numpy.ndarray object
    mc = metrics.confusion_matrix(y,y_hat)
    #"negative" is the first row (index 0) of the matrix
    import numpy
    res = mc[0,0]/numpy.sum(mc[0,:])
    #return the specificity
    return res
#

# make the function usable as a scorer object
specificite = metrics.make_scorer(specificity,greater_is_better=True)

#using the new scorer object
#modele is the classifier fitted on the training set (see page 9)
sp = specificite(modele,X_test,y_test)
print(sp) # 0.915 = 184 / (184 + 17)
```

Note: Use the package like a simple toolbox is one thing, programming in Python is another. This skill is essential if we want to go further.

Confusion matrix =

```
[[184  17]
 [ 45  54]]
```

# CROSS VALIDATION

Measuring performance on small dataset

Cross-validation with scikit-learn

**Issue:** When dealing with a small file, the subdivision of data into learning and test samples is penalizing. Indeed, we will have less instances to build an effective model, and the estimate of the error will be unreliable because based on too few observations.

**Solution:** (1) Learning the classifier using the whole dataset. (2) Evaluate the performance of this classifier using the cross-validation mechanism.

```
#import the LogisticRegression class
from sklearn.linear_model import LogisticRegression

#instantiate and initialize the object
lr = LogisticRegression()

#fit on the whole dataset (X,y)
modele_all = lr.fit(X,y)

#print the coefficients and the intercept
print(modele_all.coef_,modele_all.intercept_)
# [[ 1.17056955e-01 -1.69020125e-02 7.53362852e-04 5.96780492e-02 6.77559538e-01 7.21222074e-03 2.83668010e-02 -6.41169185e-04]] [-5.8844014]
# !!! Of course, the coefficients and the intercept are not the same as the ones estimated on the training set !!!

#import the model_selection module
from sklearn import model_selection

#10-fold cross-validation to evaluate the success rate
succes = model_selection.cross_val_score(lr,X,y,cv=10,scoring='accuracy')

#details of the results for each fold
print(succes)

#mean of the success rate = cross-validation estimation of the success rate of modele_all
print(succes.mean()) # 0.767
```

| |
|---|
| 0.74025974 |
| 0.75324675 |
| 0.79220779 |
| 0.72727273 |
| 0.74025974 |
| 0.74025974 |
| 0.81818182 |
| 0.79220779 |
| 0.73684211 |
| 0.82894737 |

# SCORING

Gains chart

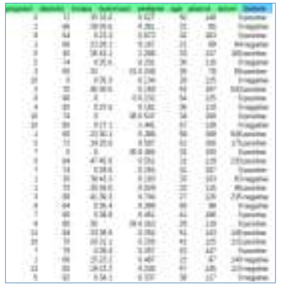
# Scoring

<u>Ex. of direct marketing:</u> identify the likely responders to a mailing (1)

<u>Goal:</u> contact the fewest people, get the max of purchases

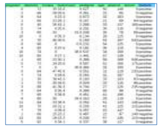
<u>Process:</u> assign a "probability of responding" score to individuals, sort them in a decreasing way (high score = high probability to purchase), estimate the number of purchases for a given target size (number of customer to contact) using the gain chart

<u>Note:</u> The idea can be transposed to other areas (e.g. disease screening)



Dataset

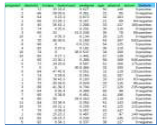
Training set



Construction of the classifier f(.) which can calculate the probability (or any value proportional to the probability) on an instance to be positive (the class of interest)

$Y = f(X1, X2, \ldots) + \varepsilon$

Calculate the score of instances in the test set

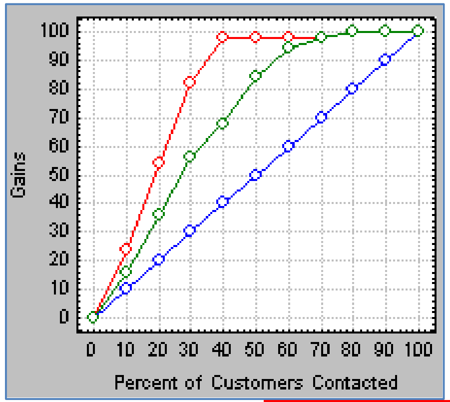


Test set

$(Y, score)$

Y : observed class values
score : probability of responding computed by f(.)

Measuring the performance using the gain chart



Gains chart (1/3)

```
#Logistic Regression class
from sklearn.linear_model import LogisticRegression
#instantiate and initialize the object
lr = LogisticRegression()
#fit the model to the training sample
modele = lr.fit(X_app,y_app)
#calculate the posterior probabilities for the test sample
probas = lr.predict_proba(X_test)
#score for 'presence' (positive class value)
score = probas[:,1] # [0.86238322 0.21334963 0.15895063 …]
#transforming in 0/1 (dummy variables) the Y_test vector
pos = pandas.get_dummies(y_test).as_matrix()
#get the second column (index = 1)
pos = pos[:,1] # [ 1 0 0 1 0 0 1 1 …]
#number of "positive" instances
import numpy
npos = numpy.sum(pos) # 99 – there are 99 "positive" instances into the test set
```

Class membership probabilities
Negative, Positive

```
[ 0.13761678,  0.86238322],
[ 0.78665037,  0.21334963],
[ 0.84104937,  0.15895063],
[ 0.39960826,  0.60039174],
[ 0.81646421,  0.18353579],
[ 0.91705129,  0.08294871],
[ 0.32575719,  0.67424281],
[ 0.27436772,  0.72563228],
[ 0.56763049,  0.43236951],
```

Class membership
Negative, Positive

```
[ 0.,  1.],
[ 1.,  0.],
[ 1.,  0.],
[ 0.,  1.],
[ 1.,  0.],
[ 1.,  0.],
[ 0.,  1.],
[ 0.,  1.],
```

Gains chart (2/3)

The individual n°55 has the lowest score, then the n°45, … , the individual n°159 has the highest score.

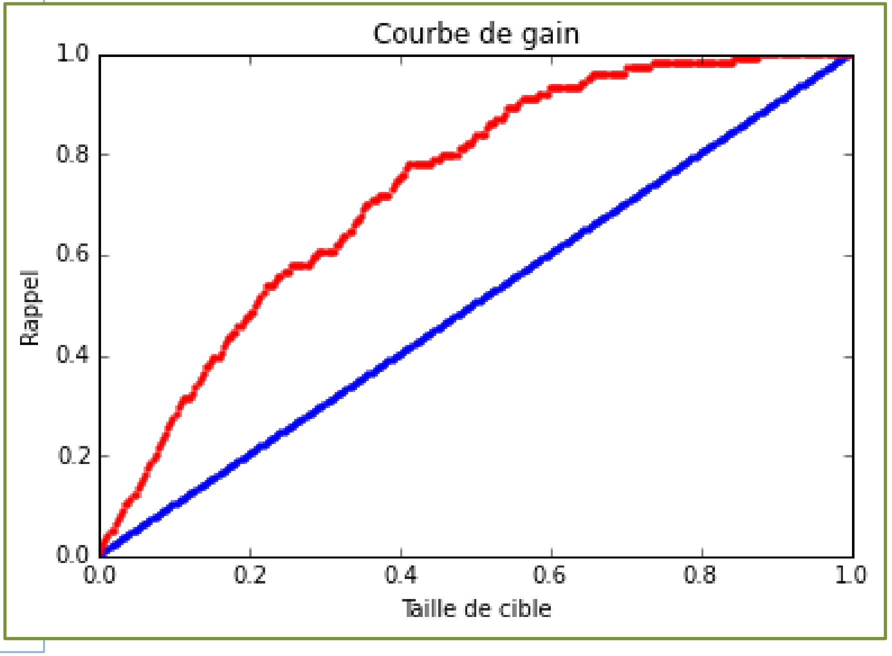
```
#indices that would sort according to the score
index = numpy.argsort(score) # [ 55 45 265 261 … 11 255 159]
#invert the indices, first the instances with the highest score
index = index[::-1] # [ 159 255 11 … 261 265 45 55 ]
#sort the class membership according to the indices
sort_pos = pos[index] # [ 1 1 1 1 1 0 1 1 …]
#cumulated sum
cpos = numpy.cumsum(sort_pos) # [ 1 2 3 4 5 5 6 7 … 99]
#recall column
rappel = cpos/npos # [ 1/99 2/99 3/99 4/99 5/99 5/99 6/99 7/99 … 99/99]
#nb. of instances into the test set
n = y_test.shape[0] # 300, il y a 300 ind. dans l'éch. test
#target size
taille = numpy.arange(start=1,stop=301,step=1) # [1 2 3 4 5 …  300]
#target size in percentage
taille = taille / n # [ 1/300 2/300 3/300 … 300/300 ]
```

The "scores" computed by the model seem quite good. There are a majority of positive instances for the highest scores.

# Gains chart (3/3)

```
#graphical representation with matplotlib
import matplotlib.pyplot as plt

#title and axis labels
plt.title('Courbe de gain')
plt.xlabel('Taille de cible')
plt.ylabel('Rappel')

#limits in horizontal and vertical axes
plt.xlim(0,1)
plt.ylim(0,1)

#tricks to represent the diagonal
plt.scatter(taille,taille,marker='.',color='blue')

#gains curve
plt.scatter(taille,rappel,marker='.',color='red')

#show the chart
plt.show()
```

The x-coordinate of the chart shows the percentage of the cumulative number of sorted data records according to the decreasing score value. The y-coordinate shows the percentage of the number of records that actually contain the selected target field value for the appropriate amount of records on the x-coordinate (see Gains chart).



# GRID SEARCH

Searching for estimator parameters

## Dependencies of the learning algorithms to their parameters

```
#support vector machine
from sklearn import svm

#by default: RBF kernel and C = 1.0
mvs = svm.SVC()

#fit the model to the training sample
modele2 = mvs.fit(X_app,y_app)

#prediction on the test set
y_pred2 = modele2.predict(X_test)

#confusion matrix
print(metrics.confusion_matrix(y_test,y_pred2))

#success rate on the test set
print(metrics.accuracy_score(y_test,y_pred2)) # 0.67
```

Issue: Many machine learning algorithms are dependent to parameters that are not always obvious to determine to obtain the best performance on our dataset. E.g. SVM.

*class* sklearn.svm.SVC(*C=1.0, kernel='rbf', degree=3, gamma=0.0, coef0=0.0, shrinking=True, probability=False, tol=0.001, cache_size=200, class_weight=None, verbose=False, max_iter=-1, random_state=None*)

The method is not better than the default classifier (systematically predict the majority class value "negative"). Confusion matrix:

```
[[201   0]
 [ 99   0]]
```

The (SVM) method is unsuitable or the settings are not appropriate?

## Grid search for searching the best parameters

#import the class
from sklearn import model_selection

#combination of parameters to evaluate
parametres = [{'C':[0.1,1,10],'kernel':['rbf','linear']}]

#cross-validation for 3 x 2 = 6 combinations
#accuracy rate is the performance measurement used
#mvs is the object form the svm.SVC class (cf. previous page)

We indicate the parameters to vary, scikit-learn combines them and measures performance in cross-validation for each combination.

- grid = model_selection.GridSearchCV(estimator=mvs,param_grid=parametres,scoring='accuracy')
- # launch searching - the calculations can be long grille = grid.fit(X_app,y_app)
- #result for each combination print(pandas.DataFrame.from_dict(grille.cv_results_).loc[:,["params",

| | params | mean_test_score |
|---|---|---|
| 0 | {'C': 0.1, 'kernel': 'rbf'} | 0.638889 |
| 1 | {'C': 0.1, 'kernel': 'linear'} | 0.752137 |
| 2 | {'C': 1, 'kernel': 'rbf'} | 0.638889 |
| 3 | {'C': 1, 'kernel': 'linear'} | 0.747863 |
| 4 | {'C': 10, 'kernel': 'rbf'} | 0.638889 |
| 5 | {'C': 10, 'kernel': 'linear'} | 0.756410 |

- # the best combination of C and kernel for our dataset print(grille.best_params_)
  # {'C' : 10, 'kernel' : 'linear'}
- # the performance of the best combination (success rate measured in cross-validation)
- print(grille.best_score_) # 0.7564
- #prediction with this best model i.e. {'C' : 10, 'kernel' : 'linear'}
- y_pred3 = grille.predict(X_test)
- #success rate on the test set
- print(metrics.accuracy_score(y_test,y_pred3)) # 0.7833, the performance is similar to the one of logistic regression

# FEATURE SELECTION

Selecting the most relevant features in a model

Attribute selection (1/2)

Initial features (predictive attributes): pregnant, diastolic, triceps, bodymass, pedigree, age, plasma, serum.

```
#import the LogisticRegression class
from sklearn.linear_model import LogisticRegression

#instantiate an object
lr = LogisticRegression()

#function for feature selection.
from sklearn.feature_selection import RFE
selecteur = RFE(estimator=lr)

#launch the selection process
sol = selecteur.fit(X_app,y_app)

#number of selected attributes
print(sol.n_features_) # 4 → 4 = 8 / 2 variables sélectionnées

#list of selected features
print(sol.support_) # [True False False True True False True False ]

# order of deletion
print(sol.ranking_) # [1 2 4 1 1 3 1  5]
```

Goal: detecting the subset of relevant features in order to obtain a simpler model, for a better interpretation, a shorter training time, and an enhanced generalization performance (1).

Approach: The RFE (recursive feature elimination) approach selects the features by recursively considering smaller and smaller sets of features. For the linear model, it is based on the value of the coefficients (the lowest one in absolute value is removed). The process continues until we reach the desired number of features. The variables must scaled (standardized or normalized) if we want to compare the coefficients.

Selected attributes: pregnant, bodymass, pedigree, plasma.

**Serum** was removed first, then **triceps**, then **age**, then **diastolic**. The remaining variables are indexed **1**.

## Attribute selection (2/2)

```
# matrix for the selected attributes - training set
# we use the boolean vector sol.support_
X_new_app = X_app[:,sol.support_]
print(X_new_app.shape) # (468, 4) → 4 variables restantes

# fit the model on the selected attributes
modele_sel = lr.fit(X_new_app,y_app)

# matrix for the selected attributes – test set
X_new_test = X_test[:,sol.support_]
print(X_new_test.shape) # (300, 4)

# prediction on the test set
y_pred_sel = modele_sel.predict(X_new_test)

# success rate
print(metrics.accuracy_score(y_test,y_pred_sel)) # 0.787
```

The resulting classifier is as good as (almost, 0793) the original model, but with half the number of attributes.