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This document describes how to use functions from the R (R Core Team, 2023) packages dae (Brien, 2023b) and odw (Butler, 2022) to produce layouts for experiments and to check some of their properties. An introduction to the approach used in the document is given by Brien et al. (2023).

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Topic 0 Introduction for the workshop and the software to be used

0.1 Installed software

The following software should be installed on your computer:

- R (4.1.x or later preferable)
- RStudio
- Packages (you can check the version using the packageVersion function.)
 - dae (Version 3.2-15 or later from CRAN (https://cran.at.r-project.org/package=dae/) or http: //chris.brien.name/rpackages)
 - odw (Version 2.1.4) from https://mmade.org/optimaldesign/)

0.2 Programme

0.2.1 Day 1

12:00–13:00: 1. Concepts in experimental design: Experiment description, randomization by permutation based on the nesting an crossing, canonical analysis of a design and formulating allocation-based mixed models for orthogonal designs, including those with multiple errors.

13:00-13:45: Lunch.

13:45-14:30 1. (cont'd) Orthogonal experimental design in R: using dae to generate orthogonal designs for experiments.

14:30–15:30: 2. Nonorthogonal experimental design: Using the concepts in the context of balanced and unbalanced experiments; canonical efficiency factors and the alphabet of efficiency measures; the effects of covariates and missing observations.

15:30-16:00: Afternoon tea.

16:00-17:00: 2. (cont'd) Nonorthogonal experimental design in R: using dae and odw to produce nonorthogonal designs for experiments.

0.2.2 Day 2

13:00–14:00: 3. Miscellaneous topics in experimental design: systematic allocation and pseudoreplication, block-treatment interaction, designing animal grazing experiments, and nested factorials.

14:00-15:00: 3. (cont'd) Miscellaneous experimental design topics in R: further use of dae and odw.

15:00–15:15: Afternoon tea.

0.3 Packages and the functions to be used

0.3.1 dae

The package dae provides functions useful in the design and anova of experiments (Brien, 2023b). There are around 90 functions that fall into the following categories and those that will be used in this course are described:

1. Data

BIBDWheat.dat Data for a balanced incomplete block experiment.

Cabinet1.des A design for one of the growth cabinets in an experiment with 50 lines and 4 harvests.

Casuarina.dat Data for an experiment with rows and columns from Williams et al. (2002).

Exp249.munit.des Systematic, main-unit design for an experiment to be run in a greenhouse.

Fac4Proc.dat Data for a 2⁴ factorial experiment.

LatticeSquare_t49.des A Lattice square design for 49 treatments.

McIntyreTMV.dat The design and data from McIntyre (1955) two-phase experiment.

Oats.dat Data for an experiment to investigate nitrogen response of 3 oats varieties from Yates (1937).

Sensory3Phase.dat Data for the three-phase sensory evaluation experiment in Brien and Payne (1999).

Sensory3PhaseShort.dat Data for the three-phase sensory evaluation experiment in Brien and Payne (1999), but with short factor names.

SPLGrass.dat Data for an experiment to investigate the effects of grazing patterns on pasture composition.

2. Factor manipulation functions

fac.gen: Generate all combinations of several factors and, optionally, replicate them.

fac.recast: Recasts a factor by modifying the values in the factor vector and/or the levels attribute, possibly combining some levels into a single level.

fac.uselogical: Forms a two-level factor from a logical object.

fac.combine: Combines several factors into one.

fac.divide: Divides a factor into several separate factors.

fac.multinested: Creates several factors, one for each level of a nesting fac and each of whose values are either generated within those of the level of nesting fac or using the values of a nested fac.

fac.nested: Creates a factor, the nested factor, whose values are generated within those of a nesting factor.

3. Design functions

designAnatomy: Given the layout for a design, obtain its anatomy via the canonical analysis of its projectors to show the confounding and aliasing inherent in the design.

designLatinSqrSys: Generate a systematic plan for a Latin Square design.

designBlocksGGPlot: Adds block boundaries to a plot produced by designGGPlot.

designGGPlot: A graphical representation of an experimental design based on labels stored in a data.frame using ggplot2.

designRandomize: Takes a systematic design and randomizes it according to the nesting (and crossing) relationships between the recipient(unit) factors for the randomization.

no.reps: Computes the number of replicates for an experiment.

summary.pcanon: Summarizes the anatomy of a design, being the decomposition of the sample space based on its canonical analysis, as produced by designAnatomy. The table produced includes the degrees of freedom and summary statistics of the canonical efficiency factors.

efficiencies.pcanon: Extracts the canonical efficiency factors from a **pcanon.object** produced by **designation**.

- 4. ANOVA functions
- 5. Matrix functions
- 6. Projector and canonical efficiency functions
- 7. Miscellaneous functions.

0.3.2 odw

The package odw generates optimal experimental designs (Butler, 2022). It does this based on an *anticipated* mixed model and obtains a design that minimizes the average variance of pairwise differences (AVPD). It more than 30 functions; the two primary functions for this course are as follows:

odw: Generates optimal designs for comparative experiments under a general linear mixed model.

odw.options: Sets or displays various options that affect the behaviour of odw.

Documentation for each of these functions is available from the user manual for the relevant package. In general this can be found in the doc subdirectory of the directory in which the package is installed or from the help for the function once the package has been installed. For the latter, to see the manual for package foo, enter help(package="foo") and click on the link User guides, package vignettes and other documentation.

For dae, the manual is available via vignette("dae-manual", package="dae") and there are some notes that show how to use the functions that are available via vignette("DesignNotes", package="dae").

0.4 Notation used for mixed models

The general form for a mixed model is:

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u} + \mathbf{e},$$

where β is the vector of fixed parameters, \mathbf{u} is the vector of random effects, and \mathbf{e} is the vector of residuals corresponding to each observation. The matrices \mathbf{X} and \mathbf{Z} are the design matrices for the fixed and random effects, respectively. Generally, \mathbf{X} and $\boldsymbol{\beta}$ are conformably partitioned so that there is a separate submatrix and subvector for each fixed term. Similarly, \mathbf{Z} and \mathbf{u} are conformably partitioned according to the random terms.

A mixed model is expressed in symbolic form by list of the fixed terms, followed by a '|', and then a list of the random terms. Terms contributing to the residual variation are underlined.

Topic 1 Orthogonal experimental design in R

This class of experiments covers the orthogonal standard or textbook experiments, those that involve a single randomization, in the sense that the randomization can be achieved with a single permutation. Hence there will be two sets of factors, or tiers, an allocated set that is allocated to a recipient set. These two sets are also referred to as the unit and treatment factors, respectively.

Firstly, initialize by loading the dae library. Also check the version that is loaded.

```
library(dae)
packageVersion("dae")
```

1.1 Two potential designs for a 5×5 grid of plots

Suppose an experiment to investigate five treatments is to be conducted on 25 plots, the 25 plots being arranged in a 5×5 grid. Two possible designs are a randomized complete-block design (RCBD) or a Latin square design (LSqD). The factor-allocation diagram (Brien et al., 2023) for the RCBD is in Figure 1 and that for the LSqD is in Figure 2.

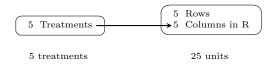


Figure 1: Factor-allocation diagram for an RCBD: treatments are allocated to units; the arrow indicates that the factor Treatments is randomized to Columns; Columns in R indicates that the Columns are considered to be nested within Rows for this randomization; R = Rows.

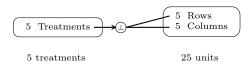


Figure 2: Factor-allocation diagram for an LSqD: treatments are allocated to units; the arrow indicates that the allocation is randomized; the '①' at the end of the arrow indicates that an orthogonal design is used; the two lines from '①' indicates that the Treatments are allocated to the combinations of Rows and Columns using the design.

1.1.1 Produce the randomized layout for an RCBD

Use designRandomize to randomize the treatments according to an RCBD. The arguments to designRandomize that need to be set are (i) allocated, (ii) recipient, (iii) nested.recipients, and optionally, (iv) seed. The allocated factors are also referred to as treatment factors and the recipient factors as block or unit factors. A systematic arrangement of the allocated factors, corresponding to the values of the recipient factors, needs to be supplied and there are a number of ways of doing this.

Our general approach is to set up a systematic design in a data.frame to separate this aspect of constructing a design from the randomizing of a design. The naming convention used is that the name of the data.frame containing the systematic design ends in .sys. This data.frame should contain the values of both the recipient and the allocated factors, the latter in a systematic order that is appropriate for the design. The dae function fac.gen will be used to generate the values of the recipient factors in standard order and often will also be used to generate the values of the allocated factors.

Then the allocated and recipient factors are supplied to designRandomize by subsetting the columns of the data.frames to just the appropriate factors for each argument. Note that the Treatments could also be supplied as a factor and the recipient factors can be specified directly to the recipient argument as a list, e.g. list(Rows=b, Columns=t). A data.frame containing the recipient and randomized allocated factors is produced and, in these notes, the name for the data.frame with the randomized layout will end in .lay.

The randomization is controlled by nested.recipients: nested recipient factors are permuted within those factors that nest them. Only the nesting is specified: it is assumed that that if two factors are not nested then they must be crossed. So for this example, given that the nested.recipients has Columns nested within Rows, the randomized layout is obtained by permuting (i) Rows and (ii) Columns within Rows. Then the permuted Rows and Columns and the systematic Treatments are sorted so that Rows and Columns are in standard order.

In this example, the allocated factor is Treatments, with 5 levels, and the recipient factors are Rows and Columns, both with 5 levels. Suppose that Rows are to form the blocks.

Use the following R code to obtain and display the layout:

```
b <- 5
t <- 5
#'## Set up a systematic design
RCBD.sys <- cbind(fac.gen(generate = list(Rows=b, Columns=t)),</pre>
                  fac.gen(generate = list(Treatments = LETTERS[1:t]),
                          times = b))
#'## Obtain the randomized layout
                                              = RCBD.sys["Treatments"],
RCBD.lay <- designRandomize(allocated</pre>
                            recipient
                                              = RCBD.sys[c("Rows", "Columns")],
                            nested.recipients = list(Columns = "Rows"),
                                               = 1134)
#'## Output the layout
RCBD.lav
#'## Plot the layout
designGGPlot(RCBD.lay, labels = "Treatments", cellalpha = 0.75,
             blockdefinition = cbind(1,t))
```

The function fac.gen is from the package dae and generates the factors in the list in standard order with the specified numbers of levels or the levels in supplied character or numeric vectors. The seed is specified to ensure that the same design is produced whenever designRandomize is run with these argument settings.

1.1.2 Produce the randomized layout for an LSqD

Use designRandomize to randomize the treatments according to an LSqD, having obtained the systematic design using fac.gen and designLatinSqrSys. For this design, Rows and Columns are crossed; there are no nested factors. Consequently, the nested.recipients argument is omitted so that designRandomize assumes that the recipient factors are crossed. The layout can be obtained using the following R code:

The function fac.gen is from the package dae and generates the factors in the list in standard order with the specified numbers of levels or the levels in supplied character or numeric vectors. The seed is specified to ensure that the same design is produced whenever designRandomize is run with these arguments.

1.1.3 Check the properties of the designs

The properties of the designs can be investigated using designAnatomy.

Because these experiments involve a single randomization, they are two-tiered. That is, there are just two sets of factors involved in the randomization. As we have seen, the first set of factors is the set of allocated (treatment) factors and the second set is the set of recipient (unit) factors. Further there will be a set of projectors associated with each tier and designAnatomy is used to do an eigenanalysis of the relationships between the two sets of projectors. The sets of projectors are specified to designAnatomy via model formulae, the formula for the recipient factors coming first in the list for formulae.

For both the RCBD and LSqD the two sets of factors are (i) {Rows, Columns} and (ii) {Treatments}. What differs between the two designs is the nesting/crossing relationship between Rows and Columns and this will be expressed in the formulae.

Use the commands given below to produce the anatomies (like skeleton-anova tables but produced from an eigenanalysis) for the RCBD and LSqD that have been obtained. Note that the 'Mean' source has been omitted from these tables, but can be included using grandMean = TRUE when calling designAnatomy.

Get the mixed-model terms for the analysis by rerunning the summary function with the labels.swap argument set to TRUE.

```
#'## Term-based anatomy for the RCBD
summary(RCBD.canon, labels.swap = TRUE)
#'## Term-based anatomy for the LSqD
summary(LSqD.canon, labels.swap = TRUE)
```

1.1.4 Questions

- 1. What is the advantage of specifying a seed in designRandomize?
- 2. With what unit source is Treatments confounded in these designs and what is the difference between the designs in the interpretation of these units sources?
- 3. What would determine which of these two designs is used for a particular experiment?

1.2 Split-unit from Kaps and Lamberson (2004)

Kaps and Lamberson (2004, p.344) describes a split-unit experiment that investigates the effects of four different pasture treatments and two mineral supplements on the milk yield of cows. The Pasture treatments are assigned to the main units formed from large plots using a randomized complete-block design with 3 blocks and the Mineral supplements are randomly assigned to the subunits (smaller plots) in each main unit. The factor-allocation diagram for the experiment is in Figure 3.

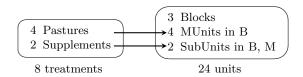


Figure 3: Factor-allocation diagram for a split-plot design: treatments are allocated to units; the arrows indicates that the factors Pastures and Supplements are randomized to MUnits and SubUnits, respectively; MUnits in B indicates that the MUnits are considered to be nested within Blocks for this randomization; SubUnits in B, M indicates that the SubUnits are considered to be nested within Blocks and MUnits for this randomization; B = Blocks, M = MUnits

1.2.1 Produce the randomized experimental layout

Use fac.gen to obtain a systematic layout and then designRandomize to obtain a randomized layout for this experiment. Check the properties of the design, as illustrated in the following R code:

```
#'## Set up the systematic design
Milk.sys <- cbind(fac.gen(list(Blocks=3, MUnits=4, SubUnits=2)),</pre>
                  fac.gen(list(Pastures=LETTERS[1:4],
                               Supplements=2), times=3))
#'## Obtain the randomized layout
Milk.lay <- designRandomize(allocated</pre>
                                               = Milk.sys[c("Pastures", "Supplements")],
                                               = Milk.sys[c("Blocks", "MUnits", "SubUnits")],
                            recipient
                            nested.recipients = list(MUnits = "Blocks",
                                                      SubUnits = c("MUnits", "Blocks")),
                            seed
                                               = 580523)
#'## Plot design produced, first combining Pastures and Supplements so plot on 2 lines per cell
Milk.lay$Treatments <- with(Milk.lay, fac.combine(list(Pastures, Supplements),
                                                   combine.levels = TRUE, sep = "\n")
designGGPlot(Milk.lay, labels = "Treatments",
             row.factors = c("Blocks", "MUnits"), column.factors = "SubUnits",
             cellfillcolour.column = "Pastures", cellalpha = 0.75,
             blockdefinition = rbind(c(1,2)))
#'## Check its properties
Milk.canon <- designAnatomy(formulae = list(unit = ~ Blocks/MUnits/SubUnits,
                                             trt = ~ Pastures*Supplements),
                            data
                                     = Milk.lay)
summary(Milk.canon, which.criteria = c("aeff", "order"))
```

1.2.2 Questions

- 1. In what sense does this design involve a single randomization?
- 2. What is the initial allocated mixed model for this design? Is it equivalent to a randomization model?
- 3. A factorial RCBD would involve randomizing the $3 \times 4 = 12$ treatments to the 12 subunits within each block. What is the effect on treatment comparisons of using the split-unit design as compared to a factorial RCBD?

1.3 Split-unit design with criss-cross design on the subunits from Mead (1990)

Mead (1990, Example 14.1) describes an experiment to investigate the effects of grazing patterns on pasture composition. It is available in dae as SPLGrass.dat.

The design for the experiment is a split-unit design with a criss-cross or strip-unit design on the subunits. The main units are arranged in 3 Rows \times 3 Columns. Each main unit is split into 2 SubRows x 2 SubColumns.

The factor Period, with levels 3, 9 and 18 days, is assigned to the main units using a 3×3 Latin square. The two-level factors Spring and Summer are assigned to subunits using a criss-cross or strip-unit design that is randomized within each main unit; Spring is randomized to SubRows and Summer is randomized to SubColumns. The levels of each of Spring and Summer are two different grazing patterns in its season. The response variable is Main. Grass.

Use data(SPLGrass.dat) to load the design (and the data). Plot the design: create a factor Treats by combining the factors Period, Spring and Summer using fac.combine with the argument combine.levels set to TRUE and then use designGGPlot with cellfillcolour.column set to "Period" and cellalpha set to about 0.4. Also, investigate the properties of the design using designAnatomy.

1.3.1 Questions

- 1. Describe the confounding that is inherent in this design.
- 2. Draw a factor-allocation diagram for this experiment.
- 3. What is the initial allocated mixed model for this design?

1.4 A design for the petrol additives experiment

Box et al. (2005, Section 4.4) describes a car emission experiment that investigates 4 additives. It involves 4 cars being driven by 4 drivers. Here we investigate increasing the replication by repeating the experiment on two occasions. Suppose that the 4 cars differ between occasions.

In a data.frame called LSRepeat.sys, generate a systematic design using two 4×4 Latin squares for allocating the 4 Additives to the 32 tests, being the combinations of the 2 Occasions x 4 Drivers x 4 Cars. Make sure that a Latin square is used for each Occasion.

Now a comparison is made of two different ways of randomizing this design. Firstly, we retain the factors Occasions, Drivers and Cars from the systematic design. The factor-allocation diagram is in Figure 4.

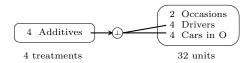


Figure 4: Factor-allocation diagram for repeated LSqDs: treatments are allocated to units; the arrow indicates that the allocation is randomized; the '①' at the end of the arrow indicates that an orthogonal design is used; the two lines from '①' indicates that the Additives are allocated to the combinations of Drivers and Cars within Occasions using the design.

```
#'## Obtain a randomized layout with Cars nested within Occasions
LSRepeat2b.lay <- designRandomize(allocated
                                                    = LSRepeat.sys["Additives"],
                                  recipient
                                                    = LSRepeat.sys[c("Occasions", "Drivers",
                                                                      "Cars")],
                                  nested.recipients = list(Cars="Occasions"),
                                                    = 194)
#'## Plot the layout
designGGPlot(LSRepeat2b.lay, row.factors = "Cars", column.factors = c("Occasions", "Drivers"),
             labels = "Additives", cellalpha = 0.75, blockdefinition = cbind(4,4))
#'## Get the anatomy of the layout
LSRepeat2b.canon <- designAnatomy(formulae = list(unit = ~ (Occasions/Cars)*Drivers,
                                                  trt = ~ Additives),
                                  data
                                           = LSRepeat2b.lay)
```

summary(LSRepeat2b.canon)

Secondly, we use only Drivers and Cars to do the randomization, but still attempt to include Occasions in the analysis. The new factor-allocation diagram is in Figure 5.

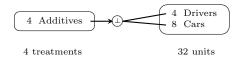


Figure 5: Factor-allocation diagram for repeated LSqDs: treatments are allocated to units; the arrow indicates that the allocation is randomized; the '①' at the end of the arrow indicates that an orthogonal design is used; the two lines from '①' indicates that the Additives are allocated to the combinations of Drivers and Cars using the design.

```
#'## Obtain a randomized layout
LSRepeat.D8.sys <- LSRepeat.sys
LSRepeat.D8.sys$Cars <- with(LSRepeat.D8.sys, fac.combine(list(Occasions, Cars)))
LSRepeat.D8.sys <- with(LSRepeat.D8.sys, LSRepeat.D8.sys[order(Drivers,Cars),])
LSRepeat2b.D8.lay <- designRandomize(allocated = LSRepeat.D8.sys["Additives"],
                                    recipient = LSRepeat.D8.sys[c("Drivers", "Cars")],
                                               = 149)
                                    seed
#'## Plot the layout
designGGPlot(LSRepeat2b.D8.lay, row.factors = "Drivers", column.factors = "Cars",
             labels = "Additives", cellfillcolour.column = "Additives",
             cellalpha = 0.75, blockdefinition = cbind(4,8))
#'## Get the anatomy of the layout
LSRepeat2.D8.canon <- designAnatomy(formulae = list(unit = ~ Drivers*Cars,
                                                    trt = ~ Additives),
                                    data
                                             = LSRepeat2b.D8.lay)
summary(LSRepeat2.D8.canon)
#'## Add Occasions to the analysis
LSRepeat2b.D8.lay$Occasions <- fac.recast(LSRepeat2b.D8.lay$Cars,
                                          newlevels = rep(1:2, each=4))
LSRepeat2b.D8.lay
LSRepeat2b.D8.canon <- designAnatomy(formulae = list(unit = ~ (Occasions + Cars)*Drivers,
                                                     trt = ~ Additives),
                                    data
                                              = LSRepeat2b.D8.lay)
summary(LSRepeat2b.D8.canon)
```

1.4.1 Questions

- 1. The Residual degrees of freedom for a single 4×4 Latin square are 6. Has the use of two 4×4 Latin squares had the desired effect of increasing the Residual df? What other advantage does the use of two Latin squares have over the use of a single Latin square?
- 2. What is the difference between the two randomizations?
- 3. How do the two anatomies that include Occasions differ?
- 4. What effect does including Occasions#Drivers have on the anatomy?

Topic 2 Nonorthogonal experimental design in R

This class of experiments covers the nonorthogonal standard or textbook experiments and these experiments must be single phase because they involve a single randomization.

Firstly, initialize by loading the libraries that will be used and setting the output width.

```
library(dae, quietly = TRUE)
library(odw)
packageVersion("odw")
options(width=100)
```

2.1 Twenty treatments in an alpha design

The following table gives an alpha design for 20 treatments, taken from Williams et al. (2002, p.128). The design has 3 replicates, each of which contains 5 blocks of 4 plots. It is a resolved design in that each replicate contains a complete set of the treatments.

Table 1: Unrandomized alpha design for 20 treatments

							Re	eplica	te							
			1					2						3		
Block	1	2	3	4	5	1	2	3	4	5		1	2	3	4	5
	1	2	3	4	5	1	2	3	4	5	-	1	2	3	4	5
	6	7	8	9	10	7	8	9	10	6		8	9	10	6	7
	11	12	13	14	15	13	14	15	11	12		15	11	12	13	14
	16	17	18	19	20	19	20	16	17	18		17	18	19	20	16

The factor-allocation diagram for the experiment is in Figure 6.

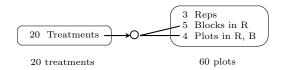


Figure 6: Factor-allocation diagram for the alpha design: treatments are allocated to units; the arrow indicates that the allocation is randomized; the 'O' at the end of the arrow indicates that a nonorthogonal design is used; the two lines from 'O' indicate that the Treatments are allocated to the combinations of Blocks and Plots using the design; Blocks in R indicates that the Blocks are considered to be nested within Reps for this randomization; Plots in R, B indicates that the Plots are considered to be nested within Reps and Blocks for this randomization; R = Reps; B = Blocks.

2.1.1 Produce the randomized layout for the alpha design and check its properties

Use designRandomize to obtain the randomized layout and designAnatomy to check its properties.

The summary table shows us a number of summary statistics calculated from the canonical efficiency factors. They are:

aefficiency: the harmonic mean of the nonzero canonical efficiency factors.

mefficiency: the mean of the nonzero canonical efficiency factors.

eefficiency: the minimum of the nonzero canonical efficiency factors.

sefficiency: the variance of the nonzero canonical efficiency factors.

xefficiency: the maximum of the nonzero canonical efficiency factors.

order: the order of balance and is the number of unique nonzero canonical efficiency factors.

dforthog: the number of canonical efficiency factors that are equal to one.

For this example it can be seen that (i) an average 74.47%, as measured by the harmonic mean, or 78.95%, as measured by the arithmetic mean, of the information about Treats is confounded with the differences between plots within the reps-blocks combinations and (ii) there are 3 different efficiency factors associated with the 19 Treats degrees of freedom estimated from Plots[Reps:Blocks], the smallest of which is 0.5833 and 7 of which are one. In this case, where the treatments are equally replicated, it can be concluded that the mean variance of a normalized treatment contrast is inversely proportional to the harmonic mean of the canonical efficiency factors (A), that is, to 0.7447. In particular, AVPD = 2/(rA).

```
AVPD <- designAmeasures(mat.Vpredicts(target = ~ Treats - 1,
	fixed = ~ Reps/Blocks,
	design = alpha.lay))[[1]]
Aeff <- summary(alpha.canon, which.criteria = "aeff")$decomp$aefficiency[3]
(measures <- c(AVPD, Aeff, 2/(3*Aeff)))
```

Get the mixed-model terms for the analysis by rerunning the summary function with the labels.swap argument set to TRUE.

```
#'## Obtain the terms for the design
summary(alpha.canon, which.criteria = "all", labels.swap = TRUE)
```

2.1.2 Questions

- 1. What is the randomization-based mixed model for this experiment?
- 2. In a mixed-model analysis, which unit terms might you fit as fixed terms? Why?

2.2 Balanced incomplete-block design from Joshi (1987)

Joshi (1987) gives an experiment to investigate six varieties of wheat that employs a balanced incomplete-block design with 10 blocks, each consisting of three plots. The factor-allocation diagram for the experiment is in Figure 7.

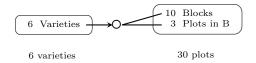


Figure 7: Factor-allocation diagram for the balanced incomplete-block design: treatments are allocated to units; the arrow indicates that the allocation is randomized; the 'O' at the end of the arrow indicates that a nonorthogonal design is used; the two lines from 'O' indicates that the Varieties are allocated to the combinations of Blocks and Plots using the design; Plots in B indicates that the Plots are considered to be nested within Blocks for this randomization; B = Blocks.

2.2.1 Load the design and check its of the design

Use the following R code to input the data for the experiment and check its properties.

From this it is clear that 80% of the information about Varieties is available from the Plots[Blocks] source; that is, 80% of the Varieties information is confounded with differences between plots within blocks. Of course, the remaining 20% is confounded with Blocks.

Calculate the AVPD and check that AVPD = 2/(rA)

2.2.2 What if two observations are missing?

Set the two observations that are not the Control to missing and obtain the anatomy The greatest effect is surprisingly on the comparison between the Control and New.

2.2.3 Questions

- 1. What is the value of xefficiency for Varieties when confounded with Plots[Blocks] for the original design? Why?
- 2. How many nonzero eigenvalues does $\mathbf{Q}_{V}\mathbf{Q}_{BP}\mathbf{Q}_{V}$ have?
- 3. What is the effect of the missing values on the efficiency for Varieties when confounded with Plots[Blocks]?

2.3 A design with rows and columns for a Casuarina trial

Williams et al. (2002, p.144) provide an example of a tree experiment that investigated differences between 60 provenances of a species of Casuarina tree, these provenances coming from 18 countries; the trees were inoculated prior to planting at two different times. The design used was a split-unit design comprised of four rectangles each of six rows by ten columns; the rectangles are located next to each other so that they are contiguous along the rows. The two inoculation times were randomized to the rectangles (main units). The provenances were randomized to the subunits using a resolved, latinized, row-column design, the rectangles forming replicates of the Provenances. The latinization was by columns and was necessary because differences between Columns (across Reps) was anticipated; it served to avoid multiple occurrences of a provenance in a column. At 30 months, diameter at breast height (Dbh) was measured.

The factor-allocation diagram for the experiment is in Figure 8.

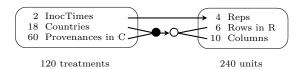


Figure 8: Factor-allocation diagram for the balanced lattice design: treatments are allocated to units; the arrows indicates that the allocations are randomized; the two lines leading to the '•' indicate that it is is the combinations of Countries and Provenances that is allocated; the 'O' at the end of the lower arrow indicates that a nonorthogonal design is used; the two lines from 'O' indicates that the Countries and Provenances are allocated to the combinations of Rows and Columns using the design; Rows in B indicates that the Rows are considered to be nested within Reps for this randomization; R = Reps.

2.3.1 Input the design and check the properties of the design

Use the following R code to input the design and check its properties.

Firstly, note that designAnatomy has automatically detected that Provenances is nested within Countries, even though Provenances has 60 unique levels: the sources for these two terms are Countries and Provenances [Countries] and these have 17 and 42 degrees of freedom when estimated from Rows # Columns [Reps], respectively. The total of these degrees of freedom is 59, one less than the number of Provenances, as expected.

Secondly, the partial aliasing evident in this design reflects a lack of (structure) balance between the treatment sources within each units source. This is an undesirable, but unavoidable, feature of the design for this experiment.

2.3.2 Questions

- 1. What is it about the design that makes it resolved for Provenances?
- 2. What is the disadvantage of allocating InocTimes to Reps?

2.4 A resolved design for the wheat experiment that is near-A-optimal under a mixed model

Gilmour et al. (1995) provides an example of a wheat experiment for 25 Varieties in which a balanced lattice square design was employed, it being a resolved row-column design.

The factor-allocation diagram for the experiment is in Figure 9.

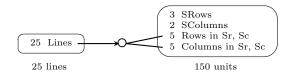


Figure 9: Factor-allocation diagram for the balanced lattice square design: treatments are allocated to units; the arrows indicates that the allocations are randomized; the 'O' at the end of the lower arrow indicates that a nonorthogonal design is used; the two lines from 'O' indicates that the Lines are allocated to the combinations of Rows and Columns using the design; Rows (Columns) in Sr, Sc indicates that the Rows (Columns) are considered to be nested within SRows and SColumns for this randomization; Sr = S(uper)Rows; Sc = S(uper)Columns.

In the lectures it was stated that, while the design is optimal for a fixed model, it is not optimal for a mixed model. In this exercise, a search will be made for a resolved design that is near-A-optimal under a mixed model.

2.4.1 Input the design and check the properties of the design

Use the following R code to input and extract the design, plot it and check its properties. The R package asremlPlus Brien (2023a) can be used to access the data set or it is available in an rda data file. Because we are going to use the design to produce a new design for another experiment, we rerandomize the design using the randomization appropriate to the balanced lattice square design. Being a valid randomization in that it corresponds to the randomization model, the properties of the design will be unchanged.

```
#'## Get the design
library(asremlPlus)
data(Wheat.dat)
latt.lay <- cbind(fac.gen(list(SRows = 2, Rows = 5, SColumns = 3, Columns = 5)),</pre>
                  Wheat.dat["Variety"])
#'## Rerandomize the design for a new experiment
latt.lay <- designRandomize(allocated = latt.lay["Variety"],</pre>
                             recipient = latt.lay[c("SRows", "Rows", "SColumns", "Columns")],
                             nested.recipients = list(Rows = "SRows",
                                                       Columns = "SColumns"),
                             seed = 63146)
#'## Add row and column factors that have a unique level for each row and each column (needed for ar1)
latt.lay <- cbind(fac.gen(list(ARows = 10, AColumns = 15)),latt.lay)</pre>
#'## Plot the design
#+ "LattDesign"
library(scales)
cell.colours <- hue_pal()(25)</pre>
designGGPlot(latt.lay, labels = "Variety",
             row.factors = c("SRows", "Rows"), column.factors = c("SColumns", "Columns"),
             colour.values = cell.colours, cellalpha = 0.75, size = 6,
             blockdefinition = cbind(5,5))
#'## Check the properties of the design
latt.canon <- designAnatomy(formulae = list(units = ~ (SRows:SColumns)/(Rows*Columns),</pre>
```

2.4.2 Search for a near-A-optimal design

Use odw to search for a near-A-optimal design under a mixed model for a crossed row-column design with autocorrelations, as opposed to a nested row-column design with independent errors. In this case the "tabu+rw" search method is to be used. Further, the odw options are to be set to values that I have found by trail-and-error to be successful. The options are

P: the probability of accepting a non-improving design; the default is P=0.005.

localSearch: the number of steps in the random walk local search strategy of the "tabu+rw" search option; the default is 10000.

tabuStop: if the number of consecutive tabu loops with no change in the objective function exceeds tabuStop, then tabu optimization terminates (the default is 4).

```
#'## Set odw options
maxit <- 25
search <- "tabu+rw"</pre>
odw.options(P = 0.10, localSearch = 10000, tabuStop = 100)
#'## Set up the values of the variance components and autocorrelation for the random terms
params \leftarrow c(2.5, 1, 0.1, 0.1, 0.5, 1, 0.6, 0.4)
names(params) <- c("g.sRR", "g.sCC", "g.sRsCR", "g.sRsCC", "g.u", "g.aRaC", "rho.R", "rho.C")</pre>
#'### Set the values in odw
Wheat.start <- odw(fixed
                            = ~ SRows*SColumns + Variety,
                            = ~ SRows:Rows + SColumns:Columns +
                                    SRows:SColumns:(Rows + Columns) + units,
                   residual = " ar1(ARows):ar1(AColumns),
                   permute = ~ Variety, swap = ~ SRows:SColumns,
                   data
                             = latt.lay, start.values = TRUE)
vp.table <- Wheat.start$vparameters.table</pre>
vp.table$Value <- params</pre>
print(vp.table)
#'### Generate the near-A-optimal design
Wheat.odw <- odw(fixed = ~ SRows*SColumns + Variety,
                 random = "SRows:Rows + SColumns:Columns +
                               SRows:SColumns:(Rows + Columns) + units,
                 residual = ~ ar1(ARows):ar1(AColumns),
                 permute = " Variety, swap = " SRows:SColumns,
                 G.param = vp.table, R.param = vp.table,
                 maxit
                           = maxit, search = search,
                 data
                          = latt.lay)
Wheat.lay <- Wheat.odw$design
Wheat.lay$unit <- factor(1:nrow(Wheat.lay))</pre>
```

Given that this is a spatial design, it cannot be now randomized. However, the initial design from which it was derived was randomized, thereby guarding against systematic patterns that might have been artefacts from a systematic input design.

2.4.3 Checking the properties of the designs

Now calculate the A-measure for the original lattice-square design and the near-optimal design produce by odw. Also, produce the anatomy for the near-optimal design.

```
#'### Calculate the A-measure for the lattice square design under a mixed model
latt.lay$unit <- factor(1:nrow(latt.lay))</pre>
(A.latt <- designAmeasures(mat.Vpredicts(target = ~ Variety - 1,
                                         fixed = ~ SRows*SColumns - 1,
                                         random = ~ SRows:Rows + SColumns:Columns +
                                                    SRows:SColumns:(Rows + Columns) + unit - 1,
                                                = as.list(params[1:5]),
                                                 = kronecker(mat.ar1(params["rho.R"], 10),
                                                        mat.ar1(params["rho.C"], 15)),
                                         design = latt.lay))[[1]])
#'### Check the A-value for the near-optimal design
(A.wht <- designAmeasures(mat.Vpredicts(target = ~ Variety - 1,
                                        fixed = ~ SRows*SColumns - 1,
                                        random = ~ SRows:Rows + SColumns:Columns +
                                                   SRows: SColumns: (Rows + Columns) + unit - 1,
                                               = as.list(params[1:5]),
                                        R.
                                               = kronecker(mat.ar1(params["rho.R"], 10),
                                                      mat.ar1(params["rho.C"], 15)),
                                        design = Wheat.lay))[[1]])
(A.wht/A.latt)
#'## Check the properties of the design
Wheat.canon <- designAnatomy(formulae = list(unit = ~ (SRows:SColumns)/(Rows*Columns),
                                             trt = ~ Variety),
                             data
                                      = Wheat.lay)
summary(Wheat.canon, which.criteria = c("aeff", "meff", "xeff", "eeff", "order"))
```

2.4.4 Questions

- 1. How do the AVPD values calculated by odw and those calculated using designAmeasures and mat. Vpredicts compare?
- 2. Summarize the differences between the original balanced lattice square design and the odw design. Is the increased precision of the odw design worthwhile?

Topic 3 Miscellaneous experimental design topics in R

This section includes examples covering the recognition pseudoreplication, grazing trials and the use of nested factorials.

Firstly, initialize by loading the libraries that will be used and setting the output width.

```
library(dae, quietly = TRUE)
library(odw)
packageVersion("odw")
options(width=100)
```

3.1 An animal feeding experiment

Suppose an animal scientist wants to investigate the effect on the weight gain of calves fed four different feed mixtures. They have four pens available for the experiment and they randomize the mixtures to these pens. Each pen has six calves and the weight gain of the each calf is obtained. The factor-allocation diagram for the experiment is in Figure 10.

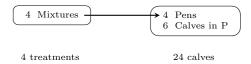


Figure 10: Factor-allocation diagram for the animal feeding experiment: treatments are allocated to calves; the arrow indicates that the factor Mixtures is randomized to Pens; Calves in P indicates that the Calves are nested within Pens; P = Pens.

Obtain the randomized layout for this experiment and check its properties.

```
#'## Set up the systematic design and obtain the layout
Feed.sys <- cbind(fac.gen(list(Pens=4, Calves=6)),</pre>
                  Mixtures = factor(rep(LETTERS[1:4], each=6)))
Feed.lay <- designRandomize(allocated
                                               = Feed.sys["Mixtures"],
                            recipient
                                              = Feed.sys[c("Pens", "Calves")],
                            nested.recipients = list(Calves = "Pens"),
                                               = 872159)
                            seed
#'## plot the design
designGGPlot(Feed.lay, labels = "Mixtures",
             row.factors = "Pens", column.factors = "Calves",
             cellalpha = 0.75, size = 6, blockdefinition = cbind(1,6))
#'## Check its properties
Feed.canon <- designAnatomy(formulae = list(unit = "Pens/Calves,
                                             trt = "Mixtures),
                            data
                                      = Feed.lay)
summary(Feed.canon)
```

3.1.1 Questions

- 1. How is the pseudoreplication involved in this experiment manifested in the anatomy?
- 2. The randomization-based mixed model for the experiment is Mixtures | Pens + Pens:Calves. What difficulties do you anticipate in attempting to fit this model? How could the model be modified so that a fit

can be obtained? Brien and Demétrio (2009) call models formed by removing terms to enable a fit to be achieved 'models of convenience'. What dangers do you foresee in basing conclusions on the fitted model of convenience?

3.2 Grazing experiments

Consider an experiment in which weaners are to be fed on of the three pasture regimens. The pasture regimens are to be assigned to plot in a field using a generalized randomized block design that has four blocks, each with six plots. There are 24 weaners to be assigned one to a plot.

Obtain the randomized layout for a design in which the weaners are divided into four Classes of six Weaners each, based on initial weight, and the Classes are to be assigned to the Blocks and the Weaners within a Class are to be assigned to the Plots within a Block, as described in Kaps and Lamberson (2004, p. 280–1).

```
n <- 24 #number of weaners
b <- 4 #number of blocks
t <- 3 #number of treatments
a <- 2
         #number of weaners per block-treatment
#'### Generate a systematic GRBD for assigning treatments to plots
GRBD.sys <- cbind(fac.gen(list(Blocks = b, Plots = t*a)),</pre>
                  fac.gen(list(Regimens = t, a), times = b))
#'### Randomize treatments to plots
GRBD.lay <- designRandomize(recipient = GRBD.sys[c("Blocks", "Plots")],</pre>
                            allocated = GRBD.sys["Regimens"],
                            nested.recipients = list(Plots = "Blocks"),
                            seed = 158211)
#'### Generate animals factors
Animal.C2B.sys <- fac.gen(list(Classes = b, Weaners = t*a))
#'### Randomize the plots and treatments to animals
GRBD.C2B.lay <- designRandomize(recipient = Animal.C2B.sys,</pre>
                                 allocated = GRBD.lay,
                                 nested.recipients = list(Weaners = "Classes"),
                                 seed = 82572)
#'### Plot the layout
#+ WeanerGRBD_C2B
GRBD.C2B.lay$TreatClass <- with(GRBD.C2B.lay, fac.combine(list(Regimens, Classes),</pre>
                                                           combine.levels = TRUE))
designGGPlot(GRBD.C2B.lay, labels = "TreatClass", label.size = 6,
             title = "Plot of Regimens, Classes",
             row.factors = "Plots", column.factors = "Blocks",
             cellfillcolour.column = "Regimens", cellalpha = 0.75,
             blockdefinition = cbind(t*a, 1))
```

Check the properties of the layout using an anatomy.

Obtain a second randomized layout for the grazing experiment in which two Weaners, one from each of two Classes based on initial weight, are assigned to the two plots within each Block that received the same Regimen, as discussed by Roberts (1975) and Brien and Demétrio (1998). Use GRBD.sys for the field desifn from the first grazing experiment,

```
#'### Generate animals factors, generate pseudofactors and randomize P2
Animal.C2P.sys <- fac.gen(list(Weaners = b*t, Classes = a))
GRBD.lay <- cbind(with(GRBD.lay, GRBD.lay[order(Blocks,Regimens),]),</pre>
                  fac.gen(list(P1 = t, P2 = a), each = b))
GRBD.lay <- designRandomize(allocated = GRBD.lay[c("Plots", "Regimens")],</pre>
                             recipient = GRBD.lay[c("Blocks", "P1", "P2")],
                             nested.recipients = list(P2 = c("Blocks", "P1")),
                             except = c("Blocks", "P1"),
                             seed = 75415)
GRBD.lay <- GRBD.lay[c("Blocks", "Plots", "Regimens")]</pre>
#'### Randomize treatments and plots to animals (using reordered GRBD)
GRBD.C2P.lay <- designRandomize(recipient = Animal.C2P.sys,</pre>
                                 allocated = GRBD.lay,
                                 nested.recipients = list(Weaners = "Classes"),
                                 seed = 158211)
#'### Plot the layout
#+ WeanerGRBD_C2P
GRBD.C2P.lay$TreatClass <- with(GRBD.C2P.lay, fac.combine(list(Regimens, Classes),</pre>
                                                            combine.levels = TRUE))
designGGPlot(GRBD.C2P.lay, labels = "TreatClass", label.size = 6,
             title = "Plot of Regimens, Classes",
             row.factors = "Plots", column.factors = "Blocks",
             cellfillcolour.column = "Regimens", cellalpha = 0.75,
             blockdefinition = cbind(t*a, 1))
#'### Check the properties using an anatomy
GRBD.C2P.canon <- designAnatomy(formula = list(anim = ~ Classes/Weaners,
                                                plot = ~ Blocks/Plots,
                                                trt = ~ Regimens*(Classes+Blocks)),
                                 data = GRBD.C2P.lay)
summary(GRBD.C2P.canon, which.criteria = c("aeff", "order"))
```

3.2.1 Questions

- 1. How is the assignment of Classes to Plots or Blocks achieved in the R code?
- 2. How does the aliasing reported in the output arise in the case in which Classes are randomized to Blocks?
- 3. What advantages does assigning Classes to Plots have over assigning Classes to Blocks? Are there any disadvantages?

3.3 A detergent experiment

Mead et al. (2012) describe an experiment to investigate nine detergent formulations that were compared by washing plates one at a time until they were clean. There were only 3 basins available at any one time and so a BIBD with 12 blocks was used to assign formulations to washing instances. Each basin has a different operator who washed at the same rate at each time of washing. The response is the number of plates washed before the foam disappears.

The treatments involve two bases, four additive amounts and a control; they are:

- 1. base I +three parts additive
- 2. base I + two parts additive
- 3. base I + one part additive
- 4. base I
- 5. base II + three parts additive
- 6. base II + two parts additive
- 7. base II + one part additive
- 8. base II
- 9. Control

The factor-allocation diagram for the experiment is in Figure 11.

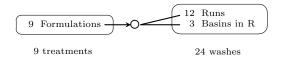


Figure 11: Factor-allocation diagram for the detergent experiment: treatments are allocated to washes; the arrow indicates that the allocation is randomized; the 'O' at the end of the arrow indicates that a nonorthogonal design is used; the two lines from 'O' indicate that the Treatments are allocated to the combinations of Runs and Basins using the design; Basins in R indicates that the Basins are considered to be nested within Runs for this randomization; R = Runs.

The systematic incomplete-block design is shown in Table 2.

Table 2: Systematic balanced incomplete-block design for 9 treatments in blocks of 3

	Basin					
Run	1	2	3			
1	1	2	3			
2	4	5	6			
3	7	8	9			
4	1	4	7			
5	2	5	8			
6	3	6	9			
7	1	5	9			
8	2	6	7			
9	3	4	8			
10	1	6	8			
11	2	4	9			
12	3	5	7			

3.3.1 Produce the randomized layout for the BIBD and check its properties

```
2, 5, 8,
                                          3, 6, 9,
                                          1, 5, 9,
                                          2, 6, 7,
                                          3, 4, 8,
                                          1, 6, 8,
                                         2, 4, 9,
                                         3, 5, 7)))
#'## Randomize the systematic design
BIBD.lay <- designRandomize(allocated
                                             = BIBD.sys["Formulations"],
                           recipient = BIBD.sys[c("Runs", "Basins")],
                           nested.recipients = list(Basins = "Runs"),
                                             = 64686)
#'### Check properties of the BIBD
BIBD.canon <- designAnatomy(formulae = list(wash = ~ Runs/Basins,
                                           form = ~ Formulations),
                            data
                                    = BIBD.lay)
summary(BIBD.canon, which.criteria = c('aeff', 'order'))
```

3.3.2 Add nested factors and check the decomposition using them

3.3.3 Leave out Types and try decomposition with Bases and Additives in both orders

```
BIBD.nest2.canon <- designAnatomy(formulae = list(wash = ~ Runs/Basins, form = ~ Bases*Additives),

data = BIBD.lay)

summary(BIBD.nest2.canon, which.criteria = c('aeff', 'order'))

BIBD.nest2.canon <- designAnatomy(formulae = list(wash = ~ Runs/Basins, form = ~ Additives*Bases),

data = BIBD.lay)

summary(BIBD.nest2.canon, which.criteria = c('aeff', 'order'))
```

3.3.4 Questions

- 1. What do you conclude about the properties of the design both without and with the nested factors?
- 2. What is the effect of removing the Types factor?
- 3. What is the advantage of using nested factors for this experiment?
- 4. Is there any reason to think that a row-column design might be better than a block design for this experiment?

3.4 An experiment to investigate the effects of spraying Sultana grapes

Clingeleffer et al. (1977) report an experiment to investigate the effects of tractor speed and spray pressure on the quality of dried sultanas. The response was the lightness of the dried sultanas which is measured using a Hunterlab D25 L colour difference meter. Lighter sultanas are considered to be of better quality and these will have a higher lightness measurement (L). There were three tractor speeds and two spray pressures resulting in 6 treatment combinations which were applied to 6 plots, each consisting of 12 vines, using a randomized complete-block design with three blocks. However, these 6 treatment combinations resulted in only 4 rates of spray application as indicated in the following table.

Table 3: Application rates for the sprayer experiment

	Tractor speed (km hr^{-1})							
Pressure (kPa)	3.6	2.6	1.8					
140	2090	2930	4120					
330	2930	4120	5770					

That is, there are 4 different rates of application, two of which have different combinations of Tractor speed and Spray pressure. So, a factor, Rates, with four levels is set up to compare the means of the four rates and then separate nested factors for each rate are generated.

We set up the RCBD for Speed and Pressure then derive the Rate factors.

```
b <- 3
t <- 6
#'## Construct a systematic layout
RCBD.sys <- cbind(fac.gen(generate = list(Blocks=b, Plots=t)),
                  fac.gen(generate = list(Pressure = c("140", "330"),
                                            Speed = c("3.6", "2.6", "1.8")), times = b))
#'## Obtain the randomized layout
RCBD.lay <- designRandomize(allocated</pre>
                                                = RCBD.sys[c("Pressure", "Speed")],
                                                = RCBD.sys[c("Blocks", "Plots")],
                             recipient
                             nested.recipients = list(Plots = "Blocks"),
                             seed
                                                = 353441)
#'## Add nested factors
RCBD.lay <- within(RCBD.lay,</pre>
                      Treatments <- fac.combine(list(Pressure, Speed), combine.levels = TRUE)</pre>
                      Rates <- fac.recast(Treatments,</pre>
                                           newlevels = c("2090", "2930", "4120".
                                                          "2930", "4120", "5770"))
```

Now check the properties of the design with the nested factors.

3.4.1 Questions

- 1. What is the prior allocation model for this design?
- 2. How does the prior allocation model differ from the randomization model for this design?
- 3. Why are terms involving Rate2090 and Rate5770 not included in the prior allocation model?

3.5 A Control treatment for an incomplete-block design

An incomplete-block design for 6 treatments in 6 blocks of size 4 is required. A design is obtained from Cochran and Cox (1957, p. 379).

Input the design.

Randomize the design and check its properties

Investigate the effect of designating a treatment to be a Control and including a Control factor in the fixed model. It is noted that, in this case at least, it does not matter which treatment is designated to be the control.

Now use odw, to obtain a near-A-optimal under a fixed model using a randomization of the treatment to the plots within incomplete blocks for the initial design.

Randomize the design obtained using odw and check its properties

- 1. Why must the Control source be balanced?
- 2. How do the Cochran and Cox design and the design obtained with odw compare?

3.6 The Casuarina experiment (continued)

In Section 2.3 an exploration was made of the properties of the split-unit design for an experiment to investigate the differences between 60 provenances of a species of Casuarina tree, these provenances coming from 18 countries; the trees were inoculated prior to planting at two different times.

The experiment involves nested factors in that the provenances came from 12 countries so that the factor Provenances is nested within Countries. Here we investigate a model that has separate terms for each country that model differences between provenances from each country. Use the dae function fac.multinested to generate the individual nested factors for each country.

This example has two difficulties that need to be dealt with. Firstly, a number of Countries contribute only one Provenance and terms for differences among provenances from those countries are superfluous. Secondly, because of the large number of terms and considerable nonothogonality in the design, it is difficult to get a full decomposition. To overcome this, the following measures are taken:

- Leave out nested terms for countries with only a single provenance;
- Reduce the tolerances on testing for idempotency using the function set.daeTolerance;
- Do not attempt to partition the InocTimes#Provenances[Countries] interaction.

3.6.1 Questions

1. How does this analysis compare with that conducted in Section 2.3?

Topic 4 Using R for advanced experimental design

Firstly, initialize by loading the libraries that will be used and setting the output width.

```
library(dae)
library(odw)
options(width=100)
```

4.1 Athletic examples based on Brien et al. (2011)

Brien et al. (2011) give several designs for an athletic experiment that illustrate the basic principles to be employed in designing multiphase experiments. Here designs for two different multiphase scenarios are considered, both being based on a first-phase that is the testing phase and employs a split-unit design.

4.1.1 A standard single-phase athlete training experiment

First, a split-unit design is generated for an experiment in which the performance of an athlete when subject to nine different training conditions is tested. The nine training conditions are the combinations of three surfaces and three intensities of training. Also, assume that the prime interest is in surface differences, with intensities included to observe the surfaces over a range of intensities. The experiment is to involve 12 athletes, three per month for four consecutive months; each athlete undergoes three tests. The heart rate of the athlete is to be taken immediately upon completion of a test.

A split-plot design is to be employed for the experiment: the three intensities are randomized to the three athletes in each month and the three surfaces are randomized to the three tests that each athlete is to undergo. The factor-allocation diagram is shown in Figure 12. Generate a randomized layout for the experiment.

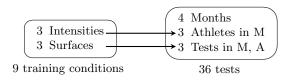


Figure 12: Factor-allocation diagram for the standard athlete training experiment: training conditions are randomized to tests; the two left-hand arrows indicate that the levels of Intensities and Surfaces are randomized to Athletes and Tests, respectively; M = Months; A = Athletes.

```
#'## Phase 1: Construct a systematic layout and generate a randomized layout for the first phase
split.sys <- cbind(fac.gen(list(Months = 4, Athletes = 3, Tests = 3)),</pre>
                    fac.gen(list(Intensities = LETTERS[1:3], Surfaces = 3),
                            times = 4))
split.lay <- designRandomize(allocated</pre>
                                                 = split.sys[c("Intensities", "Surfaces")],
                                                 = split.sys[c("Months", "Athletes", "Tests")],
                              recipient
                              nested.recipients = list(Athletes = "Months",
                                                         Tests = c("Months", "Athletes")),
                              seed
                                                 = 2598)
#'## Plot the design
#+ "SplitDes_v2"
split.lay <- within(split.lay,</pre>
                     Conditions <- fac.combine(list(Intensities, Surfaces),</pre>
                                                combine.levels = TRUE))
plt <- designGGPlot(split.lay, labels = "Conditions",</pre>
                     row.factors = "Tests", column.factors = c("Months", "Athletes"),
```

Question

1. Why was a split-plot design chosen for this experiment?

4.1.2 A simple two-phase athlete training experiment

Multiphase experiments differ from those previously presented in that they employ two or more randomizations or allocations, each to a different type of unit. As a result, there will be three or more sets of factors, or tiers, to deal with; further, when there are three sets of factors, three formula will need to be supplied to designAnatomy.

Suppose that, in addition to heart rate taken immediately upon completion of a test, the free haemoglobin is to be measured using blood specimens taken from the athletes after each test and transported to the laboratory for analysis. That is, a second laboratory phase is required to obtain the new response. In this phase, because the specimens become available monthly, the batch of specimens for one month are to be processed, in a random order, before those for the next month are available. The factor-allocation diagram for this experiment is in Figure 13, the dashed line indicating that Months are systematically allocated to Batches. The randomizations in this diagram are composed (Brien and Bailey, 2006) and is one of the two types of randomizations in a chain (Bailey and Brien, 2016). This means that the second-phase randomization only need to consider how the tests factors are to be assigned to locations; training conditions can be ignored in determining the combined-units design.

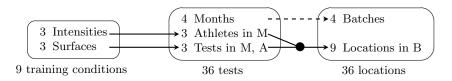


Figure 13: Factor-allocation diagram for the two-phase athlete training experiment: training conditions are randomized to tests and tests are allocated to locations; the two left-hand arrows indicate that the levels of Intensities and Surfaces are randomized to Athletes and Tests, respectively; the dashed arrow indicates that Months are systematically allocated to Batches; the ${}^{\bullet}$ indicates that the combinations of the levels of Athletes and Tests are randomized to the Locations; M = Months; A = Months;

Using the following R code, obtain a layout for the second phase and check the properties of the layout. In doing this, the first-phase layout is randomized. However, because Months is not randomized to Batches, the argument except in designRandomize is used to effect the systematic allocation.

```
nested.recipients = list(Locations = "Batches"),
                                             = "Batches",
                           seed
                                             = 71230)
eg1.lay
#'## Plot the layout
#+ Athlete_eq1lay
eg1.lay$Conditions <- with(eg1.lay, fac.combine(list(Intensities, Surfaces),
                                                 combine=TRUE, sep=","))
designGGPlot(eg1.lay, labels = "Conditions",
             row.factors = "Locations", column.factors = "Batches",
             cellfillcolour.column = "Athletes", cellalpha = 0.75, size = 6,
             title = "Randomized Intensities-Surfaces combinations",
             blockdefinition = rbind(c(9,1)),
             ggplotFuncs = list(xlab("Batches (Months)"),
                                theme(legend.position = "right")))
```

Check the properties of the design.

Questions

- 1. What would be the allocation-based mixed model for this experiment, an allocation-based mixed model having the same terms as the randomization-based mixed model that would apply if all the allocations had been made by randomizing. Do you anticipate any problem in fitting it?
- 2. Compare the units for the two phases in this experiment?
- 3. What are the outcomes for the two phases for this experiment?

4.1.3 Allowing for lab processing order in the athletic training example

Brien (2017) discusses a design, and its properties, that differs in the second phase from that described in Section 4.1.2: it assumes that lab processing order within a batch is important and so the second-phase are now crossed; hence a row-column design is required for this phase. However, one cannot consider a design for just Months, Athletes and Tests and ignore Intensities and Surfaces, as was done in the previous design. Indeed prime consideration needs to be given to Intensities and Surfaces. That is, a suitable cross-phase design for allocating Intensities and Surfaces to Batches and Locations is needed. However, the combined-units design that allocates Months, Athletes and Tests to Batches and Locations has to be considered in that it must account for the split-unit nature of the first-phase design.

For the combined-units design, the Months are associated with Batches. Then each triple of consecutive locations in a batch are associated with a single athlete, one of those for the month associated with the batch. This leaves tests to be assigned to locations within triples. Thus, the cross-phase design will need to allocate efficiently an intensity to a location triple and surface to the locations within a triple.

The cross-phase design is a balanced factorial design (Hinkelmann and Kempthorne, 2005, Section 12.5) and can be constructed using two extended Latin squares (ELS) as follows:

1. a 3×4 ELS, formed from a 3×3 Latin square by repeating one of its columns, will be used to allocate Intensities to the 3 Locations triples \times 4 Months.

- 2. A 3×4 ELS will be used to allocate Surfaces to the 3 Locations \times 4 Months within a triple; the same ELS is used for the three triples.
- 3. To ensure no repeat Intensities-Surfaces combinations for a Location, the two Batches to which the repeated columns of the ELS for Intensities are assigned must be different from the two Batches to which repeated columns of the ELS for Surfaces are assigned.

The factor-allocation diagram, for this design, is in Figure 14. In this diagram, the training conditions and tests panels are surrounded by a dashed rectangle and genotypes go from the training conditions sources to the genotypes from the test sources. This indicates that the result of the allocation in the first phase needs to be explicitly taken into account in the second-phase allocation. The randomizations involved have been called randomized-inclusive randomizations (Brien and Bailey, 2006) and are one of the two types of randomizations in a chain (Bailey and Brien, 2016). Because Batches and Locations are crossed, the second phase randomization is achieved by independently permuting the Batches and Locations. A design with the same properties had been previously constructed by Rosemary Bailey (pers. comm.).

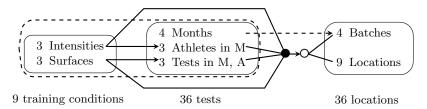


Figure 14: Factor-allocation diagram for the two-phase athlete training experiment with a row-column design on the second-phase units: training conditions are randomized to tests, then training conditions and tests are randomized to locations; the ' \bullet ' indicates that the observed combinations of the levels of Intensities, Surfaces, Athletes and Tests are randomized to locations; the ' \bullet ' indicates that a nonorthogonal design was used in this randomization to the combinations of the levels of Batches and Locations; the dashed arrow indicates that Months were systematically allocated to Batches; the dashed oval indicates that all factors from the first phase form a pseudotier and all are actively involved in determining the allocation to locations; M = M on the sand M = M of the second-phase units:

Use the following R code to obtain a layout for the new second phase design.

```
#'## Generate a systematic cross-phase design for Intensities and Surfaces
#' It is based on (i) an extended Latin square design (ELSqD) for allocating Intensities to
#' Locations triples x Batches and (ii) the same ELSqD for each triple, the ELSqD being used to
#' allocate Surfaces to the three Locations within each triple by four Batches.
#' The Batches to which the repeated columns of the ELSqD for Intensities are assigned must be
#' different from the Batches to which repeated columns of the ELSqD for Surfaces are assigned.
#+ Athlete_eq2sys_v3
eg2.phx.sys <- cbind(fac.gen(list(Batches = 4, Locations = 9)),
                     data.frame(Intensities = factor(rep(c(designLatinSqrSys(3), c(3,2,1)),
                                                         each = 3), labels = LETTERS[1:3]),
                                Surfaces = factor(c(rep(1:3, times = 3),
                                                    rep(1:3, times = 3),
                                                    rep(c(2,3,1), times = 3),
                                                    rep(c(3,1,2), times = 3)))))
eg2.phx.sys$Conditions <- with(eg2.phx.sys, fac.combine(list(Intensities, Surfaces),
                                                        combine.levels = TRUE))
designGGPlot(eg2.phx.sys, labels = "Conditions",
             row.factors = "Locations", column.factors = "Batches",
             cellfillcolour.column = "Intensities", cellalpha = 0.75, size = 6,
             title = "Intensities-Surfaces for systematic cross-phase design",
             blockdefinition = rbind(c(9,1)),
             ggplotFuncs = list(xlab("Batches (Months)"),
                                theme(legend.position = "right")))
```

```
#'## Two-phase design
#'## Generate a systematic two-phase design by bringing in first-phase recipient factors
eg2.phx.sys$Months <- eg2.phx.sys$Batches
eg2.sys <- merge(split.lay, eg2.phx.sys) #merge on common factors Months, Intensities & Surfaces
eg2.sys <- with(eg2.sys, eg2.sys[order(Batches,Locations),])
designGGPlot(eg2.sys, labels = "Conditions",
             row.factors = "Locations", column.factors = "Batches",
             cellfillcolour.column = "Athletes", cellalpha = 0.75, size = 6,
             title = "Intensities-Surfaces for systematic two-phase design ",
             blockdefinition = rbind(c(9,1)),
             ggplotFuncs = list(xlab("Batches (Months)"),
                                theme(legend.position = "right")))
#'## Allocate to the second-phase units
eg2.lay <- designRandomize(allocated = eg2.sys[c("Months", "Athletes", "Tests",
                                                 "Intensities", "Surfaces")],
                           recipient = eg2.sys[c("Batches", "Locations")],
                           except = "Batches",
                           seed
                                     = 243526)
head(eg2.lay)
#'## Plot the layout
#+ Athlete_eq2lay_v3
eg2.lay$Conditions <- with(eg2.lay, fac.combine(list(Intensities, Surfaces),
                                                combine=TRUE, sep=","))
designGGPlot(eg2.lay, labels = "Conditions",
             row.factors = "Locations", column.factors = "Batches",
             cellfillcolour.column = "Athletes", cellalpha = 0.75, size = 6,
             title = "Randomized Intensities-Surfaces combinations",
             blockdefinition = rbind(c(9,1)),
             ggplotFuncs = list(xlab("Batches (Months)"),
                                theme(legend.position = "right")))
```

Check the properties of the design.

It is clear that Athletes [Months] and Tests [Months: Athletes] are not orthogonal to Locations and Batches #Locations, because the former sources are confounded with both of the latter sources. To examine the nature of the nonorthogonality, the anatomy for just the tests and locations tiers is obtained.

Questions

1. What do you conclude about the confounding of Athletes[Months] and Tests[Months:Athletes] with Locations?

- 2. Are the designs proposed for this experiment first-order balanced?
- 3. What has been the cost of allowing for order of processing in the lab? Is the cost acceptable? Why?

4.2 McIntyre's (1955) two-phase example

McIntyre (1955) reports an investigation of the effect of four light intensities on the synthesis of tobacco mosaic virus in leaves of tobacco *Nicotiana tabacum* var. Hickory Pryor. It is a two-phase experiment: the first phase is a treatment phase, in which the four light treatments are randomized to the tobacco leaves, and the second phase is an assay phase, in which the tobacco leaves are randomized to the half-leaves of assay plants.

In the first phase, four successive leaves at defined positions on the stem were taken from each of eight plants of comparable age and vigour that had been inoculated with the virus. Arbitrarily grouping the plants into two sets of four, the four treatments were applied to the leaves, which had been separated from the plants and were sustained by flotation on distilled water, in a Latin square design for each set with tobacco plants as columns and leaf positions as rows; see Figure 16.

In the second phase, virus content of each tobacco leaf was assayed by expressing sap and inoculating half leaves of the assay plants, $Datura\ stramonium$, on which countable lesions would appear. Lots of eight sap samples were formed from pairs of tobacco plants, the pairs being comprised of a plant from each set in the treatment phase. The eight samples from a lot were assigned to four assay plants using one of four 4×4 Graeco-Latin square designs, with the leaves from a single tobacco plant assigned using one of the alphabets and the second tobacco plant using the other (see Figure 17). Actually, this design is a semi-Latin square (Bailey, 1992).

The factor-allocation diagram for the experiment is in Figure 15. Unfortunately, the randomization for this experiment was not described by McIntyre (1955). Because there are multiple squares in both phases, there are several possible randomizations depending on the effects anticipated as possible in the experiment. As shown by the nesting relations in the factor-allocation diagram, I have assumed that randomization to NicPlant was within Sets and to Posn was across Sets. Similarly, I have assumed that randomization to DatPlant was within Lot and to AssPosn across Lot. In the factor-allocation diagram, N_1 is a factor for the pairs of tobacco plants formed by taking a plant from each set in the first phase.

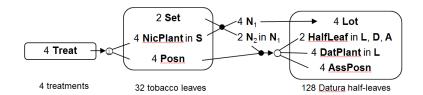


Figure 15: Factor-allocation diagram for McIntyre's (1955) two-phase experiment: treatments are randomized to tobacco leaves and tobacco leaves are randomized to Datura half-leaves; the arrow to the ' \bigcirc ', the ' \bigcirc ' and the two genotypes from the ' \bigcirc ' indicate that Treat is randomized to the combinations of NicPlant and Posn using an orthogonal design; N_1 is a pseudofactor indexing the pairs of tobacco plants formed by taking a plant from each set in the first phase and N_2 is a pseudofactor indexing the tobacco plants within the pairs formed by taking a plant from each set in the first phase; N_1 is randomized to Lot in the second phase; the combinations of N_2 and Posn is randomized to the combinations of HalfLeaf, DatPlant and AssPosn using a nonorthogonal design, the latter indicated by the 'O'; S = Set; L = Lot; D = DatPlant; A = AssPosn.

Figure 16: Layout for the first phase of McIntyre's (1955) experiment[†]

				j	Nicotiana Plai	$_{ m nts}$			
	1	2	3	4		1	2	3	4
Leaf					Leaf				
Position					Position				
1	a	b	c	d		a	b	c	d
	1	5	9	13		17	21	25	29
2	b	a	d	С		С	d	a	b
	2	6	10	14		18	22	26	30
3	c	d	a	b		d	С	b	a
	3	7	11	15		19	23	27	31
4	d	c	b	a		b	a	d	c
	4	8	12	16		20	24	28	32

 † The letter in each cell refers to the light intensity to be applied to the unit and the number to the unit.

Figure 17: Layout for the second phase of McIntyre's (1955) experiment[†]

Assay Leaf Position	1	2	3	4	Datura Plants Assay Leaf Position	5	6	7	8
1	1	2	3	4		5	6	7	8
	17	20	18	19		23	22	24	21
2	2	1	4	3		8	7	6	5
	18	19	17	20		22	23	21	24
3	3	4	1	2		7	8	5	6
	19	18	20	17		21	24	22	23
4	4	3	2	1		6	5	8	7
	20	17	19	18		24	21	23	22
Assay Leaf Position	9	10	11	12	Datura Plants Assay Leaf Position	13	14	15	16
1	9	10	11	12		13	14	15	16
	28	25	27	26		30	31	29	32
2	10	9	12	11		16	15	14	13
	27	26	28	25		31	30	32	29
3	11	12	9	10		15	16	13	14
	26	27	25	28		32	29	31	30
4									
	12	11	10	9		14	13	16	15

†The numbers in the cell refer to the units from the first phase (tobacco leaves) to be assigned to the two half-leaves of the assay plant; they are in standard order for Set, then NicPlant followed by Position.

4.2.1 Check the properties of the randomized layout

Load the data and use designTwophaseAnatomies to check the properties of the design.

4.2.2 Questions

n <- r*c

no. plots

- 1. Summarize the properties of the four design species for this example.
- 2. Is the variance matrix for this experiment based on two sets of terms that are orthogonal?
- 3. What are the advantages and disadvantages of a mixed-model analysis of the data from this experiment, as opposed to an anova?

4.3 A p-rep design for a field experiment with 576 Genotypes

A field experiment is to be conducted on a grid of $60 \text{ rows} \times 12 \text{ columns}$. Of the 576 Genotypes, 144 are to be duplicated and the remaining 432 are to be unreplicated. In the lecture, the field-phase design was optimized under a model in which Genotypes was assumed to be random. However, in the resulting design, all border plots were occupied by duplicated lines. As Sermarini et al. (2020) note, this can be avoided by assuming Genotypes to be fixed with little loss in precision. Here we use odw to obtain a near-optimal design under a model with fixed Genotypes. The factor-allocation diagram is in Figure 18.

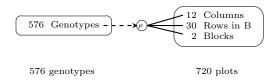


Figure 18: Factor-allocation diagram for the p-rep design for a field experiment with 576 Genotypes: genotypes are allocated to plots; the dashed arrow on the left indicates that the allocation of Genotypes is not randomized; the '@' at the end of the arrow indicates that Genotypes are allocated to combinations of the levels of Blocks, Rows and Columns, using a design that takes into account correlation between plots; B = Blocks.

4.3.1 Generate the starting design and check the properties of the design

Use the following R code to generate a balanced-lattice design and to check its properties.

```
#'# This script generates a p-rep design for 576 genotypes, 144 of which are replicated and Genotypes a
#'### It is the first-phase design of a two-phase design a la Smith et al. (2006)

#'## Set up constants
g <- 576  # no. genotypes
ndup <- 144 # no. duplicated genotypes
b <- 2  # no. blocks
r <- 60  # no. rows
c <- 12  # no. columns</pre>
```

```
#'## Generate a simple lattice for Genotypes 1:144
# 1
#' 1:144 are replicated twice 145:q are replicated once
latt.mat <- matrix(1:ndup, nrow = 12, ncol = 12)</pre>
blk1.genos <- sample((ndup+1):g, (g-ndup)/2)
                                                 #randomly select half undup Genotypes for Block 1
blk2.genos <- ((ndup+1):g)[!((ndup+1):g %in% blk1.genos)] #rest in Block 2
latt.lay <- fac.gen(list(Blocks = 2, WRows = 30, Columns = 12))</pre>
latt.lay <- within(latt.lay,</pre>
                   Genotypes <- factor(c(latt.mat, blk1.genos,</pre>
                                          t(latt.mat),blk2.genos)))
#'### Randomize the initial design
latt.lay <- designRandomize(allocated</pre>
                                             = latt.lay["Genotypes"],
                            recipient
                                            = latt.lay[c("Blocks", "WRows", "Columns")],
                            nested.recipients = list(WRows = "Blocks"),
                                              = 64058)
                            seed
latt.lay <- within(latt.lay,</pre>
                   Rows <- fac.combine(list(Blocks, WRows)))</pre>
#'### Check properties
latt.canon <- designAnatomy(formulae = list(plot = ~ (Blocks + Rows)*Columns,
                                            trt = ~ Genotypes),
                            data
                                    = latt.lay)
summary(latt.canon, which.criteria = c("aeff", "meff", "eeff", "order", "dfor"))
```

4.3.2 Search for a near-A-optimal design

Use odw to search for a near-A-optimal design under a mixed model with Genotypes assumed fixed.

```
#'## Set odw options
maxit <- 10
search <- "tabu+rw"</pre>
odw.options(P = 0.10, localSearch = 10000, tabuStop = 100)
#'## Set up variance parameters (based on Smith et al (2006, p.405))
g.G <- 1
g.BR <- 0.5
g.C < -0.1
g.BC <- 0.05
g.u <- 0.5
g.BRC <- 1.0
rho.R <- 0.6
rho.C <- 0.4
residual
                                  = ~ ar1(Rows):ar1(Columns),
                       residual = ari(nows):ari(columns),
permute = ~ Genotypes, swap = ~ Blocks,
                       start.values = TRUE,
                               = latt.lay)
                       data
vp.table <- prepuar1.latt.odw$vparameters.table</pre>
vp.table$Value[c(1:4, 6:7)] <- c(g.BR, g.C, g.BC, g.u, rho.R, rho.C)</pre>
vp.table
prepuar1.latt.odw <- odw(fixed = ~ Genotypes + Blocks,</pre>
```

```
random = " Rows + Columns/Blocks + units,
                         residual = ~ ar1(Rows):ar1(Columns),
                         permute = ~ Genotypes, swap = ~ Blocks,
                         G.param = vp.table, R.param = vp.table,
                         maxit = maxit, search = search,
                         data
                                  = latt.lay)
prepuar1.latt.lay <- prepuar1.latt.odw$design</pre>
#'### Plot the design
prepuar1.latt.lay$Replication <- fac.recast(prepuar1.latt.lay$Genotypes,</pre>
                                            newlevels = rep(1:2, c(ndup, (g-ndup))))
designGGPlot(prepuar1.latt.lay, labels = "Genotypes",
             row.factors = c("Blocks", "WRows"), column.factors = "Columns",
             cellfillcolour.column = "Replication",
             colour.values = c("lightgreen", "lightcyan"),
             axis.text.size = 10, blockdefinition = cbind(30,12),
             title = NULL)
```

Obtain the anatomy of the design produced and calculate the A-value under the model for Genotypes assumed random.

```
#'### Check properties
summary(prepuar1.latt.canon <- designAnatomy(formulae = list(plot = ~ (Blocks + Rows)*Columns,</pre>
                                                             trt = ~ Genotypes),
                                                      = prepuar1.latt.lay),
                                             data
        which.criteria = c("aeff", "meff", "eeff", "order", "dfor"))
#'### Calculate the A-measure under Genotypes random
prepuar1.latt.lay$unit <- factor(1:nrow(prepuar1.latt.lay)) #factor for ASReml units
(designAmeasures(mat.Vpredicts(target = ~ Genotypes - 1,
                               Gt
                               fixed = ~ Blocks,
                               random = "Rows + Columns/Blocks + unit - 1,
                                      = as.list(c(g.BR, g.C, g.BC, g.u)),
                                      = kronecker(mat.ar1(rho.R, r),
                                                  mat.ar1(rho.C, c)),
                               design = prepuar1.latt.lay)))
```

In the values for the variance parameters, $\gamma_{\rm BC}$ was set to 0.05, thus indicating that it was thought to be small. The question then arises as to what would be the effect of leaving out the term. To check this recalculate the AVPD without it and redo the anatomy with the source omitted.

4.3.3 Questions

- 1. How do the plots of the *p*-rep designs obtained from the balanced lattice under the assumptions of fixed and random Genotypes compare?
- 2. The A-value for the design obtained with random Genotypes was 1.202. How does A-value for the design optimized with fixed Genotypes compare when random Genotypes are assumed for the model for it?
- 3. Summarize the differences between the original balanced lattice design and the odw design, both optimized under a fixed genotypes. Is the increased precision of the odw design worthwhile?
- 4. Is this design connected under a fixed model? How can you tell?

4.4 A two-phase p/q-rep design for a field experiment with 576 Genotypes

In Section 4.3, a design was constructed for a field experiment to be conducted on a grid of $60 \text{ rows} \times 12 \text{ columns}$. Of the 576 Genotypes, 144 were duplicated and the remaining 432 were unreplicated. This field experiment is the first-phase of the experiment, the second phase being a milling phase in which samples of grain are taken from the plots to be milled so that quality characteristics of the grain can be ascertained.

The factor-allocation diagram for the two-phase experiment is in Figure 19.

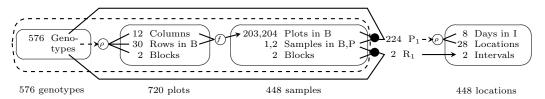


Figure 19: Factor-allocation diagram for a two-phase p/q-rep design for a field experiment with 576 Genotypes: genotypes are allocated to plots, a fraction of the plots are selected to produce samples and samples are allocated to locations; the dashed arrow on the left indicates that the allocation of Genotypes is not randomized; the '②' at the end of the arrow indicates that Genotypes are allocated to combinations of the levels of Blocks, Rows and Columns, using a design that takes into account correlation between plots; the '②' indicates the selection of a fraction of the levels of Rows and Columns from each Block; the solid lines signify that the selection is random; the dashed oval encircling the three panels on the left indicates that a pseudotier of all factors is formed in allocating samples to locations because it uses all the information about the first-phase factors; the levels of the pseudofactor R_1 groups together the blocks and samples that are to be assigned to the same interval; the pseudofactor P_1 indexes the Plots that are to occur within the same interval; the dashed arrow ending at the '②' indicates that Plots within P_1 are systematically allocated, the '②' indicates that the design allows for correlation between observations in the milling phase and the two lines leaving it indicate that the Plots are assigned to the combinations of the levels of Days and Locations within an Interval; B = Blocks; P = Plots; I = Intervals; D = Days.

4.4.1 Select the samples and assign them systematically to the milling phase

Use the following R code to select the samples from the field experiment for the milling phase, plot it and check its properties.

```
#'# This script systematically assigns sampled plots from the first-phase.
#'### It is based on an example from Smith et al. (2006)

#'## Select genotypes for milling phase, balanced between blocks
sampdupgenos <- sample(1:ndup, 37)  #select the 37 dup field genotypes
samp.blk1.undup <- sample(blk1.genos, 167)  #select the 167 undup field genotypes from blk1</pre>
```

```
samp.blk1.milldup <- sample(samp.blk1.undup, 20) #and from them select 20 genos to dup in milling phase
samp.blk2.undup <- sample(blk2.genos, 166) #select the 166 undup field qenotypes from blk1</pre>
samp.blk2.milldup <- sample(samp.blk2.undup, 21) #and from them Select 21 genos to dup in milling phase
milldup <- c(samp.blk1.milldup, samp.blk2.milldup)</pre>
millundup <- setdiff(c(samp.blk1.undup, samp.blk2.undup), milldup)</pre>
sampgenos <- c(sampdupgenos, millundup, milldup)</pre>
#'## Construct revised data.frame
ph2samp.lay <- with(prepuar1.latt.lay, prepuar1.latt.lay[Genotypes %in% sampgenos,])
#'### Plot the sampled plots
#+ "SamplesGfix_v9"
fullgrid <- merge(fac.gen(list(Blocks = 2, WRows = 30, Columns = 12)),</pre>
                    ph2samp.lay, all.x = TRUE)
fullgrid$Replication <- 1</pre>
fullgrid$Replication[as.numfac(fullgrid$Genotypes) < 145 ] <- 2</pre>
fullgrid$Replication[is.na(fullgrid$Genotypes)] <- 0</pre>
fullgrid$Replication <- factor(fullgrid$Replication)</pre>
designGGPlot(fullgrid, labels = "Genotypes",
             row.factors = c("Blocks","WRows"), column.factors = "Columns",
             cellfillcolour.column = "Replication",
             colour.values = c("grey50","lightcyan","lightgreen"),
             axis.text.size = 10, blockdefinition = cbind(30,12),
             title = NULL,
             ggplotFuncs = list(theme(legend.position = "right")))
with(fullgrid, table(Replication, Blocks))
#'## Allocate samples systematically - confounds both field and milling dups with Intervals
#'### Allocate the field plots as the first sample
ph2sys.lay <- within(ph2samp.lay,</pre>
                        Days \leftarrow factor(c(rep(1:3, each = 26), rep(4:8, each =25),
                                          rep(1:4, each = 26), rep(5:8, each = 25)))
                        Intervals <- Blocks
                        Samples <- factor(1, levels = 1:2)</pre>
#'### Add the milling duplicates in the opposite Interval to the first duplicate
ph2sys.lay <- rbind(ph2sys.lay,</pre>
                     within(prepuar1.latt.lay[prepuar1.latt.lay$Genotypes %in% milldup, ],
                              Days \leftarrow factor(c(rep(1:8, 3)[-(1:4)], rep(1:8, 3)[-(1:3)]))
                              Intervals <- Blocks
                              Intervals[Blocks == 1][1:20] <- 2
                              Intervals[Blocks == 2] <- 1</pre>
                              Samples <- factor(2, levels = 1:2)</pre>
ph2sys.lay <- within(ph2sys.lay,
                        Genotypes <- factor(Genotypes)</pre>
                        Locations <- fac.nested(fac.combine(list(Intervals,Days)))</pre>
                        xLocn <- as.numeric(Locations)</pre>
                        xLocn <- xLocn - mean(unique(xLocn))</pre>
```

```
ph2sys.lay <- with(ph2sys.lay, ph2sys.lay[order(Intervals, Days, Locations), ])</pre>
#'### Plot the design
#+ Breed576sys2phGfix_v9
designGGPlot(ph2sys.lay, labels = "Genotypes",
             row.factors = c("Locations"), column.factors = c("Intervals", "Days"),
             cellfillcolour.column = "Rows",
             axis.text.size = 10, blockdefinition = cbind(28,1),
             title = NULL)
ph2sys.lay$Replication <- "millundup"
ph2sys.lay$Replication[ph2sys.lay$Genotypes %in% sampdupgenos] <- "field"
ph2sys.lay$Replication[ph2sys.lay$Genotypes %in% milldup] <- "mill"
designGGPlot(ph2sys.lay, labels = "Genotypes",
             row.factors = c("Locations"), column.factors = c("Intervals", "Days"),
             cellfillcolour.column = "Replication",
             colour.values = c("lightgreen","lightcyan","grey50"),
             axis.text.size = 10, blockdefinition = cbind(28,1),
             title = NULL,
             ggplotFuncs = list(theme(legend.position = "bottom")))
```

4.4.2 Randomize the systematic p/q-rep design to produce an initial design

```
#'## Randomize the allocation to the second-phase units
ph2sys.lay <- with(ph2sys.lay, ph2sys.lay[order(Intervals,Days,Locations),])</pre>
ph2sys.ini <- designRandomize(allocated = ph2sys.lay[c("Blocks", "WRows", "Rows", "Columns",
                                                        "Samples", "Genotypes")],
                              recipient = ph2sys.lay[c("Intervals", "Days", "Locations")],
                              nested.recipients = list(Days = "Intervals",
                                                        Locations = c("Intervals", "Days")),
                              seed = 705865)
#'### Plot the design
designGGPlot(ph2sys.ini, labels = "Genotypes",
             row.factors = c("Locations"), column.factors = c("Intervals", "Days"),
             cellfillcolour.column = "Rows",
             axis.text.size = 10, blockdefinition = cbind(28,1),
             title = NULL)
ph2sys.ini$Replication <- "millundup"</pre>
ph2sys.ini$Replication[ph2sys.ini$Genotypes %in% sampdupgenos] <- "field"
ph2sys.ini$Replication[ph2sys.ini$Genotypes %in% milldup] <- "mill"
designGGPlot(ph2sys.ini, labels = "Genotypes",
             row.factors = c("Locations"), column.factors = c("Intervals", "Days"),
             cellfillcolour.column = "Replication",
             colour.values = c("lightgreen","lightcyan","grey50"),
             axis.text.size = 10, blockdefinition = cbind(28,1),
             title = NULL,
             ggplotFuncs = list(theme(legend.position = "bottom")))
```

4.4.3 Optimize the intial design for the two-phase model

Had to remove Rows:Columns:Samples because of singularities and Int.Days must be used in the residual model.

```
g.BRCS <- 0.25
g.ID < -0.8
g.L <- 0.2
rho.L <- 0.6
ph2sys.ini$IntDays <- with(ph2sys.ini, fac.combine(list(Intervals, Days)))</pre>
maxit <- 3
ph2sys.odw.ini <- odw(fixed
                                   = ~ Intervals,
                                 = ~ Genotypes + Rows + Columns/Blocks + Rows:Columns +
                      random
                        ar1(Rows):ar1(Columns) + Rows:Columns:Samples + Intervals:Days + Locations,
                      residual = ~ IntDays:ar1(Locations),
                                  = ~ Genotypes | Rows/Columns/Samples + Columns/Blocks,
                      permute
                                   = ~ Intervals,
                      swap
                      start.values = TRUE, data=ph2sys.ini)
vpc <- ph2sys.odw.ini$vparameters.table</pre>
vpc$Value <- c(g.G*g.BRC, g.BR*g.BRC, g.C*g.BRC, g.BC*g.BRC, g.BRC, rho.R, rho.C, g.BRCS,</pre>
               g.ID, g.L, 1, rho.L)
(vpc)
ph2sys.odw <- odw(fixed = ~ Intervals,</pre>
                  random = ~ Genotypes + Rows + Columns/Blocks + Rows:Columns +
                    ar1(Rows):ar1(Columns) + Rows:Columns:Samples + Intervals:Days + Locations,
                  residual = ~ IntDays:ar1(Locations),
                  permute = ~ Genotypes | Rows/Columns/Samples + Columns/Blocks,
                             = ~ Intervals,
                  G.param = vpc, R.param = vpc,
                  maxit = maxit, search = search, data=ph2sys.ini)
ph2sys.odw.lay <- ph2sys.odw$design
ph2sys.odw.lay <- within(ph2sys.odw.lay,
                           WRows <- fac.recast(Rows, newlevels = rep(1:30, times = 2))</pre>
                           xLocn <- as.numeric(Locations)</pre>
                           xLocn <- xLocn - mean(unique(xLocn))</pre>
                         })
#'### Check the two-phase A-measure
G.RC <- g.BRC * kronecker(mat.ar1(rho.R, r), mat.ar1(rho.C, c)) #ar1(R):ar1(C)
(designAmeasures(mat.Vpredicts(target = ~ Genotypes - 1,
                               Gt = g.G*g.BRC,
                               fixed = ^{\sim} Intervals - 1,
                               random = ~ Rows + Columns/Blocks + Rows:Columns/Samples +
                                 Intervals:Days + Locations - 1,
                                    = c(as.list(c(g.BR*g.BRC, g.C*g.BRC, g.BC*g.BRC)),
                                          list(G.RC = G.RC),
                                           as.list(c(g.BRCS, g.ID, g.L))),
                               R = with(ph2sys.odw.lay, kronecker(diag(nlevels(IntDays)),
                                                                   mat.ar1(rho.L,
                                                                           nlevels(Locations)))),
                               design = ph2sys.odw.lay)))
```

4.4.4 Plot the design

```
designGGPlot(ph2sys.odw.lay, labels = "Genotypes",
             row.factors = c("Locations"), column.factors = c("Intervals", "Days"),
             cellfillcolour.column = "Rows",
             axis.text.size = 10, blockdefinition = cbind(28,1),
             title = NULL)
#Set up a factor indicating the type of duplication
genodups <- with(ph2sys.odw.lay, table(Genotypes))</pre>
genodups <- names(genodups[genodups == 2])</pre>
ph2sys.odw.lay$Replication <- "undup"</pre>
ph2sys.odw.lay$Replication[ph2sys.odw.lay$Genotypes %in% genodups] <- "field"
ph2sys.odw.lay$Replication[ph2sys.odw.lay$Genotypes %in% milldup] <- "mill"
designGGPlot(ph2sys.odw.lay, labels = "Genotypes",
             row.factors = c("Locations"), column.factors = c("Intervals", "Days"),
             cellfillcolour.column = "Replication",
             colour.values = c("lightgreen","lightcyan","grey50"),
             axis.text.size = 10, blockdefinition = cbind(28,1),
             title = NULL,
             ggplotFuncs = list(theme(legend.position = "bottom")))
```

4.4.5 Check the properties of the optimized p/q-rep design

4.4.6 Substituting a linear Locations term for arbitrary Locations differences

4.4.7 Questions

- 1. What permutations are performed in randomizing the systematic p/q-rep design;
- 2. Where is most of the information about Rows confounded in the two-phase design?
- 3. What are the effects on the analysis of being able to describe the Locations differences in terms of a linear trend term instead of arbitrary differences between Locations?

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