NAG DMC nagdmc_knnp

Nearest Neighbours: nagdmc_knnp

Purpose

 $\mathbf{nagdmc_knnp}$ computes k-nearest neighbour approximations given a binary tree computed by $\mathbf{nagdmc_kdtree}$ using training data.

Declaration

Parameters

1: rec1 - long Input

On entry: the index in the data of the first data record used in the analysis.

Constraint: $rec1 \ge 0$.

2: nvar - long Input

On entry: the number of variables in the data.

Constraint: $\mathbf{nvar} > 1$.

3: nrec - long Input

On entry: the number of consecutive records, beginning at rec1, used in the analysis.

Constraint: $\mathbf{nrec} > 1$.

4: dblk - long Input

On entry: the total number of records in the data block.

Constraint: $dblk \ge rec1 + nrec$.

 $5: \quad data[dblk * nvar] - double$

Input

On entry: the data values for the jth variable (for $j = 0, 1, ..., \mathbf{nvar} - 1$) are stored in $\mathbf{data}[i*\mathbf{nvar} + j]$, for $i = 0, 1, ..., \mathbf{dblk} - 1$.

6: iproot - long Input

On entry: the integer value of the root node of a binary tree as returned by nagdmc_kdtree.

7: norm - int Input

On entry: the norm used to compute distances. If $\mathbf{norm} = 1$, the ℓ_1 -norm (or Manhattan distance) is used; otherwise $\mathbf{norm} = 2$ and the ℓ_2 -norm (or Euclidean distance) is used.

Constraint: $norm \in \{1, 2\}$.

8: k - long

On entry: the number of nearest neighbours used in the computation.

Constraint: $0 < \mathbf{k} < \mathbf{nrec}$.

9: res[nrec] - double

Output

On exit: $\mathbf{res}[i]$ contains the k-nearest neighbour approximation for the ith data record, for $i = 0, 1, \dots, \mathbf{nrec} - 1$.

10: $\mathbf{nn}[\mathbf{nrec}*\mathbf{k}] - \mathbf{long}$

Outnut

On exit: if **nn** is set to 0, it is not referenced; otherwise $\mathbf{nn}[i * \mathbf{k} + j]$ contains the index in the training data for the jth nearest neighbour to the ith data record, for $j = 0, 1, ..., \mathbf{k} - 1$; for $i = 0, 1, ..., \mathbf{nrec} - 1$.

11: dist[nrec*k] - double

Output

On exit: if **dist** is set to 0, it is not referenced; otherwise $\mathbf{dist}[i * \mathbf{k} + j]$ contains the distance from the *i*th data record to its *j*th nearest neighbour, for $j = 0, 1, \dots, \mathbf{k} - 1$; for $i = 0, 1, \dots, \mathbf{nrec} - 1$.

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12: info - int *

On exit: info gives information on the success of the function call:

0: the function successfully completed its task.

i; i = i = 1, 2, 3, 4, 7, 8: the specification of the *i*th formal parameter was incorrect.

57: information in the binary tree has been corrupted.

99: the function failed to allocate enough memory.

100: an internal error occurred during the execution of the function.

> 100: an error occurred in a function specified by the user.

Notation

nrec the number of data records in the analysis, n.

data the data values, X.

 \mathbf{k} the number of nearest neighbours used in the calculations, k.

res the nearest neighbour approximations \hat{y}_i , for i = 1, 2, ..., n.

Description

Let X be a set of n data records x_i , for i = 1, 2, ..., n, on p independent variables and a continuous dependent variable y. The ith data record takes a value x_{ij} on the jth independent variable.

The k-nearest neighbour approach searches a set of training data records T (i.e., data records with known values for y) to find the k-nearest data records to x_i . Nearest neighbours are found by using a binary tree search, e.g., see Bentley (1975). The proximity of x_i to a member t of T is defined by a distance calculated over the independent variables and can defined by using one of:

(a) the ℓ_1 -norm or Manhattan distance:

$$\sum_{i=1}^{p} |x_{ij} - t_j|,$$

where $|\cdot|$ denotes the modulus operator;

(b) the ℓ_2 -norm or Euclidean distance:

$$\left[\sum_{j=1}^{p} (x_{ij} - t_j)^2\right]^{1/2}.$$

Let S_i be a set containing the k-nearest neighbours in T to x_i . Then the predicted value of y for x_i , \hat{y}_i , is given by the mean of its k-nearest neighbours:

$$\hat{y}_i = \frac{1}{k} \sum_{\forall t \in S_i} t_y.$$

References and Further Reading

Bentley J L (1975) Multi-dimensional binary search trees used for associative searching Communications of the ACM 18(9) 509–517.

Duda R O and Hart P E (1972) Pattern Classification and Scene Analysis Wiley New York.

Storer J A and Cohn M (1993) Algorithms for fast vector quantization *Proc. Data Compression Conference* 381–390 IEEE Computer Society Press.

See Also

nagdmc_kdtree computes a binary tree for a nearest neighbour analysis.

nagdmc_free_kdtreenagdmc_load_kdtreeloads a binary tree from a file into memory.