Programming (FEB22012X)

6. Exercise

Deadline for submission: 2013-10-13 23:59 CET

Introduction

In this assignment you will implement a binary tree structure, k-d tree, and use it together with the k nearest neighbor algorithm (k-NN) for classifying flowers based on four attributes. Note that the k in the two names have no relation with each other.

K-d trees are a space-partitioning data structure used to store k-dimensional data points. Every non-leaf node of the tree represents a hyperplane cutting the space in two parts (i.e. in two half-spaces). The leaf nodes represent partitions of the original space. For example, a k-d tree with a root node and two children would split the space in 2 parts based on a single attribute. For more information and a graphical representation of a k-d tree, see `http://en.wikipedia.org/wiki/K-d_tree`.

In this exercise we will use the k nearest neighbor (k-NN) algorithm for classifying flowers based on their sepal length, sepal width, petal length, and petal width in three species: setosa, versicolor, and virginica. K-NN classifies unseen data points by looking at the points in the *training set*, that is, a set of flowers for which we know the species. Based on the euclidean distances between the training points and the new point, k nearest ones are located. The new point (flower) will be classified to be of the species of the majority of these k points.

A naive solution for finding a closest point would be to compute the distance from the new point to each point in the training data set. In this way, if you have 100 points to classify and a data set containing 1000 observations, you would have to do $100 \times 1000 = 100000$ distance computations. With a k-d tree this can be reduced (on average) to $100 \times \log_2 1000 = 996$.

Exercise part 1: implement a k-d tree

A k-d tree is created recursively by performing splits of the measurement space using cutting planes parallel to the axes of the space. Location of an individual split is obtained by taking mean of the observations' values on the considered dimension, resulting in optimally balanced trees. For example, at the root node of the tree, all points belonging to the left child will have smaller values than the root for the first dimension, and all points belonging to the right child larger values.

Creating a k-d tree

First, you should implement an algorithm for constructing a k-d tree. The pseudo-code for this part of the assignment is given in Algorithm 1. In the end, you should have a function called *kdtree* that takes as its input a data matrix D where the rows represent the observations and the columns the variables, and returns the root node of the constructed tree.

The algorithm starts with dimension 1 and sorts the matrix on this column. Then, the median index is determined. You should implement this in such a way that for a length of one, the first element is chosen as the median, for a length of two, the second element, for a length of three, also the second element, for a length four, the third element, etc. Next, the next dimension for splitting should be selected so, that after the last dimension the first dimension is used for splitting. For storing the node information, make a class (Point) for it with the necessary fields. The last lines in the pseudo-code perform the recursion.

Searching in a k-d tree

Now that you are able to create a k-d tree, you need to implement the search functionality for finding the the nearest point in the tree for a given query point. The search procedure is recursive and traverses the tree downwards while remembering the best point. The full pseudo-code is presented in Algorithm 2. Input for the

Algorithm 1 kdtree(D, axisIndex) - creating a k-d tree

```
Input: a $n \times k$ matrix $D$, where $n$ is the number of points and $k$ the dimensionality
Input: $axisIndex$, index of the axis to do the split (default: 1)
Output: node $ret$ (root of the build k-d (sub) tree)
1: if $|D| == 0$ then
2:    return []
3: end if
4: sort matrix D on column $axisIndex$
5: determine $medianIndex$ for column $axisIndex$ in $D$
6: determine $nextAxis$
7: initialize empty point $ret$
8: $ret.axisSplit = axisIndex$
9: $ret.val =$ the $medianIndex^{\text{th}}$ row of $D$
10: $ret.left = kdtree(D(1 : (medianIndex - 1), :), nextAxis)$
11: $ret.left = kdtree(D((medianIndex + 1) : end, :), nextAxis)$
```

function is a starting node *head* (e.g. the root) and the query point q. Output of the function is the closest point stored in the tree and its squared distance to the query point.

The algorithm first starts by computing the distance between the query point and the observation stored at the root of the tree (line 2). Then, it does a check whether or not the variables that track the best point should be updated (lines 3–4). Obviously, the first time this will always happen as the variable *bd* is initialized to be Inf (infinite). Next, the difference between the head and q is computed to check whether the left node or right node is closer (only considering the dimension used for the split), this is done on lines 6–13. The next step is to perform a recursive search where *head* becomes the node that is closer (node *close*). This recursive search should be skipped if *close* is empty (line 14). Finally, if *away* is not empty and the previously computed difference is smaller than the best distance, then another recursive search has to be performed with *head* = *away*. This last line is where the magic happens in the k-d tree search (see the animation at the k-d tree wikipedia page).

Algorithm 2 Searching in a k-d tree

```
Input: a k-d tree, represented by its root node $head$
Input: a query point $q$
Input: the best distance $bd$ (initially $Inf$)
Output: the best point $bp$
Output: the best distance $bd$
1: $headSD$ = compute Euclidean distance between the point in $head$ and $q$
2: if $headSD < bd$ then
3:    $bp \leftarrow head$
4:    $bd \leftarrow headSD$
5: end if
6: $d \leftarrow$ difference between the point in $head$ and $q$ ($= q - head$) in dimension $head.axisSplit$
7: if $d \leq 0$ then
8:    $close = head.left$
9:    $away = head.right$
10: else
11:    $close = head.right$
12:    $away = head.left$
13: end if
14: if $close$ is not empty then
15:    recursive search with $head = close$
16: end if
17: if $away$ is not empty and $d^2 < bd$ then
18:    recursive search with $head = away$
19: end if
```

Exercise part 2: classify new points based on their nearest neighbor

The k-NN algorithm requires the value for k to be specified. We will now use $k = 1$, meaning that an unseen data point will be classified to the same class as its nearest neighbor in the training data set.

Download the data set from `http://smaa.fi/static/prog2/2011/data/iris.data` into a directory accessible by Matlab. For more information on the data set, see `http://en.wikipedia.org/wiki/Iris_flower_data_set`. The data set has the following columns:

1. sepal length in cm
2. sepal width in cm
3. petal length in cm
4. petal width in cm
5. class:
    - Iris Setosa
    - Iris Versicolour
    - Iris Virginica

Make a script file, that:

1. Loads the data from iris.data and normalizes it (see function `zscore`)
2. Constructs a k-d tree with the iris.data using the four first attributes for the $k = 4$ dimensions on which the splitting is done. The actual values stored in the tree should contain the class as well.
3. Constructs 1000 points with 4 attributes having uniformly distributed values between the minimum- and maximum ones in the data (sepal and petal lengths and widths). Leave the class of these empty.
4. Uses the k-d tree searching procedure to find the closest point in the k-d tree for each of these. Assign each random point to the class of its nearest neighbor.
5. Makes two scatterplots where x-axis have the sepal length, y-axis the petal length, and the point itself color (blue, green, or red) indicating its class (setosa, versicolour, or virginica). For the first plot use the points from iris.data, and for the second one your recently classified random points. Plot according to the original vector space, not in the normalized space (i.e. the plots should have x- and y-axes in centimeters, not in z-values).