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:

<table>
<thead>
<tr>
<th>CBC</th>
<th>PSA</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>142</td>
<td>67</td>
<td>Normal</td>
</tr>
<tr>
<td>132</td>
<td>58</td>
<td>Normal</td>
</tr>
<tr>
<td>178</td>
<td>69</td>
<td>Cancer</td>
</tr>
<tr>
<td>188</td>
<td>46</td>
<td>Normal</td>
</tr>
<tr>
<td>183</td>
<td>68</td>
<td>Cancer</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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

\[ f(CBC, PSA) = 0.8 \times CBC - PSA - 20 \]

- \( f(CBC, PSA) > 0 \) \implies \text{Cancer}
- \( f(CBC, PSA) < 0 \) \implies \text{Normal}
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

<table>
<thead>
<tr>
<th>Predicted positive</th>
<th>Predicted negative</th>
</tr>
</thead>
<tbody>
<tr>
<td>Actual positive</td>
<td>TP = 10</td>
</tr>
<tr>
<td>Actual negative</td>
<td>FP = 2</td>
</tr>
<tr>
<td></td>
<td>FN = 3</td>
</tr>
<tr>
<td></td>
<td>TN = 12</td>
</tr>
</tbody>
</table>

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

```python
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**: Proportion 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).

<table>
<thead>
<tr>
<th>Actual positive</th>
<th>Predicted positive</th>
<th>Predicted negative</th>
</tr>
</thead>
<tbody>
<tr>
<td>TP = 9</td>
<td>FN = 4</td>
<td></td>
</tr>
<tr>
<td>FP = 3</td>
<td>TN = 15</td>
<td></td>
</tr>
</tbody>
</table>

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.
Decision tree in Python

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

```python
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	n, 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)
```
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

\[ \text{Sens} = \frac{TP}{TP + FN} = \frac{9}{9 + 8} = 53\% \]
\[ \text{FPR} = \frac{FP}{FP + TN} = \frac{1}{1 + 11} = 8\% \]

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

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

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

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!