Cross-validation for parameter tuning, model selection, and feature selection (video #7)

Created by Data School. Watch all 9 videos on YouTube. Download the notebooks from GitHub.

Note: This notebook uses Python 3.6 and scikit-learn 0.19.1. The original notebook (shown in the video) used Python 2.7 and scikit-learn 0.16, and can be downloaded from the archive branch.

Agenda

- What is the drawback of using the **train/test split** procedure for model evaluation?
- How does **K-fold cross-validation** overcome this limitation?
- How can cross-validation be used for selecting **tuning parameters**, choosing between **models**, and selecting **features**?
- What are some possible **improvements** to cross-validation?

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
- But, it provides a **high variance** estimate since changing which observations happen to be in the testing set can significantly change testing accuracy

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

In [ ]:
```
# read in the iris data
```

```
iris = load_iris()

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

In [ ]:
```
# use train/test split with different random_state values
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=4)

# 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)
print(metrics.accuracy_score(y_test, y_pred))
```

```
0.9736842105263158
```

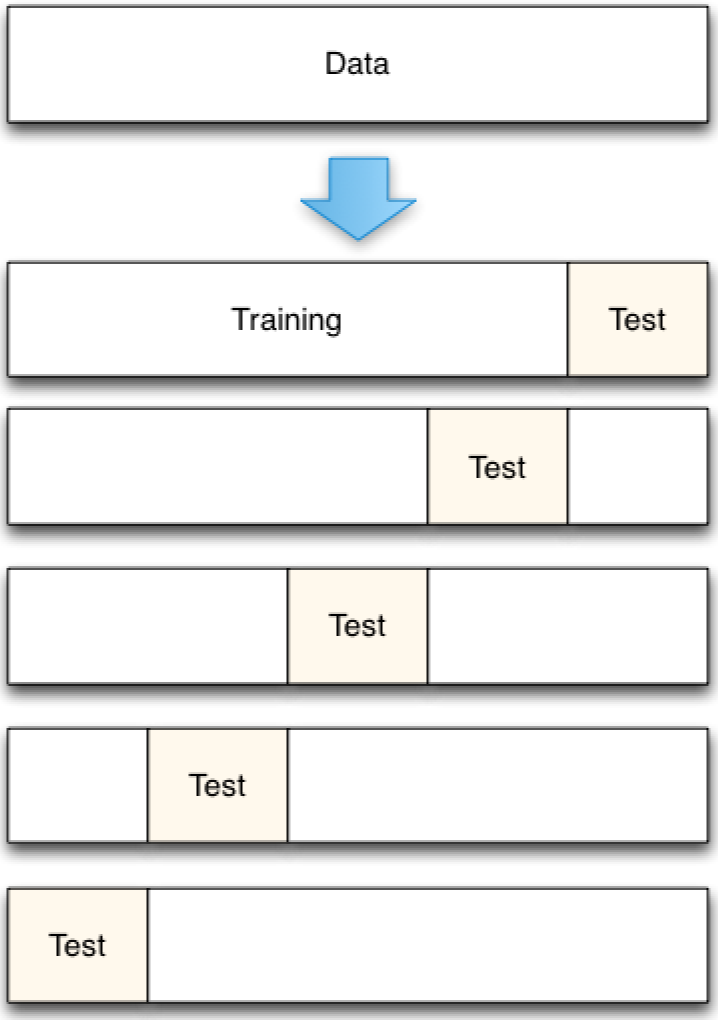
Question: What if we created a bunch of train/test splits, calculated the testing accuracy for each, and averaged the results together?

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

Steps for K-fold cross-validation

1. Split the dataset into K **equal** partitions (or "folds").
2. Use fold 1 as the **testing set** and the union of the other folds as the **training set**.
3. Calculate **testing accuracy**.
4. Repeat steps 2 and 3 K times, using a **different fold** as the testing set each time.
5. Use the **average testing accuracy** as the estimate of out-of-sample accuracy.

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



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

# print the contents of each training and testing set
print('{} {:^61} {}'.format('Iteration', 'Training set observations', 'Testi
for iteration, data in enumerate(kf, start=1):
    print('{:^9} {} {:^25}'.format(iteration, data[0], str(data[1])))
```

```
Iteration                    Training set observations                   Tes
ting 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**

Comparing cross-validation to train/test split

Advantages of **cross-validation:**

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

Advantages of **train/test split:**

- Runs K times faster than K-fold cross-validation
- Simpler to examine the detailed results of the testing process

Cross-validation recommendations

1. K can be any number, but **K=10** is generally recommended
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
   - scikit-learn's `cross_val_score` function does this by default

Cross-validation example: parameter tuning

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

In [ ]:
```
from sklearn.model_selection import cross_val_score
```

In [ ]:
```
# 10-fold cross-validation with K=5 for KNN (the n_neighbors parameter)
knn = KNeighborsClassifier(n_neighbors=5)
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 [ ]:
```
# use average accuracy as an estimate of out-of-sample accuracy
print(scores.mean())
```

```
0.9666666666666668
```

In [ ]:
```
# search for an optimal value of K for KNN
k_range = list(range(1, 31))
```

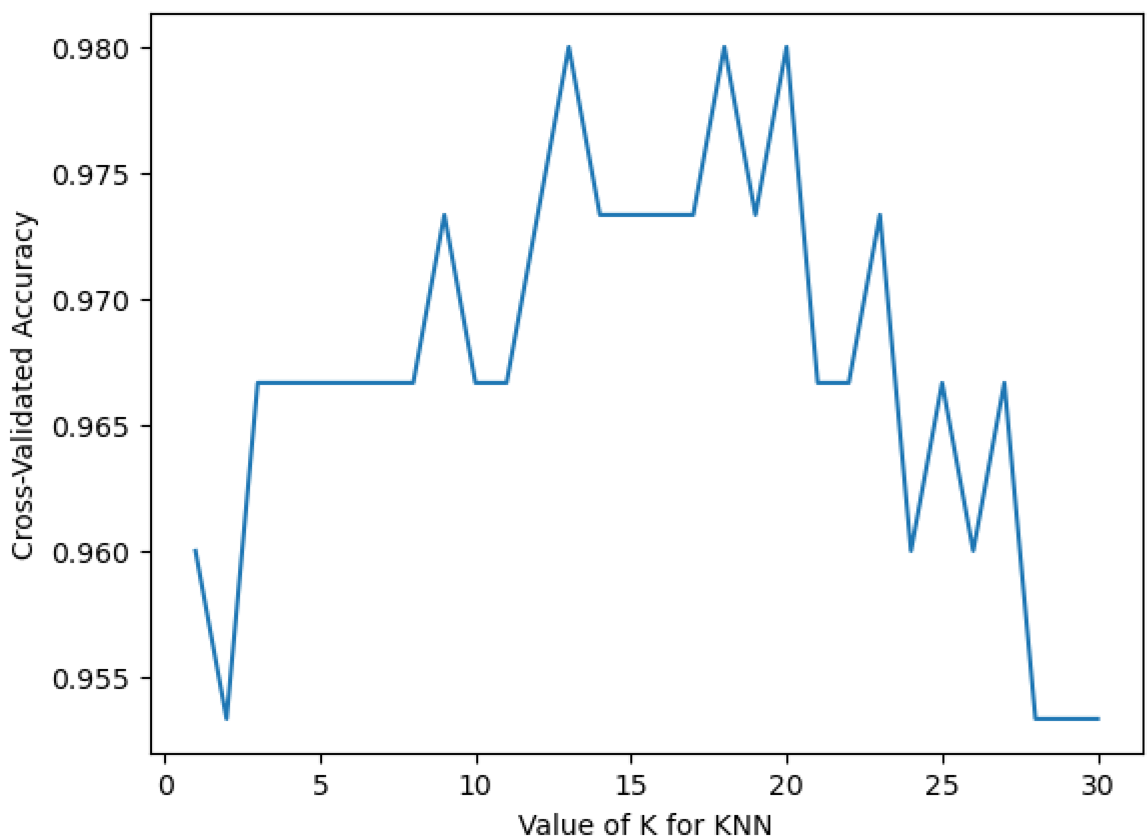
```
k_scores = []
for k in k_range:
    knn = KNeighborsClassifier(n_neighbors=k)
    scores = cross_val_score(knn, X, y, cv=10, scoring='accuracy')
    k_scores.append(scores.mean())
print(k_scores)
```

```
[0.96, 0.9533333333333334, 0.9666666666666666, 0.9666666666666666, 0.966666
6666666668, 0.9666666666666668, 0.9666666666666668, 0.9666666666666668, 0.9
733333333333334, 0.9666666666666668, 0.9666666666666668, 0.973333333333333
4, 0.9800000000000001, 0.9733333333333334, 0.9733333333333334, 0.9733333333
333334, 0.9733333333333334, 0.9800000000000001, 0.9733333333333334, 0.98000
00000000001, 0.9666666666666666, 0.9666666666666666, 0.9733333333333334, 0.
96, 0.9666666666666666, 0.96, 0.9666666666666666, 0.9533333333333334, 0.953
3333333333334, 0.9533333333333334]
```

In [ ]:
```
import matplotlib.pyplot as plt
%matplotlib inline

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

Out[ ]:
```
Text(0, 0.5, 'Cross-Validated Accuracy')
```



Cross-validation example: model selection

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

In [ ]:
```
# 10-fold cross-validation with the best KNN model
knn = KNeighborsClassifier(n_neighbors=20)
print(cross_val_score(knn, X, y, cv=10, scoring='accuracy').mean())
```

```
0.9800000000000001
```

In [ ]:
```
# 10-fold cross-validation with logistic regression
from sklearn.linear_model import LogisticRegression
logreg = LogisticRegression(max_iter=1000)
print(cross_val_score(logreg, X, y, cv=10, scoring='accuracy').mean())
```

```
0.9733333333333334
```

Cross-validation example: feature selection

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

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

In [ ]:
```
# read in the advertising dataset
data = pd.read_csv('data/Advertising.csv', index_col=0)
```

In [ ]:
```
# 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)
y = data.Sales
```

In [ ]:
```
# 10-fold cross-validation with all three features
lm = LinearRegression()
scores = cross_val_score(lm, X, y, cv=10, scoring='neg_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]
```

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

```
1.6913531708051797
```

In [ ]:
```
# 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='neg_mean_squared_er
```

```
1.6796748419090768
```

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

Resources

- scikit-learn documentation: Cross-validation, Model evaluation
- scikit-learn issue on GitHub: MSE is negative when returned by cross_val_score
- Section 5.1 of An Introduction to Statistical Learning (11 pages) and related videos: K-fold and leave-one-out cross-validation (14 minutes), Cross-validation the right and wrong ways (10 minutes)
- Scott Fortmann-Roe: Accurately Measuring Model Prediction Error

- Machine Learning Mastery: An Introduction to Feature Selection
- Harvard CS109: Cross-Validation: The Right and Wrong Way
- Journal of Cheminformatics: Cross-validation pitfalls when selecting and assessing regression and classification models

Comments or Questions?

- Email: kevin@dataschool.io
- Website: http://dataschool.io
- Twitter: @justmarkham

In [ ]:
```
from IPython.core.display import HTML
def css_styling():
    styles = open("styles/custom.css", "r").read()
    return HTML(styles)
css_styling()
```

Out[ ]: