Line H. Clemmensen
Section of Statistics and Data Analysis
DTU Compute

Exercises 02582
Module 2
Spring 2018

February 7, 2018

Topics: Model Selection

Resources for this exercise:

Listing 1: Resources in Matlab

```
Indices = crossvalind('Kfold', N, K); % create the random folds for CV
x_tr = x(Indices~=i,:); % the training data
trace(H); % trace of the matrix H
I = randi(N,M,1); % sample with replacement.
load silhouettes % load the data in silhouettes.mat (from CampusNet)
knn() % perform knn - file provided on CN
roc_gui.m % interface to play with Receiver Operator Curves (ROC)
```

Listing 2: Resources in R

```
library('cvTools') # load cvTools library (includes cvFolds)
folds <- cvFolds(n, K = 5, R = 1, type = "random") # folds for the CV
x_tr = x[folds$subsets[folds$which!=j],] # training data
library('psych') # load library psych (includes tr)
tr(H) # trace of the square matrix H
I = sample(1:n, size=n, replace = TRUE) # sample with replacement
library('class') # load library class (includes knn)
knn() # perform knn
```

Listing 3: Resources in Python

```python
import numpy as np
import matplotlib.pyplot as plt
import scipy.linalg as lng
import scipy.io
from sklearn.neighbors import KNeighborsClassifier
from sklearn.model_selection import train_test_split
from sklearn.metrics import roc_curve, auc

scipy.io.loadmat(path + '\\diabetes.mat') # load diabetes data
(i + 1) % K + 1 # use modulus K to get folds
np.random.permutation(N) # random permutation of N values
XTrain = X[i != I, :] # the training data
np.trace(outer) # trace of the matrix outer
np.random.randint(0, N, N) # sample with replacement.
scipy.io.loadmat(path + '\\Silhouettes.mat') # load silhouettes data
KNeighborsClassifier() # perform knn
```

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Exercises:

1 Perform model selection for ridge regression (for the diabetes data set):

(a) Consider using ridge-regression solutions for the diabetes data set. What is a suitable range for the shrinkage parameter λ in which to search for an optimal solution in? (Refer to question 1.3.b from last week)

(b) Select a suitable value for the regularization parameter using K-fold cross-validation. Plot the resulting optimal value of lambda on a plot of the parameter trace (i.e. a plot of the $\hat{\beta}_j$s as a function of λ).

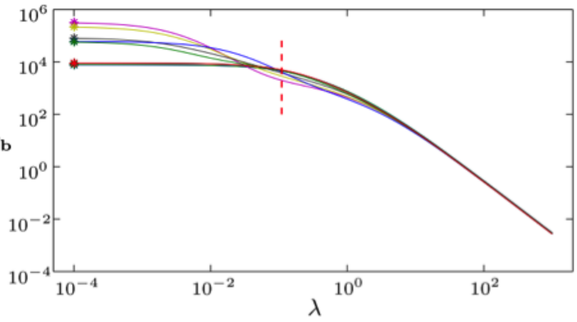
(i) Try one of the common choices $K = 5$ and $K = 10$, and run the cross-validation a couple of times. Which would you prefer and why?

(ii) What is the value of K corresponding to leave-one-out cross-validation?

(c) Find a suitable value of λ using the one-standard-error rule. What is the difference between the two strategies (cross-validation and cross-validation with one-standard-error-rule)?

(d) Select suitable values for the regularization parameter using the AIC and BIC criteria (cf. 7.5-7.7 in ESL). What are the advantages and disadvantages of using cross-validation vs. information criteria?

(e) Use the bootstrap to estimate the variance of the parameters of the solution (β) for each value of lambda in exercise 1a. Plot the variance estimates as a function of lambda. A plot of the analytical variances is seen below and can be used for



comparison.

2 Perform model selection for KNN classification (for the silhouette data):

(a) Load the dataset and plot the silhouettes.

(i) Matlab hint: Plot the silhouettes using `plot(Xa(:,1:65)', Xa(:,66:end)', '-')`. The variables Male and Fem contain row indices to male and female silhouettes.

(ii) R hint: Plot the silhouettes using `plot(X[1,1:65], X[1,66:p], type='l')`. The variable class contains information on whether it is a male or female silhouette.

(iii) Python hint: Plot the silhouettes using `plot(Xa[Fem,:65].T, Xa[Fem, 65:].T)`. The variables Male and Fem contain row indices to male and female silhouettes (with some adjustment, mat['Fem'].ravel() - 1, from Matlab indexing).

(b) What size of fold would you use for cross-validation for the silhouette data set? Why?

(c) Select a suitable number K for KNN classification on the silhouette profiles data using leave-one-out cross-validation.

3 Use the receiver operator curve (ROC) and determine specificity and sensitivity (currently only has a solution and help files in Matlab):

(a) Make a function `[sens, spec] = roc_data( y, y_true, cut)` that takes as input the estimated response y, the true response y_{true} and the cut off value *cut*, and outputs the sensitivity and specificity.

(i) Matlab hint: `function [sens spec] = roc_data(y, y_true, cut)`.

(ii) R hint: The gui is currently not available in R (but calculate sensitivity and specificity anyway).

(iii) Python hint: The gui is currently not available in Python (but calculate sensitivity and specificity anyway).

(iv) General hint: compute TP, TN, FP and FN. From there, sensitivity and specificity is easily computed.

(b) Run the function `roc_gui.m` which takes your `roc_data` function as input. The output plot illustrates the data for the next exercise, and gives you a tool to adjust the cut off value for the classification rule, which is also plotted in the figure.

(c) Assume you are developing a mammography system for General Electrics, and that the GUI is showing the two features you have extracted to find suspicious image regions. GE has ordered the system to have a sensitivity of 95% to make sure very few lesions go undetected. Discuss this solution with your mates. What are you sacrificing to get such a sensitive system? Which sensitivity would you recommend based on the given data?

End of exercise