COMP 204

Intro to machine learning with scikit-learn (part two)

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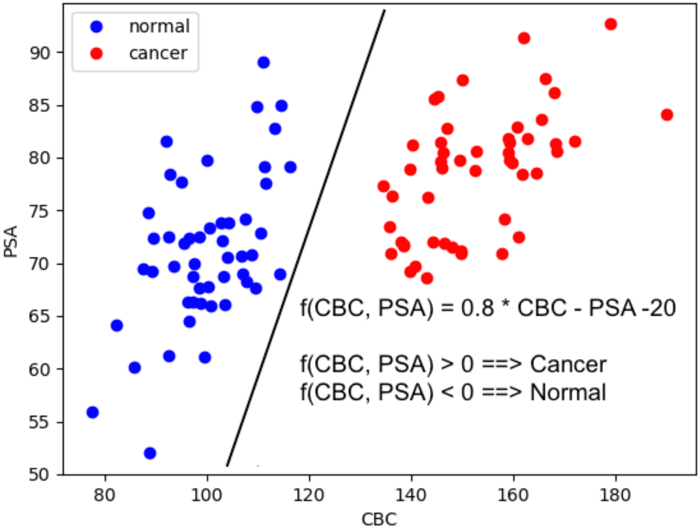
Return to our prostate cancer prediction problem

Suppose you want to learn to predict if a person has a prostate cancer based on two easily-measured variables obtained from blood sample: Complete Blood Count (CBC) and Prostate-specific antigen (PSA). We have collected data from patients known to have or not have prostate cancer:

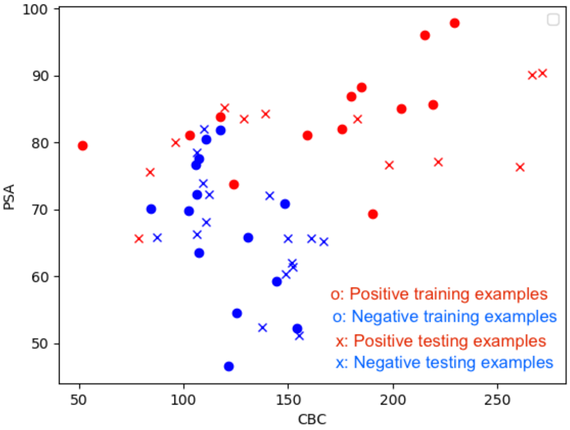
CBC	PSA	Status
142	67	Normal
132	58	Normal
178	69	Cancer
188	46	Normal
183	68	Cancer
...		

Goal: Train classifier to predict the class of new patients, from their CBC and PSA.

A perfect classifier



More realistic data



Here, it is impossible to cleanly separate positive and negative examples with a straight line.

→ We will be bound to make classification errors.

True/false positives and negatives

True positive (TP)

Positive example that is predicted to be positive

- A person who is predicted to have cancer and actually has cancer

False positive (FP)

Negative example that is predicted to be positive

- A person who is predicted to have cancer and but doesn't have cancer

True negative (TN)

Negative example that is predicted to be negative

- A person who is predicted to not have cancer and actually doesn't have cancer

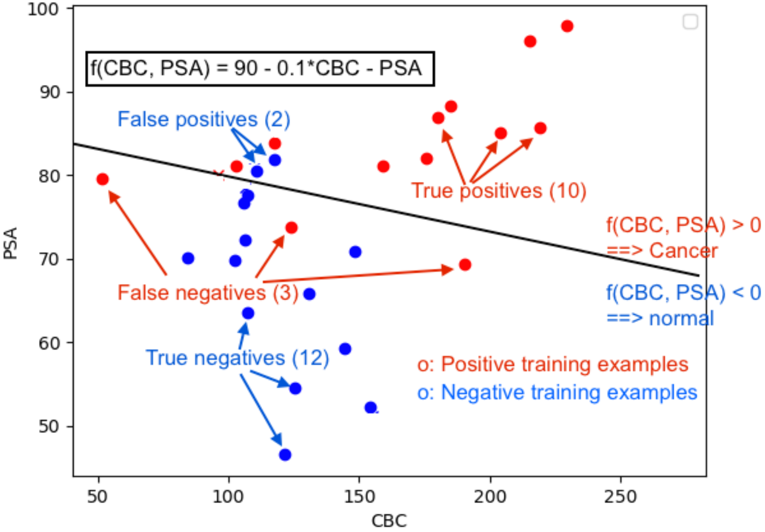
False negative (FN)

Positive example that is predicted to be negative

- A person who is predicted to not have cancer and but actually has cancer

More realistic data

Here: TP $= 10$, TN $= 12$, FP $= 2$, FN $= 3$.



Confusion matrices

Confusion matrix: A table describing the counts of TPs, FPs, TNs, and FNs

	Predicted positive	Predicted negative
Actual positive	TP = 10	FN = 3
Actual negative	FP = 2	TN = 12

In scikit-learn, we can get the confusion matrix for the SVC by:

```
from sklearn.metrics import confusion_matrix

clf = svm.SVC()
clf.fit(X_train, y_train)
preds = clf.predict(X_test)
tn, fp, fn, tp = confusion_matrix(y_test, preds).ravel()
```

True/false positive rates

Sensitivity: Pproportion of positive examples that are predicted to be positive

- Fraction of cancer patients who are predicted to have cancer

$$Sensitivity = \frac{TP}{TP + FN} = \frac{10}{10 + 3} = 77\%$$

Specificity: Proportion of negative examples that are predicted to be negative

- Fraction of healthy patients who are predicted to be healthy

$$Specificity = \frac{TN}{FP + TN} = \frac{12}{2 + 12} = 86\%$$

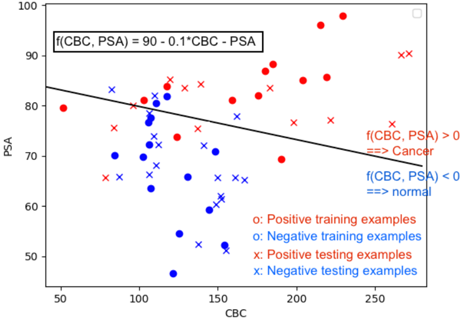
False-positive rate (FPR): Proportion of negative examples that are predicted to be positive

- Fraction of healthy patients who are predicted to have cancer

$$FPR = \frac{FP}{FP + TN} = 1 - specificity = \frac{2}{2 + 12} = 14\%$$

Accuracy on training vs testing sets

To get an unbiased estimation of the accuracy of a predictor, we need to evaluate it against our test data (not used for the training).



	Predicted positive	Predicted negative
Actual positive	TP $= 9$	FN $= 4$
Actual negative	FP $= 3$	TN $= 15$

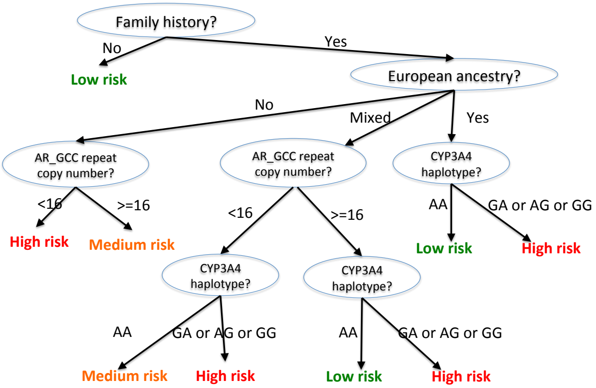
$Sens = \frac{TP}{TP+FN} = \frac{9}{9+4} = 69\%$, $FPR = \frac{FP}{FP+TN} = \frac{3}{3+15} = 17\%$

Decision tree

Linear classifiers are limited in how well they can match the training data.

Another type of classifier is called a decision tree.

http://scikit-learn.org/stable/modules/tree.html

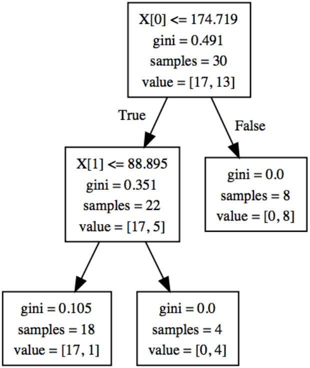


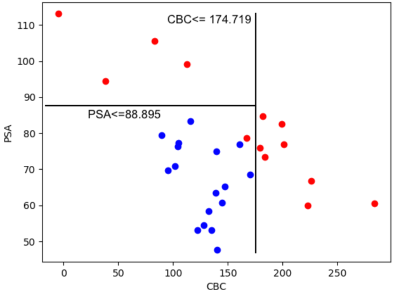
Decision tree in Python

Note: Requires installing graphviz by running "pip install graphviz"

```
import graphviz
from sklearn import model_selection
from sklearn.metrics import confusion_matrix
from sklearn import model_selection,tree

depth = 3
clf = tree.DecisionTreeClassifier(max_depth=depth)
clf.fit(X_train, y_train)
p_train = clf.predict(X_train)
p_test = clf.predict(X_test)

#plot tree
dot_data = tree.export_graphviz(clf, out_file=None)
graph = graphviz.Source(dot_data)
graph.render("prostate_tree_depth_"+str(depth))

# calculate training and testing error
tn,fp,fn,tp = confusion_matrix(y_train,p_train).ravel()
print("Training data:",tn,fp,fn,tp)
tn,fp,fn,tp = confusion_matrix(y_test,p_test).ravel()
print("Test data:",tn,fp,fn,tp)
```

Decision tree

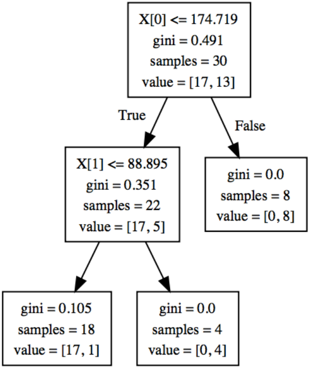


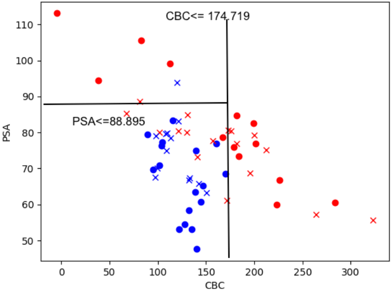


$$Sens = \frac{TP}{TP+FN} = \frac{12}{12+1} = 92\%, \; FPR = \frac{FP}{FP+TN} = \frac{0}{0+17} = 0\%$$

Great accuracy on training set!

Decision tree

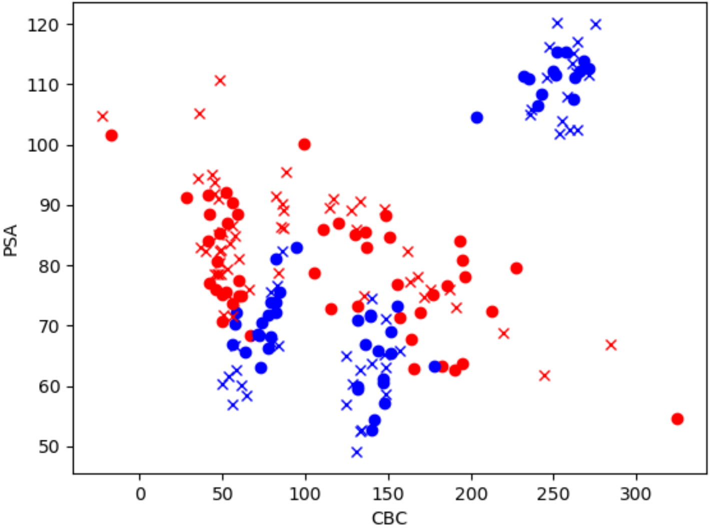




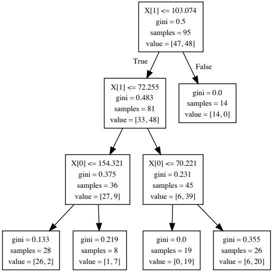
$$Sens = \frac{TP}{TP+FN} = \frac{9}{9+8} = 53\%, \ FPR = \frac{FP}{FP+TN} = \frac{1}{1+11} = 8\%$$

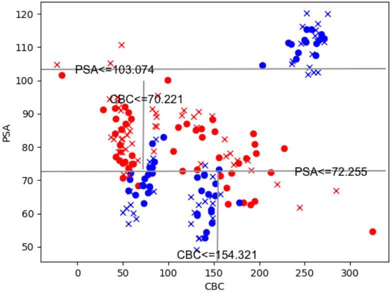
Not so good on the test set...

A harder example



Decision tree (max_depth = 3)

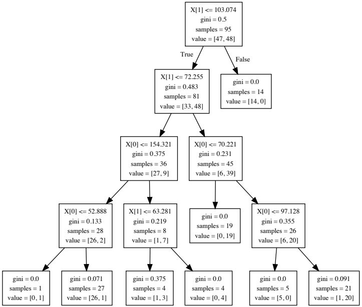


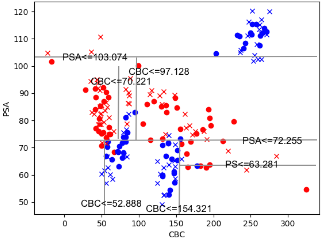


$$sens(train) = \frac{TP}{TP+FN} = \frac{41}{41+6} = 87\%,$$
$$FPR(train) = \frac{FP}{FP+TN} = \frac{9}{9+39} = 19\%$$

$$sens(test) = \frac{TP}{TP+FN} = \frac{36}{36+7} = 84\%,$$
$$FPR(test) = \frac{FP}{FP+TN} = \frac{8}{8+44} = 15\%$$

Deeper trees - max_depth = 4





$$sens(train) = \frac{TP}{TP+FN} = \frac{45}{45+2} = 96\%,$$
$$FPR(train) = \frac{FP}{FP+TN} = \frac{1}{1+47} = 2\%$$

$$sens(test) = \frac{TP}{TP+FN} = \frac{37}{37+6} = 86\%,$$
$$FPR(test) = \frac{FP}{FP+TN} = \frac{11}{11+41} = 21\%$$

Accuracy on training data is much higher than on testing data: overfitting! We've gone too far!

ML - closing comments

Very powerful algorithms exist and are available in scikit-learn:

- Decision trees and decision forests
- Support vector machines
- Neural networks
- etc. etc.

These algorithms can be used for classification / regression based on all kinds of data:

- Arrays of numerical values
- Images, video, sound
- Text
- etc. etc.

Applications in life sciences

- Medical diagnostic
- Interpretation of genetic data
- Drug design, optimization of medical devices
- Modeling of ecosystems
- etc. etc.

Experiment with different approaches/problems!