# NAG Library Function Document nag outlier peirce (g07gac)

## 1 Purpose

nag\_outlier\_peirce (g07gac) identifies outlying values using Peirce's criterion.

# 2 Specification

## 3 Description

nag outlier peirce (g07gac) flags outlying values in data using Peirce's criterion. Let

y denote a vector of n observations (for example the residuals) obtained from a model with p parameters,

m denote the number of potential outlying values,

 $\mu$  and  $\sigma^2$  denote the mean and variance of y respectively,

 $\tilde{y}$  denote a vector of length n-m constructed by dropping the m values from y with the largest value of  $|y_i - \mu|$ ,

 $\tilde{\sigma}^2$  denote the (unknown) variance of  $\tilde{y}$ ,

 $\lambda$  denote the ratio of  $\tilde{\sigma}$  and  $\sigma$  with  $\lambda = \frac{\tilde{\sigma}}{\sigma}$ .

Peirce's method flags  $y_i$  as a potential outlier if  $|y_i - \mu| \ge x$ , where  $x = \sigma^2 z$  and z is obtained from the solution of

$$R^m = \lambda^{m-n} \frac{m^m (n-m)^{n-m}}{n^n} \tag{1}$$

where

$$R = 2 \exp\left(\left(\frac{z^2 - 1}{2}\right)(1 - \Phi(z))\right) \tag{2}$$

and  $\Phi$  is the cumulative distribution function for the standard Normal distribution.

As  $\tilde{\sigma}^2$  is unknown an assumption is made that the relationship between  $\tilde{\sigma}^2$  and  $\sigma^2$ , hence  $\lambda$ , depends only on the sum of squares of the rejected observations and the ratio estimated as

$$\lambda^2 = \frac{n - p - mz^2}{n - p - m}$$

which gives

$$z^{2} = 1 + \frac{n - p - m}{m} (1 - \lambda^{2})$$
(3)

A value for the cutoff x is calculated iteratively. An initial value of R=0.2 is used and a value of  $\lambda$  is estimated using equation (1). Equation (3) is then used to obtain an estimate of z and then equation (2) is used to get a new estimate for R. This process is then repeated until the relative change in z between consecutive iterations is  $\leq \sqrt{\epsilon}$ , where  $\epsilon$  is **machine precision**.

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By construction, the cutoff for testing for m+1 potential outliers is less than the cutoff for testing for m potential outliers. Therefore Peirce's criterion is used in sequence with the existence of a single potential outlier being investigated first. If one is found, the existence of two potential outliers is investigated etc.

If one of a duplicate series of observations is flagged as an outlier, then all of them are flagged as outliers.

#### 4 References

Gould B A (1855) On Peirce's criterion for the rejection of doubtful observations, with tables for facilitating its application *The Astronomical Journal* **45** 

Peirce B (1852) Criterion for the rejection of doubtful observations The Astronomical Journal 45

# 5 Arguments

1:  $\mathbf{n}$  - Integer Input

On entry: n, the number of observations.

Constraint:  $n \geq 3$ .

2: **p** – Integer Input

On entry: p, the number of parameters in the model used in obtaining the y. If y is an observed set of values, as opposed to the residuals from fitting a model with p parameters, then p should be set to 1, i.e., as if a model just containing the mean had been used.

Constraint:  $1 \le p \le n - 2$ .

3:  $\mathbf{y}[\mathbf{n}]$  - const double

On entry: y, the data being tested.

4: **mean** – double Input

On entry: if var > 0.0, mean must contain  $\mu$ , the mean of y, otherwise mean is not referenced and the mean is calculated from the data supplied in y.

5: **var** – double *Input* 

On entry: if  $\mathbf{var} > 0.0$ ,  $\mathbf{var}$  must contain  $\sigma^2$ , the variance of y, otherwise the variance is calculated from the data supplied in  $\mathbf{y}$ .

6: iout[n] - Integer Output

On exit: the indices of the values in y sorted in descending order of the absolute difference from the mean, therefore  $|\mathbf{y}[\mathbf{iout}[i-1] - \mu| \ge |\mathbf{y}[\mathbf{iout}[i-1] - \mu|, \text{ for } i = 2, 3, \dots, \mathbf{n}.$ 

7: **niout** – Integer \* Output

On exit: the number of potential outliers. The indices for these potential outliers are held in the first **niout** elements of **iout**. By construction there can be at most  $\mathbf{n} - \mathbf{p} - 1$  values flagged as outliers.

8: **Idiff** – Integer Input

On entry: the maximum number of values to be returned in arrays diff and llamb.

If  $\mathbf{ldiff} \leq 0$ , arrays  $\mathbf{diff}$  and  $\mathbf{llamb}$  are not referenced and both  $\mathbf{diff}$  and  $\mathbf{llamb}$  may be  $\mathbf{NULL}$ .

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# 9: **diff[ldiff**] – double

Output

On exit: if **diff** is not **NULL** then **diff**[i-1] holds  $|y-\mu|-\sigma^2z$  for observation  $\mathbf{y}[\mathbf{iout}[i-1]-1]$ , for  $i=1,2,\ldots,\min(\mathbf{ldiff},\mathbf{niout}+1,\mathbf{n-p}-1)$ .

#### 10: **llamb**[**ldiff**] – double

Output

On exit: if **llamb** is not **NULL** then **llamb**[i-1] holds  $\log (\lambda^2)$  for observation **y**[iout[i-1]-1], for  $i=1,2,\ldots,\min(\text{ldiff},\text{niout}+1,\mathbf{n}-\mathbf{p}-1)$ .

#### 11: **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 ALLOC FAIL

Dynamic memory allocation failed.

See Section 3.2.1.2 in How to Use the NAG Library and its Documentation for further information.

#### NE BAD PARAM

On entry, argument  $\langle value \rangle$  had an illegal value.

#### NE INT

```
On entry, \mathbf{n} = \langle value \rangle. Constraint: \mathbf{n} \geq 3.
```

## NE\_INT\_2

```
On entry, \mathbf{p} = \langle value \rangle and \mathbf{n} = \langle value \rangle.
Constraint: 1 \le \mathbf{p} \le \mathbf{n} - 2.
```

## 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.

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

See Section 3.6.6 in How to Use the NAG Library and its Documentation for further information.

## NE NO LICENCE

Your licence key may have expired or may not have been installed correctly. See Section 3.6.5 in How to Use the NAG Library and its Documentation for further information.

## 7 Accuracy

Not applicable.

#### 8 Parallelism and Performance

nag\_outlier\_peirce (g07gac) is not threaded in any implementation.

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#### 9 Further Comments

One problem with Peirce's algorithm as implemented in nag\_outlier\_peirce (g07gac) is the assumed relationship between  $\sigma^2$ , the variance using the full dataset, and  $\tilde{\sigma}^2$ , the variance with the potential outliers removed. In some cases, for example if the data y were the residuals from a linear regression, this assumption may not hold as the regression line may change significantly when outlying values have been dropped resulting in a radically different set of residuals. In such cases nag\_outlier\_peirce\_two\_var (g07gbc) should be used instead.

## 10 Example

This example reads in a series of data and flags any potential outliers.

The dataset used is from Peirce's original paper and consists of fifteen observations on the vertical semidiameter of Venus.

## 10.1 Program Text

```
/* nag_outlier_peirce (g07gac) Example Program.
* NAGPRODCODE Version.
* Copyright 2016 Numerical Algorithms Group.
 * Mark 26, 2016.
/* Pre-processor includes */
#include <stdio.h>
#include <math.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nagg07.h>
int main(void)
{
  /* Integer scalar and array declarations */
 Integer i, n, niout, p, exit_status, ldiff;
 Integer *iout = 0;
  /* NAG structures */
 NagError fail;
  /* Double scalar and array declarations */
 double *y = 0, *diff = 0, *llamb = 0;
  /* Let the routine calculate the mean and variance from the supplied data */
  double mean = 0.0;
  double var = 0.0;
 exit_status = 0;
  /* Initialize the error structure */
 INIT_FAIL(fail);
 printf("nag_outlier_peirce (g07gac) Example Program Results\n");
  /* Skip headings in data file */
#ifdef _WIN32
 scanf_s("%*[^\n] ");
#else
 scanf("%*[^\n] ");
#endif
  /* Read in the problem size */
#ifdef _WIN32
```

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```
scanf_s("%" NAG_IFMT " %" NAG_IFMT " %" NAG_IFMT "%*[^\n] ", &n, &p,
#else
 scanf("%" NAG_IFMT " %" NAG_IFMT " %" NAG_IFMT "%*[^\n] ", &n, &p, &ldiff);
#endif
  if (!(y = NAG\_ALLOC(n, double)) | |
      !(diff = NAG_ALLOC(ldiff, double)) ||
      !(llamb = NAG_ALLOC(ldiff, double)) || !(iout = NAG_ALLOC(n, Integer)))
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
  /* Read in the data */
  for (i = 0; i < n; i++)
#ifdef _WIN32
   scanf_s("%lf%*[^\n] ", &y[i]);
#else
   scanf("%lf%*[^\n] ", &y[i]);
#endif
  /* Use nag_outlier_peirce (g07gac) to get a list of potential outliers */
  nag_outlier_peirce(n, p, y, mean, var, iout, &niout, ldiff, diff, llamb,
                     &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_outlier_peirce (g07gac).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  /* Display the potential outliers */
  printf("\n");
printf(" Number of potential outliers: %" NAG_IFMT "\n", niout);
  if (ldiff > 0) {
    printf(" %5s %5s %8s
                                  %8s\n", "No.", "Index", "Value",
                            %8s
           "Diff", "ln(lambda^2)");
  }
  else {
   printf(" %5s %5s %8s\n", "No.", "Index", "Value");
  for (i = 0; i < niout; i++)
    if (i < ldiff) {</pre>
     printf("%5" NAG_IFMT " %5" NAG_IFMT " %10.2f %10.2f %10.2f \n", i + 1,
             iout[i], y[iout[i] - 1], diff[i], llamb[i]);
    else {
     printf("%5" NAG_IFMT " %5" NAG_IFMT " %10.2f\n", i + 1, iout[i],
             y[iout[i] - 1]);
    }
END:
 NAG_FREE(y);
  NAG_FREE (diff);
 NAG_FREE(llamb);
 NAG_FREE(iout);
  return exit_status;
}
10.2 Program Data
nag_outlier_peirce (g07gac) Example Program Data
15 2 1 :: n,p,ldiff
-0.30
0.48
0.63
-0.22
```

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```
-0.44
-0.24
-0.13
-0.05
0.39
1.01
0.06
-1.40
0.20
0.10 :: y
```

# 10.3 Program Results

nag\_outlier\_peirce (g07gac) Example Program Results

Number	of pote	ential outl	iers: 2	
No.	Index	Value	Diff	<pre>ln(lambda^2)</pre>
1	13	-1.40	0.31	-0.30
2	11	1.01		

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