Supplement Sections with a glossary, figures, R-scripts and underlying theory for Exposing the confounding in experimental designs to understand and evaluate them, and formulating linear mixed models for analyzing the data from a designed experiment

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Supplement Section A Glossary

Terms within definitions that are in blue are links to their definitions.

The **A-efficiency criterion** is the efficiency criterion that is calculated as the harmonic mean of the canonical efficiency factors of the projection matrices for two sources.

An **A-optimal design** is a design that has, for each treatments source, the minimum value, amongst designs in a defined category of designs, for the sum of the reciprocals of the nonzero eigenvalues of its information matrix under the anticipated model. For an anticipated model that is a fixed model, the A-optimal design has (i) the maximum value for the A-efficiency criterion for the treatments source when confounded with the source for the identity term for the units and (ii) the minimum average variance of differences between the estimates of all pairs of treatments effects.

An **abbreviated term/source name** consists of just the initial capital letters of the factors' names in a term/source.

An aliased source is a treatments source (units source) all of whose contrasts are the same as at least some of the contrasts for another treatments source (units source) (cf. a partially aliased source).

Aliasing is the mixing up of different treatments contrasts, or, less frequently, of different units contrasts.

The allocated factors/terms/sources are all based on the factors that have been allocated to the recipient factors, the latter indexing the units. The allocated terms are derived from the allocated factors and the allocated sources are derived from the allocated terms. They are also called treatments factors/terms/sources.

An allocation See factor allocation.

An allocation model is a model that is based on the allocations employed in an experimental design, and so can only be formulated after the design has been obtained (cf. anticipated model). The factor-allocation diagram facilitates the derivation of such models. There are two allocation models for an experimental design that are formulated in the order given: (i) the initial allocation model; and (ii) the homogeneous allocation model. The homogeneous allocation model may also be modified to form a prior allocation model.

An **anatomy** is the analysis of a design to reveal its structure. It is built on the allocations in the design and uses the terms in a linear model for the design. It is expressed in the confounding relationships between the sources derived from the terms.

An **anatomy table** summarizes the anatomy of an experimental design, displaying the confounding relations between sources in the table and thereby facilitating the study of the design's properties. For a standard design, it consists of two major columns, one for units and one for treatments, each of which contains a source column and a DF column. For designs that are not orthogonal, a column of A-efficiency criteria is added to the treatments major column. To these two major columns is added a third major column that contains the EMS.

An **ANOVA** is an analysis of variance performed on a response variable.

An **anticipated model** is a linear mixed model with terms for the effects that are anticipated to occur in an experiment and that is formulated before a design is obtained (cf. allocation models). It is used to inform the selection of a design. Deciding on the terms to include often requires consultation with the researcher and relies on the experience of both the researcher and the designer. Generally, the objective in looking for a design is to find one that is optimal for this model (see A-optimal design). However, the anticipated model is often not explicitly stated, but has a subliminal presence, and so the search for an optimal design can be an informal process.

Balanced experimental designs See Classes of experimental designs.

The **canonical efficiency factors** for two sources are the nonzero eigenvalues of the matrices of a certain product of the projection matrices of two sources, the eigenvalues lying between zero and one. The canonical efficiency factors can be used to calculate efficiency criteria.

Classes of experimental designs based on the order of balance of the design are orthogonal, (first-order) balanced and nonorthogonal designs. These classes are distinguished as follows:

Orthogonal designs are those designs for which the order of balance for all confounded sources and aliased sources is one and all of their canonical efficiency factors are equal to one.

Structure-orthogonal designs are those orthogonal designs for which there is no aliasing between treatment sources when they are confounded with the same units source. That is, the design is orthogonal given the structure imposed by the combined decomposition.

Balanced designs are those designs for which the order of balance for all confounded sources and aliased sources is one.

- Structure-balanced designs are those balanceddesigns for which there is no aliasing between treatment sources when they are confounded with the same units source. That is the design is balanced given the structure imposed by the combined decomposition.
- **Nonorthognal designs** are those designs for which at least one canonical efficiency factor for any confounded source or any aliased source is not one.
- Orthogonal designs are a subset of the balanced designs and some balanced designs are nonorthogonal. Orthogonal designs may also be structure-orthogonal and balanced designs may also be structure-balanced.
- A **combined decomposition** is the decomposition for a design of the units space that results from combining the decomposition according to the units sources with the decomposition according to the treatments sources. The combined decomposition is said to impose a structure on the units and it is summarized in an anatomy table.
- A **combined**, **units permutation** is a permutation of the units that combines several permutations, each one for groups of the units that are indexed by subsets of the factors corresponding to a units term/source. This is one way of randomly selecting a units permutation from the set of valid permutations for an experimental design and so achieving the randomization of the design.
- A **confounded source** is the blending together of all of the information for a treatments source with a single units source as a result of the allocation of treatments to units (cf. a partially confounded source).
- **Confounding** is the blending together of at least some contrasts for a treatments source with those for a units source that results from the allocation of treatments to units.
- A **decomposition** is the division of the units space into subspaces, either by the subspaces of the treatments-sources or the units-sources.
- A decomposition table is an anatomy table without the EMS. It summarizes the combined decomposition of the units space.
- The **DF** for a source is the number of degrees of freedom or dimension of a source's subspace. Mathematically, it is the rank of the projection matrix for the source and this is equal to the number of canonical efficiency factors.
- An efficiency criterion is a statistic calculated from the canonical efficiency factors of the projection matrices for two sources. They can be interpreted in terms of the amount of information for one source that is mixed up, by aliasing or confounding, with the other source.
- An **EMS** is the expected mean squares for a line of sources in an anatomy table. They are based on the terms in a linear mixed model.
- An **exhausted source** is a units source that has no Residual DF because its DF are equal to the sum of those of the treatments sources confounded with it. One consequence of this is that it is likely that some variance components are not be estimable.
- **Exhaustive confounding** occurs when there is one or more exhausted sources in a combined decomposition of the units space.
- An **experimental design** is a prescription for the randomized allocation of one of set of factors (treatments factors) to another set of factors (units factors).
- An **experimental unit** for a treatments factor is the smallest entity, identified by the units factors in a source, with which a treatment source is confounded.
- A factor is a categorical variable indexing the observational units in a design and is usually considered as an explanatory variable in an analysis of the data obtained using the design. The convention in this paper is for a factor's name to have an initial capital letter. Factors can be dichotomized into treatments factors and units factors.
- A factor allocation is the assignment of the levels of one or more treatments factors to one or more units factors using an experimental design. Types of allocations include allocation by randomization, restricted randomization, spatial allocation and systematic allocation. An outcome of an allocation is that allocated sources are confounded with certain recipient sources and this can be displayed using a anatomy table.
- The **factor-allocation paradigm** describes an experiment in terms of the two sets of factors involved in a factor allocation, along with the nesting and crossing relations among the factors within each set of factors and an indication of what allocations were made. This information can be exhibited in a factor-allocation diagram.
- A factor-allocation diagram exhibits a factor allocation for an experimental design, in which one set of factors (treatments factors) is allocated to another set of factors (units factors). It has a panel for each set of factors and solid arrows to indicate randomized allocations and dashed arrows

indicate systematic allocation. The use of a structure-orthogonal design for the factor allocation is indicated by a circle containing a 'perp' ('①') and a nonorthogonal design is indicated by a an empty circle ('O').

A fixed model is a model in which the only random term is the identity term for the units.

A fixed term is a term that contributes to the model for the expectation and whose parameters are allowed to take arbitrary values (cf. random term).

A homogeneous allocation model is the second of two allocation models to produce in formulating the linear mixed model for a designed experiment. Convert the initial allocation model to the homogeneous allocation model by (i) adding block-treatment interactions that are thought to be needed, and (ii) deciding if any terms need to be swapped from a fixed term to random term and vice versa. The model is homogeneous in the sense that all the fixed terms have a parameter for each combination of the observed levels of the factors comprising the term and the effects for each random term are assumed to be independent and identically distributed.

An identity term is a term whose constituent factors uniquely index the observational units.

Inextricably confounded sources occur when a treatments source is confounded with a units source and the DF for the two sources are the same, so that separate estimates of the parameters for both terms are impossible.

An **initial allocation model** is the first of two allocation models to produce in formulating the linear mixed model for a designed experiment. It is obtained directly from the factor-allocation diagram by forming terms from all possible combinations of the factors within a panel, subject to the restriction that terms involving a nested factor must include all its nesting factors. The fixed terms are those that come from the factors in a panel that were allocated; the remaining terms are the random terms.

A longitudinal experiment is an experiment that involves times and/or locations whose differences are of interest and to which treatments are not allocated. Longitudinal experiments are a subclass of the repeated-measurements experiments.

Marginality is the relationship between two terms derived from the same panel. A term is said to be marginal to another term if the column space of its indicator matrix is a subspace of the indicator matrix of the other term. Marginality is also referred to as the hierarchy of terms.

A model of convenience is a prior allocation model that does not include all the terms in the homogeneous allocation model, usually to remove random terms to make the model nonsingular so that it can be fitted using mixed model software.

Nonorthogonal experimental designs See Classes of experimental designs.

An **observational unit** is a unit from which a single value of a response variable is obtained. Observational units are never allocated.

The **order of balance** for two sources is the number of different values of the canonical efficiency factors computed from a particular product of their projections matrices.

Orthogonal experimental designs See Classes of experimental designs.

A panel contains the set of factors that were either allocated together (treatments) or were jointly (potential) recipients of factors being allocated. The panel also exhibits the nesting relations between the factors; if a factor is not nested within another factor, then the two factors are crossed, i.e. the crossing of factors in the panel is implicit.

A partially aliased source is the blending together of a part of the information for some or all contrasts for a treatments source with those for more than one treatments sources, or, less frequently, of units contrasts with other units contrasts. The amount of aliasing of one source with another source can be measured using the an efficiency criterion (cf. an aliased source).

A partially confounded source is the blending together of a part of the information for some or all contrasts for a treatments source with those for more than one units source as a result of the allocation of treatments to units (cf. a confounded source).

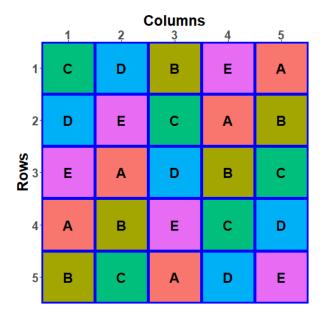
A prior allocation model is a third allocation model to produce in formulating the linear mixed model for a designed experiment. Derive it from the homogeneous allocation model by (i) changing the parameterization of those random terms for which it is to be assumed that their effects display unequal variance or are correlated, (ii) consider removing random terms because of potential singularities in the variance matrix, and (iii) reparameterize those fixed terms for which linear or curved trends are to be fitted.

A random term is a term whose effects are assumed to behave in a manner such that it is appropriate to characterize them by a probability distribution. Usually they contribute a variance component to the variance model (cf. fixed term).

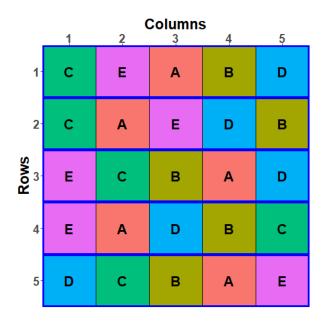
- A randomization is the random assignment, according to an experimental design, of the levels of the allocated (treatments) factors to the units to which the recipient factors belong. One way to randomize a design is to randomly choose a combined, units permutation from a (restricted) set of valid combined, units permutations and apply it to the units.
- The recipient factors/terms/sources are all based on the units factors, to which the allocated factors are allocated (see also factor allocation). The recipient terms are derived from the recipient factors and the recipient sources are derived from the recipient terms. They are also called units factors/terms/sources.
- Repeated-measurements experiments are experiments in which observations are made on a set of entities over time and/or space. They can be subdivided into longitudinal experiments and experiments in which differences between times and/or space are not of interest per se. Thus, cross-over experiments are not longitudinal experiments, because treatments are allocated to the different times and there is no specific interest in the differences between times.
- The set of terms for a panel is comprised of the terms formed from all combinations of the factors within that panel, except that nested factors cannot occur in a term without the factors that nest them. They give rise to the allocated or treatments terms and the recipient or units terms.
- A skeleton-ANOVA is an ANOVA table for an experiment that includes sources for all of the terms in a linear mixed model for a response variable from an experiment. Traditionally, it is used to establish the form of the ANOVA to be employed in analyzing data from an experiment and its sources are listed as a single sequence; generally they do not involve the full set of units factors, instead including a Residual source as the final source in the list.
- A source is the subspace for the main, interaction or nested effects associated with a term, it being the subspace of the column space for the term that has been made orthogonal to terms that are marginal to the term. The notation we use for sources is that given in Brien and Demétrio (2009, Table 1). A source is orthogonalized for all marginal terms. The name of the source for each term is derived as follows: of the factors in a term, only those that nest any of the other factors must be in the square brackets joined by ':'; the rest are put to the left of the square brackets and joined by '#s'. That is, those factors in square brackets nest the remaining factors that interact.
- A standard experimental design is defined to be an experimental design obtained from allocating one set of objects, to be called the treatments, to a second set of objects, to be called the units. Examples are randomized complete-block and split-unit designs.
- **Statistics for canonical efficiency factors** that are used in this paper are: i) the A-efficiency criterion; and (ii) the order of balance.
- Structure-balanced experimental designs See Classes of experimental designs.
- Structure-orthogonal experimental designs See Classes of experimental designs.
- A symbolic model expresses the model as the sum of abbreviated term names, with the names of the fixed terms to the left of a vertical straight line (|) and the random terms to its right. It is understood that the formal linear mixed model replaces each of the abbreviated term names with an indicator matrix multiplied by a vector of fixed-effects parameters or random effects.
- A **term** is derived from the observed levels combinations of one or more of the factors in the experiment. For example, suppose that A, B and C are factors with a, b and c levels, respectively, and all combinations of the three factors are observed. Then A:B:C is the term with abc levels formed from all combinations of the levels of the three factors. It is represented in a model by an indicator matrix, all of whose elements are either zero or one.
- A **treatment** is a, perhaps conceptual, object that is allocated to one or more units and may be based on a combination of the levels of several factors.
- The treatments factors/terms/sources are all associated with the treatments and are the allocated factors/terms/sources in a factor allocation. The treatments terms are derived from the treatments factors in the treatments panel and the treatments sources are derived from the treatments terms.
- The units for an experimental design form a set of objects, the observational units, that are indexed by the units factors. For a standard design, a set of factors, called the treatments factors, are allocated to the units factors.
- The units factors/terms/sources are the recipient factors/terms/sources in a factor allocation. The units factors belong to the units and describe them (cf. treatments factors); they are commonly referred to as the block factors, although it is necessary to be careful to include all factors for the identity term. The units terms are derived from the units factors in the units panel and the units sources are derived from the units terms.
- The units space is the vector space \mathbb{R}^n where n is the number of (observational) units in a design.

A universally optimal design is a design that is A-, D- and E-optimal. A-optimality is generally considered to be the most appropriate form of optimality for designs that compare treatments, although the other forms are also used.

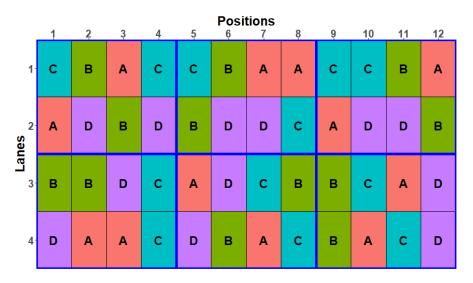
Supplement Section B Supplement Figures showing the randomized layouts for the examples



SUPPLEMENT FIGURE 1 A randomized layout of Varieties in an LSqD on a 5×5 grid of plots from Section 2.1 of Brien et al. (2023).



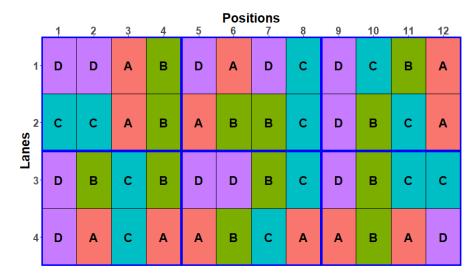
SUPPLEMENT FIGURE 2 A randomized layout of Varieties in an RCBD on a 5×5 grid of plots from Section 2.2 of Brien et al. (2023); blue lines encompass a block.



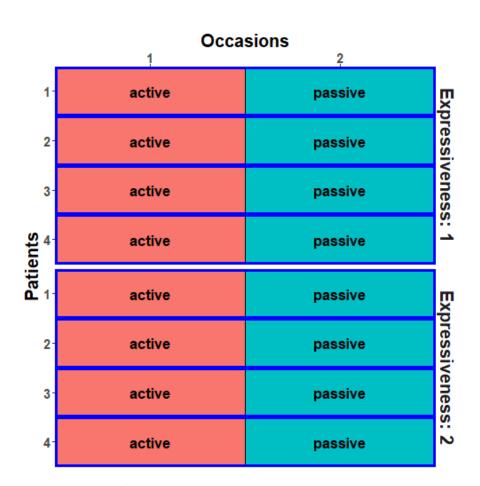
SUPPLEMENT FIGURE 3 A randomized layout of Zinc levels in a GRBD on a 4×12 grid of pots from Section 3.2 of Brien et al. (2023); blue lines encompass a block.

	Lanes				
	1	2	3	4	
1	2,5	4,5	2,1	3,1	
2	1,5	3,5	1,1	4,1	
3	3,4	4,4	3,2	4,2	
4		2,4	1,2	2,2	
5	3,3	1,3	3,5	2,5	
6	2,3	4,3	4,5	1,5	
7	2,2	1,2	4,4	2,4	
8	3,2	4,2	1,4	3,4	
9		4,1	4,3	3,3	
10		2.1	1.3	2.3	
11		2,2	2,2	1,2	
12	3,2	2,2 1,2	4,2	3,2	
13 14	3,5	1,5	2,4	1,4	
14	2,5	4,5	4,4	3,4	
15 16 17 0 18	3,4	1,4	3,5	4,5	
16	2,4	4,4	1,5	2,5	
17	4,1	1,1	1,3	2,3	
ω 18·	3,1	2,1	4,3	3,3	
⊆ 19	2,3	3,3	3,1	4,1	
Positions 51 18 18 18 18		1.3	2.1	1.1	
# 21	4,3	2,3	3,2	2,2	
22	3,3	1,3	1,2	4,2	
23	1,4	3,4	1,3	3,3	
24	4,4	2,4	4,3	2,3	
25	4,1	1,1	1,1	3,1	
26	2,1	3,1	4,1	2,1	
27	4,2	2,2	1,5	4,5	
28	1,2	3,2	2,5	3,5	
29	2,5	4,5	4,4	1,4	
30		3.5	3.4	2.4	
31		4,3	3,3	4,3	
32		1,3	1,3	2,3	
33		2,1	3,1	4,1	
34		1,1	1,1	2,1	
35		1,2 2,2	1,4	3,4	
36			2,4	4,4	
37	3,4	4,4	3,2	4,2	
38	2,4	1,4	1,2	2,2	
39		1,5	2,5	1,5	
40		3.5	3.5	4.5	

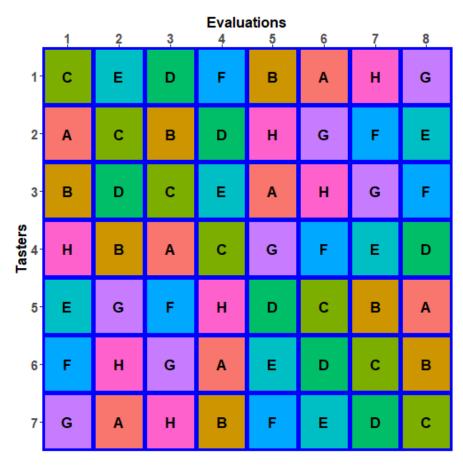
SUPPLEMENT FIGURE 4 A randomized layout for an experiment with Weeks randomized; each cell gives the randomized values of the Zinc and Week levels from Section 4.1 of Brien et al. (2023); blue lines encompass a block and main units are coloured for Weeks.



SUPPLEMENT FIGURE 5 A randomized layout for a longitudinal GRBD for a 4×12 grid of pots from Section 4.2 of Brien et al. (2023); blue lines encompass a block.



SUPPLEMENT FIGURE 6 A layout for the Farewell and Herzberg pain experiment from Section 4.3 of Brien et al. (2023); each cell gives the motion to be performed on an Occasion; blue lines encompass a patient.



Supplement Section C R scripts for generating, plotting and evaluating designs

The R scripts given in this section are available in files in the supplementary zip file. The scripts use the function designRandomize to obtain randomized layouts, the function designGGPlot to plot the design, and the function designAnatomy to obtain anatomy tables, without EMSs, for the layouts for all the examples in the paper. These functions are available from dae (Brien, 2023), a package for the R statistical computing environment (R Core Team, 2023). The package is available on CRAN and at http:\\chris.brien.name\rpackages, the latter being updated more often than CRAN.

In all cases, the R scripts contain the following line:

#knitr::spin("filename")

Provided that you have the packages knitr, dae and ggplot2 installed, you can produce a 'html' file with the output for an example using the R script for the example in the supplementary zip file by executing all of this line, except the '#'. This will also produce a markdown file from which a pdf file can be produced using the function 'rmarkdown:render'.

Otherwise, all the comment lines (beginning with '#') can be ignored and the remaining lines executed manually.

Supplement Section C.1 R-script for an LSqD on a 5×5 grid of plots from Section 2.1 of Brien et al. (2023)

This script produces the randomized layout in Supplement Figure 1 and the anatomy on which Table 1 of Brien et al. (2023) is based. The script and its output files are available in the file Sect2-1_LSqDGridr5c5.r in the supplementary zip file.

```
#'# Script to generate and evaluate an LSqD for a 5 x 5 grid of plots
# To execute the script and produce a html file with the output,
# select all of the line, except for the hash ('#'),
# that starts with '#knitr::spin' and then 'Run the selection'.
#'## Initialize
library(knitr)
#knitr::spin("Sect2-1_LSqDGridr5c5.r
packageVersion("knitr")
packageVersion("dae")
packageVersion("ggplot2")
b <- 5
t <- 5
#'## Construct a systematic design and obtain the randomized layout
LSqD.sys <- cbind(fac.gen(list(Rows = b, Columns = t)),
                  Varieties = factor(designLatinSqrSys(t), labels = LETTERS[1:t]))
LSqD.lay <- designRandomize(allocated
                                             = LSqD.sys["Varieties"],
                                             = LSqD.sys[c("Rows", "Columns")],
                            recipient
                            seed
                                              = 141)
#'## Output the layout
LSqD.lay
#'## Plot the layout
#| "Sect2-1_LSqDGridr5c5", fig.path = "figures/",
#| fig.cap = "Randomized layout for Sect2-1_LSqDGridr5c5"
designGGPlot(LSqD.lay, labels = "Varieties", size = 8,
             title = NULL, title.size = 25, axis.text.size = 20,
             blockdefinition = cbind(1,1)
#'## Get the anatomy of the layout
LSqD.canon <- designAnatomy(formulae = list(units = ~ Rows*Columns,
                                            trts = ~ Varieties),
                            grandMean = TRUE, data = LSqD.lay)
summary(LSqD.canon)
```

Supplement Section C.2 R-script for an RCBD on a 5×5 grid of plots from Sections 2.2 and 3.1 of Brien et al. (2023)

This script produces the randomized layout in Supplement Figure 2 and the anatomies on which Tables 2 and 3a of Brien et al. (2023) are based. The script and its output files are available in the file Sect2-2_3-1_RCBDGridr5c5.r in the supplementary zip file.

```
#'# Script to generate and evaluate an RCBD for a 5 x 5 grid of plots
# To execute the script and produce a html file with the output,
# select all of the line, except for the hash ('#'),
# that starts with '#knitr::spin' and then 'Run the selection'.
#'## Initialize
library(knitr)
#knitr::spin("Sect2-2_3-1_RCBDGridr5c5.r")
library(dae)
packageVersion("knitr")
packageVersion("dae")
packageVersion("ggplot2")
b <- 5
t <- 5
#'## Construct a systematic design and obtain the randomized layout
RCBD.sys <- cbind(fac.gen(list(Rows = b, Columns = t)),</pre>
                  fac.gen(list(Varieties = LETTERS[1:t]), times = b))
RCBD.lay <- designRandomize(allocated</pre>
                                              = RCBD.sys["Varieties"],
                                              = RCBD.sys[c("Rows", "Columns")],
                            recipient
                            nested.recipients = list(Columns = "Rows"),
                            seed
                                               = 1134)
#'## Output the layout
RCBD.lay
#'## Plot the layout
#| "Sect2-2_3-1_RCBDGridr5c5", fig.path = "figures/",
#| fig.cap = "Randomized layout for Sect2-2_3-1_RCBDGridr5c5"
designGGPlot(RCBD.lay, labels = "Varieties", size = 8,
             title = NULL, title.size = 25, axis.text.size = 20,
             blockdefinition = cbind(1,5))
#'## Get the anatomy of the layout for the initial allocation model
RCBD.canon <- designAnatomy(formulae = list(units = ~ Rows/Columns,
                                            trts = ~ Varieties),
                            grandMean = TRUE, data = RCBD.lay)
summary(RCBD.canon)
#'## Get the anatomy of the layout for the homogeneous allocation model with a block-treatment int
RCBD.RV.canon <- designAnatomy(formulae = list(units = ~ Rows/Columns,
                                                trtblks = ~ Rows*Varieties),
                               grandMean = TRUE, data = RCBD.lay)
summary(RCBD.RV.canon)
```

Supplement Section C.3 R-script for a GRBD on a 4×12 grid of pots from Section 3.2 of Brien et al. (2023)

This script produces the randomized layout in Supplement Figure 3 and the anatomy on which Table 4 of Brien et al. (2023) is based. The script and its output files are available in the file Sect3-2_GRBDGridr4c12.r in the supplementary zip file.

```
#'# Script to generate and evaluate a GRBD for a 4 x 12 grid of pots
# To execute the script and produce a html file with the output,
# select all of the line, except for the hash ('#'),
# that starts with '#knitr::spin' and then 'Run the selection'.
#'## Initialize
library(knitr)
#knitr::spin("Sect3-2_GRBDGridr4c12.r")
library(dae)
packageVersion("knitr")
packageVersion("dae")
packageVersion("ggplot2")
b <- 6
k <- 8
t <- 4
#'## Construct a systematic design and obtain the randomized layout
GRBD.sys <- cbind(fac.gen(list(Blocks = b, Pots = k)),</pre>
                  fac.gen(list(Zinc = LETTERS[1:t]), times = b*k/t))
GRBD.lay <- designRandomize(allocated</pre>
                                               = GRBD.sys["Zinc"],
                                               = GRBD.sys[c("Blocks", "Pots")],
                             recipient
                             nested.recipients = list(Pots = "Blocks"),
                                                = 5733)
#'## Add factors for Lane and Position
GRBD.lay <- cbind(with(GRBD.lay, fac.divide(Blocks,</pre>
                                             factor.names = list(PLanes = 2,
                                                                  QPositions = 3))),
                  with(GRBD.lay, fac.divide(Pots,
                                             factor.names = list(Lanes = 2,
                                             Positions = 4))),
                  GRBD.lav)
GRBD.lay <- within(GRBD.lay,</pre>
                     Lanes <- fac.combine(list(PLanes, Lanes))</pre>
                     Positions <- fac.combine(list(QPositions, Positions))</pre>
                   })
GRBD.lay <- GRBD.lay[, -match(c("PLanes", "QPositions"), names(GRBD.lay))]</pre>
#'## Output the layout
GRBD.lay
#'## Plot the layout
#| "Sect3-2_GRBDGridr4c12", fig.width = 12, fig.path = "figures/",
#| fig.cap = "Randomized layout for Sect3-2_GRBDGridr4c12"
designGGPlot(GRBD.lay, row.factors = "Lanes", column.factors = "Positions",
             labels = "Zinc", size = 8,
             title = NULL, title.size = 25, axis.text.size = 20,
             blockdefinition = cbind(2,4))
```

Supplement Section C.4 R-script for an experiment with Weeks randomized from Section 4.1 of Brien et al. (2023)

This script produces the randomized layout in Supplement Figure 4 and the anatomy on which Table 5 of Brien et al. (2023) is based. The script and its output files are available in the file Sect4-1_SUDTimeRand.r in the supplementary zip file.

```
#'# Script to generate and evaluate a Split-unit design (SUD) with Weeks randomized
# To execute the script and produce a html file with the output,
# select all of the line, except for the hash ('#'),
# that starts with '#knitr::spin' and then 'Run the selection'.
#'## Initialize
library(knitr)
#knitr::spin("Sect4-1_SUDTimeRand.r")
library(dae)
packageVersion("knitr")
packageVersion("dae")
packageVersion("ggplot2")
r <- 8
a <- 5
b <- 4
#'## Construct a systematic layout and obtain the randomized layout
SUD.sys <- cbind(fac.gen(list(Blocks = r, MainUnits = a, Pots = b)),
fac.gen(list(Weeks = a, Zinc = b), times = r))
SUD.lay <- designRandomize(allocated</pre>
                                              = SUD.sys[c("Zinc", "Weeks")],
                                              = SUD.sys[c("Blocks", "MainUnits", "Pots")],
                           recipient
                           nested.recipients = list(MainUnits = "Blocks",
                                                     Pots = c("MainUnits", "Blocks")),
                                              = 3116)
                            seed
#'## Output the layout
head(SUD.lay, n = a*b)
summary(SUD.lay)
#'## Locate the design in the glasshouse and plot
#| "Sect4-1_SUDTimeRand.r", fig.height = 10, fig.width = 5, fig.path = "figures/",
#| fig.cap = "Randomized layout for Sect4-1_SUDTimeRand.r"
SUD.lay <- cbind(SUD.lay,
with(SUD.lay, fac.divide(Pots, list(PLane = 2, PPosn = 2))),
with(SUD.lay, fac.divide(Blocks, list(BLane = 2, BPosn = 4))))
SUD.lay <- within(SUD.lay,
                  {
                    Lanes <- fac.combine(list(BLane, PLane))</pre>
                    Positions <- fac.combine(list(BPosn, MainUnits, PPosn))</pre>
                    Treatments <- fac.combine(list(Zinc, Weeks), combine.levels = TRUE)</pre>
                  })
SUD.lay <- SUD.lay[c("Lanes", "Positions", "Blocks", "MainUnits", "Pots",
                      "Zinc", "Weeks", "Treatments")]
designGGPlot(SUD.lay, labels = "Treatments", size = 5,
             row.factors = "Positions", column.factors = "Lanes",
             cellfillcolour.column = "Weeks",
             title = NULL, title.size = 18, axis.text.size = 15,
             blockdefinition = cbind(10,2))
```

Supplement Section C.5 R-script for a longitudinal GRBD for a 4×12 grid of pots from Section 4.2 of Brien et al. (2023)

This script produces the randomized layout in Supplement Figure 5 and the anatomy on which Table 6 of Brien et al. (2023) is based. The script and its output files are available in the file Sect4-2_GRBDlongi.r in the supplementary zip file.

```
#'# Script to generate and evaluate a longitudinal GRBD for a 4 x 12 grid of pots
# To execute the script and produce a html file with the output,
# select all of the line, except for the hash ('#'),
# that starts with '#knitr::spin' and then 'Run the selection'.
#'## Initialize
library(knitr)
#knitr::spin("Sect4-2_GRBDlongi.r")
library(dae)
packageVersion("knitr")
packageVersion("dae")
packageVersion("ggplot2")
b <- 6
k <- 8
t < -4
d <- 14
#'## Construct a systematic design and obtain the randomized layout
longi.sys <- cbind(fac.gen(list(Blocks = b, Pots = k, Days = d)),</pre>
                   fac.gen(list(Zinc = LETTERS[1:t]), times = b*(k/t), each = d))
longi.lay <- designRandomize(allocated</pre>
                                                = longi.sys["Zinc"],
                                                 = longi.sys[c("Blocks", "Pots", "Days")],
                              recipient
                              nested.recipients = list(Pots = "Blocks"),
                                                 = 5733)
                              seed
#'## Add factors for Lane and Position
longi.lay <- cbind(with(longi.lay, fac.divide(Blocks,</pre>
                                                factor.names = list(PLanes = 2,
                                                                    QPositions = 3))),
                   with(longi.lay, fac.divide(Pots,
                                                factor.names = list(Lanes = 2,
                                                                    Positions = 4))),
                   longi.lay)
longi.lay <- within(longi.lay,</pre>
Lanes <- fac.combine(list(PLanes, Lanes))</pre>
Positions <- fac.combine(list(QPositions, Positions))</pre>
longi.lay <- longi.lay[, -match(c("PLanes", "QPositions"), names(longi.lay))]</pre>
#'## Output the layout
head(longi.lay, n = 75)
#'## Plot the layout
#| "Sect4-2_GRBDlongi", fig.width = 12, fig.path = "figures/",
#| fig.cap = "Randomized layout for Sect4-2_GRBDlongi"
designGGPlot(subset(longi.lay, Days == "1"),
             row.factors = "Lanes", column.factors = "Positions",
             labels = "Zinc", size = 8,
             title = NULL, title.size = 25, axis.text.size = 20,
```

blockdefinition = cbind(2,4))

Supplement Section C.6 R-script for the Farewell and Herzberg pain experiment from Section 4.3 of Brien et al. (2023)

This script produces the randomized layout in Supplement Figure 6 and the anatomies on which Table 7 of Brien et al. (2023) is based. The script and its output files are available in the file Sect4-3_FHPain.r in the supplementary zip file.

```
#'# Script to generate and evaluate a design the Farewell and Herzberg pain experiment
# To execute the script and produce a html file with the output,
# select all of the line, except for the hash ('#'),
# that starts with '#knitr::spin' and then 'Run the selection'.
#'## Initialize
library(knitr)
#knitr::spin("Sect4-3_FHPain.r")
library(dae)
packageVersion("knitr")
packageVersion("dae")
packageVersion("ggplot2")
#'## Construct the systematic layout
Pain.lay <- cbind(fac.gen(list(Expressiveness = 2, Patients = 4, Occasions = 2)),
                  fac.gen(list(Motions = c("active", "passive")), times = 8))
#'## Output the layout
Pain.lay
#'## Plot the layout
#| "Sect4-3_FHPain", fig.width = 12, fig.path = "figures/",
#| fig.cap = "Randomized layout for Sect4-3_FHPain"
designGGPlot(Pain.lay, labels = "Motions", size = 6,
             row.factors = c("Expressiveness", "Patients"),
             column.factors = "Occasions",
             title = NULL, title.size = 20, axis.text.size = 15,
             blockdefinition = cbind(1,5))
#'## Get the anatomy of the layout for the initial allocation model
Pain.canon <- designAnatomy(formulae = list(units =</pre>
                                               ~ (Expressiveness/Patients)*Occasions,
                                             trts = ~ Motions),
                            grandMean = TRUE, data = Pain.lay)
summary(Pain.canon)
#'## Get the anatomy of the layout for the homogeneous allocation model
Pain.ME.canon <- designAnatomy(formulae = list(units</pre>
                                                  ~ (Expressiveness/Patients)*Occasions,
                                                trtblks = ~ Motions*Expressiveness),
                               grandMean = TRUE, data = Pain.lay)
summary(Pain.ME.canon)
#'## Get the anatomy of the layout under the assumption of nested Occasions
Pain.nest.canon <- designAnatomy(formulae = list(units</pre>
                                                    ~ Expressiveness/Patients/Occasions,
                                                  trtblks = ~ Motions*Expressiveness),
                                 grandMean = TRUE, data = Pain.lay)
summary(Pain.nest.canon)
```

Supplement Section C.7 R-script for the YSD for 8 treatments from Section 5 of Brien et al. (2023)

This script produces the randomized layout in Supplement Figure 7 and the anatomies on which Table 8 of Brien et al. (2023) is based. The script and its output files are available in the file Sect5_YSDr7c8.r in the supplementary zip file.

```
#'# Script to generate and evaluate a YSD for 8 treatments in 7 rows x 8 columns
# To execute the script and produce a html file with the output,
# select all of the line, except for the hash ('#'),
# that starts with '#knitr::spin' and then 'Run the selection'.
#'## Initialize
library(knitr)
#knitr::spin("Sect5_YSDr7c8.r")
library(dae)
packageVersion("knitr")
packageVersion("dae")
packageVersion("ggplot2")
r <- 7
c <- 8
t <- 8
#'## Construct a systematic design and obtain the randomized layout
YSD.sys <- cbind(fac.gen(list(Tasters = r, Evaluations = c)),
                  Products = factor(designLatinSqrSys(t)[1:(r*c)],
                                    labels = LETTERS[1:t]))
YSD.lay <- designRandomize(allocated = YSD.sys["Products"],</pre>
                           recipient = YSD.sys[c("Tasters", "Evaluations")],
                                     = 6142)
#'## Output the layout
YSD.lay
#'## Plot the layout
#+ "Sect5_YSDr7c8", fig.path = "figures/",
#+ fig.cap = "Randomized layout for Sect5_YSDr7c8"
designGGPlot(YSD.lay, labels = "Products", size = 6,
             row.factors = "Tasters", column.factors = "Evaluations",
             title = NULL, title.size = 16, axis.text.size = 15,
             blockdefinition = cbind(1,1)
#'## Get the anatomy of the layout for the initial allocation model
YSD.canon <- designAnatomy(formulae = list(units = ~ Tasters*Evaluations,
                                           trts = ~ Products),
                           grandMean = TRUE, data = YSD.lay)
summary(YSD.canon)
#'## Get the anatomy of the layout for the homogeneous allocation model
YSD.JP.canon <- designAnatomy(formulae = list(units = ~ Tasters*Evaluations,
                                               trtblks = ~ Tasters*Products),
                              grandMean = TRUE, data = YSD.lay)
summary(YSD.JP.canon)
```

Supplement Section D Constructing the anatomy table, without EMS, for a design that is structure-balanced

The material in this section is based on Brien and Bailey (2009, Sections 3 and 4)

Let \mathcal{F} be the set of units (recipient) terms and assume that a poset (partially ordered set) structure is defined on the units, which is the case for most experiments conducted in practice and all the examples in Brien et al. (2023). Let \mathcal{G} be the set of treatments (allocated) terms, possibly with some terms from \mathcal{F} included in \mathcal{G} to ensure that a poset structure is defined on the treatments. Denote by $\mathcal{F}^{(s)}$ and $\mathcal{G}^{(s)}$ the sets of sources such that, for each of the elements F and G in the sets \mathcal{F} and G, there is an element $F^{(s)}$ and a $G^{(s)}$ in each of the sets $\mathcal{F}^{(s)}$ and $\mathcal{G}^{(s)}$.

A poset structure (also referred to as a poset block structure) is a decomposition of the data space derived from a set of factors that can be ordered based on their nesting relations, i.e. the set of factors forms a partially ordered set, the order being provided by the nesting of the factors. The elements of the decomposition correspond to a set of terms that consist of all combinations of the factors, subject to the restriction that a term that includes a nested factor must also include its nesting factors. The terms must include a factor that is marginal to all terms, which we refer to as the Mean term, and a term to which all terms are marginal, the maximal term.

For example, consider the LSqD in Section 2.1 of Brien et al. (2023). In addition to the Mean factor, the units involves two factors, Rows and Columns that are crossed. Hence the sets of terms derived from these factors are $\mathcal{F} = \{\text{Mean}, R, C, R:C\}$. The treatments are indexed by Varieties and so $\mathcal{G} = \{\text{Mean}, V\}$. The sets of sources are $\mathcal{F}^{(s)} = \{\text{Mean}, R, C, R \# C\}$ and $\mathcal{G}^{(s)} = \{\text{Mean}, V\}$.

Given a poset of factors indexing the set of n units, there is a poset structure on the units specified by a set, \mathcal{P} say, of mutually orthogonal projection matrices that sum to \mathbf{I}_n , there being a matrix for each source in $\mathcal{F}^{(s)}$ that is the matrix that projects onto the subspace for the source. This set of subspaces is referred to as the structure on the units.

Similarly, given a poset of factors indexing the treatments, there is a structure on the treatments defined by a set of mutually orthogonal projection matrices being denoted by Q. The matrices in Q needs to have been suitably redefined to project on the full unit space, as described in Brien and Bailey (2009, Section 4).

An anatomy table without EMS consists of two major columns, one for units and the other for treatments. The units major column contains a source and a DF column for the units. The treatments major column contains (i) a column of A-efficiency criteria values that are not equal to one, if any, and (ii) a source and a DF column.

To construct the anatomy for a design, it is necessary to determine the confounding between pairs of sources, one being a units source from $\mathcal{F}^{(s)}$ and the other a treatments source from $\mathcal{G}^{(s)}$. The confounding between pairs of sources can be determined by applying the following rule to every such pair of sources.

Rule 1 (Confounding). For treatment source $G^{(s)}$ in $\mathcal{G}^{(s)}$ and units source $F^{(s)}$ in $\mathcal{F}^{(s)}$, consider $\mathbf{P}_F \mathbf{Q}_G$, where \mathbf{P}_F is the element of \mathcal{P} for $F^{(s)}$ and \mathbf{Q}_G is the element of \mathcal{Q} for $G^{(s)}$.

If $\mathbf{P}_F \mathbf{Q}_G$ is nonzero then there is confounding of $G^{(s)}$ with $F^{(s)}$, otherwise there is not confounding between the pair.

In order to construct an anatomy table, in addition to the sources and their confounding, the canonical efficiency factors and the degrees of freedom to the sources are needed.

Rule 2 (Canonical efficiency factors). The canonical efficiency factors for a treatment source (partially) confounded with a units source are the nonzero eigenvalues of the matrix product $\mathbf{Q}_G \mathbf{P}_F \mathbf{Q}_G$ for this pair of sources. A single value summary of the canonical efficiency factors is the A-efficiency criterion, calculated as their harmonic mean.

The canonical efficiency factors can be used to determine the balance of a design.

Rule 3 (Balance). A structure-balanced design is one for which any treatments source confounded with a units source has (i) canonical efficiency factors that are all equal and (ii) there is no partial aliasing between treatments sources when both are confounded with the same units source (Brien and Bailey, 2009). A structure-balanced design for which all canonical efficiency factors are equal to one is said to be structure orthogonal. If all treatments sources have canonical efficiency factors that all are

equal, but there is partial aliasing, then the design is first-order balanced; if in addition, the values of the canonical efficiency factors are one then the design is (first-order) orthogonal. Any design that has one or more canonical efficiency factors that are not equal to one is said to be nonorthogonal.

The balance properties of a design can be ascertained using the designAnatomy function from the R package dae (Brien, 2023), because the efficiency criteria it produces are, like the A-efficiency criterion, simple statistics calculated from the canonical efficiency factors. The order of balance is also amongst that statistics that can be reported.

Having determined the confounding, the sources in the anatomy table can be tabulated. List down the units sources and their DF in a pair of columns and then form another pair of columns with the treatments sources and DF, lining up each treatment source and DF with the units source(s) and DF(s) with which it is confounded. If the design is nonorthogonal, but structure-balanced, add a column before the column of treatment sources that contains the values of the A-efficiency criterion that are not one.

The DF for sources in an anatomy table are the ranks of projection matrices that specify an orthogonal decomposition of the units space. For the units column in the anatomy table, the decomposition is that corresponding to \mathcal{P} . For the treatments column, the decomposition is that resulting from combining the elements of \mathbf{Q} with \mathbf{P} to specify the orthogonal projection matrices for the joint decomposition of the units space. The set of projection matrices of this decomposition are those resulting from the refinement of elements of \mathcal{P} by elements of \mathcal{Q} and is denoted $\mathcal{P} \triangleright \mathcal{Q}$ by Brien and Bailey (2009, Section 4).

There are three types of projection matrices in the set $\mathcal{P} \triangleright \mathcal{Q}$.

- 1. The first type is the projection matrix for a combined source for a treatment source $G^{(s)}$ confounded with a units source $F^{(s)}$; the projection matrix is denoted by $\mathbf{P}_F \triangleright \mathbf{Q}_G$ and it projects onto the part of \mathbf{P}_F pertaining to \mathbf{Q}_G .
- 2. The second type of projection matrix is for a Residual source resulting from a units source $F^{(s)}$ whose subspace has not been accounted for in its entirety by treatments sources, $G^{(s)}$ s, confounded with it; the Residual source is denoted by $\mathbf{P}_F \vdash \mathcal{Q}$ and it projects onto the part of \mathbf{P}_F orthogonal to all \mathbf{Q}_G in \mathcal{Q} .
- 3. The final type of projection matrix is a for a complete units source $F^{(s)}$ that has no treatments source $G^{(s)}$ confounded with it, it being denoted by \mathbf{P}_F and having the property that $\mathbf{P}_F \mathbf{Q}_G = \mathbf{0}$ for all \mathbf{Q}_G in \mathcal{Q} .

Since it is being assumed that Q is structure-balanced in relation to \mathcal{P} (Brien and Bailey, 2009), the expressions for the first two types of projection matrices in terms of the elements of \mathcal{P} and \mathcal{Q} are:

$$\begin{split} \mathbf{P}_{F} \rhd \mathbf{Q}_{G} &= \lambda_{F^{(s)} \leftarrow G^{(s)}}^{-1} \mathbf{P}_{F} \mathbf{Q}_{G} \mathbf{P}_{F}, \\ \mathbf{P}_{F} \vdash \mathcal{Q} &= \mathbf{P}_{F} - \sum_{\substack{G \in \mathcal{G} \\ \lambda_{F^{(s)} \leftarrow G^{(s)}} \neq 0}} \mathbf{P}_{F} \rhd \mathbf{Q}_{G}, \end{split}$$

for \mathbf{P}_F in \mathcal{P} and \mathbf{Q}_G in \mathcal{Q} and where $\lambda_{F^{(s)}\leftarrow G^{(s)}}$ is the canonical efficiency factor for $G^{(s)}$ when confounded with $F^{(s)}$ (Brien and Bailey, 2009); $\lambda_{F^{(s)}\leftarrow G^{(s)}}$ is the value of all nonzero eigenvalues of $\mathbf{Q}_G\mathbf{P}_F\mathbf{Q}_G$, there being only one value for structure-balanced designs. Note that, for $\lambda_{F^{(s)}\leftarrow G^{(s)}}$ equal to one, $\mathbf{P}_F \rhd \mathbf{Q}_G$ is equal to \mathbf{Q}_G .

Rule 4 (DF). The DF for the units column in an anatomy table are the ranks of the projection matrices in \mathcal{P} and those for the treatments column are the ranks of those projection matrices in $\mathcal{P} \rhd \mathcal{Q}$ that are not equal to an element of \mathcal{P} i.e projection matrices of types 1 and 2 in the set $\mathcal{P} \rhd \mathcal{Q}$.

There are four units sources in the anatomy table in Table 1 of (Brien et al., 2023), viz. Mean, Rows, Columns and R#C with DFs 1, 4, 4 and 16. The decomposition of units refined by treatments is specified by the five lines in the body of the anatomy table: (i) Mean confounded with Mean, (ii) Rows, (iii) Columns, (iv) Varieties confounded with R#C and (v) Residual for R#C. Given that the design is structure orthogonal, the elements of $\mathcal{P} \rhd \mathcal{Q}$ are (i) $\mathbf{P}_0 \rhd \mathbf{Q}_0 = \mathbf{Q}_0$ (type 1), (ii) \mathbf{P}_R (type 3), (iii) \mathbf{P}_C (type 3), (iv) $\mathbf{P}_{RC} \rhd \mathbf{Q}_V = \mathbf{P}_{RC} \mathbf{Q}_V \mathbf{P}_{RC} = \mathbf{Q}_V$ (type 1), and (v) $\mathbf{P}_{RC} \vdash \mathcal{Q} = \mathbf{P}_{RC} - \mathbf{Q}_V$ (type 2). The entries in the treatments column are for (i) Mean confounded with Mean, (ii) Varieties confounded with R#C and (111) Residual for R#C and the ranks of the corresponding projection matrices are 1, 4 and 12. Because the design in structure orthogonal, all eigenvalues are one, and so in all cases a DF is the number of eigenvalues of a projection matrix equal to one and the A-efficiency criterion is also one.

Supplement Section E Deriving the EMSs under a homogeneous allocation model that may include block-treatment interactions for a design that is structure-balanced

The rules for obtaining the expected mean squares (EMSs) are presented in Appendix of Brien et al. (2023). The derivation, provided here, of these rules uses the techniques of Brien and Bailey (2009) and Bailey and Brien (2016), although in terms of variance components instead of canonical covariance components (for a justification, see Speed, 1986). The notation from Supplement Section D is used. However, because EMSs are now involved, a model is required, unlike in Supplement Section D.

Supplement Section E.1 Introduction

Let \mathcal{F} be the set of terms for the units (recipient) factors in a homogeneous allocation model and again assume that a poset structure is defined on the units. Let \mathcal{G} be the set of terms for the treatments (allocated) factors in a homogeneous allocation model, possibly with some terms from \mathcal{F} included in \mathcal{G} to ensure that a poset structure is defined on the treatments. Denote by $\mathcal{F}^{(s)}$ and $\mathcal{G}^{(s)}$ the sets of sources such that, for each of the elements F and G in the sets \mathcal{F} and G, there is an element $F^{(s)}$ and a $G^{(s)}$ in each of the sets $\mathcal{F}^{(s)}$ and $\mathcal{G}^{(s)}$. Further, suppose that \mathcal{Q} is structure-balanced in relation to \mathcal{P} (see Supplement Section D).

As a device, assume initially that all terms are random. A linear mixed model in marginal form can be expressed in terms of three different sets of parameters: (i) the variance components, (ii) the covariances between pairs of observations, and (iii) the spectral components. Each of the elements of one of the three sets of parameters is a linear combination of the elements of the other sets.

The *initial all-random model*, in terms of the variance components, is:

$$\mathbb{E}[\mathbf{Y}] = \boldsymbol{\psi} = \mathbf{0} \quad \text{and}$$

$$\operatorname{Var}[\mathbf{Y}] = \mathbf{V} = \mathbf{V}_{\mathcal{F}} + \mathbf{V}_{\mathcal{G}} = \sum_{F \in \mathcal{F}} \sigma_F^2 \mathbf{R}_F + \sum_{G \in \mathcal{G}} \sigma_G^2 \mathbf{S}_G$$
(1)

where $\mathbf{V}_{\mathcal{F}}$ and $\mathbf{V}_{\mathcal{G}}$ are the variance matrices for terms in \mathcal{F} and \mathcal{G} , each \mathbf{R} and \mathbf{S} is obtained from the indicator matrix for its term, \mathbf{Z} , as $\mathbf{Z}\mathbf{Z}^{\top}$, and σ_{\cdot}^{2} is a variance component for term F or G.

The variance matrices can be written in terms of any one of the three sets of parameters.

$$\mathbf{V}_{\mathcal{F}} = \sum_{F \in \mathcal{F}} \gamma_F \mathbf{B}_F = \sum_{F \in \mathcal{F}} \sigma_F^2 \mathbf{R}_F = \sum_{F \in \mathcal{F}} \eta_F \mathbf{P}_F$$

$$\mathbf{V}_{\mathcal{G}} = \sum_{G \in \mathcal{G}} \gamma_G \mathbf{C}_G = \sum_{G \in \mathcal{G}} \sigma_G^2 \mathbf{S}_G = \sum_{G \in \mathcal{G}} \eta_G \mathbf{Q}_G,$$
(2)

where γ_F for term F in \mathcal{F} is the covariance between pairs observations that share the same combinations of the levels of the factors in F, but do not share such combinations for any other F' in \mathcal{F} to which F is marginal (similarly for γ_G for term G in \mathcal{G}); \mathbf{B}_F and \mathbf{C}_G are incidence matrices whose elements are zero or one, a one indicating observations that share the same covariance; η_F for source $F^{(s)}$ corresponding to F in F and g for source $G^{(s)}$ corresponding to G in g are the spectral components for sources $F^{(s)}$ and $G^{(s)}$; \mathbf{P}_F and \mathbf{Q}_G are orthogonal projection matrices that project onto subspaces for sources $F^{(s)}$ and $G^{(s)}$. The elements of each of the sets \mathcal{B}_F and \mathcal{C}_G sum to \mathbf{J}_n , where \mathbf{J}_n is the $n \times n$ matrix of ones. The spectral components are the eigenvalues of \mathbf{V}_F and \mathbf{V}_G , and are the contributions of the various sources to the EMSs; \mathbf{P}_F and \mathbf{Q}_G project onto the eigenspaces of \mathbf{V}_F and \mathbf{V}_G .

In the present context, expressions for the contributions of the sources to the EMSs in terms of the variance components are the objective. This can be achieved using expressions for the spectral components in terms of the variance components. Firstly, write F < D for F and D in F and F marginal to D and G < H for G and H in G and G marginal to G. Also, let G and G be the common number of replicates of the combinations of the levels of the factors in term G and in term G. Then, the EMS contributions, the spectral components G0, in terms of the variance components, G1, for the initial all-random model are as follows.

$$\eta_F = \sum_{D \ge F} k_D \sigma_D^2 \quad \text{and} \quad \eta_G = \sum_{H \ge G} k_H \sigma_H^2.$$
(3)

For the LSqD in Section 2.1 of Brien et al. (2023), the spectral components for the units sources in terms of the variance components are:

- 1. $\eta_{\text{Mean(u)}} = \sigma_{\text{RC}}^2 + 5\sigma_{\text{R}}^2 + 5\sigma_{\text{C}}^2 + 25\sigma_{\mu(u)}^2$,
- 2. $\eta_{\rm R} = \sigma_{\rm RC}^2 + 5\sigma_{\rm R}^2$, 3. $\eta_{\rm C} = \sigma_{\rm RC}^2 + 5\sigma_{\rm C}^2$, and
- 4. $\eta_{RC} = \sigma_{RC}^2$.

Each of these spectral components is the random contribution of a units source to the EMSs.

Supplement Section E.2 Obtaining the EMSs

An EMS for a source is expected value of the sum of squares of the projection of the response variable Y into the subspace for a source, divided by the dimensions of the subspace. If A is the projection matrix for a source and $\nu_{\mathbf{A}}$ is its rank or degrees of freedom, then its EMS is

$$\mathbb{E}\left[\left(\mathbf{A}\mathbf{Y}\right)^{\top}\left(\mathbf{A}\mathbf{Y}\right)/\nu_{\mathbf{A}}\right] = \mathbb{E}\left[\mathbf{Y}^{\top}(\mathbf{A}/\nu_{\mathbf{A}})\mathbf{Y}\right].$$
(4)

That is, the EMS is the sum of squares of **AY** divided by $\nu_{\mathbf{A}}$, which is a quadratic form in **Y**; the matrix of the quadratic form is the scaled projection matrix $\mathbf{A}/\nu_{\mathbf{A}}$. Let $\mathbb{E}[\mathbf{Y}] = \boldsymbol{\psi}$ and $\mathrm{Var}[\mathbf{Y}] = \mathbf{V}$. Then, the general form of an EMS for a source (Searle, 1971, Section 2.5) is:

$$\mathbb{E}\left[\mathbf{Y}^{\top}(\mathbf{A}/\nu_{\mathbf{A}})\mathbf{Y}\right] = \operatorname{trace}(\{\mathbf{A}/\nu_{\mathbf{A}}\}\mathbf{V}) + \boldsymbol{\psi}^{\top}(\mathbf{A}/\nu_{\mathbf{A}})\boldsymbol{\psi}. \tag{5}$$

So an EMS for a source is made up of two parts, a random contribution, trace($\{A/\nu_A\}V$), and a fixed contribution, $\psi^{\top}(\mathbf{A}/\nu_{\mathbf{A}})\psi$. The fixed contribution is denoted by θ and is itself a quadratic form in ψ . The random contribution is a function of the variance components, the σ^2 s.

The expressions in (2) for $V_{\mathcal{F}}$ and $V_{\mathcal{G}}$ in terms of the sets of matrices \mathcal{P} and \mathcal{Q} can be used to obtain the EMSs to include in an anatomy table because the decomposition for a design combines these sets of matrices, as described in Supplement Section D. The sources for which EMS are required, the EMS sources, are those resulting from the refinement of \mathcal{P} by \mathcal{Q} and whose set of projection matrices is $\mathcal{P} \triangleright \mathcal{Q}$. The projection matrices in $\mathcal{P} \triangleright \mathcal{Q}$ are the A matrices given in (4) and so, divided by their rank, they become the matrices of the quadratic forms for the EMSs based on the all-random model in (1).

Now, for the all-random model in (1), in which $\psi = 0$, the expression for the EMS for a source reduces to

$$\mathbb{E}\left[\mathbf{Y}^{\top}(\mathbf{A}/\nu_{\mathbf{A}})\mathbf{Y}\right] = \operatorname{trace}(\mathbf{A}\mathbf{V})/\nu_{\mathbf{A}}.$$
(6)

It can be shown, assuming Q is structure-balanced in relation to P and the all-random model in (1), that:

for
$$\mathbf{A} = \mathbf{P}_F \rhd \mathbf{Q}_G$$
, $\mathbb{E}\left[\mathbf{Y}^{\top}(\mathbf{A}/\nu_{\mathbf{A}})\mathbf{Y}\right] = \eta_F + \lambda_{F^{(s)} \leftarrow G^{(s)}} \eta_G$;
for a Residual source
or a units source with

no confounded treatment source, $\mathbb{E}\left[\mathbf{Y}^{\top}(\mathbf{A}/\nu_{\mathbf{A}})\mathbf{Y}\right] = \eta_{F}$.

However, expressions for the EMSs under a homogeneous allocation model are required. That is, the designations of terms as fixed and random in the homogeneous allocation model are allowed to differ from the designations in the initial all-random model. While the overall expression for an EMS for a source in (7) applies to both models, the expressions for the EMS contributions must be modified as described below. Let \mathcal{T} and $\mathcal{T}^{(s)}$ be the sets of fixed terms and sources, respectively, and \mathcal{U} and $\mathcal{U}^{(s)}$ be the sets of random terms and sources, respectively. Then, the homogeneous allocation model in the form of a marginal linear mixed model is:

$$\mathbb{E}[\mathbf{Y}] = \boldsymbol{\psi} = \sum_{T \in \mathcal{T}} \mathbf{X}_T \boldsymbol{\tau}_T \quad \text{and} \quad \operatorname{Var}[\mathbf{Y}] = \mathbf{V} = \sum_{U \in \mathcal{F} \cap \mathcal{U}} \sigma_U^2 \mathbf{R}_U + \sum_{U \in \mathcal{G} \cap \mathcal{U}} \sigma_U^2 \mathbf{S}_U, \tag{8}$$

where \mathbf{X}_T is the design matrix for the terms T in \mathcal{T} , $\boldsymbol{\tau}_T$ is the vector of fixed parameters for T.

Rule 5 (Random EMS contributions). The random EMS contributions for the sources corresponding to the terms U in $\mathcal{U} \cap (\mathcal{F} \cup \mathcal{G})$ are obtained by setting to zero the variance components in (3) for each T in $\mathcal{T} \cap \mathcal{F}$ or in $\mathcal{T} \cap \mathcal{G}$, as well as for each G in $\mathcal{G} \cap \mathcal{F} \cap \mathcal{U}$. That is, for terms F, G in \mathcal{U} , they become:

$$\eta_F = \sum_{\substack{D \ge F \\ D \in (\mathcal{F} \cap \mathcal{U})}} k_D \sigma_D^2 \quad \text{and} \quad \eta_G = \sum_{\substack{H \ge G \\ H \in (\mathcal{G} \cap \mathcal{U} \setminus \mathcal{F})}} k_H \sigma_H^2, \tag{9}$$

and, for sources corresponding to the terms F, G in \mathcal{T} , they become:

$$\eta_F = \sum_{\substack{D > F \\ D \in (\mathcal{F} \cap \mathcal{U})}} k_D \sigma_D^2 \quad \text{and} \quad \eta_G = \sum_{\substack{H > G \\ H \in (\mathcal{G} \cap \mathcal{U} \setminus \mathcal{F})}} k_H \sigma_H^2. \tag{10}$$

where the subscript $\mathcal{G} \cap \mathcal{U} \setminus \mathcal{F}$ indicates the intersection of the sets \mathcal{G} and \mathcal{U} from which is subtracted any element of the set \mathcal{F} in $\mathcal{G} \cap \mathcal{U}$. The difference between (9) and (10), is that only (9) includes components σ_F^2 and σ_G^2 .

Rule 6 (The EMS for an EMS source). The EMS for an EMS source is obtained by combining the random contributions in (9) and (10) using the expressions in (7), and, if the EMS source involves one or more sources for fixed terms, adding a θ with a subscript as follows:

Source $A^{(s)} \in \mathcal{G}^{(s)}$ confounded with source $B^{(s)} \in \mathcal{F}^{(s)}$:

both terms A and B fixed: $\theta_{B^{(s)}\leftarrow A^{(s)}}$, for $A\in\mathcal{T}\cap\mathcal{G},\,B\in\mathcal{T}\cap\mathcal{F};$ term A only fixed: $\theta_{B^{(s)*}\leftarrow A^{(s)}}$, or, if $\lambda_{B^{(s)}\leftarrow A^{(s)}}=1,\,\theta_{A^{(s)}}$, for $A\in\mathcal{T}\cap\mathcal{G},\,B\in\mathcal{U}\cap\mathcal{F};$ term B only fixed: $\theta_{B^{(s)}\leftarrow A^{(s)*}}$, for $A\in\mathcal{U}\cap\mathcal{G},\,B\in\mathcal{T}\cap\mathcal{F};$

both terms A **and** B **random:** no θ applicable for $A \in \mathcal{U} \cap \mathcal{G}$, $B \in \mathcal{U} \cap \mathcal{F}$.

No confounding with source $B^{(s)} \in \mathcal{F}^{(s)}$:

term B fixed: $\theta_{B^{(s)}}$, for $B \in \mathcal{T} \cap \mathcal{F}$.

A Residual source for $B^{(s)} \in \mathcal{F}^{(s)}$:

term B fixed: $\theta_{B_{\vdash}^{(s)}}$, for $B \in \mathcal{T} \cap \mathcal{F}$, where $B_{\vdash}^{(s)}$ means that part of the recipient source $B^{(s)}$ that is orthogonal to all allocated sources.

For any case in which $A^{(s)}$ is confounded with $B^{(s)}$, the quadratic form is given by

$$\theta_{B^{(s)} \leftarrow A^{(s)}} = \psi^{\top} \left(\nu_{B^{(s)} \leftarrow A^{(s)}}^{-1} \lambda_{B^{(s)} \leftarrow A^{(s)}}^{-1} \mathbf{P}_B \mathbf{Q}_A \mathbf{P}_B \right) \psi, \tag{11}$$

perhaps with the addition of an asterisk to one of the sources to indicate that there is a random term involved. If a term is random, it does not contribute to ψ and affects the fixed contribution $\theta_{B^{(s)}\leftarrow A^{(s)}}$ only through the matrix of the quadratic form and its associated scalar. If only $A^{(s)}$ is fixed and $\lambda_{B^{(s)} \leftarrow A^{(s)}}$ is one, $\theta_{B^{(s)} \leftarrow A^{(s)}}$ in (11) simplifies to $\psi^{\top}(\mathbf{Q}_A/\nu_{A^{(s)}})\psi$; that is, the term B has no influence on the fixed contribution.

EMSs for the GRBD in Section 3.2 of Brien et al. Supplement Section E.3 (2023)

Consider the homogeneous allocation model for the GRBD in Section 3.2 of Brien et al. (2023):

$$Mean + Z \qquad | \qquad Mean + B + B:Z + \underline{B:P}. \tag{12}$$

The sets of terms that give rise to poset structures are $\mathcal{F} = \{\text{Mean}(u), B, B:P\}$ and $\mathcal{G} = \{\text{Mean}(t), B, Z, B:Z\}$. Note that only in Supplement Section E, because the initial all-random model is used, is it necessary to distinguish between the Mean term from the units, Mean(u), and the mean term from the treatments, Mean(t). In the homogeneous allocation models, the Mean term from the units is assumed random and that from the treatments is assumed fixed and so there is not the ambiguity that is present here.

Under the all-random model in (1), we have for \mathcal{F} ,

- 1. $\eta_{\text{Mean(u)}} = \sigma_{\text{BP}}^2 + 8\sigma_{\text{B}}^2 + 48\sigma_{\mu(u)}^2$, 2. $\eta_{\text{B}} = \sigma_{\text{BP}}^2 + 8\sigma_{\text{B}}^2$, and 3. $\eta_{\text{BP}} = \sigma_{\text{BP}}^2$;

and for \mathcal{G} ,

1. $\eta_{\mathrm{Mean(t)}} = 2\sigma_{\mathrm{BZ}}^2 + 8\sigma_{\mathrm{B}}^2 + 12\sigma_{\mathrm{Z}}^2 + 48\sigma_{\mu(t)}^2$, 2. $\eta_{\mathrm{B}} = 2\sigma_{\mathrm{BZ}}^2 + 8\sigma_{\mathrm{B}}^2$, 3. $\eta_{\mathrm{Z}} = 2\sigma_{\mathrm{BZ}}^2 + 12\sigma_{\mathrm{Z}}^2$, and 4. $\eta_{\mathrm{BZ}} = 2\sigma_{\mathrm{BZ}}^2$. The fixed terms are the Mean and Z in the set $\mathcal G$ and so σ_{Z}^2 and $\sigma_{\mu(t)}^2$ are set to zero, as is σ_{B}^2 , because it is also in the set $\mathcal F$. Thus, for $\mathcal G$, $\eta_{\mathrm{Mean}} = 2\sigma_{\mathrm{BZ}}^2$ and $\eta_{\mathrm{B}} = \eta_{\mathrm{Z}} = \eta_{\mathrm{BZ}} = 2\sigma_{\mathrm{BZ}}^2$ under the homogeneous allocation model

To form the EMS, all canonical efficiencies are one and so an η_G is added to the η_F with which it is confounded. The fixed contributions $\theta_{\mu(t)}$ and θ_Z are added to the EMS for the Mean and Zinc. The EMS for the one Residual source in Table 4 of Brien et al. (2023) is $\eta_{\rm BP} = \sigma_{\rm BP}^2$.

Supplement Section F Deriving the EMSs for a design that is nonorthogonal, but structure-balanced, except for the inclusion of an identity

term for the treatments

The notation used in Supplement Section D and Supplement Section E is employed here. Thus, \mathcal{F} and \mathcal{G} are the sets of terms for units (recipient) and treatments (allocated) factors in an initial all-random model. \mathcal{P} and \mathcal{Q} are the sets of source projections matrices defining the poset structures on the units and treatments, respectively. Additionally, assume that both sets have an identity term, assumed to be random, that uniquely indexes the observational units and that there are n observational units. Denote these identity terms by F_I in \mathcal{F} and G_I in \mathcal{G} . Suppose that a subset of terms \mathcal{G}^* that does not include G_I can be identified such that (i) the corresponding subset \mathcal{Q}^* of \mathcal{Q} is a poset structure that is structure-balanced in relation to \mathcal{P} and (ii) the two sets of terms \mathcal{F} and \mathcal{G}^* jointly contain all of the terms in the model for homogeneous allocation model, except G_I . Let $\mathcal{F}^* = \mathcal{F} \setminus F_I$.

In the example in Section 5 of Brien et al. (2023), $\mathcal{F} = \{\text{Mean}, \text{T}, \text{E}, \text{T:E}\}\$ and $\mathcal{G} = \{\text{Mean}, \text{T}, \text{P}, \text{T:P}\}\$ and so F_I and G_I are T:E and T:P. Further, if $\mathcal{G}^* = \{\text{Mean}, \text{P}\}$, then \mathcal{Q}^* , based on \mathcal{G}^* , is a poset structure that is structure-balanced in relation to \mathcal{P} . Further, $\mathcal{F} \cup \mathcal{G}^*$ contains all of the terms in the model for the homogeneous allocation model, except T:P.

For the present situation of random identity terms for both units and treatments, the initial all-random model in (1) and the homogeneous allocation model in (8) apply. However, the implications of two identity terms is that $\mathbf{R}_{F_I} = \mathbf{S}_{G_I} = \mathbf{I}_n$, where \mathbf{I}_n is the identity matrix of order n. Consequently, the all-random model in (1) can be rewritten with a modified variance matrix \mathbf{V} that does not involve \mathbf{S}_{G_I} as follows:

$$\psi = \mathbf{0},$$

$$\mathbf{V} = \sum_{F \in \mathcal{F}^*} \sigma_F^2 \mathbf{R}_F + (\sigma_{F_I}^2 + \sigma_{G_I}^2) \mathbf{R}_{F_I} + \sum_{G \in \mathcal{G}^*} \sigma_G^2 \mathbf{S}_G.$$
(13)

Since \mathcal{P} and \mathcal{Q}^* are poset structures, the variance matrix in (13) can be rewritten as follows:

$$\mathbf{V} = \sum_{F \in \mathcal{F}^*} \eta_F \mathbf{P}_F + (\sigma_{F_I}^2 + \sigma_{G_I}^2) \mathbf{P}_{F_I} + \sum_{G \in \mathcal{G}^*} \eta_G \mathbf{Q}_G.$$

Let \mathcal{T} and $\mathcal{T}^{(s)}$ be the sets of fixed terms and sources, respectively, and \mathcal{U} and $\mathcal{U}^{(s)}$ be the sets of random terms and sources, respectively, for the homogeneous allocation model. Then, the homogeneous allocation model for present case is derived from (13) to yield a model similar to that in (8):

$$\psi = \sum_{T \in \mathcal{T}} \mathbf{X}_T \boldsymbol{\tau}_T \quad \text{and} \quad \mathbf{V} = \sum_{U \in \mathcal{F}^* \cap \mathcal{U}} \sigma_U^2 \mathbf{R}_U + (\sigma_{F_I}^2 + \sigma_{G_I}^2) \mathbf{R}_{F_I} + \sum_{U \in \mathcal{G}^* \cap \mathcal{U}} \sigma_U^2 \mathbf{S}_U.$$
(14)

Now this variance matrix is of the same form as that given in (8), except that \mathbf{R}_{F_I} has coefficient $\sigma_{F_I}^2 + \sigma_{G_I}^2$. Consequently, the rules derived in Supplement Section E and summarized in Appendix of Brien et al. (2023) can be used to obtain the EMS, with the proviso that the contribution for F_I ($\sigma_{F_I}^2$) is replaced with $\sigma_{F_I}^2 + \sigma_{G_I}^2$ throughout and η_{G_I} removed.

Note that the EMS remain valid when $G_I^{(s)}$ (T # P in the example) is included in the decomposition, because the subspace of the source $G_I^{(s)}$ is a subspace of the source $F_{I}^{(s)}$ (T # E_{\(\)}), it having canonical efficiency one. Because all contrasts in the subspace of $F_I^{(s)}$ have the same expectation, those corresponding to $G_I^{(s)}$ have the same expectation as $F_I^{(s)}$, viz. $\sigma_{F_I}^2 + \sigma_{G_I}^2$ ($\sigma_{\text{TE}}^2 + \sigma_{\text{TP}}^2$ for the example). Thus, when there is an identity term G_I in $\mathcal G$ and (i) two sets of sources, $\mathcal P$ and $\mathcal Q^*$, can be identified

Thus, when there is an identity term G_I in \mathcal{G} and (i) two sets of sources, \mathcal{P} and \mathcal{Q}^* , can be identified such that one is structure-balanced in relation to the other, yet there is a source for all terms in the homogeneous allocation model other than G_I , and (ii) the source for G_I has a subspace that is orthogonally confounded with the source for F_I , then EMSs for the combined decomposition of \mathcal{P} and \mathcal{Q} can be obtained using the combined decomposition of \mathcal{P} and \mathcal{Q}^* by including the sum of the variance components for G_I and F_I as the random EMS contribution for F_I .

Supplement Section F.1 EMSs for the YSD in Section 5 of Brien et al. (2023)

Consider the homogeneous allocation model for the YSD in Section 5 of Brien et al. (2023):

$$Mean + E + P \qquad Mean + T + T:P + T:E. \tag{15}$$

The sets of terms that give rise to poset structures are $\mathcal{F} = \{\text{Mean}, \text{T}, \text{E}, \text{T:E}\}\$ and $\mathcal{G} = \{\text{Mean}, \text{T}, \text{P}, \text{T:P}\}\$. However, the poset structure for \mathcal{G} is not structure balanced in relation to that for \mathcal{F} . The set of terms \mathcal{G} is replaced with $\mathcal{G}^* = \{\text{Mean}, P\}$. Now, (i) the poset structure for \mathcal{G}^* is structure balanced in relation to that for \mathcal{F} and (ii) \mathcal{G}^* and \mathcal{F} incorporate the same terms as the original poset structures, except for T:P.

Under the all-random model in (13), we have for \mathcal{F} ,

- 1. $\eta_{\text{Mean(u)}} = (\sigma_{\text{TE}}^2 + \sigma_{\text{TP}}^2) + 8\sigma_{\text{T}}^2 + 7\sigma_{\text{E}}^2 + 56\sigma_{\mu(u)}^2,$ 2. $\eta_{\text{T}} = (\sigma_{\text{TE}}^2 + \sigma_{\text{TP}}^2) + 8\sigma_{\text{T}}^2,$ 3. $\eta_{\text{E}} = (\sigma_{\text{TE}}^2 + \sigma_{\text{TP}}^2) + 7\sigma_{\text{E}}^2,$ and 4. $\eta_{\text{TE}} = (\sigma_{\text{TE}}^2 + \sigma_{\text{TP}}^2);$ and for \mathcal{G}^* ,

- 1. $\eta_{\text{Mean(t)}} = 7\sigma_{\text{P}}^2 + 56\sigma_{\mu(t)}^2$,
- 2. $\eta_{\rm P} = 7\sigma_{\rm P}^2$, and

The fixed terms are E in the set \mathcal{F} and the Mean and P in the set \mathcal{G}^* .

For \mathcal{F} , $\sigma_{\rm E}^2$ is set to zero and so

- 1. $\eta_{\text{Mean(u)}} = (\sigma_{\text{TE}}^2 + \sigma_{\text{TP}}^2) + 8\sigma_{\text{T}}^2 + 56\sigma_{\mu(\text{u})}^2$
- 2. $\eta_{\rm T} = (\sigma_{\rm TE}^2 + \sigma_{\rm TP}^2) + 8\sigma_{\rm T}^2,$ 3. $\eta_{\rm E} = (\sigma_{\rm TE}^2 + \sigma_{\rm TP}^2),$ and 4. $\eta_{\rm TE} = (\sigma_{\rm TE}^2 + \sigma_{\rm TP}^2);$

For \mathcal{G} , $\sigma_{\rm P}^2$ and $\sigma_{\mu(t)}^2$ are set to zero and so no variance terms remain. Only the Mean(t) and P remain as treatments terms and these are fixed.

There are two fixed treatment sources: Mean(t) and P. The fixed contribution to the EMS for the treatments Mean source is simply $\theta_{\text{Mean(t)}}$. However, the fixed source P is confounded with the fixed, units source Evaluations and the random, units source T # E. Thus, there are two EMS sources for P, for both of which P makes fixed contributions that are denoted by $\theta_{E\leftarrow P}$ and $\theta_{TE^*\leftarrow P}$.

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