Package 'soptdmaeA'

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Title Sequential Optimal Designs for Two-Colour cDNA Microarray
Experiments

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

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Description Computes sequential A-, MV-, D- and E-optimal or near-optimal block and row-
column designs for two-colour cDNA microarray experiments using the linear fixed ef-
fects and mixed effects models where the interest is in a comparison of all possible elemen-
tary treatment contrasts. The package also provides an optional method of using the graphi-
cal user interface (GUI) R package 'tcltk' to ensure that it is user friendly.

NeedsCompilation no

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R topics documented:

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cmatbrcd.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 block or row-column design.

Usage

```
cmatbrcd.mae(trt.N, blk.N, theta, des, dtype)
```

Arguments

trt.N	integer, specifying number of treatments v of design des.
blk.N	integer, specifying number of arrays (blocks or columns) b of design des.
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 block or row-column design with b arrays and v treatments.
dtype	character, specifying the design type. For block designs, dtype = ″blkd″ and for row-column deigns, dtype = ″rcd″.

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. 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

soptdmaeA, fixparsoptd.mae

Examples

```
##Information matrix

    trt.N <- 4
    blk.N <- 4
    theta <- 0.3
    dsgn <- rbind(1:4,c(2:4,1))
    dtype <- "rcd"

    cmatbrcd.mae(trt.N = 4, blk.N = 4, theta = 0.2, des = dsgn, dtype = "rcd")
```

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fixparsoptd.mae	*Sets parametric values and initial design*

Description

Creates a [tcltk](#) window that allow the users to set or fix values for the parametric combinations and initial optimal or near-optimal design to compute sequential optimal or near-optimal block or row-column designs.

Usage

```
fixparsoptd.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 designs,
                 respectively.

Details

fixparsoptd.mae creates a pop-up tcltk window that allow the users to set the parametric combinations and initial optimal or near-optimal designs to compute optimal or near-optimal block or row-column 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, number of added treatments strt, number of added arrays sary and a button that allows users to insert initial optimal or near-optimal design des0 by typing into a pop-up sheet that will occur when clicking on the 'Insert' button. The users are not restricted to a specific dimension of the initial design, thus, the dimension of the initial design des0 can be 2 x blk.N or blk.N x 2. The default initial design des0 is a 3 x 2 loop/cyclic design.

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 sequential optimal or near-optimal block or row-column design, to make a choice between the two design types (block design and row-column designs) and to print the summary of the resultant sequential optimal or near-optimal 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 [soptdmaeA](), the summary of the resultant sequential optimal or near-optimal design will be saved in the current working directory in .csv format. The graphical layout of resultant sequential optimal or near-optimal design together with that of the initial optimal or near-optimal design will also be displayed on R console.

Value

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

Author(s)

Dibaba Bayisa Gemechu, Legesse Kassa Debusho, and Linda Haines

See Also

[soptdmaeA](), [mmenusoptd.mae](), [tcltk](), [TkWidgets]()

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graphsoptd.mae   *Creates the graphical layout of resultant sequential optimal design*

Description

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

Usage

```
graphsoptd.mae(trt.N, blk.N, theta, soptdesF, Optcrit, strt, sary, dtype)
```

Arguments

trt.N	integer, specifying number of treatments v of resultant sequential optimal design, `soptdesF`.
blk.N	integer, specifying number of arrays b of resultant sequential optimal design, `soptdesF`.
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.
soptdesF	matrix, a 2 x b obtained sequential optimal or near-optimal block or 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 block or row-column designs, respectively.
strt	a non-negative integer, specifying number of added treatments/conditions to the initial design.

sary	a non-negative integer, specifying number of added arrays to the initial design.
dtype	character, specifying the design type. For block designs, dtype = ″blkd″ and for row-column deigns, dtype = ″rcd″.

Details

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

Value

Returns the graphical layout of the resultant sequential optimal or near-optimal block or row-column design 'soptdesF' on a separate pop-up window with the new edges (arrays) and vertices (treatments) added to the initial design coloured in red and brown, respectively, for separation purpose. Furthermore, the function graphsoptd.mae saves the graphical layout of the initial des0 and resultant sequential optimal or near-optimal 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](#)

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mmenusoptd.mae	*Creates the main menu tcltk window*

Description

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

Usage

```
mmenusoptd.mae()
```

Details

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

Author(s)

Dibaba Bayisa Gemechu, Legesse Kassa Debusho, and Linda Haines

See Also

`soptdmaeA`, `fixparsoptd.mae`, `tcltk`, `TkWidgets`

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soptdmaeA	*Sequential optimal designs for two-colour cDNA microarray experiments*

Description

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

Usage

```
soptdmaeA(trt.N, blk.N, theta, nrep, strt, sary, des0, dtype, Optcrit = "", ...)


## Default S3 method:
soptdmaeA(trt.N, blk.N, theta, nrep, strt, sary, des0, dtype, Optcrit = "",...)
## S3 method for class 'soptdmaeA'
print(x, ...)
## S3 method for class 'soptdmaeA'
summary(object, ...)
```

Arguments

trt.N	integer, specifying number of treatments v of initial design, des0.
blk.N	integer, specifying number of arrays (blocks or columns) b of initial design, des0.
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.

strt	a non-negative integer, specifying number of added treatments/conditions to the initial design.
sary	a non-negative integer, specifying number of added arrays to the initial design.
des0	matrix, a 2 x blk.N or blk.N x 2 initial block or row-column design. The initial design must be treatment connected and the number of treatments and arrays should also coincides with trt.N and blk.N inserted by the user, if this conditions are not satisfied, the package will stop running with an error message.
dtype	character, specifying the design type. For block designs, dtype = "blkd" and for row-column deigns, dtype = "rcd".
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 or row-column designs, respectively.
x	the object to be printed.
object	an object of class "soptdmaeA".
...	not used.

Details

soptdmaeA computes sequential optimal or near-optimal block or row-column designs for the two-colour cDNA microarray experiments where the interest is in a comparison of all possible elementary treatment contrasts for a given initial optimal or near-optimal designs. The function computes sequential A-, MV-, D- and E-optimal or near optimal block or row-column designs via calling of four sub-functions [seqAoptbrcd.maeA](), [seqMVoptbrcd.maeA](), [seqDoptbrcd.maeA](), and [seqEoptbrcd.maeA](), respectively. These functions uses the array exchange algorithm of Debusho, Gemechu and Haines (2016). Thus, once the parametric combinations of interest are sated, these functions will first compute, randomly, a new connected initial design with a new number of arrays and, optionally, a new number of treatments. Then they 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. The candidate arrays are lists of possible arrays with different treatment combinations and their lists are dependent of the number of arrays and treatments added to the initial optimal or near-optimal design. For example, if only one treatment and one array are to be added to the initial optimal or near-optimal design, then the candidate arrays will be only those arrays that consists of a new treatment together with the old treatments in the initial optimal or near-optimal design with or without considering their position within the array for row-column or block designs, respectively.

The minimum value of trt.N and blk.N is 3 and trt.N should be less than or equal to blk.N - 1. Thus, the least initial design should be of a design with 3 number of treatments and number of arrays. The minimum number of sary and strt are 1 and 0, respectively, and sary should be greater than or equal to strt. The linear fixed effects model results for given parametric combinations and initial design are obtained by setting theta = 0.0.

nrep takes a value of greater than or equal to 1. However, to ensure optimality of the resultant design, for sary - strt > 0, the nrep should be greater than or equal to 10. In addition, as trt.N or blk.N or sary and/or strt or all of them increase, to ensure optimality of resultant design, it is advised to further increase the value of nrep up to greater than or equal to 50. However, it has to be noted that as trt.N or blk.N or nrep or all of them increase, computer time required to generate sequential optimal or near-optimal design increases.

Value

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

call	the method call.
v	number of treatments of obtained sequential design.
b	number of arrays of obtained sequential design.
theta	theta value.
nrep	number of replications of the optimization procedure.
strt	number of added treatments.
sary	number of added arrays.
Optcrit	optimality criteria.
optdes0	a 2 x blk.N initial optimal or near-optimal block or row-column design.
optcrtsv0	score value of the optimality criteria 'Optcrit' of the initial optimal or near-optimal block or row-column design 'optdes0'.
soptdesF	a 2 x blk.N obtained sequential optimal or near-optimal block or row-column design.
soptcrtsv	score value of the optimality criteria 'Optcrit' of the resultant sequential optimal or near-optimal block design 'soptdesF'.
file_loc, file_loc2	
	location where the summary of the resultant optimal or near-optimal block design is saved in .csv format.
equireplicate0	logical value indicating whether the initial optimal or near-optimal block or row-column design is equireplicate or not.
vtrtrep0	vector of treatment replication of the initial optimal or near-optimal block or row-column design.
equireplicate	logical value indicating whether the resultant sequential optimal or near-optimal block or row-column design is equireplicate or not.
vtrtrep	vector of treatment replication of the resultant sequential optimal or near-optimal block or row-column design.
Cmat	the C-matrix or treatment information matrix of the obtained sequential optimal or near-optimal block or row-column design.

The output also includes graphical layouts of the initial and resultant sequential optimal or near-optimal block or row-column design. The new edges (arrays) and vertices (treatments) added to the initial design are coloured in red and brown, respectively, for identification purpose.

NB: The function soptdmaeA also saves the summary of the initial and resultant sequential optimal or near-optimal block or row-column design in .csv format in the working directory. Furthermore, the function reports only one final sequential optimal or near-optimal block or row-column design, however, there is a possibility of more than one sequential optimal or near-optimal block or row-column designs for a given parametric combination. The function graphsoptd.mae can be used to

view and rearrange the graphical layout of the resultant sequential optimal or near-optimal block or row-column design on `tcltk` window. Alternative to the function `soptdmaeA`, a GUI tcltk window can be used to generate sequential optimal or near-optimal block or row-column designs, see `mmenusoptd.mae` and `fixparsoptd.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

`mmenusoptd.mae`, `fixparsoptd.mae`

Examples

```
##To obtain sequential A-optimal or near-optimal block design for a given
##initial A-optimal or near-optimal block design, set

trt.N <- 3  #Number of treatments
blk.N <- 3  #Number of blocks
theta <- 0  #theta value
nrep <- 10  #Number of replications
strt <- 2   #Number of added treatments
sary <- 3   #Number of added arrays
des0 <- rbind(1:3, c(2, 3, 1)) #Initial design
dtype = "blkd" #Design type
Optcrit <- "A"   #Optimality criteria

seqAoptbd <- soptdmaeA(trt.N = 3, blk.N = 3, theta = 0, nrep = 10,
                          strt = 2, sary = 3, des0, dtype = "blkd", Optcrit = "A")

summary(seqAoptbd)

##To obtain sequential A-optimal or near-optimal row-column design for a given
##initial A-optimal or near-optimal row-column design des0 (stated above), set

dtype = "rcd" #Design type

seqAoptrcd <- soptdmaeA(trt.N = 3, blk.N = 3, theta = 0, nrep = 10,
                          strt = 2, sary = 3, des0, dtype = "rcd", Optcrit = "A")
```

```
    summary(seqAoptrcd)
```

---

soptdmaeA-internal   *Internal functions*

Description

Functions for internal usage only.

Usage

```
## Computes A-optimal or near-optimal block or row-column designs
## using array exchange algorithm
seqAoptbrcd.maeA(trt.N, blk.N, theta, nrep, strt, sary, des0, dtype)

## Computes MV-optimal or near-optimal block or row-column designs
## using array exchange algorithm
seqMVoptbrcd.maeA(trt.N, blk.N, theta, nrep, strt, sary, des0, dtype)

## Computes A-optimal or near-optimal block or row-column designs
## using array exchange algorithm
seqDoptbrcd.maeA(trt.N, blk.N, theta, nrep, strt, sary, des0, dtype)

## Computes A-optimal or near-optimal block or row-column designs
## using array exchange algorithm
seqEoptbrcd.maeA(trt.N, blk.N, theta, nrep, strt, sary, des0, dtype)
```

Arguments

trt.N	integer, specifying number of treatments v of initial design, des0.
blk.N	integer, specifying number of arrays b of initial design, des0.
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.
strt	a non-negative integer, specifying number of added treatments/conditions to the initial design.

sary   a non-negative integer, specifying number of added arrays to the initial design.

des0   matrix, a `2 x blk.N` or `blk.N x 2` initial block or row-column design. The initial design must be treatment connected and the number of treatments and arrays should also coincides with `trt.N` and `blk.N` inserted by the user, if this conditions are not satisfied, the package will stop running with an error message.

dtype   character, specifying the design type. For block designs, `dtype = "blkd"` and for row-column deigns, `dtype = "rcd"`.

Details

These functions are handled via a generic function [soptdmaeA](#). Please refer to the [soptdmaeA](#) 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

[soptdmaeA](#)

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