# NAG Toolbox for MATLAB g04bb

# 1 Purpose

g04bb computes the analysis of variance and treatment means and standard errors for a randomized block or completely randomized design.

# 2 Syntax

```
[gmean, bmean, tmean, tabl, c, irep, r, ef, ifail] = g04bb(y, iblock, nt, it, tol, irdf, 'n', n)
```

## 3 Description

In a completely randomized design the experimental material is divided into a number of units, or plots, to which a treatment can be applied. In a randomized block design the units are grouped into blocks so that the variation within blocks is less than the variation between blocks. If every treatment is applied to one plot in each block it is a complete block design. If there are fewer plots per block than treatments then the design will be an incomplete block design and may be balanced or partially balanced.

For a completely randomized design, with t treatments and  $n_t$  plots per treatment, the linear model is

$$y_{ij} = \mu + \tau_j + e_{ij}, \quad j = 1, 2, \dots, t \text{ and } i = 1, 2, \dots, n_j,$$

where  $y_{ij}$  is the *i*th observation for the *j*th treatment,  $\mu$  is the overall mean,  $\tau_j$  is the effect of the *j*th treatment and  $e_{ij}$  is the random error term. For a randomized block design, with *t* treatments and *b* blocks of *k* plots, the linear model is

$$y_{ii(l)} = \mu + \beta_i + \tau_l + e_{ij}, \quad i = 1, 2, \dots, b, j = 1, 2, \dots, k \text{ and } l = 1, 2, \dots, t,$$

where  $\beta_i$  is the effect of the *i*th block and the ij(l) notation indicates that the *l*th treatment is applied to the *i*th plot in the *j*th block.

The completely randomized design gives rise to a one-way analysis of variance. The treatments do not have to be equally replicated, i.e., do not have to occur the same number of times. First the overall mean,  $\hat{\mu}$ , is computed and subtracted from the observations to give  $y'_{ij} = y_{ij} - \hat{\mu}$ . The estimated treatment effects,  $\hat{\tau}_j$  are then computed as the treatment means of the mean adjusted observations,  $y'_{ij}$ , and the treatment sum of squares can be computed from the sum of squares of the treatment totals of the  $y'_{ij}$  divided by the number of observations per treatment total,  $n_j$ . The final residuals are computed as  $r_{ij} = y'_{ij} - \hat{\tau}_j$ , and, from the residuals, the residual sum of squares is calculated.

For the randomized block design the mean is computed and subtracted from the observations to give  $y'_{ij(l)} = y_{ij(l)} - \hat{\mu}$ . The estimated block effects, ignoring treatment effects,  $\hat{\beta}_i$ , are then computed using the block means of the  $y'_{ij(l)}$  and the unadjusted sum of squares computed as the sum of squared block totals for the  $y'_{ij(l)}$  divided by number of plots per block, k. The block adjusted observations are then computed as  $y''_{ij(l)} = y'_{ij(l)} = \hat{\beta}_i$ . In the case of the complete block design, with the same replication for each treatment within each block, the blocks and treatments are orthogonal, and so the treatment effects are estimated as the treatment means of the block adjusted observations,  $y''_{ij(l)}$ . The treatment sum of squares is computed as the sum of squared treatment totals of the  $y''_{ij(l)}$  divided by the number of replicates to the treatments, r = bk/t. Finally the residuals, and hence the residual sum of squares, are given by  $r_{ij(l)} = y''_{ij(l)} - \hat{\tau}_l$ .

For a design without the same replication for each treatment within each block the treatments and the blocks will not be orthogonal, so the treatments adjusted for blocks need to be computed. The adjusted treatment effects are found as the solution to the equations

$$(R - NN^{\mathrm{T}}/k)\hat{\tau} = q,$$

where q is the vector of the treatment totals for block adjusted observations,  $y''_{ij(l)}$ , R is a diagonal matrix with  $R_{ll}$  equal to the number of times the lth treatment is replicated, and  $\mathbf{n}$  is the t by b incidence matrix, with  $N_{lj}$  equal to the number of times treatment l occurs in block j. The solution to the equations can be written as

$$\hat{\tau} = \Omega q$$

where  $\Omega$  is a generalized inverse of  $(R-NN^{\rm T}/k)$ . The solution is found from the eigenvalue decomposition of  $(R-NN^{\rm T}/k)$ . The residuals are first calculated by subtracting the estimated treatment effects from the block adjusted observations to give  $r'_{ij(l)} = y''_{ij(l)} - \hat{\tau}_l$ . However, since only the unadjusted block effects have been removed and blocks and treatments are not orthogonal, the block means of the  $r'_{ij(l)}$  have to be subtracted to give the correct residuals,  $r_{ij(l)}$  and residual sum of squares.

The mean squares are computed as the sum of squares divided by the degrees of freedom. The degrees of freedom for the unadjusted blocks is b-1, for the completely randomized and the complete block designs the degrees of freedom for the treatments is t-1. In the general case the degrees of freedom for treatments is the rank of the matrix  $\Omega$ . The F-statistic given by the ratio of the treatment mean square to the residual mean square tests the hypothesis

$$H_0: \tau_1 = \tau_2 = \cdots = \tau_t = 0.$$

The standard errors for the difference in treatment effects, or treatment means, for the completely randomized or the complete block designs, are given by:

$$\operatorname{se}(\tau_j - \tau_{j*}) = \left(\frac{1}{n_j} + \frac{1}{n_{j*}}\right) s^2$$

where  $s^2$  is the residual mean square and  $n_j = n_{j*} = b$  in the complete block design. In the general case the variances of the treatment effects are given by

$$\operatorname{var}(\tau) = \Omega s^2$$

from which the appropriate standard errors of the difference between treatment effects or the difference between adjusted means can be calculated.

In the complete block design all the information on the treatment effects is given by the within block analysis. In other designs there may be a loss of information due to the non-orthogonality of treatments and blocks. The efficiency of the within block analysis in these cases is given by the (canonical) efficiency factors, these are the nonzero eigenvalues of the matrix  $(R - NN^T/k)$ , divided by the number of replicates in the case of equal replication, or by the mean of the number of replicates in the unequally replicated case, see John 1987. If more than one eigenvalue is zero then the design is said to be disconnected and some treatments can only be compared using a between block analysis.

## 4 References

Cochran W G and Cox G M 1957 Experimental Designs Wiley

Davis O L 1978 The Design and Analysis of Industrial Experiments Longman

John J A 1987 Cyclic Designs Chapman and Hall

John J A and Quenouille M H 1977 Experiments: Design and Analysis Griffin

Searle S R 1971 Linear Models Wiley

## 5 Parameters

## 5.1 Compulsory Input Parameters

1: y(n) - double array

The observations in the order as described by iblock and nt.

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#### 2: iblock – int32 scalar

Indicates the block structure.

```
abs(iblock) \leq '1'
```

There are no blocks, i.e., it is a completely randomized design.

## iblock $\geq 2$

There are **iblock** blocks and the data should be input by blocks, i.e., y must contain the observations for block 1 followed by the observations for block 2, etc.

## iblock < -2

There are abs(iblock) blocks and the data is input in parallel with respect to blocks, i.e., y(1) must contain the first observation for block 1, y(2) must contain the first observation for block  $2 \cdots y(abs(iblock))$  must contain the first observation for block abs(iblock), y(abs(iblock + 1)) must contain the second observation for block 1, etc.

Constraint: **iblock** = 1, 2 or -2.

## 3: nt - int32 scalar

the number of treatments. If only blocks are required in the analysis then set  $\mathbf{nt} = 1$ .

Constraints:

```
if abs(iblock) \ge 2, nt \ge 1; nt \ge 2 otherwise.
```

## 4: it(\*) - int32 array

Note: the dimension of the array it must be at least n if  $nt \ge 2$ , and at least 1 otherwise.

it(i) indicates which of the **nt** treatments plot i received, for i = 1, 2, ..., n. If nt = 1, it is not referenced.

```
Constraint: 1 \leq it(i) \leq nt, for i = 1, 2, ..., n.
```

#### 5: tol – double scalar

The tolerance value used to check for zero eigenvalues of the matrix  $\Omega$ . If tol = 0.0 a default value of  $10^{-5}$  is used.

Constraint:  $tol \ge 0.0$ .

#### 6: irdf – int32 scalar

An adjustment to the degrees of freedom for the residual and total.

## $irdf \ge 1$

The degrees of freedom for the total is set to  $\mathbf{n} - \mathbf{irdf}$  and the residual degrees of freedom adjusted accordingly.

irdf = 0

the total degrees of freedom for the total is set to n-1, as usual.

Constraint:  $irdf \ge 0$ .

## 5.2 Optional Input Parameters

## 1: n - int32 scalar

*Default*: The dimension of the arrays  $\mathbf{r}$ ,  $\mathbf{y}$ . (An error is raised if these dimensions are not equal.) the number of observations.

Constraint:  $n \ge 2$  and if  $abs(iblock) \ge 2$ , n must be a multiple of abs(iblock).

## 5.3 Input Parameters Omitted from the MATLAB Interface

ldtabl, ldc, wk

## 5.4 Output Parameters

1: gmean – double scalar

The grand mean,  $\hat{\mu}$ .

2: bmean(\*) - double array

**Note**: the dimension of the array **bmean** must be at least  $max(1, abs^{arg} iblock)$ .

If  $abs(iblock) \ge 2$ , bmean(j) contains the mean for the jth block,  $\hat{\beta}_j$  for j = 1, 2, ..., b.

3: tmean(nt) – double array

If  $\mathbf{nt} \geq 2$ ,  $\mathbf{tmean}(l)$  contains the (adjusted) mean for the lth treatment,  $\hat{\mu}^* + \hat{\tau}_l$ , for  $l = 1, 2, \dots, t$ , where  $\hat{\mu}^*$  is the mean of the treatment adjusted observations,  $y_{ij(l)} - \hat{\tau}_l$ .

4: tabl(ldtabl,5) - double array

The analysis of variance table. Column 1 contains the degrees of freedom, column 2 the sum of squares, and where appropriate, column 3 the mean squares, column 4 the *F*-statistic and column 5 the significance level of the *F*-statistic. Row 1 is for Blocks, row 2 for Treatments, row 3 for Residual and row 4 for Total. Mean squares are computed for all but the Total row; *F*-statistics and significance are computed for Treatments and Blocks, if present. Any unfilled cells are set to zero.

5: c(ldc,nt) - double array

If  $\mathbf{nt} \geq 2$ , the upper triangular part of  $\mathbf{c}$  contains the variance-covariance matrix of the treatment effects, the strictly lower triangular part contains the standard errors of the difference between two treatment effects (means), i.e.,  $\mathbf{c}(i,j)$  contains the covariance of treatment i and j if  $j \geq i$  and the standard error of the difference between treatment i and j if j < i for  $i = 1, 2, \dots, t$ ;  $j = 1, 2, \dots, t$ .

6: irep(nt) - int32 array

If  $\mathbf{nt} \geq 2$ , the treatment replications,  $R_{ll}$ , for  $l = 1, 2, \dots, \mathbf{nt}$ .

7: r(n) – double array

The residuals,  $r_i$ , for  $i = 1, 2, \dots \mathbf{n}$ .

8: ef(nt) - double array

If  $nt \ge 2$ , the canonical efficiency factors.

9: ifail – int32 scalar

0 unless the function detects an error (see Section 6).

## 6 Error Indicators and Warnings

Note: g04bb may return useful information for one or more of the following detected errors or warnings.

# ifail = 1

```
On entry, \mathbf{n} < 2, or \mathbf{nt} \le 0, or \mathbf{nt} = 1 and abs(\mathbf{iblock}) \le 1, or \mathbf{ldtabl} < 4, or \mathbf{ldc} < \mathbf{nt},
```

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```
or \mathbf{tol} < 0.0, or \mathbf{irdf} < 0.
```

#### ifail = 2

On entry,  $abs(iblock) \ge 2$  and **n** is not a multiple of abs(iblock).

#### ifail = 3

```
On entry, \mathbf{it}(i) < 1 or \mathbf{it}(i) > \mathbf{nt} for some i when \mathbf{nt} \ge 2, or no value of \mathbf{it} = j for some j = 1, 2, ..., \mathbf{nt}, when \mathbf{nt} \ge 2.
```

## ifail = 4

On entry, the values of y are constant.

## ifail = 5

A computed standard error is zero due to rounding errors, or the eigenvalue computation failed to converge. Both are unlikely error exits.

## ifail = 6

The treatments are totally confounded with blocks, so the treatment sum of squares and degrees of freedom are zero. The analysis of variance table is not computed, except for block and total sums of squares and degrees of freedom.

#### ifail = 7

The residual degrees of freedom or the residual sum of squares are zero, columns 3, 4 and 5 of the analysis of variance table will not be computed and the matrix of standard errors and covariances,  $\mathbf{c}$ , will not be scaled by s or  $s^2$ .

## ifail = 8

The design is disconnected; the standard errors may not be valid. The design may be nested.

# 7 Accuracy

The algorithm used by g04bb, described in Section 3, achieves greater accuracy than the traditional algorithms based on the subtraction of sums of squares.

## **8 Further Comments**

To estimate missing values the Healy and Westmacott procedure or its derivatives may be used, see John and Quenouille 1977. This is an iterative procedure in which estimates of the missing values are adjusted by subtracting the corresponding values of the residuals. The new estimates are then used in the analysis of variance. This process is repeated until convergence. A suitable initial value may be the grand mean  $\hat{\mu}$ . When using this procedure **irdf** should be set to the number of missing values plus one to obtain the correct degrees of freedom for the residual sum of squares.

For designs such as Graeco–Latin squares one or more of the blocking factors has to be removed in a preliminary analysis before the final analysis using calls to g04bb or g04bc. The residuals from the preliminary analysis are then input to g04bb. In these cases **irdf** should be set to the difference between **n** and the residual degrees of freedom from preliminary analysis. Care should be taken when using this approach as there is no check on the orthogonality of the two analyses.

For analysis of covariance the residuals are obtained from an analysis of variance of both the response variable and the covariates. The residuals from the response variable are then regressed on the residuals from the covariates using, say, g02cb or g02da. The results from those functions can be used to test for the significance of the covariates. To test the significance of the treatment effects after fitting the covariate, the residual sum of squares from the regression should be compared with the residual sum of squares obtained from the equivalent regression but using the residuals from fitting blocks only.

# 9 Example

```
y = [1;
     5;
     4;
     5;
     10;
     6;
     2;
     9;
     3;
     4;
     8;
     6;
     2;
     4;
     7;
     6;
     7;
     5;
     5;
     7;
     2;
     7;
     2;
     4;
     8;
     4;
     2;
     10;
     8;
     7];
iblock = int32(10);
nt = int32(6);
it = [int32(1);
     int32(2);
     int32(3);
     int32(1);
     int32(2);
     int32(4);
     int32(1);
     int32(3);
     int32(5);
     int32(1);
     int32(4);
     int32(6);
     int32(1);
     int32(5);
     int32(6);
     int32(2);
     int32(3);
     int32(6);
     int32(2);
     int32(4);
     int32(5);
     int32(2);
     int32(5);
     int32(6);
     int32(3);
     int32(4);
     int32(5);
     int32(3);
     int32(4);
     int32(6)];
tol = 5e-06;
irdf = int32(0);
[gmean, bmean, tmean, table, c, irep, r, ef, ifail] = g04bb(y, iblock,
nt, it, tol, irdf)
```

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```
gmean =
   5.3333
bmean =
    3.3333
    7.0000
    4.6667
    6.0000
    4.3333
    6.0000
    4.6667
    4.3333
    4.6667
    8.3333
tmean =
    2.5000
    7.2500
    8.0833
    5.9167
    2.9167
    5.3333
table =
                                             0.0039
    9.0000
             60.0000
                        6.6667
                                  4.7872
    5.0000
            101.7778
                       20.3556
                                  14.6170
                                             0.0000
            20.8889
                         1.3926
                                        Ω
   15.0000
                                                  Ω
   29.0000
           182.6667
                                        0
                                                  0
                       -0.0580
                                  -0.0580
    0.2901
             -0.0580
                                            -0.0580
                                                       -0.0580
                       -0.0580
    0.8344
             0.2901
                                  -0.0580
                                            -0.0580
                                                       -0.0580
    0.8344
              0.8344
                        0.2901
                                  -0.0580
                                            -0.0580
                                                       -0.0580
    0.8344
              0.8344
                        0.8344
                                  0.2901
                                            -0.0580
                                                       -0.0580
                        0.8344
                                            0.2901
    0.8344
              0.8344
                                  0.8344
                                                       -0.0580
    0.8344
              0.8344
                        0.8344
                                   0.8344
                                             0.8344
                                                       0.2901
irep =
           5
           5
           5
           5
r =
    1.1111
   0.3611
   -1.4722
   0.7222
   0.9722
   -1.6944
   -0.6667
   0.7500
   -0.0833
    0.0833
   0.6667
   -0.7500
   -1.2500
    0.3333
    0.9167
   -0.3611
   -0.1944
   0.5556
   -1.5556
    1.7778
   -0.2222
   0.5833
   -0.0833
   -0.5000
   0.8889
   -0.9444
    0.0556
    0.0278
    0.1944
   -0.2222
```

```
ef =

0
0.8000
0.8000
0.8000
0.8000
0.8000
0.8000
ifail =
```

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