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Cross-Validation

> **Summary:** Cross-Validation for Parameter Tuning, Model Selection, and Feature Selection

Topics

1. Review of model evaluation procedures
2. Steps for K-fold cross-validation
3. Comparing cross-validation to train/test split
4. Cross-validation recommendations
5. Cross-validation example: parameter tuning
6. Cross-validation example: model selection
7. Cross-validation example: feature selection
8. Improvements to cross-validation
9. Resources

This tutorial is derived from Data School's Machine Learning with scikit-learn tutorial. I added my own notes so anyone, including myself, can refer to this tutorial without watching the videos.

1. Review of model evaluation procedures

Motivation: Need a way to choose between machine learning models

- Goal is to estimate likely performance of a model on **out-of-sample data**

Initial idea: Train and test on the same data

- But, maximizing **training accuracy** rewards overly complex models which **overfit** the training data

Alternative idea: Train/test split

- Split the dataset into two pieces, so that the model can be trained and tested on **different data**
- **Testing accuracy** is a better estimate than training accuracy of out-of-sample performance
- Problem with train/test split
    - It provides a **high variance** estimate since changing which observations happen to be in the testing set can significantly change testing accuracy
    - Testing accuracy can change a lot depending on a which observation happen to be in the testing set

In [1]:
```
from sklearn.datasets import load_iris
from sklearn.cross_validation import train_test_split
from sklearn.neighbors import KNeighborsClassifier
from sklearn import metrics
```

In [2]:
```
# read in the iris data
iris = load_iris()

# create X (features) and y (response)
X = iris.data
y = iris.target
```

In [3]:
```
# use train/test split with different random_state values
# we can change the random_state values that changes the accuracy scores
# the accuracy changes a lot
# this is why testing accuracy is a high-variance estimate
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=6)

# check classification accuracy of KNN with K=5
knn = KNeighborsClassifier(n_neighbors=5)
knn.fit(X_train, y_train)
y_pred = knn.predict(X_test)
metrics.accuracy_score(y_test, y_pred)
```

Out[3]:
```
0.97368421052631582
```

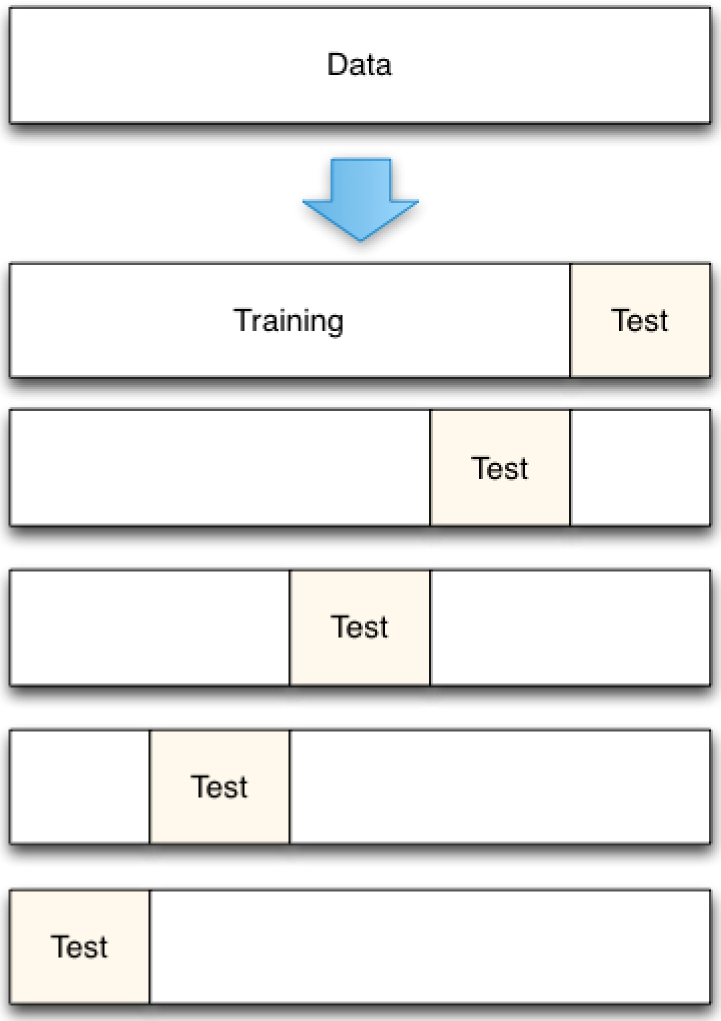
Question: What if we created a bunch of train/test splits, calculated the testing accuracy for each, and averaged the results together?

Answer: That's the essense of cross-validation!

2. Steps for K-fold cross-validation

1. Split the dataset into K **equal** partitions (or "folds")
    - So if k = 5 and dataset has 150 observations
    - Each of the 5 folds would have 30 observations
2. Use fold 1 as the **testing set** and the union of the other folds as the **training set**
    - Testing set = 30 observations (fold 1)
    - Training set = 120 observations (folds 2-5)
3. Calculate **testing accuracy**
4. Repeat steps 2 and 3 K times, using a **different fold** as the testing set each time
    - We will repeat the process 5 times
    - 2nd iteration
        - fold 2 would be the testing set
        - union of fold 1, 3, 4, and 5 would be the training set
    - 3rd iteration
        - fold 3 would be the testing set
        - union of fold 1, 2, 4, and 5 would be the training set
    - And so on...
5. Use the **average testing accuracy** as the estimate of out-of-sample accuracy

Diagram of **5-fold cross-validation:**



In [4]:
```
# simulate splitting a dataset of 25 observations into 5 folds
from sklearn.cross_validation import KFold
kf = KFold(25, n_folds=5, shuffle=False)


# print the contents of each training and testing set
# ^ - forces the field to be centered within the available space
# .format() - formats the string similar to %s or %n
# enumerate(sequence, start=0) - returns an enumerate object
print('{} {:^61} {}'.format('Iteration', 'Training set obsevations', 'Testing set observations'))
for iteration, data in enumerate(kf, start=1):
    print('{!s:^9} {} {!s:^25}'.format(iteration, data[0], data[1]))
```

```
Iteration                   Training set obsevations                   Testing set observations
    1     [ 5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24]        [0 1 2 3 4]
    2     [ 0  1  2  3  4 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24]        [5 6 7 8 9]
    3     [ 0  1  2  3  4  5  6  7  8  9 15 16 17 18 19 20 21 22 23 24]     [10 11 12 13 14]
    4     [ 0  1  2  3  4  5  6  7  8  9 10 11 12 13 14 20 21 22 23 24]     [15 16 17 18 19]
    5     [ 0  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19]     [20 21 22 23 24]
```

- Dataset contains **25 observations** (numbered 0 through 24)
- 5-fold cross-validation, thus it runs for **5 iterations**
- For each iteration, every observation is either in the training set or the testing set, **but not both**
- Every observation is in the testing set **exactly once**

3. Comparing cross-validation to train/test split

Advantages of **cross-validation:**

- More accurate estimate of out-of-sample accuracy
- More "efficient" use of data
    - This is because every observation is used for both training and testing

Advantages of **train/test split:**

- Runs K times faster than K-fold cross-validation
    - This is because K-fold cross-validation repeats the train/test split K-times
- Simpler to examine the detailed results of the testing process

4. Cross-validation recommendations

1. K can be any number, but **K=10** is generally recommended
    - This has been shown experimentally to produce the best out-of-sample estimate
2. For classification problems, **stratified sampling** is recommended for creating the folds
    - Each response class should be represented with equal proportions in each of the K folds
        - If dataset has 2 response classes
            - Spam/Ham
            - 20% observation = ham
            - Each cross-validation fold should consist of exactly 20% ham
    - scikit-learn's `cross_val_score` function does this by default

5. Cross-validation example: parameter tuning

Goal: Select the best tuning parameters (aka "hyperparameters") for KNN on the iris dataset

- We want to choose the best tuning parameters that best generalize the data

In [5]:
```
from sklearn.cross_validation import cross_val_score
```

In [6]:
```
# 10-fold cross-validation with K=5 for KNN (the n_neighbors parameter)
# k = 5 for KNeighborsClassifier
knn = KNeighborsClassifier(n_neighbors=5)

# Use cross_val_score function
# We are passing the entirety of X and y, not X_train or y_train, it takes care of splitting the dat
# cv=10 for 10 folds
# scoring='accuracy' for evaluation metric - althought they are many
scores = cross_val_score(knn, X, y, cv=10, scoring='accuracy')
print(scores)
```

```
[ 1.          0.93333333  1.          1.          0.86666667  0.93333333
  0.93333333  1.          1.          1.        ]
```

- In the first iteration, the accuracy is 100%
- Second iteration, the accuracy is 93% and so on

cross_val_score executes the first 4 steps of k-fold cross-validation steps which I have broken down to 7 steps here in detail

1. Split the dataset (X and y) into K=10 **equal** partitions (or "folds")
2. Train the KNN model on union of folds 2 to 10 (training set)
3. Test the model on fold 1 (testing set) and calculate testing accuracy
4. Train the KNN model on union of fold 1 and fold 3 to 10 (training set)
5. Test the model on fold 2 (testing set) and calculate testing accuracy
6. It will do this on 8 more times
7. When finished, it will return the 10 testing accuracy scores as a numpy array

In [7]:
```
# use average accuracy as an estimate of out-of-sample accuracy
# numpy array has a method mean()
print(scores.mean())
```

```
0.966666666667
```

Our goal here is to find the optimal value of K

In [8]:
```
# search for an optimal value of K for KNN

# range of k we want to try
k_range = range(1, 31)
# empty list to store scores
k_scores = []

# 1. we will loop through reasonable values of k
for k in k_range:
    # 2. run KNeighborsClassifier with k neighbours
    knn = KNeighborsClassifier(n_neighbors=k)
    # 3. obtain cross_val_score for KNeighborsClassifier with k neighbours
    scores = cross_val_score(knn, X, y, cv=10, scoring='accuracy')
    # 4. append mean of scores for k neighbors to k_scores list
    k_scores.append(scores.mean())


print(k_scores)
```

```
[0.95999999999999996, 0.95333333333333337, 0.96666666666666656, 0.96666666666666656, 0.96666666666666679, 0.966666
66666666679, 0.96666666666666679, 0.96666666666666679, 0.97333333333333338, 0.96666666666666679, 0.966666666666666
79, 0.97333333333333338, 0.98000000000000009, 0.97333333333333338, 0.97333333333333338, 0.97333333333333338, 0.973
33333333333338, 0.98000000000000009, 0.97333333333333338, 0.98000000000000009, 0.96666666666666656, 0.966666666666
66656, 0.97333333333333338, 0.95999999999999996, 0.96666666666666656, 0.95999999999999996, 0.96666666666666656, 0.
95333333333333337, 0.95333333333333337, 0.95333333333333337]
```

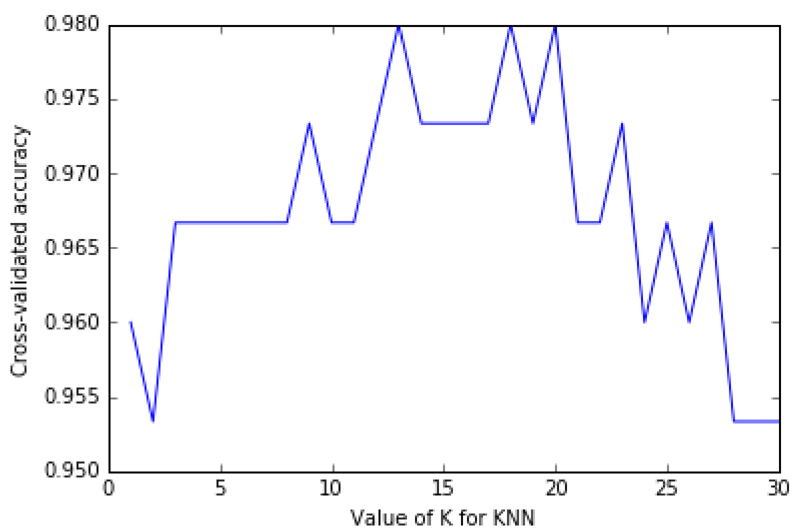
In [9]:
```
# in essence, this is basically running the k-fold cross-validation method 30 times because we want to run through K values from 1 to 30
# we should have 30 scores here
print('Length of list', len(k_scores))
print('Max of list', max(k_scores))
```

```
Length of list 30
Max of list 0.98
```

In [10]:
```
# plot how accuracy changes as we vary k
import matplotlib.pyplot as plt
%matplotlib inline

# plot the value of K for KNN (x-axis) versus the cross-validated accuracy (y-axis)
# plt.plot(x_axis, y_axis)
plt.plot(k_range, k_scores)
plt.xlabel('Value of K for KNN')
plt.ylabel('Cross-validated accuracy')
```

Out[10]:
```
<matplotlib.text.Text at 0x111cb07b8>
```



The maximum cv accuracy occurs from k=13 to k=20

- The general shape of the curve is an upside down yield
  - This is quite typical when examining the model complexity and accuracy
  - This is an example of bias-variance trade off
    - Low values of k (low bias, high variance)
      - The 1-Nearest Neighbor classifier is the most complex nearest neighbor model
      - It has the most jagged decision boundary, and is most likely to overfit
    - High values of k (high bias, low variance)
      - underfit
    - Best value is the middle of k (most likely to generalize out-of-sample data)
      - just right
- The best value of k
  - Higher values of k produce less complex model
    - So we will choose 20 as our best KNN model

6. Cross-validation example: model selection

Goal: Compare the best KNN model with logistic regression on the iris dataset

In [11]:
```
# 10-fold cross-validation with the best KNN model
knn = KNeighborsClassifier(n_neighbors=20)

# Instead of saving 10 scores in object named score and calculating mean
# We're just calculating the mean directly on the results
print(cross_val_score(knn, X, y, cv=10, scoring='accuracy').mean())
```

```
0.98
```

In [12]:
```
# 10-fold cross-validation with logistic regression
from sklearn.linear_model import LogisticRegression
logreg = LogisticRegression()
print(cross_val_score(logreg, X, y, cv=10, scoring='accuracy').mean())
```

```
0.953333333333
```

We can conclude that KNN is likely a better choice than logistic regression

7. Cross-validation example: feature selection

Goal: Select whether the Newspaper feature should be included in the linear regression model on the advertising dataset

In [13]:
```
import pandas as pd
import numpy as np
from sklearn.linear_model import LinearRegression
```

In [14]:

```
# read in the advertising dataset
data = pd.read_csv('http://www-bcf.usc.edu/~gareth/ISL/Advertising.csv (http://www-bcf.usc.edu/~gareth/ISL/Advertising.csv)', i
ndex_col=0)
```

In [15]:

```
# create a Python list of three feature names
feature_cols = ['TV', 'Radio', 'Newspaper']

# use the list to select a subset of the DataFrame (X)
X = data[feature_cols]

# select the Sales column as the response (y)
# since we're selecting only one column, we can select the attribute using .attribute
y = data.Sales
```

In [16]:

```
# 10-fold cross-validation with all three features
# instantiate model
lm = LinearRegression()

# store scores in scores object
# we can't use accuracy as our evaluation metric since that's only relevant for classification problems
# RMSE is not directly available so we will use MSE
scores = cross_val_score(lm, X, y, cv=10, scoring='mean_squared_error')
print(scores)
```

```
[-3.56038438 -3.29767522 -2.08943356 -2.82474283 -1.3027754  -1.74163618
 -8.17338214 -2.11409746 -3.04273109 -2.45281793]
```

MSE should be positive

- But why is the MSE here negative?
- MSE is a loss function
    - It is something we want to minimize
    - A design decision was made so that the results are made negative
    - The best results would be the largest number (the least negative) so we can still maximize similar to classification accuracy
- Classification Accuracy is a reward function
    - It is something we want to maximize

In [17]:
```
# fix the sign of MSE scores
mse_scores = -scores
print(mse_scores)
```

```
[ 3.56038438  3.29767522  2.08943356  2.82474283  1.3027754   1.74163618
  8.17338214  2.11409746  3.04273109  2.45281793]
```

In [18]:
```
# convert from MSE to RMSE
rmse_scores = np.sqrt(mse_scores)
print(rmse_scores)
```

```
[ 1.88689808  1.81595022  1.44548731  1.68069713  1.14139187  1.31971064
  2.85891276  1.45399362  1.7443426   1.56614748]
```

In [19]:
```
# calculate the average RMSE
print(rmse_scores.mean())
```

```
1.69135317081
```

In [20]:
```
# 10-fold cross-validation with two features (excluding Newspaper)
feature_cols = ['TV', 'Radio']
X = data[feature_cols]
print(np.sqrt(-cross_val_score(lm, X, y, cv=10, scoring='mean_squared_error')).mean())
```

```
1.67967484191
```

Without Newspaper

- Average RMSE = 1.68
- lower number than with model with Newspaper
    - RMSE is something we want to minimize
    - So the model excluding Newspaper is a better model

8. Improvements to cross-validation

Repeated cross-validation

- Repeat cross-validation multiple times (with **different random splits** of the data) and average the results
- More reliable estimate of out-of-sample performance by **reducing the variance** associated with a single trial of cross-validation

Creating a hold-out set

- "Hold out" a portion of the data **before** beginning the model building process
- Locate the best model using cross-validation on the remaining data, and test it **using the hold-out set**
- More reliable estimate of out-of-sample performance since hold-out set is **truly out-of-sample**

Feature engineering and selection within cross-validation iterations

- Normally, feature engineering and selection occurs **before** cross-validation
- Instead, perform all feature engineering and selection **within each cross-validation iteration**
- More reliable estimate of out-of-sample performance since it **better mimics** the application of the model to out-of-sample data

9. Resources

- scikit-learn documentation: Cross-validation (http://scikit-learn.org/stable/modules/cross_validation.html), Model evaluation (http://scikit-learn.org/stable/modules/model_evaluation.html)
- scikit-learn issue on GitHub: MSE is negative when returned by cross_val_score (https://github.com/scikit-learn/scikit-learn/issues/2439)
- Section 5.1 of An Introduction to Statistical Learning (http://www-bcf.usc.edu/~gareth/ISL/) (11 pages) and related videos: K-fold and leave-one-out cross-validation (https://www.youtube.com/watch?v=nZAM5OXrktY) (14 minutes), Cross-validation the right and wrong ways (https://www.youtube.com/watch?v=S06JpVoNaA0) (10 minutes)
- Scott Fortmann-Roe: Accurately Measuring Model Prediction Error (http://scott.fortmann-roe.com/docs/MeasuringError.html)
- Machine Learning Mastery: An Introduction to Feature Selection (http://machinelearningmastery.com/an-introduction-to-feature-selection/)
- Harvard CS109: Cross-Validation: The Right and Wrong Way (https://github.com/cs109/content/blob/master/lec_10_cross_val.ipynb)
- Journal of Cheminformatics: Cross-validation pitfalls when selecting and assessing regression and classification models (http://www.jcheminf.com/content/pdf/1758-2946-6-10.pdf)

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KELVIN TAN • a year ago

I am using Python 3.6, and having this error:
C:\Users\xxx\Anaconda3\lib\site-packages\sklearn\metrics\scorer.py:100: DeprecationWarning: Scoring method mean_squared_error was renamed to neg_mean_squared_error in version 0.18 and will be removed in 0.20.
sample_weight=sample_weight)
when run the line:
scores = cross_val_score(lm, X, y, cv=10, scoring='mean_squared_error'), so I change to
scores = cross_val_score(lm, X, y, cv=10, scoring='neg_mean_squared_error'), and it works.

also 'Radio' should be 'radio' and 'Newspaper' should be 'newspaper'.
y = data.Sales should be y = data.sales

Can you also explain why 31 in
k_range = range(1, 31) ?

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