

# Package ‘optbdmaeAT’

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**Title** Optimal Block Designs for Two-Colour cDNA Microarray Experiments

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**Depends** R (>= 3.3.1), MASS, Matrix, igraph, tcltk

**License** GPL-2

**Description** Computes A-, MV-, D- and E-optimal or near-optimal block designs for two-colour cDNA microarray experiments using the linear fixed effects and mixed effects models where the interest is in a comparison of all possible elementary treatment contrasts. The algorithms used in this package are based on the treatment exchange and array exchange algorithms of Debusho, Gemechu and Haines (2016, unpublished). The package also provides an optional method of using the graphical user interface (GUI) R package tcltk to ensure that it is user friendly.

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`cmatbd.mae`*Computes the treatment information matrix*

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### Description

Computes the information matrix (C-matrix) for treatment effects under either the linear fixed effects model or the linear mixed effects model setting for a given block design of size 2.

### Usage

```
cmatbd.mae(trt.N, blk.N, theta, des)
```

### Arguments

<code>trt.N</code>	integer, specifying number of treatments, $v$ .
<code>blk.N</code>	integer, specifying number of arrays, $b$ .
<code>theta</code>	numeric, representing a function of the ratio of random array variance and random error variance. It takes any value between 0 and 1, inclusive.
<code>des</code>	matrix, a $2 \times b$ block design with $b$ blocks of size $k = 2$ and $v$ treatments.

### Value

Returns a  $v \times v$  treatment information matrix (C-matrix).

### Author(s)

Dibaba Bayisa Gemechu, Legesse Kassa Debusho, and Linda Haines

### References

Debusho, L. K., Gemechu, D. B., and Haines, L. M. (2016). Algorithmic construction of optimal block designs for two-colour cDNA microarray experiments using the linear mixed model. Under review.

Gemechu D. B., Debusho L. K. and Haines L. M. (2014). A-optimal designs for two-colour cDNA microarray experiments using the linear mixed effects model. *Peer-reviewed Proceedings of the Annual Conference of the South African Statistical Association for 2014 (SASA 2014), Rhodes University, Grahamstown, South Africa.* pp 33-40, ISBN: 978-1-86822-659-7.

### See Also

[optbdmaeAT](#), [fixparbd.mae](#), [intcbd.mae](#)

## Examples

```
##Information matrix

trt.N <- 3
blk.N <- 3
theta <- 0.2
dsgn <- intcbd.mae(trt.N = 3, blk.N = 3)

cmatbd.mae(trt.N = 3, blk.N = 3, theta = 0.2, des = dsgn)
```

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fixparbd.mae	<i>Sets parametric values</i>
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## Description

Creates a `tcltk` widow that allow the users to set or fix values for the parametric combinations to compute optimal or near-optimal block designs.

## Usage

```
fixparbd.mae(Optcrit)
```

## Arguments

Optcrit	character, specifying the optimality criteria to be used. Optcrit takes the letter "A", "MV", "D" and "E" for A-, MV-, D- and E-optimal or near-optimal block designs, respectively.
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## Details

`fixparbd.mae` creates a pop-up `tcltk` window that allow the users to set the parametric combinations to compute optimal or near-optimal block designs. The parameters include the number of treatments `trt.N`, number arrays `blk.N`, theta value `theta`, number of replications of the optimization procedure `nrep` and number of iterations required during exchange procedure `itr.cvrgval`. Furthermore, on this window, the checkbox options that allow the users to choose whether or not they need to have the graphical layout of the resultant optimal or near-optimal block design, to make a choice between the two-alternative algorithms (treatment exchange and array exchange algorithms) and to print the summary of the resultant optimal or near-optimal block design on R-console directly are available.

After setting all the required parametric combinations and selecting the algorithm of interest, clicking on the search button on the set parametric combinations `tcltk` window, similar to the results that can be obtained when using the function `optbdmaeAT`, the summary of the resultant optimal or near-optimal block design will be saved in the current working directory in `.csv` format and it will also be displayed on R console with graphical layout of the resultant optimal or near-optimal block designs.

**Value**

The `fixparbd.mae` function creates a pop-up tcltk window that allow the users to set the parametric combinations to compute optimal or near-optimal block designs.

**Author(s)**

Dibaba Bayisa Gemechu, Legesse Kassa Debusho, and Linda Haines

**See Also**

[optbdmaeAT](#), [mmenubd.mae](#), [tcltk](#), [TkWidgets](#)

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graphoptbd.mae

*Creates the graphical layout of resultant optimal design*

---

**Description**

Creates the graphical layout of resultant A-, MV-, D- or E-optimal or near-optimal block design on a separate pop-up GUI tcltk window.

**Usage**

```
graphoptbd.mae(trt.N, blk.N, theta, OptdesF, Optcrit, cbVal2)
```

**Arguments**

<code>trt.N</code>	integer, specifying number of treatments, $v$ .
<code>blk.N</code>	integer, specifying number of arrays, $b$ .
<code>theta</code>	numeric, representing a function of the ratio of random array variance and random error variance. It takes any value between 0 and 1, inclusive.
<code>OptdesF</code>	matrix, a $2 \times b$ obtained optimal or near-optimal block design.
<code>Optcrit</code>	character specifying the optimality criteria to be used. Thus, <code>Optcrit</code> takes the letter "A", "MV", "D" and "E" for A-, MV-, D- and E-optimal or near-optimal block designs, respectively.
<code>cbVal2</code>	checkbox value. It takes a value of zero or one. The default value of <code>cbVal2</code> is 0. Thus, if <code>cbVal2 = 0</code> , the function will display the graphical layout of the resultant optimal design generated using the treatment exchange algorithm. Similarly, if <code>cbVal = 1</code> , the function will display the graphical layout of the resultant optimal design generated using the array exchange algorithm.

**Details**

Detail discussions concerning the constructions of a graphs can be found in [igraph](#) R package.

**Value**

Returns the graphical layout of the resultant optimal or near-optimal block design 'OptdesF' on a separate pop-up window. Furthermore, the function graphoptbd.mae saves the graphical layout of the resultant optimal or near-optimal block design in .pdf format in a working subdirectory.

**Note**

When closing a pop-up window for graphical layout of the resultant designs (Graph plot), if the window is closed by clicking on the red button with "X" sign (top-right), the warning message "Warning message: In rm(list = cmd, envir = .tkplot.env): object 'tkp ...' not found" will occur in R console irrespective of what command is executed next. To resolve this warning message, click on "close" menu that is located at the top-left of the graph plot pop-up window when closing this window.

**Author(s)**

Dibaba Bayisa Gemechu, Legesse Kassa Debusho, and Linda Haines

**See Also**

[igraph](#)

**Examples**

```
##To create the graphical layout of the D-optimal block design
##obtained using the treatment exchange algorithm for
trt.N <- 10 #Number of treatments
blk.N <- 10 #Number of blocks
theta <- 0.2 #theta value
OptdesF <- rbind(1:10, c(2:10,1)) #D-optimal design (loop design)

graphoptbd.mae(trt.N = 10, blk.N = 10, theta = 0.2, OptdesF, Optcrit = "D", cbVal2 = 0)
```

---

intcbd.mae

*Generates initial connected block design*

---

**Description**

Generates a random initial connected block design for a given number of blocks b of size k = 2 and the number of treatments v.

**Usage**

```
intcbd.mae(trt.N, blk.N)
```

**Arguments**

trt.N            integer, specifying number of treatments, v.  
blk.N            integer, specifying number of arrays, b.

**Value**

Returns a  $2 \times b$  connected block design with  $b$  blocks of size  $k = 2$  and number of treatments  $v$ .

**Author(s)**

Dibaba Bayisa Gemechu, Legesse Kassa Debusho, and Linda Haines

**References**

Debusho, L. K., Gemechu, D. B., and Haines, L. M. (2016). Algorithmic construction of optimal block designs for two-colour cDNA microarray experiments using the linear mixed model. Under review.

Gemechu D. B., Debusho L. K. and Haines L. M. (2014). A-optimal designs for two-colour cDNA microarray experiments using the linear mixed effects model. *Peer-reviewed Proceedings of the Annual Conference of the South African Statistical Association for 2014 (SASA 2014), Rhodes University, Grahamstown, South Africa.* pp 33-40, ISBN: 978-1-86822-659-7.

**See Also**

[optbdmaeAT](#), [cmatbd.mae](#)

**Examples**

```
#Initial connected block design for
trt.N <- 4 #Number of treatments
blk.N <- 4 #Number of blocks

intcbd.mae(trt.N = 4, blk.N = 4)
```

---

mmenubd.mae

*Creates the main menu tcltk window*

---

**Description**

Alternative to directly using the function [optbdmaeAT](#) on the R console, the function `mmenubd.mae` creates the main menu tcltk window with the list of four optimality criteria (A, MV, D and E) for search of optimal or near-optimal block designs for two-colour cDNA microarray experiments.

**Usage**

```
mmenubd.mae()
```

**Details**

The main menu window created using the function `mmenubd.mae` contains the list of four optimality criteria (the A-, MV -, D- and E) for block designs that allows user to choose an optimality criterion of interest. The function will then call for a function `fixpar.mae` for further option regarding the setup of parametric combinations and output, see `fixpar.mae` documentation.

**Author(s)**

Dibaba B. Gemechu, Legesse K. Debusho, and Linda M. Haines

**See Also**

[optbdmaeAT](#), [fixparbd.mae](#), [tcltk](#), [TkWidgets](#)

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optbdmaeAT

*Optimal block designs for two-colour cDNA microarray experiments*

---

**Description**

Used to compute A-, MV-, D- or E-optimal or near-optimal block designs for two-colour cDNA microarray experiments under either the linear fixed effects model or the linear mixed effects model settings using either the array exchange or treatment exchange algorithms of Debusho, Gemechu and Haines (2016).

**Usage**

```
optbdmaeAT(trt.N, blk.N, theta, nrep, itr.cvrval, Optcrit = "", Alg = "", ...)

## Default S3 method:
optbdmaeAT(trt.N, blk.N, theta, nrep, itr.cvrval, Optcrit = "", Alg = "", ...)
## S3 method for class 'optbdmaeAT'
print(x, ...)
## S3 method for class 'optbdmaeAT'
summary(object, ...)
```

**Arguments**

trt.N	integer, specifying number of treatments, v.
blk.N	integer, specifying number of arrays, b.
theta	numeric, representing a function of the ratio of random array variance and random error variance. It takes any value between 0 and 1, inclusive.
nrep	integer, specifying number of replications of the optimization procedure.
itr.cvrval	integer, specifying number of iterations required for convergence during the exchange procedure.
Optcrit	character, specifying the optimality criteria to be used. Optcrit takes the letter "A", "MV", "D" and "E" for A-, MV-, D- and E-optimal or near-optimal block designs, respectively.
x	the object to be printed.
object	an object of class "optbdmaeAT".
Alg	character string used to specify the algorithm to be used. Possible values of Alg are Alg="trtE" for the treatment exchange algorithm and Alg="arrayE" for the array exchange algorithm: see 'Details'.
...	not used.

## Details

optbdmaeAT computes optimal or near-optimal block design for the two-colour cDNA microarray experiments where the interest is in a comparison of all possible elementary treatment contrasts. The function computes A-, MV-, D- and E-optimal or near optimal block designs via calling of eight sub-functions `Aoptbd.maeT`, `Aoptbd.maeA`, `MVoptbd.maeT`, `MVoptbd.maeA`, `Doptbd.maeT`, `Doptbd.maeA`, `Eoptbd.maeT` and `Eoptbd.maeA`, respectively. Each function requires an initial connected block designs, generated using the function `intcbd.mae`.

The minimum value of `trt.N` and `blk.N` is 3 and `trt.N` should be less than or equal to `blk.N - 1`. The linear fixed effects model results for given `trt.N` and `blk.N` are obtained by setting `theta = 0.0`.

`Alg` specifies the exchange algorithm of Debusho, Gemechu and Haines (2016). If `Alg = "trtE"`, the function optbdmaeAT perform the treatment exchange procedure through deletion and addition of treatments at a time and selects a design with best treatment exchange with respect to the optimality criterion value. If `Alg = "arrayE"`, the function optbdmaeAT perform the array exchange procedure through deletion and addition of candidate arrays at a time and selects a design with best array exchange with respect to the optimality criterion value.

`nrep` takes a value of greater than or equal to 2. However, to ensure optimality of the resultant design, the `nrep` should be greater than or equal to 10 and in addition, as `trt.N` and `blk.N` increase, to ensure optimality of resultant design, it is advised to further increase the value of `nrep` up to greater than or equal to 100. However, it has to be noted that as `trt.N` or `blk.N` or `nrep` or all of them increases, computer time required to generate optimal or near-optimal block design increases.

`itr.cvrval` number of iterations during exchange procedure. It takes a value between 2 and `blk.N`. It is used to speedup the computer search time by setting how long should the user should wait for the exchange process to obtain any different (if any) design than the one that was produced as the result of the preceding exchange of the current array in the initial design with candidate array. This is mainly effective if `blk.N` is very large. For example `itr.cvrval = 2`, means the exchange procedure will jump to the next array test if the exchange of the two preceding arrays with candidate arrays results with the same efficient designs. The function will not give error message if the users set `itr.cvrval > blk.N` and it will automatically set `itr.cvrval = blk.N`. The smaller the `itr.cvrval` means the faster the exchange procedure is, but this will reduce the chance of getting optimal block design and users are advised to set `itr.cvrval` closer to `blk.N`.

## Value

Returns the resultant A-, MV-, D- or E-optimal or near-optimal block design with its corresponding score value and parametric combination saved in excel file in a working directory. In addition, the function optbdmaeAT displays the graphical layout of the resultant optimal or near-optimal block designs. Specifically:

<code>call</code>	the method call.
<code>v</code>	number of treatments.
<code>b</code>	number of blocks
<code>theta</code>	theta value.
<code>nrep</code>	number of replications of the optimization procedure.
<code>itr.cvrval</code>	number of iterations required for convergence during the exchange procedure.



Optcrit	optimality criteria.
Alg	algorithm used.
OptdesF	a $2 \times \text{blk.N}$ obtained optimal or near-optimal block design.
Optcrtsv	score value of the optimality criteria 'Optcrit' of the resultant optimal or near-optimal block design 'OptdesF'.
file_loc, file_loc2	location where the summary of the resultant optimal or near-optimal block design is saved in .csv format.
equireplicate	logical value indicating whether the resultant optimal or near-optimal block design is equireplicate or not.
vtrtrep	vector of treatment replication of the resultant optimal or near-optimal block design.
Cmat	the C-matrix or treatment information matrix of the optimal or near-optimal block design.

The graphical layout of the resultant optimal or near-optimal block design.

NB: The function `optbdmaeAT` also saves the summary of the resultant optimal or near-optimal block design in .csv format in the working directory. Furthermore, the function reports only one final optimal or near-optimal block design, however, there is a possibility of more than one optimal or near-optimal block designs for a given parametric combination. The function [graphoptbd.mae](#) can be used to view and rearrange the graphical layout of the resultant optimal or near-optimal block design on tcltk window. Alternative to the function `optbdmaeAT`, a GUI tcltk window can be used to generate optimal or near-optimal block designs, see [mmenubd.mae](#) and [fixparbd.mae](#).

### Author(s)

Dibaba Bayisa Gemechu, Legesse Kassa Debusho, and Linda Haines

### References

Debusho, L. K., Gemechu, D. B., and Haines, L. M. (2016). Algorithmic construction of optimal block designs for two-colour cDNA microarray experiments using the linear mixed model. Under review.

Gemechu D. B., Debusho L. K. and Haines L. M. (2014). A-optimal designs for two-colour cDNA microarray experiments using the linear mixed effects model. *Peer-reviewed Proceedings of the Annual Conference of the South African Statistical Association for 2014 (SASA 2014), Rhodes University, Grahamstown, South Africa.* pp 33-40, ISBN: 978-1-86822-659-7.

### See Also

[mmenubd.mae](#), [fixparbd.mae](#), [intcbd.mae](#)

### Examples

```
##To obtain the A-optimal or near-optimal block design using treatment exchange algorithm, set
trt.N <- 3 #Number of treatments
```

```

blk.N <- 3 #Number of blocks
theta <- 0 #theta value
nrep <- 5 #Number of replications
itr.cvrval <- 6 #Number of iterations required during the exchange procedure
Optcrit <- "A" #Optimality criteria
Alg <- "trtE" #Algorithm

Aoptexample <- optbdmaeAT(trt.N = 3, blk.N = 3, theta = 0, nrep = 5,
                        itr.cvrval = 6, Optcrit = "A", Alg = "trtE")

summary(Aoptexample)

```

---

optbdmaeAT-internal    *Internal functions*

---

### Description

Functions for internal usage only.

### Usage

```

## Computes A-optimal or near-optimal block designs
## using array exchange algorithm
Aoptbd.maeA(trt.N, blk.N, theta, nrep, itr.cvrval)

## Computes A-optimal or near-optimal block designs
## using treatment exchange algorithm
Aoptbd.maeT(trt.N, blk.N, theta, nrep, itr.cvrval)

## Computes MV-optimal or near-optimal block designs
## using array exchange algorithm
MVOptbd.maeA(trt.N, blk.N, theta, nrep, itr.cvrval)

## Computes MV-optimal or near-optimal block designs
## using treatment exchange algorithm
MVOptbd.maeT(trt.N, blk.N, theta, nrep, itr.cvrval)

## Computes D-optimal or near-optimal block designs
## using array exchange algorithm
Doptbd.maeA(trt.N, blk.N, theta, nrep, itr.cvrval)

## Computes D-optimal or near-optimal block designs
## using treatment exchange algorithm
Doptbd.maeT(trt.N, blk.N, theta, nrep, itr.cvrval)

## Computes E-optimal or near-optimal block designs

```

```
## using array exchange algorithm
Eoptbd.maeA(trt.N, blk.N, theta, nrep, itr.cvrgval)

## Computes E-optimal or near-optimal block designs
## using treatment exchange algorithm
Eoptbd.maeT(trt.N, blk.N, theta, nrep, itr.cvrgval)
```

### Arguments

trt.N	integer, specifying number of treatments, v.
blk.N	integer, specifying number of arrays, b.
theta	numeric, representing a function of the ratio of random array variance and random error variance. It takes any value between 0 and 1, inclusive.
nrep	integer, specifying number of replications of the optimization procedure.
itr.cvrgval	integer, specifying number of iterations required for convergence during the exchange procedure. See <a href="#">optbdmaeAT</a> documentation for details.

### Details

These functions are handled via a generic function [optbdmaeAT](#). Please refer to the [optbdmaeAT](#) documentation for details.

### Author(s)

Dibaba Bayisa Gemechu, Legesse Kassa Debusho, and Linda Haines

### References

- Debusho, L. K., Gemechu, D. B., and Haines, L. M. (2016). Algorithmic construction of optimal block designs for two-colour cDNA microarray experiments using the linear mixed model. Under review.
- Gemechu D. B., Debusho L. K. and Haines L. M. (2014). A-optimal designs for two-colour cDNA microarray experiments using the linear mixed effects model. *Peer-reviewed Proceedings of the Annual Conference of the South African Statistical Association for 2014 (SASA 2014), Rhodes University, Grahamstown, South Africa.* pp 33-40, ISBN: 978-1-86822-659-7.

### See Also

[optbdmaeAT](#)

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