NAG DMC nagdmc_reg_tree

Decision Tree: nagdmc_reg_tree

Purpose

nagdmc_reg_tree approximates data by using a binary regression tree.

Declaration

Parameters

1: $\mathbf{rec1} - \mathbf{long}$

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: $dblk \ge rec1 + nrec$.

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

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

for $i = 0, 1, ..., \mathbf{dblk} - 1$.

On entry: the number of independent variables. If $\mathbf{nxvar} = 0$ then all variables in the data, excluding \mathbf{yvar} and, if $\mathbf{iwts} \ge 0$, \mathbf{iwts} , are treated as independent variables.

Constraint: $0 \le \mathbf{nxvar} < \mathbf{nvar}$.

7: xvar[nxvar] - long

Input

Input

On entry: the indices indicating the position in **data** in which values of the independent variables are stored. If $\mathbf{nxvar} = 0$ then \mathbf{xvar} must be 0, and the indices of independent variables are given by $j = 0, 1, \dots, \mathbf{nvar} - 1$; $j \neq \mathbf{yvar}$ and $j \neq \mathbf{iwts}$.

Constraints: if $\mathbf{nxvar} > 0$, $0 \le \mathbf{xvar}[i] < \mathbf{nvar}$, for $i = 0, 1, \dots, \mathbf{nxvar} - 1$; otherwise \mathbf{xvar} must be 0.

8: yvar - long Input

On entry: the index in data in which values of the dependent variable are stored.

Constraints: 0 < yvar < nvar; if nxvar > 0, $yvar \neq xvar[i]$, for i = 0, 1, ..., nxvar - 1.

9: iwts - long Input

On entry: if iwts = -1, no weights are used; otherwise iwts is the index in data in which the weights are stored.

Constraints: $-1 \le \text{iwts} < \text{nvar}$; iwts $\ne \text{yvar}$; and if nxvar > 0, iwts $\ne \text{xvar}[i]$, for $i = 0, 1, \dots, \text{nxvar} - 1$.

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10: ncat[nvar] - long

Input

On entry: $\mathbf{ncat}[i]$ contains the number of categories in the *i*th variable, for $i = 0, 1, \dots, \mathbf{nvar} - 1$. If the *i*th variable is continuous, $\mathbf{ncat}[i]$ must be set equal to zero.

Constraints: $\mathbf{ncat}[i] \ge 0$, for $i = 0, 1, \dots, \mathbf{nvar} - 1$, $(i \ne \mathbf{yvar})$; $\mathbf{ncat}[\mathbf{yvar}] = 0$.

11: bcat[nvar] - long

Input

On entry: $\mathbf{bcat}[i]$ contains the base level value for the $\mathbf{ncat}[i]$ categories on the ith variable. If $\mathbf{ncat}[i] > 0$, for $i = 0, 1, \dots, \mathbf{nvar} - 1$, the categorical values on the ith variable are given by $\mathbf{bcat}[i] + j$, for $j = 0, 1, \dots, \mathbf{ncat}[i] - 1$; otherwise $\mathbf{bcat}[i]$ is not referenced. If the base level for each categorical variable is zero, \mathbf{bcat} can be 0.

12: **mns** - long

Input

On entry: if the number of data records at a node is greater than or equal to **mns**, a partition of data is attempted; otherwise a leaf node is forced.

Constraint: 1 < mns < nrec.

13: mnc - long

Input

On entry: during the search for an optimal partition of data at a node each candidate partition must contain at least **mnc** data records.

Constraint: $1 \leq \mathbf{mnc} \leq \mathbf{mns}/2$.

14: alpha - double

Input

On entry: the value of the pruning constant used in the binary tree.

Constraint: $alpha \ge 0.0$.

15: iproot - long *

Output

On exit: **iproot** is an integer cast of the memory location pointing to the root node in the tree. This value is passed to the functions described in 'See Also'. Information on the detail of a decision tree can be found by using the value of **iproot**.

Detail of partitions in a binary regression tree are available by using in a C program the code:

RTNode *proot;

proot = (RTNode *)iproot;

where RTNode is a C structure with the following members:

type – int

if the node is a leaf, type is set to one; otherwise type is set to zero;

ndata - long

the number of data records at this node;

ybar - double

the estimate of the mean of the dependent variable over data records at the node.

yvar - double

the variance of ybar;

parent - RTNode *

if this node is not the root of a binary tree, a pointer to the parent node; otherwise parent is set equal to zero.

If type = 1, the remaining structure members are set equal to dummy values and should not be referenced; otherwise the following information is available:

svar - long

the index in the data of the variable on which records are partitioned;

ncats - long

if independent variable **svar** is categorical, the number of categories on variable j^* ; otherwise zero:

 ${\tt sval}-{\tt double}$

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if ncats = 0, sval gives the scalar value of the test on variable svar; otherwise sval is not referenced:

```
lr - char []
```

if ncats = 0, 1r is not referenced; otherwise it is an array of ncats elements, the value of 1r[i] determines the direction in the binary tree taken by data records at the node with category bcat[svar] + i on variable svar, for i = 0, 1, ..., ncats - 1. The possible values for lr[i] are:

- '1' data records at the node with category value bcat[svar] + i on svar are sent to the left child node;
- 'r' data records at the node with category value bcat[svar] + i on svar are sent to the right child node.
- 'a' the ith category on svar is absent at this node.

```
rss - double
```

the value of the residual sum of squares;

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lchild - RTNode *
```

a pointer to left child node;

```
rchild - RTNode *
```

a pointer to right child node.

A C source code example that accesses the information in a binary regression tree is given in 'Explanatory Code'.

16: info - int * Output

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

0: the function successfully completed its task.

 $i; i = 1, 2, 3, 4, 6, 7, \dots, 10, 12, 13, 14$: the specification of the ith formal parameter was incorrect.

99: the function failed to allocate enough memory.

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

Notation

nrec the number of records, p. nxvar the number of variables, m.

the number of categories on variables, c_y and c_j , for $j=1,2,\ldots,m$. the base level categories, b_y and b_j , for $j=1,2,\ldots,m$. ncat

bcat

the minimum number of records, s, required for a partition to be attempted. mns

mnc the minimum number of records, t, at each child.

alpha the pruning constant, α .

Description

Let x_i denote the values of m independent variables and y_i the value of the dependent variable for the *i*th data record at a node A, for $i = 1, 2, \dots, p$. The *j*th independent variable can be continuous or categorical and its ith value is denoted by x_{ij} , for $j=1,2,\ldots,m$. If the jth independent variable is categorical it takes the c_j consecutive values $b_j, b_j+1, \ldots, b_j+c_j-1$, for a base level value b_j . The dependent variable is a categorical variable with c_y consecutive values $b_y, b_y+1, \ldots, b_y+c_y-1$, for a base level value b_y . Furthermore, let o denote the modal category and l_k be the number of records that belong to the kth category, for $k=1,2,\ldots,c_{y}$, over the values of the dependent variable at node A.

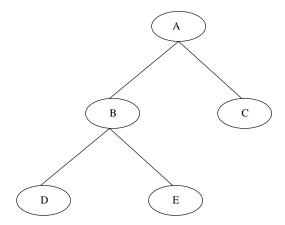


Figure 1: Graphical representation of a binary tree showing parent nodes connected by lines to their child nodes. The root node, node A, is associated with all data records and is the only node not to have a parent node. Nodes C, D and E do not have child nodes and are known as leaf nodes. Node B is neither the root node nor a leaf node and is known as an internal node. Given positive values for the scalars s and $t \leq s/2$, a partition of $p \geq s$ data records at a parent node into $q \geq t$ records at one child node and $r \geq t$ records at the other child node is based on the outcome of a test at the parent node.

Consider the case of partitioning p data records at a parent node A into child nodes B and C such that each record at node A is sent to either node B or node C (see Figure 1). Let s be the minimum number of data records at a parent node required to partition data. If p < s, a partition of data is not computed; otherwise a data partition is defined by computing a univariate test on independent variables. Two kinds of test are available. Firstly, a test on a continuous independent variable j sends the ith data record at the parent node to the left child node if $x_{ij} \le u$ and otherwise to the right child node, for a value u that minimises a criterion and sends at least t data records to left and right child nodes. Secondly, a test on a categorical independent variable j sends the ith data record at the parent node to the child node determined by the binary partition of category values that minimises a criterion and sends at least t data records to left and right child nodes. In both cases, the criterion most often used in a binary regression tree is based on a sum-of-squares criterion.

The test chosen at parent node A is the univariate test which partitions $p \ge s$ records at a node A into $q \ge t$ records at child node B and $r \ge t$ records at child node C and minimises the criterion:

$$\sum_{i \in B} \left(y_i - \bar{y}_B\right)^2 + \sum_{i \in C} \left(y_i - \bar{y}_C\right)^2,$$

where \bar{y}_B and \bar{y}_C are the means of the dependent variable of data associated with nodes B and C respectively. In order to find the test that minimises the above expression, we separate the variance in the dependent variable for data at node A into node B and node C:

Total scatter = Within-cluster scatter + Residual scatter,

where,

$$\begin{split} & \text{Total scatter} = \sum_{i \in A} \left(y_i - \bar{y}_A\right)^2, \\ & \text{Within-cluster scatter} = \sum_{i \in B} \left(y_i - \bar{y}_B\right)^2 + \sum_{i \in C} \left(y_i - \bar{y}_C\right)^2, \\ & \text{Residual scatter} = n_B \left(\bar{y}_B - \bar{y}_A\right)^2 + n_C \left(\bar{y}_C - \bar{y}_A\right)^2. \end{split}$$

Now, at node A the total scatter is a constant and, therefore, minimising the within-cluster scatter is equivalent to maximising the residual scatter, which is more efficient computationally.

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Given a successful partition of data records at node A and the value of a user-supplied scalar α , node A is forced to become a leaf node if the following condition is satisfied:

$$\frac{\displaystyle\sum_{i\in B}\left(y_{i}-\bar{y}_{B}\right)^{2}+\displaystyle\sum_{i\in C}\left(y_{i}-\bar{y}_{C}\right)^{2}}{\displaystyle\sum_{i\in A}\left(y_{i}-\bar{y}_{A}\right)^{2}}>1+\alpha.$$

Once a partition of data at a parent node into left and right child nodes has been found, the process continues recursively by considering partitions of data records at child nodes.

References and Further Reading

Brieman L. Friedman J. Olshen R. and Stone C. (1984) Classification and Regression Trees Belmont Calif.

Explanatory Code

The following C function prints the memory locations of nodes in a tree and its parent node. The type (leaf or internal) of each node is printed along with the detail of the partition at that node. If the function is called with **iproot** as its second argument, the entire tree is printed.

```
#include <stdio.h>
step_through(long bcat[], long ipnode) {
                 i, j;
*lnode = (RTNode *)ipnode;
   long
   RTNode
   if (lnode == 0)
        return;
   printf("\n Node
                      %8p"
           "\n Parent %8p"
           "\n type: %8i"
"\n svar: %8li"
           "\n sval: %8.4f"
           lnode,lnode->parent,lnode->type,lnode->svar,lnode->sval,
           lnode->rss,lnode->ybar,lnode->yvar,lnode->ndata);
   j = 0 + (bcat != 0 ? bcat[lnode->svar] : 0);
   if (lnode->ncats > 0) {
        printf("\n lr:
        for (i=0; i<lnode->ncats; ++i) {
            if (lnode->lr[i] != 'a')
                printf (" Cat. %li goes %c;",j+i,lnode->lr[i]);
        printf("\n");
   printf("\n");
   step_through(bcat,(long)(lnode->lchild));
   step_through(bcat,(long)(lnode->rchild));
}
```

See Also

nagdmc_free_reg_treenagdmc_load_reg_treenagdmc_save_reg_treenagdmc_save_reg_treenagdmc_save_reg_treereturns memory containing a binary regression tree to the operating system.loads a binary regression tree into memory.saves a binary regression tree to a binary file.

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 $reg_tree_ex.c$

nagdmc_predict_reg_tree predicts values for new data using a binary regression tree. the example calling program.