

## nag\_mv\_kmeans\_cluster\_analysis (g03efc)

### 1. Purpose

`nag_mv_kmeans_cluster_analysis (g03efc)` performs  $K$ -means cluster analysis.

### 2. Specification

```
#include <nag.h>
#include <nagg03.h>

void nag_mv_kmeans_cluster_analysis(Integer n, Integer m, double x[],
    Integer tdx, Integer isx[], Integer nvar, Integer k,
    double cmeans[], Integer tdc, double wt[],
    Integer inc[], Integer nic[], double css[],
    double csw[], Integer maxit, NagError *fail)
```

### 3. Description

Given  $n$  objects with  $p$  variables measured on each object,  $x_{ij}$  for  $i = 1, 2, \dots, n$ ;  $j = 1, 2, \dots, p$ , `nag_mv_kmeans_cluster_analysis` allocates each object to one of  $K$  groups or clusters to minimize the within-cluster sum of squares:

$$\sum_{k=1}^K \sum_{i \in S_k} \sum_{j=1}^p (x_{ij} - \bar{x}_{kj})^2,$$

where  $S_k$  is the set of objects in the  $k$ th cluster and  $\bar{x}_{kj}$  is the mean for the variable  $j$  over cluster  $k$ . This is often known as  $K$ -means clustering.

In addition to the data matrix, a  $K$  by  $p$  matrix giving the initial cluster centres for the  $K$  clusters is required. The objects are then initially allocated to the cluster with the nearest cluster mean. Given the initial allocation, the procedure is to iteratively search for the  $K$ -partition with locally optimal within-cluster sum of squares by moving points from one cluster to another.

Optionally, weights for each object,  $w_i$ , can be used so that the clustering is based on within-cluster weighted sums of squares:

$$\sum_{k=1}^K \sum_{i \in S_k} \sum_{j=1}^p w_i (x_{ij} - \tilde{x}_{kj})^2,$$

where  $\tilde{x}_{kj}$  is the weighted mean for variable  $j$  over cluster  $k$ .

The routine is based on the algorithm of Hartigan and Wong (1979).

### 4. Parameters

**n**

Input: the number of observations,  $n$ .

Constraint:  $n \geq 2$ .

**m**

Input: the number of variables in the array **x**.

Constraint:  $m \geq \mathbf{nvar}$ .

**x[n][tdx]**

Input:  $x[i-1][j-1]$  must contain the value of  $j$ th variable for the  $i$ th object for  $i = 1, 2, \dots, n$ ;  $j = 1, 2, \dots, \mathbf{m}$ .

**tdx**

Input: the last dimension of the array **x** as declared in the calling program.

Constraint:  $\mathbf{tdx} \geq \mathbf{m}$ .

**isx[m]**

Input: **isx**[ $j - 1$ ] indicates whether or not the  $j$ th variable is to be included in the analysis. If **isx**[ $j - 1$ ]  $> 0$ , then the  $j$ th variable contained in the  $j$ th column of **x** is included, for  $j = 1, 2, \dots, \mathbf{m}$ .  
 Constraint: **isx**[ $j - 1$ ]  $> 0$  for **nvar** values of  $j$ .

**nvar**

Input: the number of variables included in the sum of squares calculations,  $p$ .  
 Constraint:  $1 \leq \mathbf{nvar} \leq \mathbf{m}$ .

**k**

Input: the number of clusters,  $K$ .  
 Constraint:  $\mathbf{k} \geq 2$ .

**cmeans[k][tdc]**

Input: **cmeans**[ $i - 1$ ][ $j - 1$ ] must contain the value of the  $j$ th variable for the  $i$ th initial cluster centre, for  $i = 1, 2, \dots, K$ ;  $j = 1, 2, \dots, p$ .

Output: **cmeans**[ $i - 1$ ][ $j - 1$ ] contains the value of the  $j$ th variable for the  $i$ th computed cluster centre, for  $i = 1, 2, \dots, K$ ;  $j = 1, 2, \dots, p$ .

**tdc**

Input: the last dimension of the array **cmeans** as declared in the calling program.  
 Constraint: **tdc**  $\geq \mathbf{nvar}$ .

**wt[n]**

Input: the elements of **wt** must contain the weights to be used in the analysis. The effective number of observations is the sum of the weights. If **wt**[ $i - 1$ ] = 0.0 then the  $i$ th observation is not included in the analysis.

Constraint: **wt**[ $i - 1$ ]  $\geq 0.0$  for  $i = 1, 2, \dots, n$  and **wt**[ $i - 1$ ]  $> 0.0$  for at least two values of  $i$ .

Note: if **wt** is set to the null pointer **NULL**, i.e., (double \*)0, then **wt** is not referenced and the effective number of observations is  $n$ .

**inc[n]**

Output: **inc**[ $i - 1$ ] contains the cluster to which the  $i$ th object has been allocated, for  $i = 1, 2, \dots, n$ .

**nic[k]**

Output: **nic**[ $i - 1$ ] contains the number of objects in the  $i$ th cluster, for  $i = 1, 2, \dots, K$ .

**css[k]**

Output: **css**[ $i - 1$ ] contains the within-cluster (weighted) sum of squares of the  $i$ th cluster, for  $i = 1, 2, \dots, K$ .

**csw[k]**

Output: **csw**[ $i - 1$ ] contains the within-cluster sum of weights of the  $i$ th cluster, for  $i = 1, 2, \dots, K$ . If **wt** = **NULL** the sum of weights is the number of objects in the cluster.

**maxit**

Input: the maximum number of iterations allowed in the analysis.

Constraint: **maxit**  $> 0$ .

Suggested Value: **maxit** = 10.

**fail**

The NAG error parameter, see the Essential Introduction to the NAG C Library.

## 5. Error Indications and Warnings

**NE\_INT\_ARG\_LT**

On entry, **n** must not be less than 2: **n** =  $\langle value \rangle$ .

On entry, **k** must not be less than 2: **k** =  $\langle value \rangle$ .

On entry, **nvar** must not be less than 1: **nvar** =  $\langle value \rangle$ .

**NE\_INT\_ARG\_LE**

On entry, **maxit** must not be less than or equal to 0: **maxit** =  $\langle value \rangle$ .

**NE\_2\_INT\_ARG\_LT**

On entry, **m** =  $\langle value \rangle$  while **nvar** =  $\langle value \rangle$ .

These parameters must satisfy **m**  $\geq$  **nvar**.

On entry, **tdx** =  $\langle value \rangle$  while **m** =  $\langle value \rangle$ .

These parameters must satisfy **tdx**  $\geq$  **m**.

On entry, **tdc** =  $\langle value \rangle$  while **nvar** =  $\langle value \rangle$ .

These parameters must satisfy **tdc**  $\geq$  **nvar**.

**NE\_VAR\_INCL\_INDICATED**

The number of variables, **nvar** in the analysis =  $\langle value \rangle$ , while number of variables included in the analysis via array **isx** =  $\langle value \rangle$ .

Constraint: these two numbers must be the same.

**NE\_NEG\_WEIGHT\_ELEMENT**

On entry, **wt**[ $\langle value \rangle$ ] =  $\langle value \rangle$ .

Constraint: When referenced, all elements of **wt** must be non-negative.

**NE\_WT\_ZERO**

At least two elements of **wt** must be greater than zero.

**NE\_CLUSTER\_EMPTY**

At least one cluster is empty after the initial assignment.

Try a different set of initial cluster centres in **cmeans** and also consider decreasing the value of **k**. The empty clusters may be found by examining the values in **nic**.

**NE\_TOO\_MANY**

Too many iterations ( $\langle value \rangle$ ).

Convergence has not been achieved within the maximum number of iterations given by **maxit**.

Try increasing **maxit** and, if possible, use the returned values in **cmeans** as the initial cluster centres.

**NE\_ALLOC\_FAIL**

Memory allocation failed.

**NE\_INTERNAL\_ERROR**

An internal error has occurred in this function. Check the function call and any array sizes. If the call is correct then please consult NAG for assistance.

**6. Further Comments**

The time per iteration is approximately proportional to  $npK$ .

**6.1. Accuracy**

The routine produces clusters that are locally optimal; the within-cluster sum of squares may not be decreased by transferring a point from one cluster to another, but different partitions may have the same or smaller within-cluster sum of squares.

**6.2. References**

Everitt B S (1974) *Cluster Analysis* Heinemann.

Hartigan J A and Wong M A (1979) Algorithm AS136: A K-means clustering algorithm *Appl. Statist.* **28** 100–108.

Kendall M G and Stuart A (1976) *The Advanced Theory of Statistics (Volume 3)* Griffin (3rd Edition).

Krzanowski W J (1990) *Principles of Multivariate Analysis* Oxford University Press.

**7. See Also**

None.

## 8. Example

The data consists of observations of five variables on twenty soils (Kendall and Stuart (1976)). The data is read in, the *K*-means clustering performed and the results printed.

### 8.1. Program Text

```

/* nag_mv_kmeans_cluster_analysis (g03efc) Example Program.
 *
 * Copyright 1998 Numerical Algorithms Group.
 *
 * Mark 5, 1998.
 *
 */

#include <nag.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <nagg03.h>

#define NMAX 20
#define MMAX 5
#define KMAX 3

main()
{
    double cmeans[KMAX][MMAX], css[MMAX], csw[MMAX],
    wt[NMAX], x[NMAX][MMAX];
    double *wtptr;

    Integer nvar, i, j, k;
    Integer m, n;
    Integer inc[NMAX], isx[MMAX], nic[MMAX];
    Integer maxit;
    Integer tdc=MMAX, tdx=MMAX;

    char weight[2];

    Vprintf("g03efc Example Program Results\n\n");

    /* Skip heading in the data file */
    Vscanf("%*[^\\n]");

    Vscanf("%s",weight);
    Vscanf("%ld",&n);
    Vscanf("%ld",&m);
    Vscanf("%ld",&nvar);
    Vscanf("%ld",&k);
    Vscanf("%ld",&maxit);

    if (n <= NMAX && m <= MMAX)
    {
        if (*weight == 'W')
        {
            for (i = 0; i < n; ++i)
            {
                for (j = 0; j < m; ++j)
                    Vscanf("%lf",&x[i][j]);
                Vscanf("%lf",&wt[i]);
            }
            wtptr = wt;
        }
        else
        {
            for (i = 0; i < n; ++i)
            {
                for (j = 0; j < m; ++j)
                    Vscanf("%lf",&x[i][j]);
            }
            wtptr = 0;
        }
    }
}

```

```

    }
    for (i = 0; i < k; ++i)
    {
        for (j = 0; j < nvar; ++j)
            Vscanf("%lf",&cmeans[i][j]);
    }
    for (j = 0; j < m; ++j)
        Vscanf("%ld",&isx[j]);

    g03efc(n, m, (double *)x, tdx, isx, nvar, k, (double *)cmeans,
          tdc, wptr, inc, nic, css, csw, maxit, NAGERR_DEFAULT);

    Vprintf("\n\nThe cluster each point belongs to\n");
    for (i = 0; i < n; ++i)
        Vprintf(" %6ld%s",inc[i], (i+1)%10 ? "" : "\n");

    Vprintf("\n\nThe number of points in each cluster\n");
    for (i = 0; i < k; ++i)
        Vprintf(" %6ld",nic[i]);

    Vprintf("\n\nThe within-cluster sum of weights of each cluster\n");
    for (i = 0; i < k; ++i)
        Vprintf(" %9.2f",csw[i]);

    Vprintf("\n\nThe within-cluster sum of squares of each cluster\n\n");
    for (i = 0; i < k; ++i)
        Vprintf(" %13.4f",css[i]);

    Vprintf("\n\nThe final cluster centres\n");
    Vprintf("          1          2          3          4          5\n");
    for (i = 0; i < k; ++i)
    {
        Vprintf(" %5ld          ",i+1);
        for (j = 0; j < nvar; ++j)
            Vprintf(" %8.4f",cmeans[i][j]);
        printf("\n");
    }
    exit(EXIT_SUCCESS);
}
else
{
    Vprintf("Incorrect input value of n or m.\n");
    exit(EXIT_FAILURE);
}
}

```

## 8.2. Program Data

g03efc Example Program Data

U 20 5 5 3 10

```

77.3 13.0  9.7 1.5 6.4
82.5 10.0  7.5 1.5 6.5
66.9 20.6 12.5 2.3 7.0
47.2 33.8 19.0 2.8 5.8
65.3 20.5 14.2 1.9 6.9
83.3 10.0  6.7 2.2 7.0
81.6 12.7  5.7 2.9 6.7
47.8 36.5 15.7 2.3 7.2
48.6 37.1 14.3 2.1 7.2
61.6 25.5 12.9 1.9 7.3
58.6 26.5 14.9 2.4 6.7
69.3 22.3  8.4 4.0 7.0
61.8 30.8  7.4 2.7 6.4
67.7 25.3  7.0 4.8 7.3
57.2 31.2 11.6 2.4 6.5
67.2 22.7 10.1 3.3 6.2
59.2 31.2  9.6 2.4 6.0
80.2 13.2  6.6 2.0 5.8

```

82.2 11.1 6.7 2.2 7.2  
69.7 20.7 9.6 3.1 5.9

82.5 10.0 7.5 1.5 6.5  
47.8 36.5 15.7 2.3 7.2  
67.2 22.7 10.1 3.3 6.2

1 1 1 1 1

8.3. Program Results

g03efc Example Program Results

The cluster each point belongs to

|   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 3 | 2 | 3 | 1 | 1 | 2 | 2 | 3 |
| 3 | 3 | 3 | 3 | 3 | 3 | 3 | 1 | 1 | 3 |

The number of points in each cluster

6 3 11

The within-cluster sum of weights of each cluster

6.00 3.00 11.00

The within-cluster sum of squares of each cluster

46.5717 20.3800 468.8964

The final cluster centres

|   |         |         |         |        |        |
|---|---------|---------|---------|--------|--------|
|   | 1       | 2       | 3       | 4      | 5      |
| 1 | 81.1833 | 11.6667 | 7.1500  | 2.0500 | 6.6000 |
| 2 | 47.8667 | 35.8000 | 16.3333 | 2.4000 | 6.7333 |
| 3 | 64.0455 | 25.2091 | 10.7455 | 2.8364 | 6.6545 |