Develop k-Nearest Neighbors in Python From Scratch

by **Jason Brownlee** on October 24, 2019 in **Code Algorithms From Scratch**

Last Updated on February 24, 2020

In this tutorial you are going to learn about the **k-Nearest Neighbors algorithm** including how it works and how to implement it from scratch in Python (*without libraries*).

A simple but powerful approach for making predictions is to use the most similar historical examples to the new data. This is the principle behind the k-Nearest Neighbors algorithm.

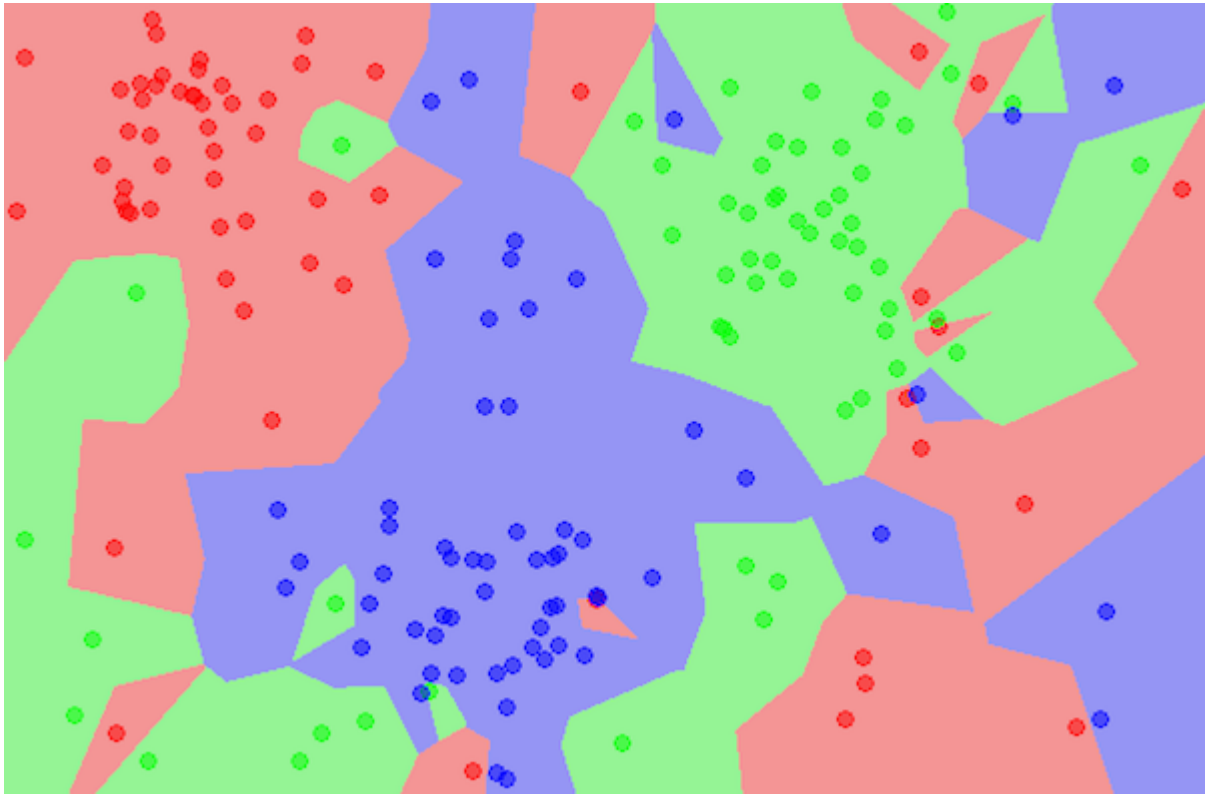
After completing this tutorial you will know:

- How to code the k-Nearest Neighbors algorithm step-by-step.
- How to evaluate k-Nearest Neighbors on a real dataset.
- How to use k-Nearest Neighbors to make a prediction for new data.

Kick-start your project with my new book Machine Learning Algorithms From Scratch, including *step-by-step tutorials* and the *Python source code* files for all examples.

Let's get started.

- **Updated Sep/2014**: Original version of the tutorial.
- **Updated Oct/2019**: Complete rewritten from the ground up.



Develop k-Nearest Neighbors in Python From Scratch
Image taken from Wikipedia, some rights reserved.

Tutorial Overview

This section will provide a brief background on the k-Nearest Neighbors algorithm that we will implement in this tutorial and the Abalone dataset to which we will apply it.

k-Nearest Neighbors

The k-Nearest Neighbors algorithm or KNN for short is a very simple technique.

The entire training dataset is stored. When a prediction is required, the k-most similar records to a new record from the training dataset are then located. From these neighbors, a summarized prediction is made.

Similarity between records can be measured many different ways. A problem or data-specific method can be used. Generally, with tabular data, a good starting point is the Euclidean distance.

Once the neighbors are discovered, the summary prediction can be made by returning the most common outcome or taking the average. As such, KNN can be used for classification or regression problems.

There is no model to speak of other than holding the entire training dataset. Because no work is done until a prediction is required, KNN is often referred to as a lazy learning method.

Iris Flower Species Dataset

In this tutorial we will use the Iris Flower Species Dataset.

The Iris Flower Dataset involves predicting the flower species given measurements of iris flowers.

It is a multiclass classification problem. The number of observations for each class is balanced. There are 150 observations with 4 input variables and 1 output variable. The variable names are as follows:

- Sepal length in cm.
- Sepal width in cm.
- Petal length in cm.
- Petal width in cm.
- Class

A sample of the first 5 rows is listed below.

```
5.1,3.5,1.4,0.2,Iris-setosa
4.9,3.0,1.4,0.2,Iris-setosa
4.7,3.2,1.3,0.2,Iris-setosa
4.6,3.1,1.5,0.2,Iris-setosa
5.0,3.6,1.4,0.2,Iris-setosa
...
```

The baseline performance on the problem is approximately 33%.

Download the dataset and save it into your current working directory with the filename "*iris.csv*".

- Download Dataset (iris.csv)

- More Information on Dataset (iris.names)

k-Nearest Neighbors (in 3 easy steps)

First we will develop each piece of the algorithm in this section, then we will tie all of the elements together into a working implementation applied to a real dataset in the next section.

This k-Nearest Neighbors tutorial is broken down into 3 parts:

- **Step 1**: Calculate Euclidean Distance.
- **Step 2**: Get Nearest Neighbors.
- **Step 3**: Make Predictions.

These steps will teach you the fundamentals of implementing and applying the k-Nearest Neighbors algorithm for classification and regression predictive modeling problems.

Note: This tutorial assumes that you are using Python 3. If you need help installing Python, see this tutorial:

- How to Setup Your Python Environment for Machine Learning

I believe the code in this tutorial will also work with Python 2.7 without any changes.

Step 1: Calculate Euclidean Distance

The first step is to calculate the distance between two rows in a dataset.

Rows of data are mostly made up of numbers and an easy way to calculate the distance between two rows or vectors of numbers is to draw a straight line. This makes sense in 2D or 3D and scales nicely to higher dimensions.

We can calculate the straight line distance between two vectors using the Euclidean distance measure. It is calculated as the square root of the sum of the squared differences between the two vectors.

- Euclidean Distance = sqrt(sum i to N (x1_i – x2_i)^2)

Where *x1* is the first row of data, *x2* is the second row of data and *i* is the index to a specific column as we sum across all columns.

With Euclidean distance, the smaller the value, the more similar two records will be. A value of 0 means that there is no difference between two records.

Below is a function named *euclidean_distance()* that implements this in Python.

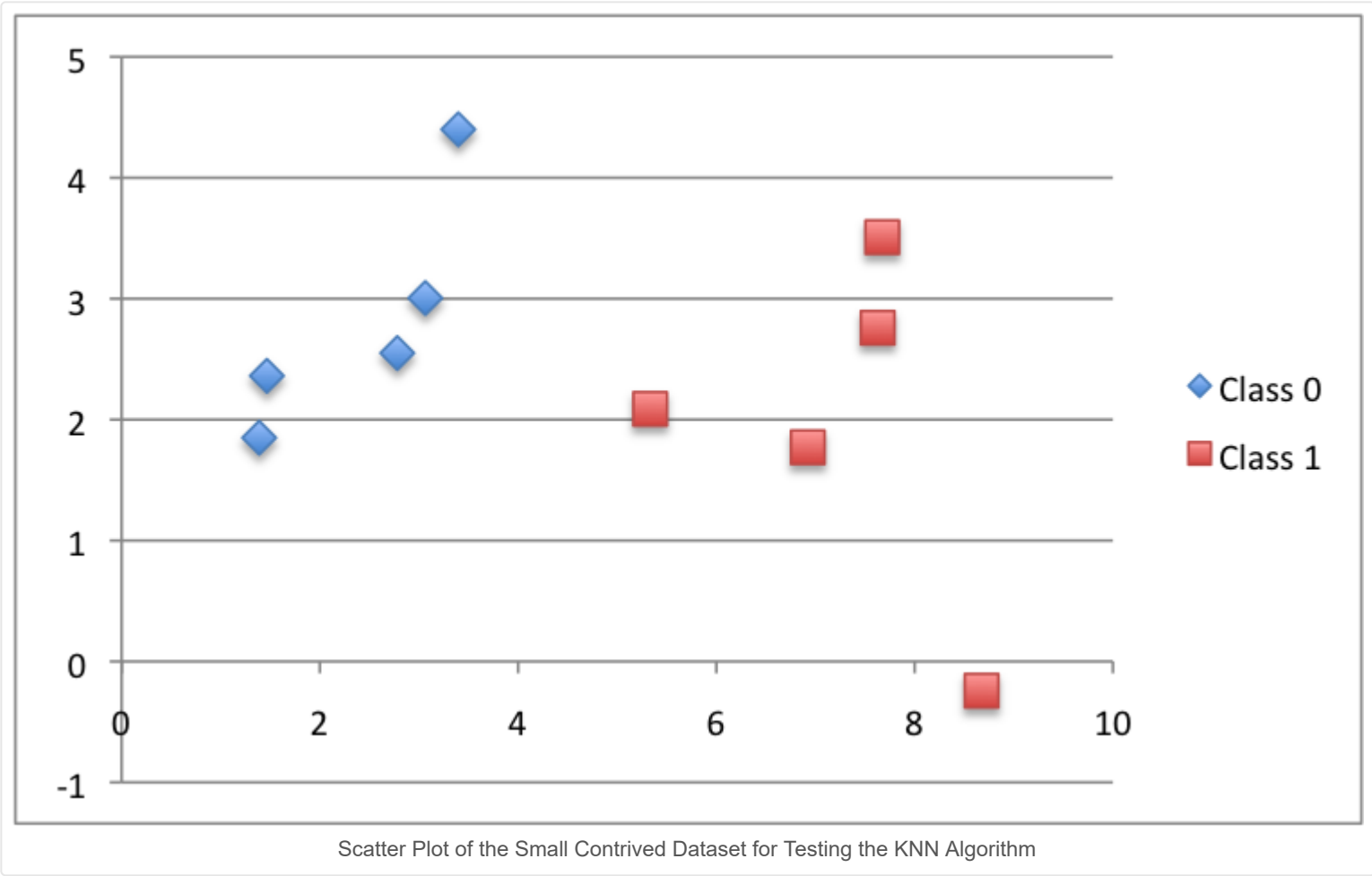
```
# calculate the Euclidean distance between two vectors
def euclidean_distance(row1, row2):
    distance = 0.0
    for i in range(len(row1)-1):
        distance += (row1[i] - row2[i])**2
    return sqrt(distance)
```

You can see that the function assumes that the last column in each row is an output value which is ignored from the distance calculation.

We can test this distance function with a small contrived classification dataset. We will use this dataset a few times as we construct the elements needed for the KNN algorithm.

```
X1                  X2                  Y
2.7810836           2.550537003         0
1.465489372         2.362125076         0
3.396561688         4.400293529         0
1.38807019          1.850220317         0
3.06407232          3.005305973         0
7.627531214         2.759262235         1
5.332441248         2.088626775         1
6.922596716         1.77106367          1
8.675418651         -0.242068655        1
7.673756466         3.508563011         1
```

Below is a plot of the dataset using different colors to show the different classes for each point.



Scatter Plot of the Small Contrived Dataset for Testing the KNN Algorithm

Putting this all together, we can write a small example to test our distance function by printing the distance between the first row and all other rows. We would expect the distance between the first row and itself to be 0, a good thing to look out for.

The full example is listed below.

```
# Example of calculating Euclidean distance
from math import sqrt

# calculate the Euclidean distance between two vectors
def euclidean_distance(row1, row2):
    distance = 0.0
    for i in range(len(row1)-1):
        distance += (row1[i] - row2[i])**2
```

```
    return sqrt(distance)

# Test distance function
dataset = [[2.7810836,2.550537003,0],
    [1.465489372,2.362125076,0],
    [3.396561688,4.400293529,0],
    [1.38807019,1.850220317,0],
    [3.06407232,3.005305973,0],
    [7.627531214,2.759262235,1],
    [5.332441248,2.088626775,1],
    [6.922596716,1.77106367,1],
    [8.675418651,-0.242068655,1],
    [7.673756466,3.508563011,1]]
row0 = dataset[0]
for row in dataset:
    distance = euclidean_distance(row0, row)
    print(distance)
```

Running this example prints the distances between the first row and every row in the dataset, including itself.

```
0.0
1.3290173915275787
1.9494646655653247
1.5591439385540549
0.5356280721938492
4.850940186986411
2.592833759950511
4.214227042632867
6.522409988228337
4.985585382449795
```

Now it is time to use the distance calculation to locate neighbors within a dataset.

Step 2: Get Nearest Neighbors

Neighbors for a new piece of data in the dataset are the *k* closest instances, as defined by our distance measure.

To locate the neighbors for a new piece of data within a dataset we must first calculate the distance between each record in the dataset to the new piece of data. We can do this using our distance function prepared above.

Once distances are calculated, we must sort all of the records in the training dataset by their distance to the new data. We can then select the top *k* to return as the most similar neighbors.

We can do this by keeping track of the distance for each record in the dataset as a tuple, sort the list of tuples by the distance (in descending order) and then retrieve the neighbors.

Below is a function named *get_neighbors()* that implements this.

```
# Locate the most similar neighbors
def get_neighbors(train, test_row, num_neighbors):
    distances = list()
    for train_row in train:
        dist = euclidean_distance(test_row, train_row)
        distances.append((train_row, dist))
    distances.sort(key=lambda tup: tup[1])
    neighbors = list()
    for i in range(num_neighbors):
        neighbors.append(distances[i][0])
    return neighbors
```

You can see that the *euclidean_distance()* function developed in the previous step is used to calculate the distance between each *train_row*and the new *test_row*.

The list of *train_row* and distance tuples is sorted where a custom key is used ensuring that the second item in the tuple (*tup[1]*) is used in the sorting operation.

Finally, a list of the *num_neighbors* most similar neighbors to *test_row* is returned.

We can test this function with the small contrived dataset prepared in the previous section.

The complete example is listed below.

```
# Example of getting neighbors for an instance
from math import sqrt

# calculate the Euclidean distance between two vectors
def euclidean_distance(row1, row2):
    distance = 0.0
    for i in range(len(row1)-1):
        distance += (row1[i] - row2[i])**2
    return sqrt(distance)

# Locate the most similar neighbors
def get_neighbors(train, test_row, num_neighbors):
    distances = list()
    for train_row in train:
```

```
        dist = euclidean_distance(test_row, train_row)
        distances.append((train_row, dist))
    distances.sort(key=lambda tup: tup[1])
    neighbors = list()
    for i in range(num_neighbors):
        neighbors.append(distances[i][0])
    return neighbors

# Test distance function
dataset = [[2.7810836,2.550537003,0],
    [1.465489372,2.362125076,0],
    [3.396561688,4.400293529,0],
    [1.38807019,1.850220317,0],
    [3.06407232,3.005305973,0],
    [7.627531214,2.759262235,1],
    [5.332441248,2.088626775,1],
    [6.922596716,1.77106367,1],
    [8.675418651,-0.242068655,1],
    [7.673756466,3.508563011,1]]
neighbors = get_neighbors(dataset, dataset[0], 3)
for neighbor in neighbors:
    print(neighbor)
```

Running this example prints the 3 most similar records in the dataset to the first record, in order of similarity.

As expected, the first record is the most similar to itself and is at the top of the list.

```
[2.7810836, 2.550537003, 0]
[3.06407232, 3.005305973, 0]
[1.465489372, 2.362125076, 0]
```

Now that we know how to get neighbors from the dataset, we can use them to make predictions.

Step 3: Make Predictions

The most similar neighbors collected from the training dataset can be used to make predictions.

In the case of classification, we can return the most represented class among the neighbors.

We can achieve this by performing the *max()* function on the list of output values from the neighbors. Given a list of class values observed in the neighbors, the *max()* function takes a set of unique class values and calls the count on the list of class values for each class value in the set.

Below is the function named *predict_classification()* that implements this.

```
# Make a classification prediction with neighbors
def predict_classification(train, test_row, num_neighbors):
    neighbors = get_neighbors(train, test_row, num_neighbors)
    output_values = [row[-1] for row in neighbors]
    prediction = max(set(output_values), key=output_values.count)
    return prediction
```

We can test this function on the above contrived dataset.

Below is a complete example.

```
# Example of making predictions
from math import sqrt

# calculate the Euclidean distance between two vectors
def euclidean_distance(row1, row2):
    distance = 0.0
    for i in range(len(row1)-1):
        distance += (row1[i] - row2[i])**2
    return sqrt(distance)

# Locate the most similar neighbors
def get_neighbors(train, test_row, num_neighbors):
    distances = list()
    for train_row in train:
        dist = euclidean_distance(test_row, train_row)
        distances.append((train_row, dist))
    distances.sort(key=lambda tup: tup[1])
    neighbors = list()
    for i in range(num_neighbors):
        neighbors.append(distances[i][0])
    return neighbors

# Make a classification prediction with neighbors
def predict_classification(train, test_row, num_neighbors):
    neighbors = get_neighbors(train, test_row, num_neighbors)
    output_values = [row[-1] for row in neighbors]
    prediction = max(set(output_values), key=output_values.count)
    return prediction

# Test distance function
dataset = [[2.7810836,2.550537003,0],
    [1.465489372,2.362125076,0],
    [3.396561688,4.400293529,0],
    [1.38807019,1.850220317,0],
    [3.06407232,3.005305973,0],
    [7.627531214,2.759262235,1],
    [5.332441248,2.088626775,1],
```

```
    [6.922596716,1.77106367,1],
    [8.675418651,-0.242068655,1],
    [7.673756466,3.508563011,1]]
prediction = predict_classification(dataset, dataset[0], 3)
print('Expected %d, Got %d.' % (dataset[0][-1], prediction))
```

Running this example prints the expected classification of 0 and the actual classification predicted from the 3 most similar neighbors in the dataset.

```
Expected 0, Got 0.
```

We can imagine how the *predict_classification()* function can be changed to calculate the mean value of the outcome values.

We now have all of the pieces to make predictions with KNN. Let's apply it to a real dataset.

Iris Flower Species Case Study

This section applies the KNN algorithm to the Iris flowers dataset.

The first step is to load the dataset and convert the loaded data to numbers that we can use with the mean and standard deviation calculations. For this we will use the helper function *load_csv()* to load the file, *str_column_to_float()* to convert string numbers to floats and *str_column_to_int()* to convert the class column to integer values.

We will evaluate the algorithm using k-fold cross-validation with 5 folds. This means that 150/5=30 records will be in each fold. We will use the helper functions *evaluate_algorithm()* to evaluate the algorithm with cross-validation and *accuracy_metric()* to calculate the accuracy of predictions.

A new function named *k_nearest_neighbors()* was developed to manage the application of the KNN algorithm, first learning the statistics from a training dataset and using them to make predictions for a test dataset.

If you would like more help with the data loading functions used below, see the tutorial:

- How to Load Machine Learning Data From Scratch In Python

If you would like more help with the way the model is evaluated using cross validation, see the tutorial:

- How to Implement Resampling Methods From Scratch In Python

The complete example is listed below.

```
# k-nearest neighbors on the Iris Flowers Dataset
from random import seed
from random import randrange
from csv import reader
from math import sqrt

# Load a CSV file
def load_csv(filename):
    dataset = list()
    with open(filename, 'r') as file:
        csv_reader = reader(file)
        for row in csv_reader:
            if not row:
                continue
            dataset.append(row)
    return dataset

# Convert string column to float
def str_column_to_float(dataset, column):
    for row in dataset:
        row[column] = float(row[column].strip())

# Convert string column to integer
def str_column_to_int(dataset, column):
    class_values = [row[column] for row in dataset]
    unique = set(class_values)
    lookup = dict()
    for i, value in enumerate(unique):
        lookup[value] = i
    for row in dataset:
        row[column] = lookup[row[column]]
    return lookup

# Find the min and max values for each column
def dataset_minmax(dataset):
    minmax = list()
    for i in range(len(dataset[0])):
        col_values = [row[i] for row in dataset]
        value_min = min(col_values)
        value_max = max(col_values)
        minmax.append([value_min, value_max])
    return minmax

# Rescale dataset columns to the range 0-1
def normalize_dataset(dataset, minmax):
    for row in dataset:
```

```
        for i in range(len(row)):
            row[i] = (row[i] - minmax[i][0]) / (minmax[i][1] - minmax[i][0])

# Split a dataset into k folds
def cross_validation_split(dataset, n_folds):
    dataset_split = list()
    dataset_copy = list(dataset)
    fold_size = int(len(dataset) / n_folds)
    for _ in range(n_folds):
        fold = list()
        while len(fold) < fold_size:
            index = randrange(len(dataset_copy))
            fold.append(dataset_copy.pop(index))
        dataset_split.append(fold)
    return dataset_split

# Calculate accuracy percentage
def accuracy_metric(actual, predicted):
    correct = 0
    for i in range(len(actual)):
        if actual[i] == predicted[i]:
            correct += 1
    return correct / float(len(actual)) * 100.0

# Evaluate an algorithm using a cross validation split
def evaluate_algorithm(dataset, algorithm, n_folds, *args):
    folds = cross_validation_split(dataset, n_folds)
    scores = list()
    for fold in folds:
        train_set = list(folds)
        train_set.remove(fold)
        train_set = sum(train_set, [])
        test_set = list()
        for row in fold:
            row_copy = list(row)
            test_set.append(row_copy)
            row_copy[-1] = None
        predicted = algorithm(train_set, test_set, *args)
        actual = [row[-1] for row in fold]
        accuracy = accuracy_metric(actual, predicted)
        scores.append(accuracy)
    return scores

# Calculate the Euclidean distance between two vectors
def euclidean_distance(row1, row2):
    distance = 0.0
    for i in range(len(row1)-1):
        distance += (row1[i] - row2[i])**2
    return sqrt(distance)
```

```
96
97  # Locate the most similar neighbors
98  def get_neighbors(train, test_row, num_neighbors):
99      distances = list()
100     for train_row in train:
101         dist = euclidean_distance(test_row, train_row)
102         distances.append((train_row, dist))
103     distances.sort(key=lambda tup: tup[1])
104     neighbors = list()
105     for i in range(num_neighbors):
106         neighbors.append(distances[i][0])
107     return neighbors
108
109 # Make a prediction with neighbors
110 def predict_classification(train, test_row, num_neighbors):
111     neighbors = get_neighbors(train, test_row, num_neighbors)
112     output_values = [row[-1] for row in neighbors]
113     prediction = max(set(output_values), key=output_values.count)
114     return prediction
115
116 # kNN Algorithm
117 def k_nearest_neighbors(train, test, num_neighbors):
118     predictions = list()
119     for row in test:
120         output = predict_classification(train, row, num_neighbors)
121         predictions.append(output)
122     return(predictions)
123
124 # Test the kNN on the Iris Flowers dataset
125 seed(1)
126 filename = 'iris.csv'
127 dataset = load_csv(filename)
128 for i in range(len(dataset[0])-1):
129     str_column_to_float(dataset, i)
130 # convert class column to integers
131 str_column_to_int(dataset, len(dataset[0])-1)
132 # evaluate algorithm
133 n_folds = 5
134 num_neighbors = 5
135 scores = evaluate_algorithm(dataset, k_nearest_neighbors, n_folds, num_neighbors)
136 print('Scores: %s' % scores)
137 print('Mean Accuracy: %.3f%%' % (sum(scores)/float(len(scores))))
```

Running the example prints the mean classification accuracy scores on each cross-validation fold as well as the mean accuracy score.

We can see that the mean accuracy of about 96.6% is dramatically better than the baseline accuracy of 33%.

```
1  Scores: [96.66666666666667, 96.66666666666667, 100.0, 90.0, 100.0]
```

```
Mean Accuracy: 96.667%
```

We can use the training dataset to make predictions for new observations (rows of data).

This involves making a call to the *predict_classification()* function with a row representing our new observation to predict the class label.

```
...
# predict the label
label = predict_classification(dataset, row, num_neighbors)
```

We also might like to know the class label (string) for a prediction.

We can update the *str_column_to_int()* function to print the mapping of string class names to integers so we can interpret the prediction made by the model.

```
# Convert string column to integer
def str_column_to_int(dataset, column):
    class_values = [row[column] for row in dataset]
    unique = set(class_values)
    lookup = dict()
    for i, value in enumerate(unique):
        lookup[value] = i
        print('[%s] => %d' % (value, i))
    for row in dataset:
        row[column] = lookup[row[column]]
    return lookup
```

Tying this together, a complete example of using KNN with the entire dataset and making a single prediction for a new observation is listed below.

```
# Make Predictions with k-nearest neighbors on the Iris Flowers Dataset
from csv import reader
from math import sqrt

# Load a CSV file
def load_csv(filename):
    dataset = list()
    with open(filename, 'r') as file:
        csv_reader = reader(file)
        for row in csv_reader:
            if not row:
                continue
            dataset.append(row)
    return dataset

# Convert string column to float
```

```
def str_column_to_float(dataset, column):
    for row in dataset:
        row[column] = float(row[column].strip())

# Convert string column to integer
def str_column_to_int(dataset, column):
    class_values = [row[column] for row in dataset]
    unique = set(class_values)
    lookup = dict()
    for i, value in enumerate(unique):
        lookup[value] = i
        print('[%s] => %d' % (value, i))
    for row in dataset:
        row[column] = lookup[row[column]]
    return lookup

# Find the min and max values for each column
def dataset_minmax(dataset):
    minmax = list()
    for i in range(len(dataset[0])):
        col_values = [row[i] for row in dataset]
        value_min = min(col_values)
        value_max = max(col_values)
        minmax.append([value_min, value_max])
    return minmax

# Rescale dataset columns to the range 0-1
def normalize_dataset(dataset, minmax):
    for row in dataset:
        for i in range(len(row)):
            row[i] = (row[i] - minmax[i][0]) / (minmax[i][1] - minmax[i][0])

# Calculate the Euclidean distance between two vectors
def euclidean_distance(row1, row2):
    distance = 0.0
    for i in range(len(row1)-1):
        distance += (row1[i] - row2[i])**2
    return sqrt(distance)

# Locate the most similar neighbors
def get_neighbors(train, test_row, num_neighbors):
    distances = list()
    for train_row in train:
        dist = euclidean_distance(test_row, train_row)
        distances.append((train_row, dist))
    distances.sort(key=lambda tup: tup[1])
    neighbors = list()
    for i in range(num_neighbors):
        neighbors.append(distances[i][0])
```

```
    return neighbors

# Make a prediction with neighbors
def predict_classification(train, test_row, num_neighbors):
    neighbors = get_neighbors(train, test_row, num_neighbors)
    output_values = [row[-1] for row in neighbors]
    prediction = max(set(output_values), key=output_values.count)
    return prediction

# Make a prediction with KNN on Iris Dataset
filename = 'iris.csv'
dataset = load_csv(filename)
for i in range(len(dataset[0])-1):
    str_column_to_float(dataset, i)
# convert class column to integers
str_column_to_int(dataset, len(dataset[0])-1)
# define model parameter
num_neighbors = 5
# define a new record
row = [5.7,2.9,4.2,1.3]
# predict the label
label = predict_classification(dataset, row, num_neighbors)
print('Data=%s, Predicted: %s' % (row, label))
```

Running the data first summarizes the mapping of class labels to integers and then fits the model on the entire dataset.

Then a new observation is defined (in this case I took a row from the dataset), and a predicted label is calculated.

In this case our observation is predicted as belonging to class 1 which we know is "*Iris-setosa*".

```
[Iris-virginica] => 0
[Iris-setosa] => 1
[Iris-versicolor] => 2
Data=[4.5, 2.3, 1.3, 0.3], Predicted: 1
```

Tutorial Extensions

This section lists extensions to the tutorial you may wish to consider to investigate.

- **Tune KNN**. Try larger and larger *k* values to see if you can improve the performance of the algorithm on the Iris dataset.
- **Regression**. Adapt the example and apply it to a regression predictive modeling problem (e.g. predict a numerical value)
- **More Distance Measures**. Implement other distance measures that you can use to find similar historical data, such as Hamming distance, Manhattan distance and Minkowski distance.

- **Data Preparation**. Distance measures are strongly affected by the scale of the input data. Experiment with standardization and other data preparation methods in order to improve results.
- **More Problems**. As always, experiment with the technique on more and different classification and regression problems.

Further Reading

- Section 3.5 Comparison of Linear Regression with K-Nearest Neighbors, page 104, An Introduction to Statistical Learning, 2014.
- Section 18.8. Nonparametric Models, page 737, Artificial Intelligence: A Modern Approach, 2010.
- Section 13.5 K-Nearest Neighbors, page 350 Applied Predictive Modeling, 2013
- Section 4.7, Instance-based learning, page 128, Data Mining: Practical Machine Learning Tools and Techniques, 2nd edition, 2005.

Summary

In this tutorial you discovered how to implement the k-Nearest Neighbors algorithm from scratch with Python.

Specifically, you learned:

- How to code the k-Nearest Neighbors algorithm step-by-step.
- How to evaluate k-Nearest Neighbors on a real dataset.
- How to use k-Nearest Neighbors to make a prediction for new data.

Next Step

Take action!

1. Follow the tutorial and implement KNN from scratch.
2. Adapt the example to another dataset.
3. Follow the extensions and improve upon the implementation.

Leave a comment and share your experiences.