Package ‘optrcdmaeAT’

May 25, 2025

Version 1.0.1

Date 2025-05-25

Title Optimal Row-Column Designs for Two-Colour cDNA Microarray Experiments

Author Dibaba Bayisa Gemechu [aut, cre],
Legesse Kassa Debusho [aut],
Linda Haines [aut]

Maintainer Dibaba Bayisa Gemechu <`diboobayu@gmail.com`>

Depends R (>= 3.3.2), MASS, Matrix, igraph, tcltk

License GPL-2

Description Computes A-, MV-, D- and E-optimal or near-optimal row-column 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 pairwise treatment contrasts. The algorithms used in this package are based on the array exchange and treatment exchange algorithms adopted from Debusho, Gemechu and Haines (2018) <doi:10.1080/03610918.2018.1429617> algorithms after adjusting for the row-column designs setup. The package also provides an optional method of using the graphical user interface (GUI) R package tcltk to ensure that it is user friendly.

NeedsCompilation no

Repository CRAN

Date/Publication 2025-05-25 04:50:04 UTC

Contents

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

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 row-column design.

Usage

```
cmatrcd.mae(trt.N, col.N, theta, des)
```

Arguments

`trt.N`	integer, specifying number of treatments, `v`.
`col.N`	integer, specifying number of arrays (columns), `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.
`des`	matrix, a `2 x b` row-column design with `b` arrays/columns of size `k = 2` and `v` treatments.

Value

Returns a `v x 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. (2018). Algorithmic construction of optimal block designs for two-colour cDNA microarray experiments using the linear mixed effects model. *Communications in Statistics - Simulation and Computation, https://doi.org/10.1080/03610918.2018.1429617.*

Gemechu, D. B., Debusho, L. K., and Haines, L. M. (2015). A-and D-optional row-column designs for two-colour cDNA microarray experiments using linear mixed effects models. *South African Statistical Journal*, 49, 153-168.

See Also

`optrcdmaeAT`, `fixparrcd.mae`, `intcrcd.mae`

Examples

```
##Information matrix

     trt.N <- 3
     col.N <- 3
     theta <- 0.1
     rcdes <- intcrcd.mae(trt.N = 3, col.N = 3)

     cmatrcd.mae(trt.N = 3, col.N = 3, theta = 0.1, des = rcdes)
```

`fixparrcd.mae` *Sets parametric values*

Description

Creates a GUI `tcltk` window that allow the users to set or fix values for the parametric combinations to compute optimal or near-optimal row-column designs.

Usage

```
fixparrcd.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 row-column designs, respectively.

Details

`fixparrcd.mae` creates a pop-up GUI tcltk window that allow the users to set the parametric combinations to compute optimal or near-optimal row-column designs. The parameters include the number of treatments `trt.N`, number arrays `col.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 row-column 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 row-column 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 `optrcdmaeAT`, the summary of the resultant optimal or near-optimal row-column 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 row-column designs.

Value

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

Author(s)

Dibaba Bayisa Gemechu, Legesse Kassa Debusho, and Linda Haines

See Also

`optrcdmaeAT`, `mmenurcd.mae`

`graphoptrcd.mae` *Creates the graphical layout of resultant optimal row-column design*

Description

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

Usage

```
graphoptrcd.mae(trt.N, col.N, theta, OptdesF, Optcrit, cbVal2)
```

Arguments

`trt.N`	integer, specifying number of treatments, `v`.
`col.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.
`OptdesF`	matrix, a `2 x b` obtained optimal or near-optimal row-column design.
`Optcrit`	character, specifying the optimality criteria to be used. Thus, `Optcrit` takes the letter `"A"`, `"MV"`, `"D"` and `"E"` for `A-`, `MV-`, `D-` and `E-`optimal or near-optimal row-column designs, respectively.
`cbVal2`	checkbox value. It takes a value of zero or one. The default value of `cbVal2` is 0. Thus, if `cbVal2 = 0`, the function will display the graphical layout of the resultant optimal design generated using the treatment exchange algorithm. Similarly, if `cbVal2 = 1`, 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 row-column design '`OptdesF`' on a separate pop-up window. Furthermore, the function `graphoptrcd.mae` saves the graphical layout of the resultant optimal or near-optimal row-column 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

Examples

```
 ##To create the graphical layout of the D-optimal row-column design
 ##obtained using the treatment exchange algorithm for

 trt.N <- 10  #Number of treatments

 col.N <- 10  #Number of arrays

 theta <- 0.2 #theta value

 OptdesF <- rbind(1:10, c(2:10, 1)) #D-optimal design (loop design)

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

`intcrcd.mae` *Generates initial connected row-column design*

Description

Generates a random initial connected row-column design for a given number of arrays `b` of size `k` = 2 and the number of treatments `v`.

Usage

```
intcrcd.mae(trt.N, col.N)
```

Arguments

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

Value

Returns a `2 x b` connected row-column design with `b` arrays 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. (2018). Algorithmic construction of optimal block designs for two-colour cDNA microarray experiments using the linear mixed effects model. *Communications in Statistics - Simulation and Computation, https://doi.org/10.1080/03610918.2018.1429617.*

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.

Gemechu, D. B., Debusho, L. K., and Haines, L. M. (2015). A-and D-optional row-column designs for two-colour cDNA microarray experiments using linear mixed effects models. *South African Statistical Journal*, 49, 153-168.

See Also

`optrcdmaeAT`, `cmatrcd.mae`

Examples

```
#Initial connected row-column design for
trt.N <- 4 #Number of treatments
col.N <- 4 #Number of arrays

intcrcd.mae(trt.N = 4, col.N = 4)
```

`mmenurcd.mae` *Creates the main menu tcltk window*

Description

Alternative to directly using the function `optrcdmaeAT` on the R console, the function `mmenurcd.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 row-column designs for two-colour cDNA microarray experiments.

Usage

```
mmenurcd.mae()
```

Details

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

Author(s)

Dibaba Bayisa Gemechu, Legesse Kassa Debusho, and Linda Haines

See Also

`optrcdmaeAT`, `fixparrcd.mae`

`optrcdmaeAT` *Optimal row-column designs for two-colour cDNA microarray experiments*

Description

Used to compute A-, MV-, D- or E-optimal or near-optimal row-column 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 (2018) <doi.org/10.1080/03610918.2018.1429617> after adjusting to the row-column setup.

Usage

```
optrcdmaeAT(trt.N, col.N, theta, nrep, itr.cvrgval, Optcrit = "", Alg = "", ...)

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

Arguments

`trt.N`	integer, specifying number of treatments, v.
`col.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.
`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 row-column designs, respectively.
`x`	the object to be printed.
`object`	an object of class `"optrcdmaeAT"`.
`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

`optrcdmaeAT` computes optimal or near-optimal row-column 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 row-column designs via calling of eight sub-functions `Aoptrcd.maeT`, `Aoptrcd.maeA`, `MVoptrcd.maeT`, `MVoptrcd.maeA`, `Doptrcd.maeT`, `Doptrcd.maeA`, `Eoptrcd.maeT` and `Eoptrcd.maeA`, respectively. Each function requires an initial connected row-column designs, generated using the function `intcrcd.mae`.

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

`Alg` specifies the array exchange and treatment exchange algorithm to be used that is adopted from Debusho, Gemechu and Haines (2018) after adjusting for the row-column designs setup. If `Alg = "trtE"`, the function `optrcdmaeAT` 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 `optrcdmaeAT` 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 `col.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 `col.N` or `nrep` or all of them increase, computer time required to generate optimal or near-optimal row-column design increases.

`itr.cvrgval` number of iterations during exchange procedure. It takes a value between 2 and `col.N`. It is used to speedup the computer search time by setting how long 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 `col.N` is very large. For example `itr.cvrgval = 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.cvrgval > col.N` and it will automatically set `itr.cvrgval = col.N`. The smaller the `itr.cvrgval` means the faster the exchange procedure is, but this will reduce the chance of getting optimal row-column design and users are advised to set `itr.cvrgval` closer to `col.N`.

Remark: After the treatment exchange or array exchange procedure is completed, a dye-flip procedure is added to the internal functions of `optrcdmaeAT` stated above to further insure the optimality of the resulting optimal or near-optimal row-column designs. Thus, the procedure will flip (interchange) the treatments position within each array (column) and select the optimal dye-flip based on the optimality criteria of interest. This step is effective only for the large number of arrays and is efficient if `itr.cvgval` < `col.N` and there is a jump in the array exchange or treatment exchange procedure as stated above under the detail description of `itr.cvrgval`.

Value

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

`call`	the method call.
`v`	number of treatments.
`b`	number of arrays.
`theta`	theta value.
`nrep`	number of replications of the optimization procedure.
`itr.cvrgval`	number of iterations required for convergence during the exchange procedure.
`Optcrit`	optimality criteria.
`Alg`	algorithm used.
`OptdesF`	a `2` `x` `col.N` obtained optimal or near-optimal row-column design.
`Optcrtsv`	score value of the optimality criteria `'Optcrit'` of the resultant optimal or near-optimal row-column design `'OptdesF'`.
`file_loc`, `file_loc2`	location where the summary of the resultant optimal or near-optimal row-column design is saved in .csv format.
`equireplicate`	logical value indicating whether the resultant optimal or near-optimal row-column design is equireplicate or not.
`vtrtrep`	vector of treatment replication of the resultant optimal or near-optimal row-column design.
`Cmat`	the C-matrix or treatment information matrix of the optimal or near-optimal row-column design.

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

NB: The function `optrcdmaeAT` also saves the summary of the resultant optimal or near-optimal row-column design in .csv format in the working directory. Furthermore, the function reports only one final optimal or near-optimal row-column design, however, there is a possibility of more than one optimal or near-optimal row-column designs for a given parametric combination. The function `graphoptrcd.mae` can be used to view and rearrange the graphical layout of the resultant optimal or near-optimal row-column design on `tcltk` window. Alternative to the function `optrcdmaeAT`, a GUI tcltk window can be used to generate optimal or near-optimal row-column designs, see `mmenurcd.mae` and `fixparrcd.mae`.

Author(s)

Dibaba Bayisa Gemechu, Legesse Kassa Debusho, and Linda Haines

References

Debusho, L. K., Gemechu, D. B. and Haines, L. (2018). Algorithmic construction of optimal block designs for two-colour cDNA microarray experiments using the linear mixed effects model. *Communications in Statistics - Simulation and Computation, https://doi.org/10.1080/03610918.2018.1429617*.

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.

Gemechu, D. B., Debusho, L. K., and Haines, L. M. (2015). A-and D-optional row-column designs for two-colour cDNA microarray experiments using linear mixed effects models. *South African Statistical Journal*, 49, 153-168.

See Also

`mmenurcd.mae`, `fixparrcd.mae`, `intcrcd.mae`

Examples

```
##To obtain the A-optimal or near-optimal row-column design
##using treatment exchange algorithm, set
trt.N <- 3 #Number of treatments
col.N <- 3 #Number of arrays
theta <- 0 #theta value
nrep <- 5  #Number of replications
itr.cvrgval <- 6 #Number of iterations required during the exchange procedure
Optcrit <- "A"   #Optimality criteria
Alg <- "trtE"    #Algorithm

Aoptrcdes <- optrcdmaeAT(trt.N = 3, col.N = 3, theta = 0, nrep = 5,
                          itr.cvrgval = 6, Optcrit = "A", Alg = "trtE")

summary(Aoptrcdes)
```

`optrcdmaeAT-internal` *Internal functions*

Description

Functions for internal usage only.

Usage

```
## Computes A-optimal or near-optimal row-column designs
## using array exchange algorithm
Aoptrcd.maeA(trt.N, col.N, theta, nrep, itr.cvrgval)

## Computes A-optimal or near-optimal row-column designs
## using treatment exchange algorithm
Aoptrcd.maeT(trt.N, col.N, theta, nrep, itr.cvrgval)

## Computes MV-optimal or near-optimal row-column designs
## using array exchange algorithm
MVoptrcd.maeA(trt.N, col.N, theta, nrep, itr.cvrgval)

## Computes MV-optimal or near-optimal row-column designs
## using treatment exchange algorithm
MVoptrcd.maeT(trt.N, col.N, theta, nrep, itr.cvrgval)

## Computes D-optimal or near-optimal row-column designs
## using array exchange algorithm
Doptrcd.maeA(trt.N, col.N, theta, nrep, itr.cvrgval)

## Computes D-optimal or near-optimal row-column designs
## using treatment exchange algorithm
Doptrcd.maeT(trt.N, col.N, theta, nrep, itr.cvrgval)

## Computes E-optimal or near-optimal row-column designs
## using array exchange algorithm
Eoptrcd.maeA(trt.N, col.N, theta, nrep, itr.cvrgval)

## Computes E-optimal or near-optimal row-column designs
## using treatment exchange algorithm
Eoptrcd.maeT(trt.N, col.N, theta, nrep, itr.cvrgval)
```

Arguments

`trt.N`	integer, specifying number of treatments, v.
`col.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 `optrcdmaeAT` documentation for details.

Details

These functions are handled via a generic function `optrcdmaeAT`. Please refer to the `optrcdmaeAT` documentation for details.

Author(s)

Dibaba Bayisa Gemechu, Legesse Kassa Debusho, and Linda Haines

References

Debusho, L. K., Gemechu, D. B. and Haines, L. (2018). Algorithmic construction of optimal block designs for two-colour cDNA microarray experiments using the linear mixed effects model. *Communications in Statistics - Simulation and Computation, https://doi.org/10.1080/03610918.2018.1429617*.

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.

Gemechu, D. B., Debusho, L. K., and Haines, L. M. (2015). A-and D-optional row-column designs for two-colour cDNA microarray experiments using linear mixed effects models. *South African Statistical Journal*, 49, 153-168.

See Also

`optrcdmaeAT`

Index