

## NAG Library Function Document

### nag\_pls\_orth\_scores\_pred (g02ldc)

#### 1 Purpose

nag\_pls\_orth\_scores\_pred (g02ldc) calculates predictions given the output from an orthogonal scores PLS regression (nag\_pls\_orth\_scores\_svd (g02lac) or nag\_pls\_orth\_scores\_wold (g02lbc)) and nag\_pls\_orth\_scores\_fit (g02lcc).

#### 2 Specification

```
#include <nag.h>
#include <nagg02.h>

void nag_pls_orth_scores_pred (Nag_OrderType order, Integer ip, Integer my,
    Nag_EstimatesOption orig, const double xbar[], const double ybar[],
    Nag_ScalePredictor iscale, const double xstd[], const double ystd[],
    const double b[], Integer pdb, Integer n, Integer mz,
    const Integer isz[], const double z[], Integer pdz, double yhat[],
    Integer pdyhat, NagError *fail)
```

#### 3 Description

nag\_pls\_orth\_scores\_pred (g02ldc) calculates the predictions  $\hat{Y}$  of a PLS model given a set  $Z$  of test data and a set  $B$  of parameter estimates as returned by nag\_pls\_orth\_scores\_fit (g02lcc).

If nag\_pls\_orth\_scores\_fit (g02lcc) returns parameter estimates for the original data scale, no further information is required.

If nag\_pls\_orth\_scores\_fit (g02lcc) returns parameter estimates for the centred, and possibly scaled, data, further information is required. The means of variables in the fitted model must be supplied. In the case of a PLS model fitted by using scaled data, the means and standard deviations of variables in the fitted model must also be supplied. These means and standard deviations are those returned by either nag\_pls\_orth\_scores\_svd (g02lac) and nag\_pls\_orth\_scores\_wold (g02lbc).

#### 4 References

None.

#### 5 Arguments

1: **order** – Nag\_OrderType *Input*

*On entry:* the **order** argument specifies the two-dimensional storage scheme being used, i.e., row-major ordering or column-major ordering. C language defined storage is specified by **order** = Nag\_RowMajor. See Section 3.2.1.3 in the Essential Introduction for a more detailed explanation of the use of this argument.

*Constraint:* **order** = Nag\_RowMajor or Nag\_ColMajor.

2: **ip** – Integer *Input*

*On entry:* the number of predictor variables in the fitted model. **ip** must take the same value as that supplied to nag\_pls\_orth\_scores\_svd (g02lac) or nag\_pls\_orth\_scores\_wold (g02lbc) to fit the model.

*Constraint:* **ip** > 1.

- 3: **my** – Integer *Input*  
*On entry:* the number of response variables in the fitted model. **my** must take the same value as that supplied to `nag_pls_orth_scores_svd` (g02lac) or `nag_pls_orth_scores_wold` (g02lbc) to fit the model.  
*Constraint:*  $\mathbf{my} \geq 1$ .
- 4: **orig** – Nag\_EstimatesOption *Input*  
*On entry:* indicates how parameter estimates are supplied.  
**orig** = Nag\_EstimatesOrig  
Parameter estimates are for the original data.  
**orig** = Nag\_EstimatesStand  
Parameter estimates are for the centred, and possibly scaled, data.  
*Constraint:* **orig** = Nag\_EstimatesStand or Nag\_EstimatesOrig.
- 5: **xbar[ip]** – const double *Input*  
*On entry:* if **orig** = Nag\_EstimatesStand, **xbar** must contain mean values of predictor variables in the model; otherwise **xbar** is not referenced.
- 6: **ybar[my]** – const double *Input*  
*On entry:* if **orig** = Nag\_EstimatesStand, **ybar** must contain the mean value of each response variable in the model; otherwise **ybar** is not referenced.
- 7: **iscale** – Nag\_ScalePredictor *Input*  
*On entry:* if **orig** = Nag\_EstimatesStand, **iscale** must take the value supplied to either `nag_pls_orth_scores_svd` (g02lac) or `nag_pls_orth_scores_wold` (g02lbc); otherwise **iscale** is not referenced.  
*Constraint:* if **orig** = Nag\_EstimatesStand, **iscale** = Nag\_PredNoScale, Nag\_PredStdScale or Nag\_PredUserScale.
- 8: **xstd[ip]** – const double *Input*  
*On entry:* if **orig** = Nag\_EstimatesStand and **iscale**  $\neq$  Nag\_PredNoScale, **xstd** must contain the scalings of predictor variables in the model as returned from either `nag_pls_orth_scores_svd` (g02lac) or `nag_pls_orth_scores_wold` (g02lbc); otherwise **xstd** is not referenced.
- 9: **ystd[my]** – const double *Input*  
*On entry:* if **orig** = Nag\_EstimatesStand and **iscale**  $\neq$  Nag\_PredNoScale, **ystd** must contain the scalings of response variables as returned from either `nag_pls_orth_scores_svd` (g02lac) or `nag_pls_orth_scores_wold` (g02lbc); otherwise **ystd** is not referenced.
- 10: **b[dim]** – const double *Input*  
**Note:** the dimension, *dim*, of the array **b** must be at least  
 $\max(1, \mathbf{pdb} \times \mathbf{my})$  when **order** = Nag\_ColMajor;  
 $\max(1, \mathbf{ip} \times \mathbf{pdb})$  when **order** = Nag\_RowMajor and **orig** = Nag\_EstimatesStand;  
 $\max(1, 1 + \mathbf{ip} \times \mathbf{pdb})$  when **order** = Nag\_RowMajor and **orig** = Nag\_EstimatesOrig.  
The (*i*, *j*)th element of the matrix *B* is stored in  
 $\mathbf{b}[(j - 1) \times \mathbf{pdb} + i - 1]$  when **order** = Nag\_ColMajor;  
 $\mathbf{b}[(i - 1) \times \mathbf{pdb} + j - 1]$  when **order** = Nag\_RowMajor.  
*On entry:* if **orig** = Nag\_EstimatesStand, **b** must contain the parameter estimate for the centred, and possibly scaled, data as returned by `nag_pls_orth_scores_fit` (g02lcc); otherwise **b** must

contain the parameter estimates for the original data as returned by `nag_pls_orth_scores_fit` (g02lcc).

11: **pdb** – Integer *Input*

*On entry:* the stride separating row or column elements (depending on the value of **order**) in the array **b**.

*Constraints:*

if **order** = Nag\_ColMajor,  
     if **orig** = Nag\_EstimatesStand, **pdb**  $\geq$  **ip**;  
     if **orig** = Nag\_EstimatesOrig, **pdb**  $\geq$  1 + **ip**.;  
 if **order** = Nag\_RowMajor, **pdb**  $\geq$  **my**.

12: **n** – Integer *Input*

*On entry:* *n*, the number of observations in the test data *Z*.

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

13: **mz** – Integer *Input*

*On entry:* the number of available predictor variables in the test data.

*Constraint:* **mz**  $\geq$  **ip**.

14: **isz[mz]** – const Integer *Input*

*On entry:* indicates which predictor variables are to be included in the model. Predictor variables included from **z** must be in the same order as those included in the fitted model.

If **isz**[*j* – 1] = 1, the *j*th predictor variable is included in the model, for *j* = 1, 2, ..., **mz**, otherwise **isz**[*j* – 1] = 0.

*Constraints:*

**isz**[*j* – 1] = 0 or 1, for *j* = 1, 2, ..., **mz**;  
 $\sum_j \mathbf{isz}[j - 1] = \mathbf{ip}$ .

15: **z[dim]** – const double *Input*

**Note:** the dimension, *dim*, of the array **z** must be at least

$\max(1, \mathbf{pdz} \times \mathbf{mz})$  when **order** = Nag\_ColMajor;  
 $\max(1, \mathbf{n} \times \mathbf{pdz})$  when **order** = Nag\_RowMajor.

Where **Z**(*i*, *j*) appears in this document, it refers to the array element

**z**[(*j* – 1)  $\times$  **pdz** + *i* – 1] when **order** = Nag\_ColMajor;  
**z**[(*i* – 1)  $\times$  **pdz** + *j* – 1] when **order** = Nag\_RowMajor.

*On entry:* **Z**(*i*, *j*) contains the *i*th observation on the *j*th available predictor variable, for *i* = 1, 2, ..., **n** and *j* = 1, 2, ..., **mz**.

16: **pdz** – Integer *Input*

*On entry:* the stride separating row or column elements (depending on the value of **order**) in the array **z**.

*Constraints:*

if **order** = Nag\_ColMajor, **pdz**  $\geq$  **n**;  
 if **order** = Nag\_RowMajor, **pdz**  $\geq$  **mz**.

17: **yhat**[*dim*] – double *Output*

**Note:** the dimension, *dim*, of the array **yhat** must be at least

$\max(1, \mathbf{pdyhat} \times \mathbf{my})$  when **order** = Nag\_ColMajor;  
 $\max(1, \mathbf{n} \times \mathbf{pdyhat})$  when **order** = Nag\_RowMajor.

Where **YHAT**(*i*, *j*) appears in this document, it refers to the array element

**yhat**[(*j* – 1) × **pdyhat** + *i* – 1] when **order** = Nag\_ColMajor;  
**yhat**[(*i* – 1) × **pdyhat** + *j* – 1] when **order** = Nag\_RowMajor.

*On exit:* **YHAT**(*i*, *j*) contains the *i*th predicted value of the *j*th *y*-variable in the model.

18: **pdyhat** – Integer *Input*

*On entry:* the stride separating row or column elements (depending on the value of **order**) in the array **yhat**.

*Constraints:*

if **order** = Nag\_ColMajor, **pdyhat** ≥ **n**;  
 if **order** = Nag\_RowMajor, **pdyhat** ≥ **my**.

19: **fail** – NagError \* *Input/Output*

The NAG error argument (see Section 3.6 in the Essential Introduction).

## 6 Error Indicators and Warnings

### NE\_ALLOC\_FAIL

Dynamic memory allocation failed.

### NE\_BAD\_PARAM

On entry, argument *<value>* had an illegal value.

### NE\_ENUM\_CHARACTER

On entry, **iscale** = *<value>*.

Constraint: if **orig** = Nag\_EstimatesStand, **iscale** = Nag\_PredNoScale, Nag\_PredStdScale or Nag\_PredUserScale.

### NE\_INT

On entry, **ip** = *<value>*.

Constraint: **ip** > 1.

On entry, **my** = *<value>*.

Constraint: **my** ≥ 1.

On entry, **n** = *<value>*.

Constraint: **n** ≥ 1.

On entry, **pdb** = *<value>*.

Constraint: **pdb** > 0.

On entry, **pdyhat** = *<value>*.

Constraint: **pdyhat** > 0.

On entry, **pdz** = *<value>*.

Constraint: **pdz** > 0.

**NE\_INT\_2**

On entry, **mz** =  $\langle value \rangle$  and **ip** =  $\langle value \rangle$ .

Constraint: **mz**  $\geq$  **ip**.

On entry, **pdb** =  $\langle value \rangle$  and **ip** + 1 =  $\langle value \rangle$ .

Constraint: if **orig** = Nag\_EstimatesOrig, **pdb**  $\geq$  1 + **ip**.

On entry, **pdb** =  $\langle value \rangle$  and **ip** =  $\langle value \rangle$ .

Constraint: if **orig** = Nag\_EstimatesStand, **pdb**  $\geq$  **ip**.

On entry, **pdb** =  $\langle value \rangle$  and **my** =  $\langle value \rangle$ .

Constraint: **pdb**  $\geq$  **my**.

On entry, **pdihat** =  $\langle value \rangle$  and **my** =  $\langle value \rangle$ .

Constraint: **pdihat**  $\geq$  **my**.

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

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

On entry, **pdz** =  $\langle value \rangle$  and **mz** =  $\langle value \rangle$ .

Constraint: **pdz**  $\geq$  **mz**.

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

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

**NE\_INT\_ARG\_CONS**

On entry, the number of elements of **isz** equal to 1 is not **ip**.

**NE\_INT\_ARRAY\_VAL\_1\_OR\_2**

On entry, **isz**[ $j - 1$ ] =  $\langle value \rangle$ ,  $j = \langle value \rangle$ .

Constraint: **isz**[ $j - 1$ ] = 0 or 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.

**7 Accuracy**

Not applicable.

**8 Parallelism and Performance**

nag\_pls\_orth\_scores\_pred (g02ldc) is not threaded by NAG in any implementation.

nag\_pls\_orth\_scores\_pred (g02ldc) makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the Users' Note for your implementation for any additional implementation-specific information.

**9 Further Comments**

nag\_pls\_orth\_scores\_pred (g02ldc) allocates internally  $3 \times \mathbf{ip} + \mathbf{my}$  elements of double storage.

**10 Example**

This example reads in parameter estimates for a fitted PLS model and prediction data, and the PLS model predictions are calculated.

## 10.1 Program Text

```

/* nag_pls_orth_scores_pred (g02ldc) Example Program.
 *
 * Copyright 2008, Numerical Algorithms Group.
 *
 * Mark 9, 2009.
 */
/* Pre-processor includes */
#include <stdio.h>
#include <math.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nagg02.h>
#include <nagx04.h>

int main(void)
{
    /*Integer scalar and array declarations */
    Integer          exit_status = 0;
    Integer          i, ip, j, l, my, mz, n;
    Integer          pdb, pdyhat, pdz;
    Integer          *isz = 0;
    /*Double scalar and array declarations */
    double          *b = 0, *xbar = 0, *xstd = 0, *ybar = 0, *yhat = 0;
    double          *ystd = 0, *z = 0;
    /*Character scalar and array declarations */
    char            siscale[40], sorig[40];
    /*NAG Types */
    Nag_OrderType   order;
    Nag_ScalePredictor iscale;
    Nag_EstimatesOption orig;
    NagError        fail;

    INIT_FAIL(fail);

    printf("nag_pls_orth_scores_pred (g02ldc) Example Program Results\n");
    /* Skip header in data file.*/
    scanf("%*[\n] ");
    /* Read data values.*/
    scanf("%ld%ld%39s %39s %ld%ld%*[\n] ",
          &ip, &my, sorig, siscale, &n, &mz);
    orig = (Nag_EstimatesOption) nag_enum_name_to_value(sorig);
    iscale = (Nag_ScalePredictor) nag_enum_name_to_value(siscale);

    #ifdef NAG_COLUMN_MAJOR
    pdb = ((orig == Nag_EstimatesStand)?ip:l+ip);
    #define B(I, J)    b[(J-1)*pdb + I-1]
    pdyhat = n;
    #define YHAT(I, J) yhat[(J-1)*pdyhat + I-1]
    pdz = n;
    #define Z(I, J)    z[(J-1)*pdz + I-1]
    order = Nag_ColMajor;
    #else
    pdb = my;
    #define B(I, J)    b[(I-1)*pdb + J-1]
    pdyhat = my;
    #define YHAT(I, J) yhat[(I-1)*pdyhat + J-1]
    pdz = mz;
    #define Z(I, J)    z[(I-1)*pdz + J-1]
    order = Nag_RowMajor;
    #endif
    if (!(b = NAG_ALLOC(pdb*(order == Nag_RowMajor?(l+ip):my), double)) ||
        !(xbar = NAG_ALLOC(ip, double)) ||
        !(xstd = NAG_ALLOC(ip, double)) ||
        !(ybar = NAG_ALLOC(my, double)) ||
        !(yhat = NAG_ALLOC(pdyhat*(order == Nag_RowMajor?n:my), double)) ||
        !(ystd = NAG_ALLOC(my, double)) ||
        !(z = NAG_ALLOC(pdz*(order == Nag_RowMajor?n:mz), double)) ||
        !(isz = NAG_ALLOC(mz, Integer)))
    {

```

```

        printf("Allocation failure\n");
        exit_status = -1;
        goto END;
    }
    /* Read prediction x-data*/
    for (i = 1; i <= n; i++)
    {
        for (j = 1; j <= mz; j++)
            scanf("%lf ", &Z(i, j));
    }
    scanf("%*[\n] ");
    /* Read elements of isz*/
    for (j = 0; j < mz; j++)
        scanf("%ld ", &isz[j]);
    scanf("%*[\n] ");
    /* Read parameter estimates*/
    l = ip;
    if (orig != Nag_EstimatesStand)
    {
        l = l+1;
    }
    for (j = 1; j <= l; j++)
    {
        for (i = 1; i <= my; i++)
            scanf("%lf ", &B(j, i));
    }
    scanf("%*[\n] ");
    /* Read means*/
    if (orig == Nag_EstimatesStand)
    {
        for (j = 0; j < ip; j++)
            scanf("%lf ", &xbar[j]);
        scanf("%*[\n] ");
        for (l = 0; l < my; l++)
            scanf("%lf ", &ybar[l]);
        scanf("%*[\n] ");
    }
    /* Read scalings*/
    if ((orig == Nag_EstimatesStand) && (iscale != Nag_PredNoScale))
    {
        for (j = 0; j < ip; j++)
            scanf("%lf ", &xstd[j]);
        scanf("%*[\n] ");
        for (l = 0; l < my; l++)
            scanf("%lf ", &ystd[l]);
        scanf("%*[\n] ");
    }
    /* Calculate predictions*/
    /*
    * nag_pls_orth_scores_pred (g02ldc)
    * Partial least-squares
    */
    nag_pls_orth_scores_pred(order, ip, my, orig, xbar, ybar, iscale, xstd,
                            ystd, b, pdb, n, mz, isz, z, pdz, yhat, pdyhat,
                            &fail);
    if (fail.code != NE_NOERROR)
    {
        printf("Error from nag_pls_orth_scores_pred (g02ldc).\n%s\n",
              fail.message);
        exit_status = 1;
        goto END;
    }
    /*
    * nag_gen_real_mat_print (x04cac)
    * Print real general matrix (easy-to-use)
    */
    fflush(stdout);
    nag_gen_real_mat_print(order, Nag_GeneralMatrix, Nag_NonUnitDiag, n, my,
                            yhat, pdyhat, "YHAT", 0, &fail);
    if (fail.code != NE_NOERROR)
    {

```

```

    printf("Error from nag_gen_real_mat_print (x04cac).\n%s\n",
           fail.message);
    exit_status = 1;
    goto END;
}

END:
NAG_FREE(b);
NAG_FREE(xbar);
NAG_FREE(xstd);
NAG_FREE(ybar);
NAG_FREE(yhat);
NAG_FREE(ystd);
NAG_FREE(z);
NAG_FREE(isz);

return exit_status;
}

```

## 10.2 Program Data

```

nag_pls_orth_scores_pred (g02ldc) Example Program Data
15 1 Nag_EstimatesStand Nag_PredStdScale 15 15 : ip, my, orig, iscale, n, mz
-2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
 1.9607 -1.6324 0.5746 1.9607 -1.6324 0.5740
 2.8369 1.4092 -3.1398
-2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
 1.9607 -1.6324 0.5746 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398
-2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
 0.0744 -1.7333 0.0902 1.9607 -1.6324 0.5746
 2.8369 1.4092 -3.1398
-2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
 0.0744 -1.7333 0.0902 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398
-2.6931 -2.5271 -1.2871 2.8369 1.4092 -3.1398
 0.0744 -1.7333 0.0902 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398
-2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
-4.7548 3.6521 0.8524 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398
-2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
 0.0744 -1.7333 0.0902 0.0744 -1.7333 0.0902
-1.2201 0.8829 2.2253
-2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
 2.4064 1.7438 1.1057 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398
-2.6931 -2.5271 -1.2871 0.0744 -1.7333 0.0902
 0.0744 -1.7333 0.0902 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398
 2.2261 -5.3648 0.3049 3.0777 0.3891 -0.0701
 0.0744 -1.7333 0.0902 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398
-4.1921 -1.0285 -0.9801 3.0777 0.3891 -0.0701
 0.0744 -1.7333 0.0902 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398
-4.9217 1.2977 0.4473 3.0777 0.3891 -0.0701
 0.0744 -1.7333 0.0902 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398
-2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
 2.2261 -5.3648 0.3049 2.2261 -5.3648 0.3049
 2.8369 1.4092 -3.1398
-2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
-4.9217 1.2977 0.4473 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398
-2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
-4.1921 -1.0285 -0.9801 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398 : z
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 : Elements of isz
-0.1383 0.0572 -0.1906 0.1238 0.0591 0.0936

```



```

-0.2842  0.4713  0.2661 -0.0914  0.1226 -0.0488
 0.0332  0.0332 -0.0332 : b
-2.6137 -2.3614 -1.0449  2.8614  0.3156 -0.2641
-0.3146 -1.1221  0.2401  0.4694 -1.9619  0.1691
 2.5664  1.3741 -2.7821 : xbar
 0.4520 : ybar
 1.4956  1.3233  0.5829  0.7735  0.6247  0.7966
 2.4113  2.0421  0.4678  0.8197  0.9420  0.1735
 1.0475  0.1359  1.3853 : xstd
 0.9062 : ystd

```

### 10.3 Program Results

nag\_pls\_orth\_scores\_pred (g02ldc) Example Program Results

```

YHAT
      1
 1      0.2132
 2      0.5152
 3      0.1437
 4      0.4459
 5      0.1716
 6      2.4809
 7      0.0964
 8      1.4475
 9     -0.1546
10     -0.5492
11      0.5393
12      0.2686
13     -1.1332
14      1.7975
15      0.4973

```

---