

## NAG Library Function Document

### 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, const double x[],
    Integer tdx, const Integer isx[], Integer nvar, Integer k,
    double cmeans[], Integer tdc, const 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  $i = 1, 2, \dots, n$  and  $j = 1, 2, \dots, p$ , nag\_mv\_kmeans\_cluster\_analysis (g03efc) 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 function is based on the algorithm of Hartigan and Wong (1979).

#### 4 References

Everitt B S (1974) *Cluster Analysis* Heinemann

Hartigan J A and Wong M A (1979) Algorithm AS 136: A  $K$ -means clustering algorithm *Appl. Statist.* **28** 100–108

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

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

## 5 Arguments

- 1: **n** – Integer *Input*  
*On entry:* the number of observations,  $n$ .  
*Constraint:*  $n \geq 2$ .
- 2: **m** – Integer *Input*  
*On entry:* the number of variables in the array **x**.  
*Constraint:*  $m \geq \mathbf{nvar}$ .
- 3: **x**[**n** × **tdx**] – const double *Input*  
*On entry:* **x**[( $i - 1$ ) × **tdx** +  $j - 1$ ] must contain the value of  $j$ th variable for the  $i$ th object, for  $i = 1, 2, \dots, n$  and  $j = 1, 2, \dots, m$ .
- 4: **tdx** – Integer *Input*  
*On entry:* the stride separating matrix column elements in the array **x**.  
*Constraint:*  $\mathbf{tdx} \geq m$ .
- 5: **isx**[**m**] – const Integer *Input*  
*On entry:* **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  $j = 1, 2, \dots, m$ .  
*Constraint:* **isx**[ $j - 1$ ] > 0 for **nvar** values of  $j$ .
- 6: **nvar** – Integer *Input*  
*On entry:* the number of variables included in the sum of squares calculations,  $p$ .  
*Constraint:*  $1 \leq \mathbf{nvar} \leq m$ .
- 7: **k** – Integer *Input*  
*On entry:* the number of clusters,  $K$ .  
*Constraint:*  $k \geq 2$ .
- 8: **cmeans**[**k** × **tdc**] – double *Input/Output*  
*On entry:* **cmeans**[( $i - 1$ ) × **tdc** +  $j - 1$ ] must contain the value of the  $j$ th variable for the  $i$ th initial cluster centre, for  $i = 1, 2, \dots, K$  and  $j = 1, 2, \dots, p$ .  
*On exit:* **cmeans**[( $i - 1$ ) × **tdc** +  $j - 1$ ] contains the value of the  $j$ th variable for the  $i$ th computed cluster centre, for  $i = 1, 2, \dots, K$  and  $j = 1, 2, \dots, p$ .
- 9: **tdc** – Integer *Input*  
*On entry:* the stride separating matrix column elements in the array **cmeans**.  
*Constraint:*  $\mathbf{tdc} \geq \mathbf{nvar}$ .
- 10: **wt**[**n**] – const double *Input*  
*On entry:* 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.  
 If weights are not provided then **wt** must be set to **NULL** and the effective number of observations is **n**.

Constraints:

$$\begin{aligned} \mathbf{wt}[i-1] &\geq 0.0, \text{ for } i = 1, 2, \dots, n; \\ \mathbf{wt}[i-1] &> 0.0 \text{ for at least two values of } i. \end{aligned}$$

- 11: **inc**[**n**] – Integer *Output*  
*On exit:* **inc**[ $i-1$ ] contains the cluster to which the  $i$ th object has been allocated, for  $i = 1, 2, \dots, n$ .
- 12: **nic**[**k**] – Integer *Output*  
*On exit:* **nic**[ $i-1$ ] contains the number of objects in the  $i$ th cluster, for  $i = 1, 2, \dots, K$ .
- 13: **css**[**k**] – double *Output*  
*On exit:* **css**[ $i-1$ ] contains the within-cluster (weighted) sum of squares of the  $i$ th cluster, for  $i = 1, 2, \dots, K$ .
- 14: **csw**[**k**] – double *Output*  
*On exit:* **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.
- 15: **maxit** – Integer *Input*  
*On entry:* the maximum number of iterations allowed in the analysis.  
*Suggested value:* **maxit** = 10.  
*Constraint:* **maxit** > 0.
- 16: **fail** – NagError \* *Input/Output*  
The NAG error argument (see Section 2.7 in How to Use the NAG Library and its Documentation).

## 6 Error Indicators and Warnings

### NE\_2\_INT\_ARG\_LT

On entry, **m** =  $\langle value \rangle$  while **nvar** =  $\langle value \rangle$ . These arguments must satisfy **m**  $\geq$  **nvar**.

On entry, **tdc** =  $\langle value \rangle$  while **nvar** =  $\langle value \rangle$ . These arguments must satisfy **tdc**  $\geq$  **nvar**.

On entry, **tdx** =  $\langle value \rangle$  while **m** =  $\langle value \rangle$ . These arguments must satisfy **tdx**  $\geq$  **m**.

### NE\_ALLOC\_FAIL

Dynamic memory allocation failed.

### 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\_INT\_ARG\_LE

On entry, **maxit** =  $\langle value \rangle$ .

Constraint: **maxit** > 0.

**NE\_INT\_ARG\_LT**

On entry, **k** =  $\langle value \rangle$ .

Constraint: **k**  $\geq 2$ .

On entry, **n** =  $\langle value \rangle$ .

Constraint: **n**  $\geq 2$ .

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

Constraint: **nvar**  $\geq 1$ .

**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 contact NAG for assistance.

**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\_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\_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\_WT\_ZERO**

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

**7 Accuracy**

`nag_mv_kmeans_cluster_analysis` (g03efc) 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.

**8 Parallelism and Performance**

`nag_mv_kmeans_cluster_analysis` (g03efc) is not threaded in any implementation.

**9 Further Comments**

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

**10 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.

## 10.1 Program Text

```

/* nag_mv_kmeans_cluster_analysis (g03efc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 *
 */

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

#define CMEANS(I, J) cmeans[(I) *tdcmeans + J]
#define X(I, J) x[(I) *tdx + J]
int main(void)
{
    Integer exit_status = 0, i, *inc = 0, *isx = 0, j, k, m, maxit, n, *nic = 0,
        nvar;
    Integer tdcmeans, tdx;
    NagError fail;
    char weight[2];
    double *cmeans = 0, *css = 0, *csw = 0, *wt = 0, *wtptr, *x = 0;

    INIT_FAIL(fail);

    printf("nag_mv_kmeans_cluster_analysis (g03efc) Example Program Results"
        "\n\n");

    /* Skip heading in the data file */
#ifdef _WIN32
    scanf_s("%*[\n]");
#else
    scanf("%*[\n]");
#endif

#ifdef _WIN32
    scanf_s("%1s", weight, (unsigned)_countof(weight));
#else
    scanf("%1s", weight);
#endif
#ifdef _WIN32
    scanf_s("%" NAG_IFMT "", &n);
#else
    scanf("%" NAG_IFMT "", &n);
#endif
#ifdef _WIN32
    scanf_s("%" NAG_IFMT "", &m);
#else
    scanf("%" NAG_IFMT "", &m);
#endif
#ifdef _WIN32
    scanf_s("%" NAG_IFMT "", &nvar);
#else
    scanf("%" NAG_IFMT "", &nvar);
#endif
#ifdef _WIN32
    scanf_s("%" NAG_IFMT "", &k);
#else
    scanf("%" NAG_IFMT "", &k);
#endif
#ifdef _WIN32
    scanf_s("%" NAG_IFMT "", &maxit);
#else
    scanf("%" NAG_IFMT "", &maxit);
#endif
}

```

```

if (n >= 2 && nvar >= 1 && m >= nvar && k >= 2) {
    if (!(cmeans = NAG_ALLOC((k) * (nvar), double)) ||
        !(css = NAG_ALLOC(k, double)) ||
        !(csw = NAG_ALLOC(k, double)) ||
        !(wt = NAG_ALLOC(n, double)) ||
        !(x = NAG_ALLOC((n) * (m), double)) ||
        !(inc = NAG_ALLOC(n, Integer)) ||
        !(isx = NAG_ALLOC(m, Integer)) || !(nic = NAG_ALLOC(k, Integer)))
    {
        printf("Allocation failure\n");
        exit_status = -1;
        goto END;
    }
    tdx = m;
    tdcmeans = nvar;
}
else {
    printf("Invalid n or nvar or m or k.\n");
    exit_status = 1;
    return exit_status;
}
if (*weight == 'W') {
    for (i = 0; i < n; ++i) {
        for (j = 0; j < m; ++j)
#ifdef _WIN32
            scanf_s("%lf", &X(i, j));
#else
            scanf("%lf", &X(i, j));
#endif
#ifdef _WIN32
            scanf_s("%lf", &wt[i]);
#else
            scanf("%lf", &wt[i]);
#endif
    }
    wtptr = wt;
}
else {
    for (i = 0; i < n; ++i) {
        for (j = 0; j < m; ++j)
#ifdef _WIN32
            scanf_s("%lf", &X(i, j));
#else
            scanf("%lf", &X(i, j));
#endif
    }
    wtptr = 0;
}
for (i = 0; i < k; ++i) {
    for (j = 0; j < nvar; ++j)
#ifdef _WIN32
        scanf_s("%lf", &CMEANS(i, j));
#else
        scanf("%lf", &CMEANS(i, j));
#endif
    }
    for (j = 0; j < m; ++j)
#ifdef _WIN32
        scanf_s("%" NAG_IFMT " ", &isx[j]);
#else
        scanf("%" NAG_IFMT " ", &isx[j]);
#endif

/* nag_mv_kmeans_cluster_analysis (g03efc).
 * K-means
 */
nag_mv_kmeans_cluster_analysis(n, m, x, tdx, isx, nvar, k, cmeans,
                               tdcmeans, wtptr, inc, nic, css, csw, maxit,
                               &fail);

if (fail.code != NE_NOERROR) {
    printf("Error from nag_mv_kmeans_cluster_analysis (g03efc).\n%s\n",

```

```

        fail.message);
    exit_status = 1;
    goto END;
}

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

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

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

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

printf("\n\nThe final cluster centres\n");
printf("          1          2          3          4          5\n");
for (i = 0; i < k; ++i) {
    printf(" %5" NAG_IFMT "%", i + 1);
    for (j = 0; j < nvar; ++j)
        printf("%8.4f", CMEANS(i, j));
    printf("\n");
}
END:
    NAG_FREE(cmeans);
    NAG_FREE(css);
    NAG_FREE(csw);
    NAG_FREE(wt);
    NAG_FREE(x);
    NAG_FREE(inc);
    NAG_FREE(isx);
    NAG_FREE(nic);
    return exit_status;
}

```

## 10.2 Program Data

nag\_mv\_kmeans\_cluster\_analysis (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
```

### 10.3 Program Results

nag\_mv\_kmeans\_cluster\_analysis (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 |

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