NAG Toolbox

nag_mv_multidimscal_ordinal (g03fc)

1 Purpose

nag_mv_multidimscal_ordinal (g03fc) performs non-metric (ordinal) multidimensional scaling.

2 Syntax

```
[x, stress, dfit, ifail] = nag_mv_multidimscal_ordinal(typ, d, x, iter, iopt,
'n', n, 'ndim', ndim)
```

```
[x, stress, dfit, ifail] = g03fc(typ, d, x, iter, iopt, 'n', n, 'ndim', ndim)
```

Note: the interface to this routine has changed since earlier releases of the toolbox:

At Mark 22: **n** was made optional.

3 Description

For a set of n objects, a distance or dissimilarity matrix D can be calculated such that d_{ij} is a measure of how 'far apart' the objects i and j are. If p variables x_k have been recorded for each observation this measure may be based on Euclidean distance, $d_{ij} = \sum_{k=1}^{p} \left(x_{ki} - x_{kj}\right)^2$, or some other calculation such as the number of variables for which $x_{kj} \neq x_{ki}$. Alternatively, the distances may be the result of a subjective assessment. For a given distance matrix, multidimensional scaling produces a configuration of n points in a chosen number of dimensions, m, such that the distance between the points in some way best matches the distance matrix. For some distance measures, such as Euclidean distance, the size of distance is meaningful, for other measures of distance all that can be said is that one distance is greater or smaller than another. For the former metric scaling can be used, see nag_mv_multidimscal_metric (g03fa), for the latter, a non-metric scaling is more appropriate.

For non-metric multidimensional scaling, the criterion used to measure the closeness of the fitted distance matrix to the observed distance matrix is known as **stress**. **stress** is given by,

$$\sqrt{\frac{\sum_{i=1}^{n}\sum_{j=1}^{i-1}\left(\hat{d}_{ij} - \tilde{d}_{ij}\right)^2}{\sum_{i=1}^{n}\sum_{j=1}^{i-1}\hat{d}_{ij}^2}}$$

where $\hat{d}_{ij}^2$ is the Euclidean squared distance between points i and j and $\tilde{d}_{ij}$ is the fitted distance obtained when $\hat{d}_{ij}$ is monotonically regressed on d_{ij}, that is $\tilde{d}_{ij}$ is monotonic relative to d_{ij} and is obtained from $\hat{d}_{ij}$ with the smallest number of changes. So **stress** is a measure of by how much the set of points preserve the order of the distances in the original distance matrix. Non-metric multidimensional scaling seeks to find the set of points that minimize the **stress**.

An alternate measure is squared **stress**, $sstress$,

$$\sqrt{\frac{\sum_{i=1}^{n}\sum_{j=1}^{i-1}\left(\hat{d}_{ij}{}^{2}-\tilde{d}_{ij}{}^{2}\right)^{2}}{\sum_{i=1}^{n}\sum_{j=1}^{i-1}\hat{d}_{ij}{}^{4}}}$$

in which the distances in **stress** are replaced by squared distances.

In order to perform a non-metric scaling, an initial configuration of points is required. This can be obtained from principal coordinate analysis, see nag_mv_multidimscal_metric (g03fa). Given an initial configuration, nag_mv_multidimscal_ordinal (g03fc) uses the optimization function nag_opt_uncon_conjgrd_comp (e04dg) to find the configuration of points that minimizes **stress** or $sstress$. The function nag_opt_uncon_conjgrd_comp (e04dg) uses a conjugate gradient algorithm. nag_mv_multidimscal_ordinal (g03fc) will find an optimum that may only be a local optimum, to be more sure of finding a global optimum several different initial configurations should be used; these can be obtained by randomly perturbing the original initial configuration using functions from Chapter G05.

4 References

Chatfield C and Collins A J (1980) *Introduction to Multivariate Analysis* Chapman and Hall

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

5 Parameters

5.1 Compulsory Input Parameters

1: **typ** – CHARACTER(1)

Indicates whether **stress** or $sstress$ is to be used as the criterion.

typ = 'T'
stress is used.

typ = 'S'
$sstress$ is used.

Constraint: **typ** = 'S' or 'T'.

2: $\mathbf{d}(\mathbf{n}\times(\mathbf{n}-\mathbf{1})/\mathbf{2})$ – REAL (KIND=nag_wp) array

The lower triangle of the distance matrix D stored packed by rows. That is $\mathbf{d}((i-1)\times(i-2)/2+j)$ must contain d_{ij}, for $i=2,3,\ldots,n$ and $j=1,2,\ldots,i-1$. If d_{ij} is missing then set $d_{ij}<0$; for further comments on missing values see Section 9.

3: $\mathbf{x}(ldx,\mathbf{ndim})$ – REAL (KIND=nag_wp) array

ldx, the first dimension of the array, must satisfy the constraint $ldx\geq\mathbf{n}$.

The ith row must contain an initial estimate of the coordinates for the ith point, for $i=1,2,\ldots,n$. One method of computing these is to use nag_mv_multidimscal_metric (g03fa).

4: **iter** – INTEGER

The maximum number of iterations in the optimization process.

iter = 0
A default value of 50 is used.

iter < 0
A default value of $\max(50, 5nm)$ (the default for nag_opt_uncon_conjgrd_comp (e04dg)) is used.

5: **iopt** – INTEGER

Selects the options, other than the number of iterations, that control the optimization.

iopt $= 0$
Default values are selected as described in Section 9. In particular if an accuracy requirement of $\epsilon = 0.00001$ is selected, see Section 7.

iopt > 0
The default values are used except that the accuracy is given by 10^{-i} where $i =$ **iopt**.

iopt < 0
The option setting mechanism of nag_opt_uncon_conjgrd_comp (e04dg) can be used to set all options except **Iteration Limit**; this option is only recommended if you are an experienced user of NAG optimization functions. For further details see nag_opt_uncon_conjgrd_comp (e04dg).

5.2 Optional Input Parameters

1: **n** – INTEGER

Default: the dimension of the array **d** and the first dimension of the array **x**. (An error is raised if these dimensions are not equal.)

n, the number of objects in the distance matrix.

Constraint: **n** $>$ **ndim**.

2: **ndim** – INTEGER

Default: the second dimension of the array **x**.

m, the number of dimensions used to represent the data.

Constraint: **ndim** ≥ 1.

5.3 Output Parameters

1: **x**(ldx, **ndim**) – REAL (KIND=nag_wp) array

The ith row contains m coordinates for the ith point, for $i = 1, 2, \ldots, n$.

2: **stress** – REAL (KIND=nag_wp)

The value of **stress** or $sstress$ at the final iteration.

3: **dfit**($\mathbf{2} \times \mathbf{n} \times (\mathbf{n} - \mathbf{1})$) – REAL (KIND=nag_wp) array

Auxiliary outputs.

If **typ** = 'T', the first $n(n-1)/2$ elements contain the distances, $\hat{d}_{ij}$, for the points returned in **x**, the second set of $n(n-1)/2$ contains the distances $\hat{d}_{ij}$ ordered by the input distances, d_{ij}, the third set of $n(n-1)/2$ elements contains the monotonic distances, $\tilde{d}_{ij}$, ordered by the input distances, d_{ij} and the final set of $n(n-1)/2$ elements contains fitted monotonic distances, $\tilde{d}_{ij}$, for the points in **x**. The $\tilde{d}_{ij}$ corresponding to distances which are input as missing are set to zero.

If **typ** = 'S', the results are as above except that the squared distances are returned.

Each distance matrix is stored in lower triangular packed form in the same way as the input matrix D.

4: **ifail** – INTEGER

ifail $= 0$ unless the function detects an error (see Section 5).

6 Error Indicators and Warnings

Errors or warnings detected by the function:

ifail $= 1$

On entry, **ndim** < 1,
or **n** $\leq$ **ndim**,
or **typ** $\neq$ 'T' or 'S',
or $ldx <$ **n**.

ifail $= 2$

On entry, all elements of **d** ≤ 0.0.

ifail $= 3$

The optimization has failed to converge in **iter** function iterations. Try either increasing the number of iterations using **iter** or increasing the value of ϵ, given by **iopt**, used to determine convergence. Alternatively try a different starting configuration.

ifail $= 4$ (*warning*)

The conditions for an acceptable solution have not been met but a lower point could not be found. Try using a larger value of ϵ, given by **iopt**.

ifail $= 5$

The optimization cannot begin from the initial configuration. Try a different set of points.

ifail $= 6$

The optimization has failed. This error is only likely if **iopt** < 0. It corresponds to **ifail** $= 4$, 7 and 9 in nag_opt_uncon_conjgrd_comp (e04dg).

ifail $= -99$

An unexpected error has been triggered by this routine. Please contact NAG.

ifail $= -399$

Your licence key may have expired or may not have been installed correctly.

ifail $= -999$

Dynamic memory allocation failed.

7 Accuracy

After a successful optimization the relative accuracy of **stress** should be approximately ϵ, as specified by **iopt**.

8 Further Comments

The optimization function nag_opt_uncon_conjgrd_comp (e04dg) used by nag_mv_multidimscal_ ordinal (g03fc) has a number of options to control the process. The options for the maximum number of iterations (**Iteration Limit**) and accuracy (**Optimality Tolerance**) can be controlled by **iter** and **iopt** respectively. The printing option (**Print Level**) is set to -1 to give no printing. The other option set is to stop the checking of derivatives (**Verify** $=$ NO) for efficiency. All other options are left at their default values. If however **iopt** < 0 is used, only the maximum number of iterations is set. All other options can be controlled by the option setting mechanism of nag_opt_uncon_conjgrd_comp (e04dg) with the defaults as given by that function.

Missing values in the input distance matrix can be specified by a negative value and providing there are not more than about two thirds of the values missing the algorithm may still work. However the function nag_mv_multidimscal_metric (g03fa) does not allow for missing values so an alternative method of obtaining an initial set of coordinates is required. It may be possible to estimate the missing values with some form of average and then use nag_mv_multidimscal_metric (g03fa) to give an initial set of coordinates.

9 Example

The data, given by Krzanowski (1990), are dissimilarities between water vole populations in Europe. Initial estimates are provided by the first two principal coordinates computed.

9.1 Program Text

```
     function g03fc_example

fprintf('g03fc example results\n\n');

% Distance matrix (lower part)
n = nag_int(14);
d = [0.099 ...
     0.033 0.022 ...
     0.183 0.114 0.042 ...
     0.148 0.224 0.059 0.068 ...
     0.198 0.039 0.053 0.085 0.051 ...
     0.462 0.266 0.322 0.435 0.268 0.025 ...
     0.628 0.442 0.444 0.406 0.240 0.129 0.014 ...
     0.113 0.070 0.046 0.047 0.034 0.002 0.106 0.129 ...
     0.173 0.119 0.162 0.331 0.177 0.039 0.089 0.237 0.071 ...
     0.434 0.419 0.339 0.505 0.469 0.390 0.315 0.349 0.151 0.430 ...
     0.762 0.633 0.781 0.700 0.758 0.625 0.469 0.618 0.440 0.538 0.607 ...
     0.530 0.389 0.482 0.579 0.597 0.498 0.374 0.562 0.247 0.383 0.387 ...
     0.084 ...
     0.586 0.435 0.550 0.530 0.552 0.509 0.369 0.471 0.234 0.346 0.456 ...
     0.090 0.038];

% Perform principal co-ordinate analysis
roots = 'l';
ndim = nag_int(2);

[x, eval, ifail] = g03fa( ...
   roots, n, d, ndim);

% Perform multi-dimensional scaling
typ = 'T';
iter = nag_int(0);
iopt = nag_int(0);
[x, stress, dfit, ifail] = g03fc( ...
   typ, d, x, iter, iopt);

fprintf('Stress = %13.4e\n\n', stress);
mtitle = 'Co-ordinates';
matrix = 'General';
diag = ' ';
[ifail] = x04ca( ...
  matrix,diag,x,mtitle);

fig1 = figure;
hold on;
xlabel('PC 1');
ylabel('PC 2');
title({'Observation numbers', 'for PC 1 and PC 2'});
axis([-0.6 0.4 -0.4 0.3]);
```

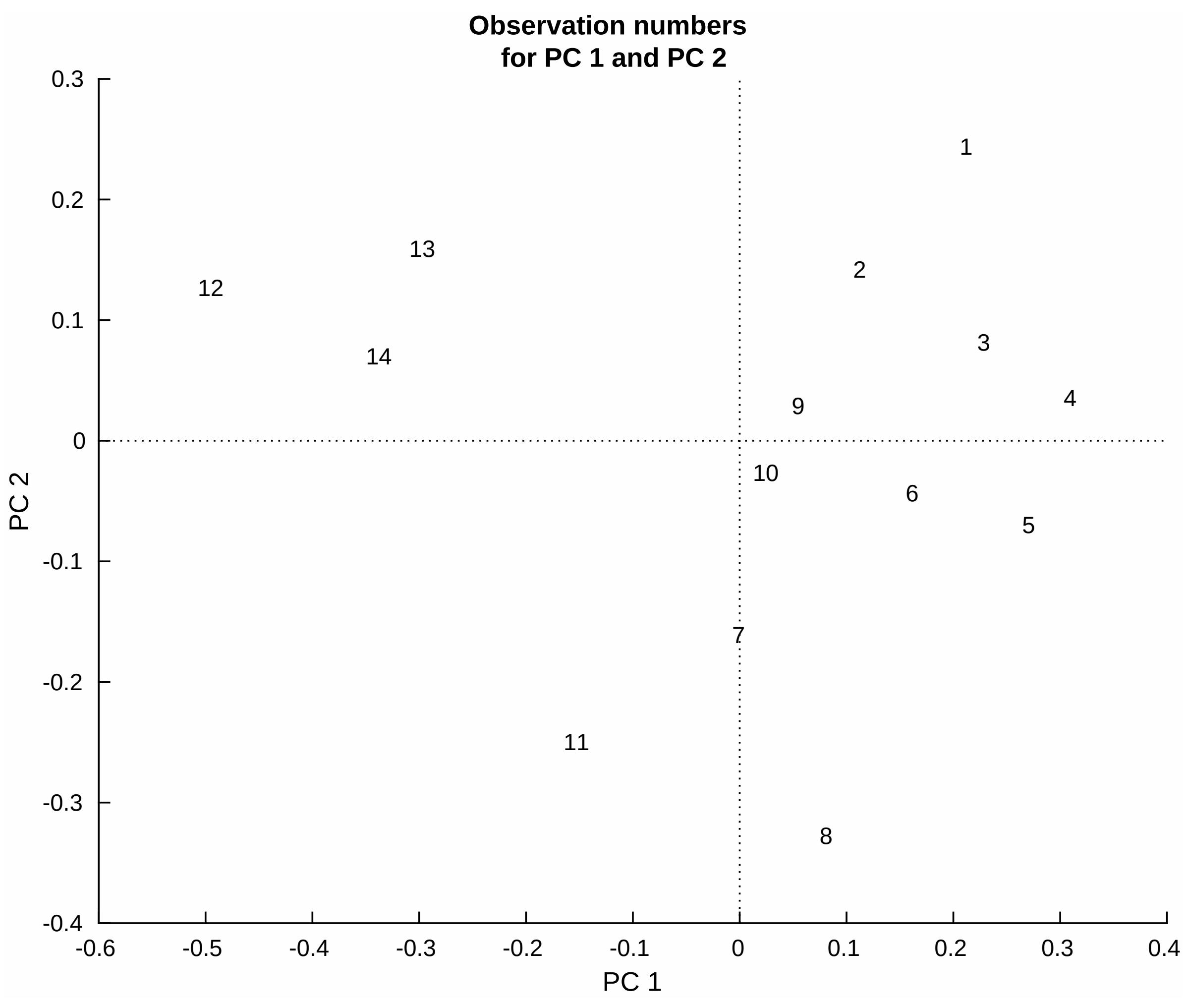
```
for j = 1:size(x,1)
  ch = sprintf('%d',j);
  text(x(j,1),x(j,2),ch);
end
plot([-0.6 0.4], [0 0], ':');
plot([0 0], [-0.4 0.3], ':');
hold off;
```

9.2 Program Results

```
     g03fc example results

Stress =    1.2557e-01

 Co-ordinates
          1       2
  1   0.2060  0.2438
  2   0.1063  0.1418
  3   0.2224  0.0817
  4   0.3032  0.0355
  5   0.2645 -0.0698
  6   0.1554 -0.0435
  7  -0.0070 -0.1612
  8   0.0749 -0.3275
  9   0.0488  0.0289
 10   0.0124 -0.0267
 11  -0.1649 -0.2500
 12  -0.5073  0.1267
 13  -0.3093  0.1590
 14  -0.3498  0.0700
```


Observation numbers
for PC 1 and PC 2
PC 1
PC 2
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
-0.6
-0.5
-0.4
-0.3
-0.2
-0.1
0
0.1
0.2
0.3
0.4
1
2
3
4
5
6
7
8
9
10
11
12
13
14