K-nearest-neighbor algorithm

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Introduction

The K-nearest-neighbor (KNN) algorithm measures the distance between a query scenario and a set of scenarios in the data set.

Suppose we have a data set of 14 scenarios, each containing 4 features and one result as displayed in Table 1.

Scenario	Outlook	Temperature	Humidity	Wind	PlayTennis
Day 1	Sunny	Hot	High	Weak	**No**
Day 2	Sunny	Hot	High	Strong	**No**
Day 3	Overcast	Hot	High	Weak	**Yes**
Day 4	Rain	Mild	High	Weak	**Yes**
Day 5	Rain	Cool	Normal	Weak	**Yes**
Day 6	Rain	Cool	Normal	Strong	**No**
Day 7	Overcast	Cool	Normal	Strong	**Yes**
Day 8	Sunny	Mild	High	Weak	**No**
Day 9	Sunny	Cool	Normal	Weak	**Yes**
Day 10	Rain	Mild	Normal	Weak	**Yes**
Day 11	Sunny	Mild	Normal	Strong	**Yes**
Day 12	Overcast	Mild	High	Strong	**Yes**
Day 13	Overcast	Hot	Normal	Weak	**Yes**
Day 14	Rain	Mild	High	Strong	**No**

Table 1

Distances

We can compute the distance between two scenarios using some distance function $d(x, y)$, where x, y are scenarios composed of N features, such that $x = \{x_1, \dots, x_N\}, y = \{y_1, \dots, y_N\}$.

Two distance functions are discussed in this summary:

- Absolute distance measuring:

$$d_A(x, y) = \sum_{i=1}^{N} |x_i - y_i|$$

Equation 1

- Euclidean distance measuring:

$$d_E(x, y) = \sum_{i=1}^{N} \sqrt{{x_i}^2 - {y_i}^2}$$

Equation 2

Because the distance between two scenarios is dependant of the intervals, it is recommended that resulting distances be scaled such that the arithmetic mean across the dataset is 0 and the standard deviation 1. This can be accomplished by replacing the scalars x, y with x', y' according to the following function:

$$x' = \frac{x - \bar{x}}{\sigma(x)}$$

Equation 3

Where x is the unscaled value, $\bar{x}$ is the arithmetic mean of feature x across the data set (see Equation 4), $\sigma(x)$ is its standard deviation (see Equation 5), and x' is the resulting scaled value.

The arithmetic mean is defined as:

$$\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$$

Equation 4

We can then compute the standard deviation as follows:

$$\sigma(x) = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_i - \bar{x})^2}$$

Equation 5

Distance functions

As stated previously, we are only considering absolute (Equation 1) and Euclidean (Equation 2) distance functions $d(x, y)$. However, we may choose to provide the original unscaled values, or use transform them using the scaling function in Equation 3.

K-nearest-neighbor

Now that we have established a measure in which to determine the distance between two scenarios, we can simply pass through the data set, one scenario at a time, and compare it to the query scenario.

We can represent our data set as a matrix $D = N \times P$, containing P scenarios $s^1, \dots, s^P$, where each scenario s^i contains N features $s^i = \{s_1^i, \dots, s_N^i\}$. A vector o with length P of output values $o = \{o^1, \dots, o^P\}$ accompanies this matrix, listing the output value o^i for each scenario s^i.

It should be noted that the vector o can also be seen as a column matrix; if multiple output values are desired, the width of the matrix may be expanded.

KNN can be run in these steps:

1. Store the output values of the M nearest neighbors to query scenario q in vector $r = \{r^1, \dots, r^M\}$ by repeating the following loop M times:
   a. Go to the next scenario s^i in the data set, where i is the current iteration within the domain $\{1, \dots, P\}$
   b. If q is not set or $q < d(q, s^i)$: $q \leftarrow d(q, s^i), t \leftarrow o^i$
   c. Loop until we reach the end of the data set (i.e. $i = P$)
   d. Store q into vector c and t into vector r
2. Calculate the arithmetic mean output across r as follows:

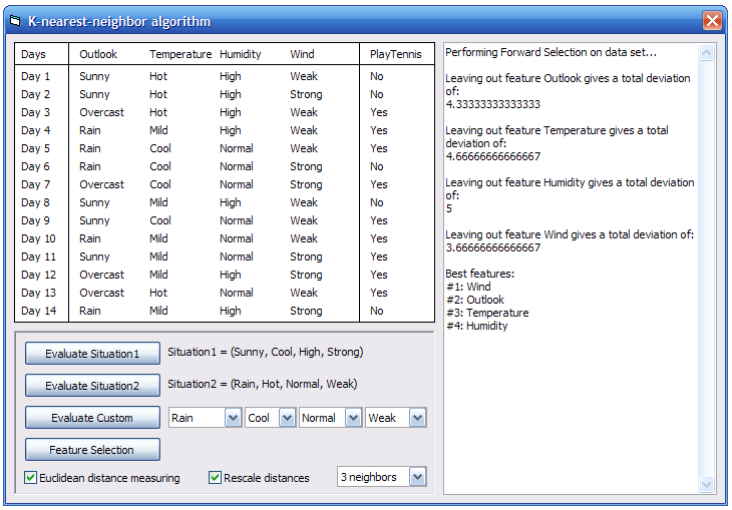
$$\bar{r} = \frac{1}{M}\sum_{i=1}^{M} r_i$$

3. Return $\bar{r}$ as the output value for the query scenario q

Demonstration application

This paper was accompanied by a demonstration application written in Visual Basic that visualizes the workings of the KNN algorithm.

The examples below can be computed using the respective evaluation buttons, or a custom query can be assembled. The three nearest neighbors are highlighted in the table and the results of evaluations appear on the right-hand pane.



Example 1

In our PlayTennis data set, we can calculate the KNN to the following query situation:

$$q_1 = \{Outlook = \text{Sunny}, Temperature = \text{Cool}, Humidity = \text{High}, Wind = \text{Strong}\}$$

We will use Absolute, unscaled distances to investigate the three nearest neighbors to q_1: $M = 3$ so that $c = \{c^1, c^2, c^3\}$. Running the algorithm as described in the previous chapter should result in the following vector c and accompanying output vector r:

$$c^1 = \{Outlook = \text{Sunny}, Temperature = \text{Hot}, Humidity = \text{High}, Wind = \text{Strong}\}$$
$$r^1 = \{PlayTennis = \text{No}\}$$
$$c^2 = \{Outlook = \text{Overcast}, Temperature = \text{Cool}, Humidity = \text{Normal}, Wind = \text{Strong}\}$$

$r^2 = \{PlayTennis = \text{Yes}\}$
$c^3 = \{Outlook = \text{Sunny}, Temperature = \text{Mild}, Humidity = \text{High}, Wind = \text{Weak}\}$
$r^3 = \{PlayTennis = \text{No}\}$

We can map the output value $PlayTennis$ from $\{\text{Yes}, \text{No}\}$ to $\{0,1\}$ for the ease of computation. The output vector r then becomes $r = \{0,1,0\}$. The arithmetic mean across r can be computed:

$$\overline{r_{q_1}} = \frac{1}{M}\sum_{i=1}^{M}\{0,1,0\} = {}^1/_3$$

Where r_{q_1} is the result for q_1. We must map this value back to the original $PlayTennis$ domain $\{\text{Yes}, \text{No}\}$:

$$\overline{r_{q_1}} = {}^1/_3$$

$$r_q = \begin{cases} \text{if } \overline{r_q} \geq {}^1/_2 \text{ then Yes} \\ \text{else No} \end{cases}$$

$$r_{q_1} = \text{No}$$

In the same fashion, we can compute KNN using the other three distance measures (Absolute scaled, Euclidean unscaled, Euclidean scaled). These results are displayed in Table 2.

	$\overline{r_{q_1}}$	r_{q_1}
Absolute unscaled distance	${}^1/_3$	$PlayTennis = \text{No}$
Absolute scaled distance	${}^1/_3$	$PlayTennis = \text{No}$
Euclidean unscaled distance	${}^2/_3$	$PlayTennis = \text{Yes}$
Euclidean scaled distance	${}^1/_3$	$PlayTennis = \text{No}$

Table 2

Example 2

For a second example, we can calculate KNN on the following query scenario:

$$q_2 = \{Outlook = \text{Rain}, Temperature = \text{Hot}, Humidity = \text{Normal}, Wind = \text{Weak}\}$$

Using the same method as in example 1, the resulting output values for q_2 using each of the four distance measures is shown in .

	$\overline{r_{q_2}}$	r_{q_2}
Absolute unscaled distance	1	$PlayTennis = \text{Yes}$
Absolute scaled distance	${}^2/_3$	$PlayTennis = \text{Yes}$
Euclidean unscaled distance	1	$PlayTennis = \text{Yes}$
Euclidean scaled distance	${}^2/_3$	$PlayTennis = \text{Yes}$

Forward selection

To improve the performance of KNN on a dataset, it is possible to evaluate each feature's deviation. The deviation is computed per feature x_j in the set of N features $x = \{x_1, \dots, x_N\}$ by calculating the sum of all differences between the calculated result $\bar{r}$ when feature x_j is left out and the actual result o^i of scenario s^i in the dataset $D = N \times P$, containing P scenarios $s^1, \dots, s^P$, where each scenario s^i contains N features $s^i = \{s_1^i, \dots, s_N^i\}$. For clarity, we'll define a new feature set y that excludes x_j, such that $y = \{x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_N\}$.

The algorithm run as follows on feature x_j, with feature set y that excludes x_j:

1. Go to the next scenario s^i in the data set, where i is the current iteration within the domain $\{1, \dots, P\}$
2. Calculate $\overline{r_{s^i}}$ over feature set y (i.e. s^i is the query scenario to compute KNN on)
3. Store the feature deviation $d_j \leftarrow d_j + \left|\overline{r_{s^i}} - o^i\right|$
4. Loop until we reach the end of the data set (i.e. $i = P$)

Note that step 3 ensures that the feature deviation d_j is always increments positively.

The forward selection computes the "best features" of the data set, i.e. features whose feature deviation is minimal.

Example 3

By performing the forward selection algorithm described above, we can compute the feature deviation for each feature in our $PlayTennis$ data set. The results, using Euclidean scaled distances, are displayed in Table 3.

Feature	Ranking	Deviation d_j
Wind	1	$3\,{}^{2}/_{3}$
Outlook	2	$4\,{}^{1}/_{3}$
Temperature	3	$4\,{}^{2}/_{3}$
Humidity	4	5

Table 3