KNN Algorithm (In Depth - Hands-on)

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1. Evaluation procedure 1 - Train and test on the entire dataset

1. Train the model on the **entire dataset**.
2. Test the model on the **same dataset**, and evaluate how well we did by comparing the **predicted** response values with the **true** response values.

In [1]:
```
# read in the iris data
from sklearn.datasets import load_iris
iris = load_iris()

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

1a. Logistic regression

In [2]:
```
# import the class
from sklearn.linear_model import LogisticRegression

# instantiate the model (using the default parameters)
logreg = LogisticRegression()

# fit the model with data
logreg.fit(X, y)

# predict the response values for the observations in X
logreg.predict(X)
```

Out[2]:
```
array([0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 2, 1, 1,
       1, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 2, 2, 2, 1, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 1, 1, 1, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 1, 2, 2, 2, 2, 2, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2])
```

In [3]:
```
# store the predicted response values
y_pred = logreg.predict(X)

# check how many predictions were generated
len(y_pred)
```

Out[3]: 150

Classification accuracy:

- **Proportion** of correct predictions
- Common **evaluation metric** for classification problems

In [4]:
```
# compute classification accuracy for the logistic regression model
from sklearn import metrics

print(metrics.accuracy_score(y, y_pred))
```

```
0.96
```

- Known as **training accuracy** when you train and test the model on the same data
- 96% of our predictions are correct

1b. KNN (K=5)

In [5]:
```
from sklearn.neighbors import KNeighborsClassifier
knn = KNeighborsClassifier(n_neighbors=5)
knn.fit(X, y)
y_pred = knn.predict(X)
print(metrics.accuracy_score(y, y_pred))
```

```
0.966666666667
```

It seems, there is a higher accuracy here but there is a big issue of testing on your training data

1c. KNN (K=1)

In [6]:
```
knn = KNeighborsClassifier(n_neighbors=1)
knn.fit(X, y)
y_pred = knn.predict(X)
print(metrics.accuracy_score(y, y_pred))
```

```
1.0
```

- KNN model
    1. Pick a value for K.
    2. Search for the K observations in the training data that are "nearest" to the measurements of the unknown iris
    3. Use the most popular response value from the K nearest neighbors as the predicted response value for the unknown iris
- This would always have 100% accuracy, because we are testing on the exact same data, it would always make correct predictions
- KNN would search for one nearest observation and find that exact same observation
    - KNN has memorized the training set
    - Because we testing on the exact same data, it would always make the same prediction

1d. Problems with training and testing on the same data

- Goal is to estimate likely performance of a model on **out-of-sample data**
- But, maximizing training accuracy rewards **overly complex models** that won't necessarily generalize
- Unnecessarily complex models **overfit** the training data

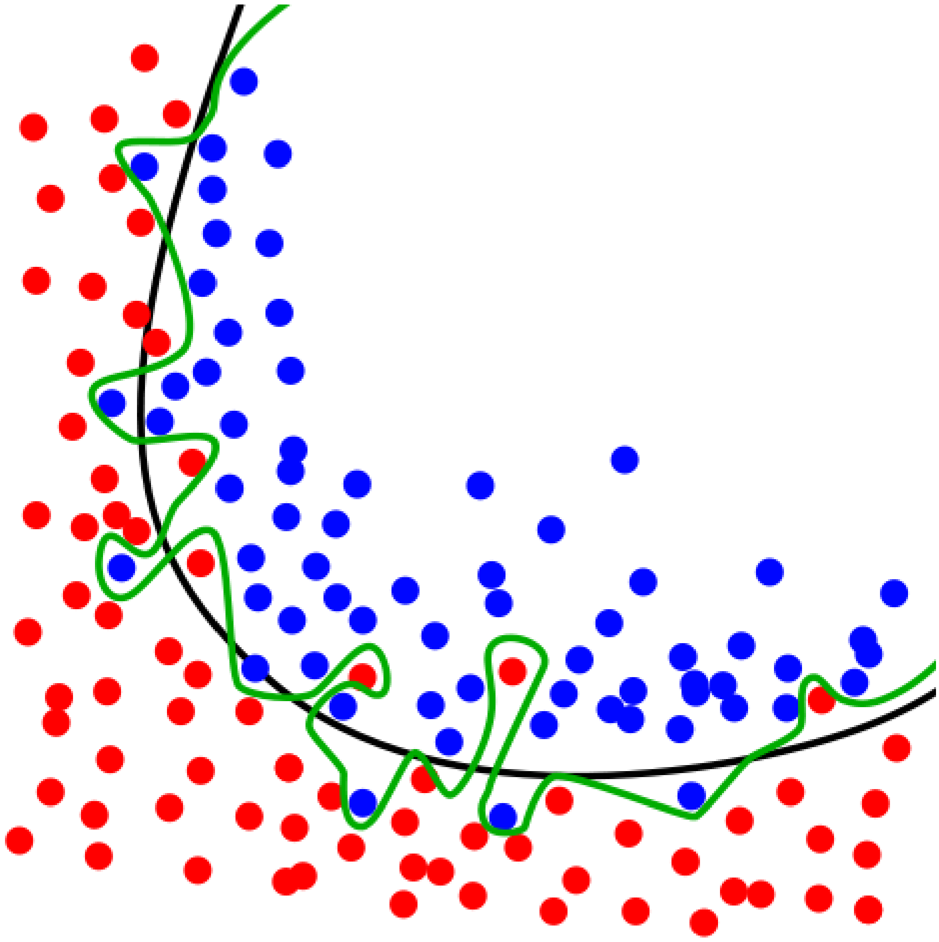


Image Credit: *[Overfitting](http://commons.wikimedia.org/wiki/File:Overfitting.svg#/media/File:Overfitting.svg)* (http://commons.wikimedia.org/wiki/File:Overfitting.svg#/media/File:Overfitting.svg) *by Chabacano. Licensed under GFDL via Wikimedia Commons.*

- Green line (decision boundary): overfit
  - Your accuracy would be high but may not generalize well for future observations
  - Your accuracy is high because it is perfect in classifying your training data but not out-of-sample data
- Black line (decision boundary): just right
  - Good for generalizing for future observations
- Hence we need to solve this issue using a **train/test split** that will be explained below

2. Evaluation procedure 2 - Train/test split

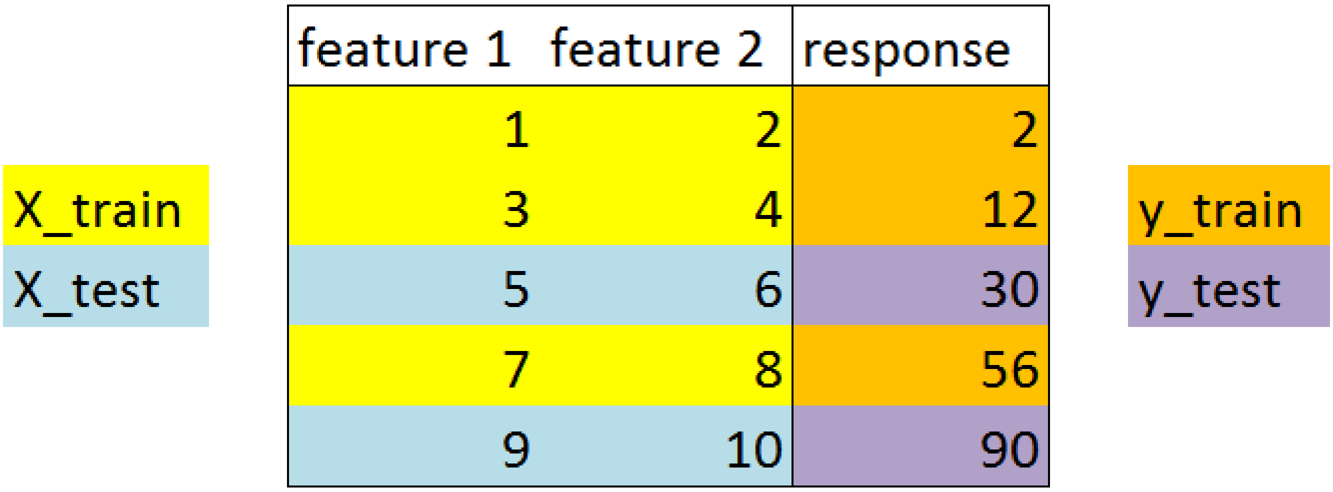
1. Split the dataset into two pieces: a **training set** and a **testing set**.
2. Train the model on the **training set**.
3. Test the model on the **testing set**, and evaluate how well we did.

In [7]:
```
# print the shapes of X and y
# X is our features matrix with 150 x 4 dimension
print(X.shape)
# y is our response vector with 150 x 1 dimension
print(y.shape)
```

```
(150, 4)
(150,)
```

In [8]:
```
# STEP 1: split X and y into training and testing sets
from sklearn.cross_validation import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.4, random_
state=4)
```

- test_size=0.4
    - 40% of observations to test set
    - 60% of observations to training set
- data is randomly assigned unless you use random_state hyperparameter
    - If you use random_state=4
        - Your data will be split exactly the same way



What did this accomplish?

- Model can be trained and tested on **different data**
- Response values are known for the testing set, and thus **predictions can be evaluated**
- **Testing accuracy** is a better estimate than training accuracy of out-of-sample performance

In [9]:
```
# print the shapes of the new X objects
print(X_train.shape)
print(X_test.shape)
```

```
(90, 4)
(60, 4)
```

In [10]:
```
# print the shapes of the new y objects
print(y_train.shape)
print(y_test.shape)
```

```
(90,)
(60,)
```

In [11]:
```
# STEP 2: train the model on the training set
logreg = LogisticRegression()
logreg.fit(X_train, y_train)
```

Out[11]:
```
LogisticRegression(C=1.0, class_weight=None, dual=False, fit_intercept=True,
          intercept_scaling=1, max_iter=100, multi_class='ovr', n_jobs=1,
          penalty='l2', random_state=None, solver='liblinear', tol=0.0001,
          verbose=0, warm_start=False)
```

In [12]:
```
# STEP 3: make predictions on the testing set
y_pred = logreg.predict(X_test)

# compare actual response values (y_test) with predicted response values (y_pre
d)
print(metrics.accuracy_score(y_test, y_pred))
```

```
0.95
```

Repeat for KNN with K=5:

In [13]:
```
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))
```

```
0.966666666667
```

Repeat for KNN with K=1:

In [14]:
```
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))
```

```
0.966666666667
```

Can we locate an even better value for K?

In [15]:
```
# try K=1 through K=25 and record testing accuracy
k_range = range(1, 26)

# We can create Python dictionary using [] or dict()
scores = []

# We use a loop through the range 1 to 26
# We append the scores in the dictionary
for k in k_range:
    knn = KNeighborsClassifier(n_neighbors=k)
    knn.fit(X_train, y_train)
    y_pred = knn.predict(X_test)
    scores.append(metrics.accuracy_score(y_test, y_pred))

print(scores)
```

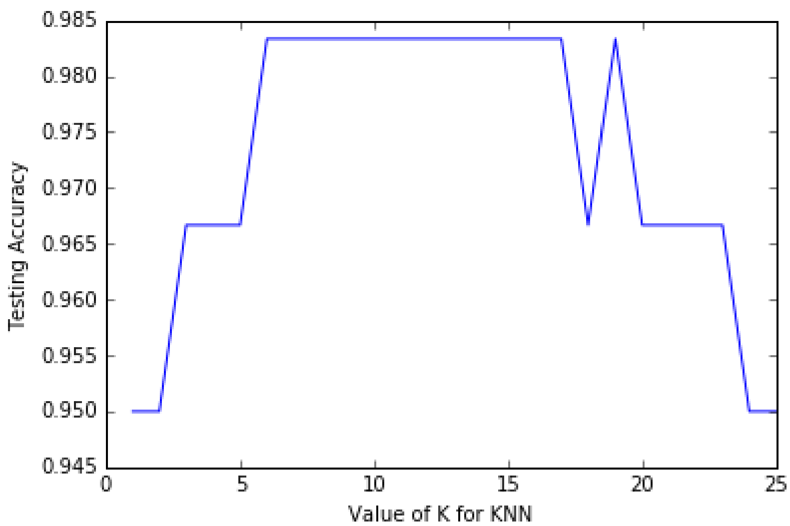
```
[0.94999999999999996, 0.94999999999999996, 0.96666666666666667, 0.96666666666666
667, 0.96666666666666667, 0.98333333333333328, 0.98333333333333328, 0.9833333333
3333328, 0.98333333333333328, 0.98333333333333328, 0.98333333333333328, 0.983333
33333333328, 0.98333333333333328, 0.98333333333333328, 0.98333333333333328, 0.98
333333333333328, 0.98333333333333328, 0.96666666666666667, 0.98333333333333328,
0.96666666666666667, 0.96666666666666667, 0.96666666666666667, 0.966666666666666
67, 0.94999999999999996, 0.94999999999999996]
```

In [16]:
```
# import Matplotlib (scientific plotting library)
import matplotlib.pyplot as plt

# allow plots to appear within the notebook
%matplotlib inline

# plot the relationship between K and testing accuracy
# plt.plot(x_axis, y_axis)
plt.plot(k_range, scores)
plt.xlabel('Value of K for KNN')
plt.ylabel('Testing Accuracy')
```

Out[16]: <matplotlib.text.Text at 0x111d43ba8>



- **Training accuracy** rises as model complexity increases
- **Testing accuracy** penalizes models that are too complex or not complex enough
- For KNN models, complexity is determined by the **value of K** (lower value = more complex)

3. Making predictions on out-of-sample data

In [17]:
```
# instantiate the model with the best known parameters
knn = KNeighborsClassifier(n_neighbors=11)

# train the model with X and y (not X_train and y_train)
knn.fit(X, y)

# make a prediction for an out-of-sample observation
knn.predict([3, 5, 4, 2])
```

```
/Users/ritchieng/anaconda3/envs/py3k/lib/python3.5/site-packages/sklearn/utils/v
alidation.py:386: DeprecationWarning: Passing 1d arrays as data is deprecated in
0.17 and willraise ValueError in 0.19. Reshape your data either using X.reshape
(-1, 1) if your data has a single feature or X.reshape(1, -1) if it contains a s
ingle sample.
  DeprecationWarning)
```

Out[17]:
```
array([1])
```

4. Downsides of train/test split

- Provides a **high-variance estimate** of out-of-sample accuracy
- **K-fold cross-validation** overcomes this limitation
- But, train/test split is still useful because of its **flexibility and speed**

5. Resources

- Quora: What is an intuitive explanation of overfitting? (http://www.quora.com/What-is-an-intuitive-explanation-of-overfitting/answer/Jessica-Su)
- Video: Estimating prediction error (https://www.youtube.com/watch?v=_2ij6eaaSl0&t=2m34s) (12 minutes, starting at 2:34) by Hastie and Tibshirani
- Understanding the Bias-Variance Tradeoff (http://scott.fortmann-roe.com/docs/BiasVariance.html)
    - Guiding questions (https://github.com/justmarkham/DAT5/blob/master/homework/06_bias_variance.md) when reading this article
- Video: Visualizing bias and variance (http://work.caltech.edu/library/081.html) (15 minutes) by Abu-Mostafa