DiGGer User Book

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Chapter 1

Introduction

DiGGer is a flexible tool for finding experimental designs that are efficient for specified blocking and correlation patterns. The package DiGGer ("NSW Dpi Biometrics Software Download Page" 2018) is an add-on for the statistical computing language and environment R (R Core Team 2015). DiGGer provides object oriented methods through two additional required R packages: R.methodsS3 and R.oo. DiGGer is available for Windows 32/64, Linux and MacOSX. The versions for Mac and Linux require gfortran to be installed.

Constructor functions are used to create the instructions required for a search. Constructor functions begin with capitals while camelCase is used for function and variable names.

To create a design search DiGGer requires

- a design layout specified as
 - rowsInDesign
 - columnsInDesign
 - optionally rowsInReplicate
 - optionally columnsInReplicate
- treatment information
 - numberOfTreatments
 - optionally treatRepPerRep
 - optionally treatGroup
- objectives to be optimised with blocks, linear covariates and correlation between plots specified

• search control parameters for each search phase, giving the number of interchanges to test, optimality measure, swap restrictions and correlation block size.

From an initial design a DiGGer search when run interchanges 2 treatments and calculates a new objective measure of design efficiency. The new design is either accepted or rejected based on rules in the Reactive Tabu Search (RTS) algorithm (Battiti and Tecchiolli (1994), Coombes (2002)). The search continues until stopping rules are met. The objective measure is an A value, related to the average variance of pairwise comparisons of treatments of interest. Lower values are better for the postulated correlation pattern. After the search the DiGGer object has a component, \$dlist, containing the field book listing of the design.

The constructor functions: DiGGer, Block, Correlation, Objective and Phase may be used to construct a design search (see Section 4). Users however, will generally choose to use wrapper functions which create searches for particular design types. The wrapper functions in this version are

- corDiGGer for general block designs with correlated errors and single treatment factors
- ibDiGGer for incomplete block designs
- rcDiGGer for row-column designs
- prDiGGer for partially replicated designs which must have a number of unreplicated treatments
- facDiGGer for designs with factorial treatments
- r2dDiGGer for strict two-directional replicates
- nurseryDiGGer for replicated designs with additional high frequency check treatments

DiGGer was developed for field designs in rectangular arrays of plots so all design searches use specifications of rectangular layouts and block structures. For some of the design types listed these rectangular specifications may be nominal and may not correspond to actual physical layouts.

This version of DiGGer differs from previous versions with more uniform syntax and random number generator seeds that allow the recovery of particular designs. The random number generator is initialised in R and the current state of the random number generator is passed to the Fortran program when the search is run. The Fortran program uses a version of RTS to find near

optimal designs for the specified objective.

Section 2 gives some preliminary concepts concerning design searches. Section 3 details the constructor functions, Section 4 illustrates the use of constructor functions in creating a block design. These two sections provide background information on the internal workings of the wrapper functions and may be skipped in an initial reading. Section 5 presents the wrapper functions with some examples and Section 6 gives examples of the flexibility that DiGGer provides.

The R Help gives details of the full range of functions in the DiGGer package.

Chapter 2

Preliminary concepts

2.1 What is a design?

In DiGGer a design is a matrix of design numbers. The design numbers are consecutive, 1 to numberOfTreatments, at the appropriate replication. Each number represents a treatment applied to an experimental unit, or plot, in the trial or experiment. The matrix has rowsInDesign rows and columnsInDesign columns. Field experiments are usually physically arranged in rows and columns but many experiments can be notionally described in terms of rows and columns.

The design may be arranged in replicates in a Randomised Complete Block (RCB) design. Each replicate defined by rowsInReplicate and columnsInReplicate has treatments repeated according to treatRepPerRep.

treatRepPerRep is a vector numberOfTreatments long with the relative replication levels for each treatment in a replicate.

k*sum(treatRepPerRep)=rowsInReplicate*columnsInReplicate, k an integer. DiGGer will randomise k repeats of the replication scheme within each replicate.

The blocks with template [rowsInReplicate × columnsInReplicate] must tile evenly within the design (Figure 2.1). All blocks tile from Row 1, Column (or Range) 1.

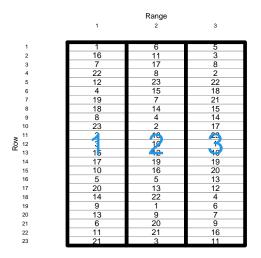


Figure 2.1: Tiling of replicates within a design

If the design is completely randomised (CR) then rowsInReplicate = rowsInDesign and columnsInReplicate = columnsInDesign.

2.2 Design properties

2.2.1 Blocks

The design may be divided into blocks. Blocks specify sections of the design with more similar experimental material. Block objects in DiGGer are defined with three parameters:

- rowsInBlock
- columnsInBlock
- blockVarianceRatio.

If the blockVarianceRatio > 0 then blocks are random, otherwise blocks are fixed. Blocks tile down and across the design from (Row 1, Column 1)

using the block template, [rowsInDesign \times columnsInDesign] (Figure 2.2). Blocks may tile unevenly:

- the final row of blocks may have fewer than rowsInBlock rows
- the final column of blocks may have fewer than columnsInBlock columns.

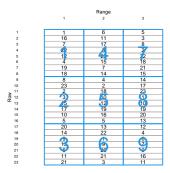


Figure 2.2: Tiling of blocks within a design. The final row of blocks (3,6,9) has one fewer row than the other blocks.

2.2.2 Blocking sequence

The blocking sequence is a list of dimension pairs

```
blockSequence = list(c(r1, c1), c(r2, c2), \ldots).
```

Each dimension pair in the list is used to create up to three sets of blocks for a search phase, the pair c(r1, c1) produces:

- Row blocks across the design with r1 rows: [r1 × columnsInDesign]
- Column blocks down the design with c1 columns: [rowsInDesign × c1]
- Intersection blocks: $[r1 \times c1]$

Redundant blocks created by the above procedure should be automatically dropped from the search specifications. Figure 2.3 shows the three sets of blocks.

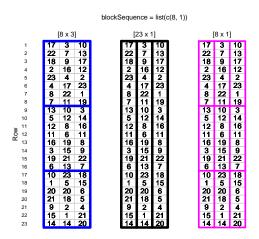


Figure 2.3: Blocking induced by blockSequence = list(c(8, 1)): $[8 \times 3]$, $[23 \times 1]$ and $[8 \times 1]$.

Note that the set of intersection blocks is nested, or completely contained, within the other blocking structures. The relative importance of these blocking structures is controlled through objectiveWeight or blockVarianceRatio specifications.

2.2.3 Correlation

Correlation may be defined across the whole of the design or within independent blocks which must tile evenly into the design. There are three models for the correlation that may occur between plots within blocks: Identity (ID), AutoRegressive (AR) and Moving Average MA.

- ID, equal correlation between plots within a block
- AR, the correlation $(\rho: -1.0 < \rho < 1.0)$ between plots decreases with the separation of plots $\rho^{|i-j|}$, with i and j either row numbers or column numbers
- MA, adjacent experimental units are correlated ($\rho: -0.5 < \rho < 0.5$) but others are not correlated.

The correlation model assumes that the row correlation model and the column correlation model represent separable processes and the overall correlation is formed by the kronecker product of these correlations. For the $AR \otimes AR$ model treatment neighbours will tend to be balanced across rows and columns. The model ensures that the same treatment is strongly discouraged from occurring next to itself in rows or columns but it encourages a treatment to occur diagonally adjacent to itself as a self-diagonal pair. One reason to introduce blocking into the design is to reduce the possibility of self-diagonals.

Although it is not possible to know the true correlation between units in an experimental design the default AR model has been shown to be appropriate in many field designs. The designs produced are robust to misspecification of the correlation parameters. The designs produced for particular AR models are only marginally less efficient for AR models with different parameters.

2.2.4 Efficiency of the design

There are a number of ways of defining the efficiency of a design. The efficiency depends on the placement of treatments in the design, the blocks in the design and the assumed correlation across the design. DiGGer uses an A efficiency measure to compare candidate designs in a search. The A-measure is the average variance of comparisons between pairs of treatments in the design. By minimising the A-measure DiGGer finds near optimal designs for given blocking and correlation structures.

Mathematically the information matrix, C, of a design adjusted for nuisance fixed effects is

$$\mathbf{C} = \mathbf{X}_1' \mathbf{\Lambda}^* \mathbf{X}_1$$

$$\mathbf{\Lambda}^* = \mathbf{\Lambda}^{-1} - \mathbf{\Lambda}^{-1} \mathbf{X}_2 (\mathbf{X}_2' \mathbf{\Lambda}^{-1} \mathbf{X}_2)^{-1} \mathbf{X}_2' \mathbf{\Lambda}^{-1}$$

$$\mathbf{\Lambda} = \sum \gamma_{b_i} \mathbf{Z}_{b_i} \mathbf{Z}_{b_i}' + \gamma_s \mathbf{\Sigma}_c \otimes \mathbf{\Sigma}_r$$

where

 X_1 is the design matrix for the treatments

 X_2 is the design matrix for nuisance fixed effects such as the overall mean, fixed blocks and linear trend in rows or columns

 Λ is the covariance matrix between plots of the design

 Λ^* is the covariance matrix adjusted for nuisance fixed effects

 \mathbf{Z}_{b_i} is the design matrix for a random block factor with variance ratio γ_{b_i}

 Σ_r is the spatial process between the rows

 Σ_c is the spatial process between the columns

 γ_s is the variance ratio associated with the spatial process.

The A value for comparing all treatments is proportional to the sum of the diagonal elements of the generalised inverse of the information matrix \mathbf{C}^- . The efficiency of the design is clearly dependent on the postulated blocking and correlation pattern in the design.

The efficiency of a design may also be calculated relative to particular treatment comparisons. Treatments may be divided into different groups of treatments and the efficiency may be based on within treatment group comparisons or between treatment group comparisons.

2.3 Searching for improvements

DiGGer is a search algorithm and requires

- an initial design
 - The initial design is a matrix of design numbers and is either generated from treatment replication and layout information or is supplied as initialDesign by the user.
- a method for changing the design
 - A design is modified by interchanging treatments that are applied to two experimental units.
 - Swap restrictions are required to preserve replicates and to preserve blocking structures that are created as part of the search. Swap restrictions may be specified by a swap block dimension pair or

may be given in matrix form using initialSwap which restricts interchanges to experimental units with the same swap code.

- an optimality/efficiency measure which depends on
 - the randomisation of the treatments
 - the correlation and blocking in the design
 - the treatments that are being compared. The default optimality is the average variance of comparisons between all pairs of treatments and is given the code A++ in DiGGer. It is 2/(numberOfTreatments 1) times the A-value of the design under the specified correlation and blocking. DiGGer aims to minimise the A-measure.
- rules to accept changes to the design
 - The algorithm in DiGGer is based on Reactive Tabu Search (RTS). It accepts any change which improves the best design in the search but allows the search to move to a poorer intermediate design when no improvement is possible from a single interchange.
 - A local minimum A-measure is reached when no treatment interchange improves the design. The search continues by choosing the best allowable interchange from a percentage of the possible interchanges as specified by the searchIntensity property of a search phase. With the default searchIntensity=100, the search for an improvement is concentrated close to the local minimum design. The lower the value of searchIntensity the more randomness is introduced into the search.
- a method to stop the search
 - a predefined maximum number of interchanges has been tested
 - a target A-measure has been bettered.

The search itself may consist of a number of component searches, or search phases.

Chapter 3

Constructor functions

The constructor functions in this version are:

- Digger which creates a Digger object with an initial design, initial swap matrix and treatment information. There is an empty slot created ready for the search specifications and results.
- Correlation defines the plot to plot correlation which may be identity, auto-regressive or moving average.
- Block defines a rectangular block factor with row, column and variance ratio properties.
- Objective defines a search objective used in the optimisation process combining correlation and block objects.
- Phase defines a search phase with swap and correlation specifications, type of optimisation measure and the objectives to be optimised.

3.1 DiGGer

The DiGGer constructor function is used to initialise a DiGGer object. It will usually be hidden within the specific design type wrapper functions but shares many function arguments with them. The arguments to DiGGer are:

- numberOfTreatments, the number of distinct treatments applied to the experimental units
- Layout information

- rowsInDesign
- columnsInDesign
- rowsInReplicate, rows in each replicate template block. If not given rowsInDesign is used.
- columnsInReplicate, columns in each replicate template block.
 If not given columnsInDesign is used.
- Treatment information
 - treatName, optional treatment label name.
 - treatNumber, optional treatment label number.
 - treatRepPerRep, vector giving the repeats of each treatment in each replicate. If not given, treatments are equally replicated.
 - treatGroup, vector of numeric codes which may be used to define comparisons of interest in the search. If not given treatments are given the same group code.
- initialDesign, an optional matrix of design numbers, 1 to numberOfTreatments, giving an initial treatment allocation. Missing plots in the matrix can be coded as a 0 design number.
- initialSwap, an optional matrix of swap codes to control allowable swaps. Treatment swaps are only possible between experimental units with the same swap code.
- rngSeeds, an optional pair of seeds for the random number generator (RNG) c(i,j) where $0 \le i \le 31328$ and $0 \le j \le 30081$. New seeds must be used to produce different designs. Best practice is to allow the DiGGer functions to create the seeds.
- rngState, the current state of the random number generator. This is useful if the search consists of a series of calls to DiGGer and the random number generator has been initialised.

After the call to DiGGer the design object will be a list with

- \$treatment a data frame with columns Name, Number, Repeats and Group and a row for each treatment.
- \$idsgn an initial design matrix.
- \$iswap an initial swap matrix.
- \$ddphase a list slot ready to be populated with search parameter information.

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3.2 Block

The Block constructor function has three parameters:

- rowsInBlock, the number of rows in a template block.
- columnsInBlock, the number of columns in a template block.
- blockVarianceRatio, the variance component ratio. If greater than zero the blocks are treated as random, otherwise blocks are treated as fixed. The use of fixed blocks with small numbers of experimental units can cause a search to crash.

The template blocks are tiled down rows and across columns of the design starting from Row 1 and Column (or Range) 1. Blocks may tile unevenly:

- the final row of blocks may have fewer than rowsInBlock rows
- the final column of blocks may have fewer than columnsInBlock columns.

3.3 Correlation

The Correlation constructor function has parameters:

- rowModel, may be "AR" for autoregressive, "MA" for moving average or "ID" for identity.
- rowParameter, for autoregressive models the parameter range is (-1,1), for moving average the parameter range is (-0.5,0.5) and the identity parameter is 0.0.
- columnModel as for the row models.
- columnParameter as for the row parameters.
- spatialVarianceRatio, the variance parameter associated with the spatial process.

3.4 Objective

The Objective constructor function combines blocks and correlation to form an objective to be optimised. The parameters to this function are:

- weight, a multiplier to give the relative importance of this objective when there are multiple objectives.
- linearCovariate, with options "ROWS", "COLUMNS" or "BOTH" to model linear trends associated with rows and columns.
- numberOfBlocks gives the number of blocking factors in the current objective.
- blocks is a list of block objects numberOfBlocks long.
- corr give a correlation object associated with the objective.

3.5 Phase

The Phase constructor combines objectives for a search and controls the search settings. The parameters of the function are:

- rowsInSwapBlock defines the number of rows in a template block in which treatment swaps are possible.
- columnsInSwapBlock defines the column dimension of the swap block.
- rowsInCorrelationBlock defines the extent of blocks with correlated experimental units. The block must tile evenly within the design layout.
- columnsInCorrelationBlock defines the column dimension of blocks with correlated experimental units.
- aType is the optimality measure used in comparing designs during a search. The default "A++" calculates an A measure using all treatment comparisons. A measures relate to the average variance of pairwise treatment comparisons. When there is more than one treatment group alternative A measures are possible. "Agg" calculates an A measure for comparisons between treatments with different group codes. Other codes: "A22" for comparisons between group 2 treatments, "A11" for comparisons between group 1 treatments, "A1+" for comparisons of group 1 treatments with others, "Aa2" for comparisons between the average of group 1 treatments with group 2 treatments and "Aaa" for the comparison between the average of group 1 and the average of group 2 treatments.
- targetAValue the objective value below which the search will stop. As the A-measures are always positive a value of 0 will not come into play as a stopping rule.

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• maxInterchanges the maximum number of treatment interchanges to test in the phase.

- searchIntensity the [0,100] percentage of swaps considered when making a non-improving treatment exchange. Zero causes a random interchange if no improvement when all possible interchanges have been considered.
- numberOfObjectives gives the number of objectives in the phase.
- objectives is a list of the objective objects.

Chapter 4

Using constructor functions

To illustrate the steps to perform a search with these functions, consider the block design in (Cochran and Cox 1957), plan 11.21, for 13 treatments in 26 blocks of 3, where the 13 by 3 blocks each contain a randomisation of three repeats of the 13 treatments. After initialising with a call to DiGGer the R object has an initial design, an initial swap matrix and the Random Number Generator (RNG) has been initialised. The block structure to be optimised is created using the Block function. There is no correlation in this design so the Correlation function creates an identity correlation object. The block and correlation objects are used in a call to the Objective function to create a search objective. The search phase is created using the Phase function. Swaps are resticted to $[13 \times 3]$ blocks. The correlation block is reduced to $[1 \times 3]$ corresponding to the size of the blocks of interest.

Besides constructor functions there are a number of modifier functions to change search settings. See the package information in the R Help for the full list. A phase may be added to the DiGGer object using one such function, addPhase(). The search may be run using the run() function.

```
b13_26x3 <- DiGGer(numberOfTreatments=13,
	rowsInDes=26, columnsInDes=3,
	rowsInRep=13, columnsInRep=3,
	rngSeeds = c(2351, 8342))
b111 <- Block(rowsInBlock=1, columnsInBlock=3,
	blockVarianceRatio=1.0)
```

The getConcurrence function tabulates the number of times that pairs of treatments occur together in blocks. For a balanced design each pair of treatments will occur together an equal number of times in blocks.

```
getConcurrence(b13_26x3)
```

```
## B RANDOM BLOCK: 1 Row by 3 Columns, VarianceRatio 1.000000
##
## Treatment-Block
##
## Number of Concurrences 0 1 2
## Number of Treatment Pairs 2 74 2
```

After 100,000 interchanges the optimal resolvable block design has not been found. Concurrences of pairs of treatments within the blocks of this design should be 0 or 1. The run() function has options for re-running or continuing the current search:

- continue=TRUE restarts the search at the current best design and repeats the final phase of the search. The tabu history is restarted.
- newpath=TRUE re-runs the search using the initial design from the original search but re-initialising the RNG so that the search path is different.
- newstart=TRUE runs the search again with a new initial design.

```
b13 26x3 <- run(b13 26x3, continue=TRUE)
getConcurrence(b13 26x3)
## B RANDOM BLOCK: 1 Row by 3 Columns, VarianceRatio 1.000000
##
## Treatment-Block
##
## Number of Concurrences
## Number of Treatment Pairs 78
The wrapper function ibDiGGer() can be used to repeat the search.
ib13 26x3 <- ibDiGGer(</pre>
    numberOfTreatments = 13,
    rowsInDesign = 26, columnsInDesign = 3,
    rowsInRep = 13, columnsInRep = 3,
    rowsInBlock = 1, columnsInBlock = 3,
    rngSeeds = c(2351, 8342))
getConcurrence(ib13 26x3)
ib13_26x3 <- run(ib13_26x3, continue=TRUE)
getConcurrence(ib13 26x3)
## B RANDOM BLOCK: 1 Row by 3 Columns, VarianceRatio 1.000000
## Treatment-Block
##
## Number of Concurrences
## Number of Treatment Pairs 78
table(getDesign(b13_26x3) - getDesign(ib13_26x3))
##
## 0
## 78
```

The designs obtained using both methods and the same RNG seeds are identical.

Chapter 5

The wrapper functions

Wrapper functions use the constructor functions to perform searches for different design types. The wrapper functions in this version are:

- corDiGGer which can perform searches for spatially adjusted incomplete block designs in the manner of the DiGGer() function in version 0.2-3.
- ibDiGGer for searches for incomplete block designs.
- rcDiGGer for row-column design searches.
- prDiGGer for partially replicated design searches.
- facDiGGer for searches for factorial and split plot designs.
- r2dDiGGer for searches with strict replication in two directions where replicates in the second set are not rectangular.
- nurseryDiGGer for replicated designs where higher frequency control treatments need to be spread regularly across the design.

5.1 General correlated designs, corDiGGer

corDiGGer is a wrapper function to perform the standard searches of the previous DiGGer versions. Standard searches consisted of a blocking phase in the absence of correlation followed by a search phase with random row and column blocks and autoregressive correlation of 0.5 between rows and between columns.

The arguments to corDiGGer are:

- numberOfTreatments
- rowsInDesign
- columnsInDesign
- rowsInReplicate
- columnsInReplicate
- blockSequence, a list of dimension pairs defining block search phases
- independentBlocks, a dimension pair defining blocks of correlated plots that must tile evenly across the design
- maxInterchanges, default 100000.
- searchIntensity, default 100. Percentage of possible interchanges to monitor when a detrimental interchange is accepted.
- aType, default "A++", compare all treatments.
- targetAValue, default 0. Search stops when A-measure falls below this value.
- runSearch, default TRUE.
- rngSeeds, default NULL.
- rngState, current state of the random number generator.
- treatName
- treatNumber
- treatRepPerRep
- treatGroup
- spatial, default TRUE, defines separable autoregressive processes for rows and columns, ("AR", 0.5), applied after the blocking search phases.
- rowColumn, default TRUE, defines random row and column blocks with variance ratio 1.0. Applied after blocking phases of the search.
- nuggetVar, default variance ratio 0.1 added for each plot in the final search phase.
- initialDesign, default NULL. Matrix of design numbers.
- initialSwap, default NULL. Dimension pair or full matrix of codes giving allowable swaps. Plots with the same code may have treatments interchanged.

The blocking phases are defined using a block sequence list, blockSequence. Each element of the list is a dimension pair, c(nr, nc) defining the shape of an individual block. Each dimension pair is combined with the overall design dimensions to define two additional block shapes:

- c(nr, nc)
 - [nr \times columnsInDesign]

```
\begin{array}{ll} - \ [{\tt rowsInDesign} \times {\tt nc}] \\ - \ [{\tt nr} \times {\tt nc}] \end{array}
```

This ensures that the strips of nr rows and the strips of nc columns can be included in the optimisation. For smaller designs these two strips define one objective and the $[nr \times nc]$ blocks define a second objective. The default weights for the objective with the larger blocks is 0.8 and the weight for the smaller block is 0.2. These weights are designed to give more emphasis to the larger blocks when replicates in two directions is the aim. The weights may need to be adjusted in cases where the block size disparity is very large or where there is unequal treatment replication. The setObjectiveWeight() function can be used to adjust weights prior to running the search. Set runSearch = FALSE in the call to corDiGGer then use the run function to run the job.

```
d18 <- corDiGGer(
  numberOfTreatments = 18,
  rowsInDesign = 18,
  columnsInDesign = 3,
  blockSequence = list(c(6,1)),
  rngSeeds = c(111, 222))
### plot(d18)</pre>
```

The desTab function calculates the frequencies of treatments occurring in blocks and shows that replicates have been set in two directions from this completely randomised initial design.

```
desTab(getDesign(d18), 18, 1)

## B1 B2 B3
## freq_1 18 18 18

desTab(getDesign(d18), 6, 3)

## B1 B2 B3
## freq 1 18 18 18
```

corDiGGer has a blockSequence = "default" option which sets up blocks that cut across replicates. The following example of 20 treatments arranged in a $[20 \times 3]$ layout with $[20 \times 1]$ replicates shows the action when replication in two directions is not possible. Four equal blocks of $[5 \times 3]$ can be formed,

equivalent to setting blockSequence = list(c(5, 1)).

```
d20 <- corDiGGer(
   numberOfTreatments = 20,
   rowsInDesign = 20, columnsInDesign = 3,
   rowsInRep = 20, columnsInRep = 1,
   blockSequence = "default",
   rngSeeds = c(111, 333))

getBlock(d20, phaseNo = 1, objectiveNo = 1,
   blockNo = 1)</pre>
```

```
## B RANDOM BLOCK: 5 Rows by 3 Columns, VarianceRatio 1.000000
getBlock(d20, 1,2,1)
```

```
## B RANDOM BLOCK: 5 Rows by 1 Column, VarianceRatio 1.000000
desTab(getDesign(d20), 5, 3)
```

```
## B1 B2 B3 B4
## freq 1 15 15 15 15
```

The treatRepPerRep parameter allows for specification of unequal replication in replicate blocks. Consider a design for 33 entries where the first treatment is replicated 4 times in each $[36 \times 1]$ replicate block in an overall $[36 \times 4]$ layout. Setting the block sequence with $[9 \times 1]$ blocks will allow for the possibility of $[9 \times 4]$ replicates with efficient $[9 \times 1]$ sub-blocks.

```
d33 <- corDiGGer(
   numberOfTreatments = 33,
   rowsInDesign = 36, columnsInDesign = 4,
   rowsInRep = 36, columnsInRep = 1,
   blockSeq = list(c(9,1)),
   treatRepPerRep= c(4,rep(1,32)),
   rngSeeds = c(111, 222))
## plot(d33)
## plot(d33, trts=1, col=2, new=FALSE)</pre>
```

```
desTab(getDesign(d33), 9, 4)
```

```
## freq 1 32 32 32 32
## freq 4 1 1
               1 1
desTab(getDesign(d33), 9, 1)
##
         B1 B2 B3 B4 B5 B6 B7 B8 B9 B10 B11 B12 B13 B14 B15 B16
## freq_1 9 9 9
                  9 9
                         9
                           9
                              9
                                 9
                                      9
                                         9
                                             9
                                                 9
                                                     9
```

The search has found replicates in two directions with each of the sixteen $[9 \times 1]$ blocks having no repeats of the higher frequency treatment.

5.2 Incomplete Block Designs, ibDiGGer

The arguments to ibDiGGer are:

- numberOfTreatments
- rowsInDesign
- columnsInDesign
- rowsInReplicate
- columnsInReplicate
- rowsInBlock
- columnsInBlock
- fixedBlocks
- blockVarianceRatio
- aType
- targetAValue
- maxInterchanges
- searchIntensity
- runSearch
- rngSeeds
- rngState
- treatName
- treatNumber
- treatRepPerRep
- treatGroup
- initialDesign
- initialSwap

Blocks to be optimised are specified by rowsInBlock and columnsInBlock. If rowsInReplicate and columnsInReplicate are supplied the design will be constrained to have replicates. Here is an example of a balanced incomplete block design. The RNG seeds have been chosen to illustrate a search which requires a continuation to find the optimum. The optimal design for random blocks with variance ratio of 1.0 was found to be 0.2857143 in a separate search. A slightly larger target A value of 0.2857145 may be specified to cause the search to stop once the A value falls below this value. The maximum interchanges to test is increased from the 100000 default to 1000000.

getConcurrence(ib19b)

```
## B RANDOM BLOCK: 1 Row by 3 Columns, VarianceRatio 1.000000
##
## Treatment-Block
##
## Number of Concurrences 0 1 2
## Number of Treatment Pairs 2 167 2
```

The getConcurrence() function tabulates the number of times that pairs of treatments occur together in blocks. If no block is specified the first block of the first objective of the first search phase is used. After this call to ibDiGGer there are 2 pairs of treatments that do not occur together in blocks and 2 pairs of treatments that occur together twice in blocks. There is an option in the run() function to continue the search with the current best design. The search history records are cleared before continuing but the current settings of the RNG, rngState, are retained for repeatability of the search.

```
ib19b <- run(ib19b, continue = TRUE)
getConcurrence(ib19b)

## B RANDOM BLOCK: 1 Row by 3 Columns, VarianceRatio 1.000000
##
## Treatment-Block

##
## Number of Concurrences 1
## Number of Treatment Pairs 171
ib19b$ddphase[[1]]$lastImprovement</pre>
```

[1] 610171

After the continuation all 171 pairs of treatments occur together once in blocks. This needed 1610171 interchanges in total.

A balanced lattice design has resolvable blocks. Again the known optimum from a previous search with random blocks can be used as a stopping rule.

```
getConcurrence(ib25s)
```

```
## B RANDOM BLOCK: 1 Row by 5 Columns, VarianceRatio 1.000000
##
## Treatment-Block
```

```
##
## Number of Concurrences 1
## Number of Treatment Pairs 300
ib25s$ddphase[[1]]$lastImprovement
## [1] 520760
```

5.3 Row-Column Designs, rcDiGGer

The arguments to the rcDiGGer function are:

- numberOfTreatments
- rowsInDesign
- columnsInDesign
- rowsInReplicate
- columnsInReplicate
- twoPhase, default TRUE, causes larger of the blocks to be optimised in the first search phase and the smaller blocks to be optimised in a second phase. The order of the optimisation can be specified as "rowThenCol" or "colThenRow". If FALSE both sets of blocks are optimised in the one search phase.
- nested, default TRUE. If TRUE block sizes are restricted to within replicates, otherwise blocks extend across the full design.
- fixedBlocks, default FALSE.
- blockGammas, default list(rGamma = 1, cGamma = 1).
- aType
- targetAValue
- maxInterchanges
- searchIntensity
- runSearch
- rngSeeds
- rngState
- treatName
- treatNumber
- treatRepPerRep
- treatGroup

- initialDesign
- initialSwap

Treatment-Block

The rows and columns may extend across the full design or they may be nested within replicates, nested = TRUE.

Row-column searches can be undertaken as two-phase searches or single phase searches. The default search action is for two-phase searches, twoPhase = TRUE. In a default two-phase search the first phase optimises the blocks, rows or columns, that are smaller. In the second phase swaps are restricted within these blocks while the other blocks are optimised. The order of optimisation can be controlled using twoPhase = "rowThenCol" or twoPhase = "colThenRow". With twoPhase = FALSE both sets of blocks are optimised in the one search phase.

These approaches are illustrated in a trial for 12 treatments in a $[3 \times 12]$ design with replicates $[3 \times 4]$. The default settings result in $[3 \times 1]$ column blocks being optimised before nested $[1 \times 4]$ row blocks. To help in efficiency calculations, fixedBlocks = TRUE.

```
test1 <- rcDiGGer(numberOfTreatments = 12,
                  rowsInDesign = 3, columnsInDesign = 12,
                  rowsInReplicate = 3, columnsInReplicate = 4,
                  maxInterchanges = 500000, fixedBlocks = TRUE,
                  rngSeeds = c(111, 222))
getConcurrence(test1, 2,1,1)
## B FIXED BLOCK: 1 Row by 4 Columns
##
## Treatment-Block
##
## Number of Concurrences
                                 1
## Number of Treatment Pairs 24 30 12
getConcurrence(test1, 2,1,2)
## B FIXED BLOCK: 3 Rows by 1 Column
##
```

[1] 0.5075503

The design efficiency is calculated from the fixed block A-measure as 2/r/A where r is the number of replicates and A is the DiGGer fixed effect aMeasure. For the test1 design it is 0.508. When row blocks are optimised before column blocks the the overall efficiency is reduced with row block concurrences better and column block concurrences worse.

```
test2 <- rcDiGGer(numberOfTreatments = 12,</pre>
                  rowsInDesign = 3, columnsInDesign = 12,
                  rowsInReplicate = 3, columnsInReplicate = 4,
                  fixedBlocks = TRUE, twoPhase = "rowThenCol",
                  rngSeeds = c(111, 222))
getConcurrence(test2, 2,1,1)
## B FIXED BLOCK: 1 Row by 4 Columns
##
## Treatment-Block
##
## Number of Concurrences
                                1 2
## Number of Treatment Pairs 21 36 9
getConcurrence(test2, 2,1,2)
## B FIXED BLOCK: 3 Rows by 1 Column
##
## Treatment-Block
##
## Number of Concurrences
                               0 1 2
## Number of Treatment Pairs 32 32 2
2/3/test2$ddphase[[2]]$aMeasures[1]
```

```
## [1] 0.5021073
```

By searching with twoPhase = FALSE the row concurrences are worse than the "rowThenCol" option. However continuing the search quickly finds an equivalent to the test1 design.

```
test3 <- rcDiGGer(numberOfTreatments = 12,
                  rowsInDesign = 3, columnsInDesign = 12,
                  rowsInReplicate = 3, columnsInReplicate = 4,
                  fixedBlocks = TRUE,
                  twoPhase = "FALSE", rngSeeds = c(111, 222))
getConcurrence(test3, 1,1,1)
## B FIXED BLOCK: 1 Row by 4 Columns
##
## Treatment-Block
##
## Number of Concurrences
                              0 1 2
## Number of Treatment Pairs 24 30 12
getConcurrence(test3, 1,1,2)
## B FIXED BLOCK: 3 Rows by 1 Column
##
## Treatment-Block
##
## Number of Concurrences
## Number of Treatment Pairs 32 32 2
2/3/test3$ddphase[[1]]$aMeasures[1]
## [1] 0.5072034
test3 <- run(test3, continue = TRUE)
getConcurrence(test3, 1,1,1)
## B FIXED BLOCK: 1 Row by 4 Columns
##
## Treatment-Block
```

[1] 0.5075503

An example of a non-resolvable row-column design for 80 entries in a $[12 \times 20]$ design is given in Venables and Eccleston (1993) with an efficiency bound of 0.8645.

[1] 0.8632279

5.4 Partially replicated designs, prDiGGer.

Partially replicated designs have some treatments that are unreplicated and rely on replicated treatments to make the trial analysable. Partially replicated design were described in Cullis, Smith, and Coombes (2006). It is recommended that at least 20% of the experimental units are occupied by replicated treatments. The aim of these experiments is usually to select promising

treatments from a set of replicated and unreplicated test treatments, with check and quality standard treatments providing the necessary replication overall to give a valid experiment.

The arguments to prDiGGer are:

- numberOfTreatments
- rowsInDesign
- columnsInDesign
- blockSequence
- betweenRowCorrModel, default "AR".
- betweenRowCorr, default 0.5.
- betweenColumnCorrModel, default "AR".
- betweenColumnCorr, default 0.5.
- treatName
- treatNumber
- treatRepPerRep
- treatGroup
- maxInterchanges, default 20000.
- targetGroup, default 1 causing "A11" optimisation in the correlation phase of the search.
- runSearch, default FALSE. Refers to the final search which spatially optimises placement of replicated treatments within blocks.
- splitOpt, default NULL. A dimension pair can be specified, c(r, c) to define blocks for sub-optimal spatial distribution of replicated entries in over-sized designs.
- rngSeeds

Group codes are used to distinguish between the different treatment types, standards and tests, with the default expectation that test treatments are coded as group 1.

prDiGGer proceeds by optimising a reduced design of replicated treatments using a scaled version of the overall block sequence. Once these blocks are established they are expanded to the size of the full design and augmented with unreplicated treatments as described in Herzberg and Jarrett (2007). The design has not been spatially optimised at this point.

The final step is to run the DiGGer object to spatially optimise the location of replicated treatments within the smallest blocks of the blocking sequence.

Deciding on the blocking sequence is a major consideration in these designs. The general recommendation is to divide the designs into blocks that correspond to the replication levels in the design.

pr293 is an unreplicated design with 288 unreplicated treatments and 5 standards each replicated 18 times. Approximately 24% of the experimental units will have replicated treatments. The block sequence has been chosen to match the replication level in the design. The $[7 \times 3]$ blocks result in 18 blocks spread across the design and should allow for each block to contain a set of the 5 standards. The sub-blocks of $[7 \times 1]$ will encourage replicated entries to be evenly placed within columns of the design.

pr118 is a partially replicated design with 56 unreplicated test treatments, 56 test treatments with two replicates and 6 standards with 4 replicates. The layout $[16 \times 12]$ suggests a nested blocking sequence:

- $[16 \times 6]$ to give 2 blocks
- $[8 \times 6]$ to give 4 blocks
- $[8 \times 1]$ to optimise column blocks.

With runSearch = TRUE the final spatial optimisation is run immediately after the blocking phase augmentation.

desTab is used to give a quick check of replication levels in each block. Notice that both the high replication treatments and the unreplicated treatments are distributed equally to the $[8 \times 6]$ blocks.

```
desTab(getDesign(pr118), 16,6)
##
          B1 B2
## freq 1 84 84
## freq 2 6 6
desTab(getDesign(pr118), 8,6)
##
          B1 B2 B3 B4
## freq 1 48 48 48 48
desTab(getDesign(pr118), 8,1)
##
          B1 B2 B3 B4 B5 B6 B7 B8 B9 B10 B11 B12 B13 B14 B15 B16 B17 B18 B19 B20
## freq 1
           8
              8
                 8
                    8
                          8
                             8
                                8
                                        8
                                            8
                                                8
                                                    8
                                                        8
                                                             8
                                                                 8
                                                                     8
                                                                         8
                       8
                                   8
                                                                                 8
          B21 B22 B23 B24
## freq 1
            8
                8
                    8
plot(pr118, trts=57:112, col=5, new=TRUE)
plot(pr118, trts=113:118, col=2, new=FALSE)
plot(pr118, trts=1:56, col=8, new=FALSE, label=FALSE)
```

Figure 5.1 shows the design. The unreplicated treatments are not labelled and can be seen to cluster close to the higher replicated treatments 113 to 118.

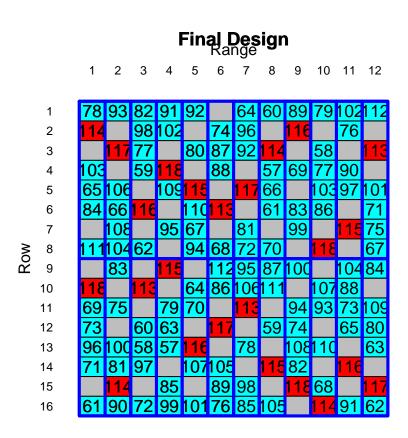


Figure 5.1: Partially replicated design for 118 treatments.

5.5 Factorial designs, facDiGGer

facDiGGer is a workaround to produce factorial designs using DiGGer. The function allocates treatment factors one at a time to the design, forming the interaction treatments at each step and using the last factor added as a group code in the search. corDiGGer is called once for each factor added. For factorial designs in general compromises are made regarding the importance of main effects and interactions in the design optimality measure. The approach used in facDiGGer is to optimise "F1", "F1:F2", ..., "F1:...:Fn" with restrictions on optimisation applied at each phase.

The arguments of facDiGGer are:

- factorNames, a text vector of factor names.
- rowsInDesign
- columnsInDesign
- rowsInReplicate
- columnsInReplicate
- mainPlotSizes, default NULL. If specified it is a sequence of block sizes defining main plot and sub-plot sizes in a split-plot design. The final pair in the list must be c(1, 1).
- treatDataFrame, gives the name of the dataframe with the factorial treatment information, see below.
- treatRepColumn, default column name in data frame "Repeats" with treatment replications per replicate.
- blockSequence
- objectiveWeight, default c(0.8, 0.2) relative weights for multiple objectives.
- searchIntensity
- chequerboard, default FALSE. Used with 2-level factors to break up the default chequerboard pattern that occurs when autoregressive correlation is present.
- spatial
- rowColumn
- designLayoutTemplate, default FALSE. An optional matrix showing replicate numbers with missing values.
- maxInterchanges
- rngSeeds

• rngState

The function expects a treatment dataframe to be supplied. The function createFactorialDF creates a dataframe ready for use by facDiGGer.

The arguments to createFactorialDF are:

- nlevelsVector
- treatName
- treatRepPerRep

After the first factor is allocated, the design for the levels of this factor is fixed. The levels of the second factor are allocated to each level of the first factor within a replicate. Treatment interchanges within replicates are restricted to interchanges between plots having the same first factor level. Before adding subsequent factors the design for the current interaction is fixed, with levels of the next factor allocated to each of the current interaction levels.

The function requires a treatment data frame with a column for each factor and the replication level of each factor combination.

A design template file may be used where there are missing plots in the rectangular design. The design template may have replicate codes which will be used to allocate replicates of the treatments from the treatment data frame. Missing plots are coded as 0.

createFactorialDF is a utility function to create treatment data frames suitable for facDiGGer.

```
DF45 <- createFactorialDF(c(3,3,5))
head(DF45)</pre>
```

```
##
      TRT F1 Fname1 F2 Fname2 F3 Fname3 Repeats
## 1
                        1
                                    1
                                           C1
        1
            1
                   Α1
                               B1
                                                      1
## 2
        2
                   Α1
                       1
                               B1
                                    2
                                           C2
                                                      1
           1
## 3
        3
                        1
                                    3
                                           C3
                                                      1
            1
                   A1
                               B1
## 4
        4
           1
                   Α1
                       1
                               B1
                                    4
                                           C4
                                                      1
## 5
        5
           1
                   A1
                        1
                               B1
                                    5
                                           C5
                                                      1
## 6
        6
           1
                   Α1
                        2
                               B2
                                    1
                                                      1
                                           C1
```

The factorNames order is the order in which factors are allocated. The allocation has better flexibility if the factors are allocated in the order of

increasing number of levels.

```
d3x3x5 <- facDiGGer(</pre>
   factorNames = c("F1", "F2", "F3"),
   rowsInDesign = 45, columnsInDesign = 3,
   rowsInRep = 45, columnsInRep = 1,
   blockSequence = list(c(15,1)),
   treatDataFrame = DF45,
   treatRepColumn = "Repeats",
   maxInt=500000, rngSeeds = c(11283, 23951))
desTab(getDesign(d3x3x5),15,3)
##
         B1 B2 B3
## freq 1 45 45 45
desTab(matrix(d3x3x5$dlist$F1,45),15,1)
##
         B1 B2 B3 B4 B5 B6 B7 B8 B9
## freq 5 3 3 3 3 3 3 3 3
desTab(matrix(d3x3x5\$dlist\$F2,45),15,1)
##
         B1 B2 B3 B4 B5 B6 B7 B8 B9
## freq 5 3 3 3 3 3 3 3 3
desTab(matrix(d3x3x5$dlist$F3,45),15,1)
##
         B1 B2 B3 B4 B5 B6 B7 B8 B9
## freq 3 5
             5
                5
                  5
                         5
                     5
                            5
                              5
```

Tabulation shows replicates in the second direction and the $[15 \times 1]$ blocks have balanced allocation of main effect levels. If the factor order is changed so that the 5 level factor is not last the third factor allocated is not balanced within 15 unit blocks (not shown).

The example in Section 3.2 of Cochran and Cox (1957) is a factorial with added control with unequally replicated treatments.

```
DF9 <- createFactorialDF(
    c(2,3,5),
    treatName=list(Control = c("Control", "Treated"),</pre>
```

	TRT	F1	Control	F2	Level	F3	Fumigant	Repeats
1	1	1	Control	1	0	1	Nil	4
22	22	2	Treated	2	1	2	CN	1
23	23	2	Treated	2	1	3	CS	1
24	24	2	Treated	2	1	4	CM	1
25	25	2	Treated	2	1	5	CK	1
27	27	2	Treated	3	2	2	CN	1
28	28	2	Treated	3	2	3	CS	1
29	29	2	Treated	3	2	4	CM	1
30	30	2	Treated	3	2	5	CK	1

Table 5.1: Data frame DF9.

```
Level = c(0,1,2),
    Fumigant = c("Nil", "CN", "CS", "CM", "CK")))
DF9 <- DF9[-c(2:15,16:20,21,26),]
DF9$Repeats <- rep(c(4,1), c(1,8))</pre>
```

Table 5.1 shows the factor order and replication levels. The argument chequerboard is used with two-level factors. When set TRUE the standard spatial model is used with two-level factors resulting in chequerboard self-diagonals of the levels. Setting blockSequence = c(1,1) is a special case which fits row and column blocks in one objective and spatial correlation in second objective.

```
test9x <- facDiGGer(
   factorNames = c("Control","Level","Fumigant"),
   rowsInDesign = 6, columnsInDesign = 8,
   rowsInRepl = 3, columnsInRep = 4,
   blockSequence = list(c(1,1)),
   chequerboard = TRUE,
   treatDataFrame=DF9, rngSeeds = c(111,444))</pre>
```

The resulting design sequence is shown in Figure 5.2. The two-level factor is allocated initially respecting replicate blocks. The second three-level factor is allocated respecting the allocated control treatments within replicates. The final treatment allocation has less flexibility as the replicates and previously

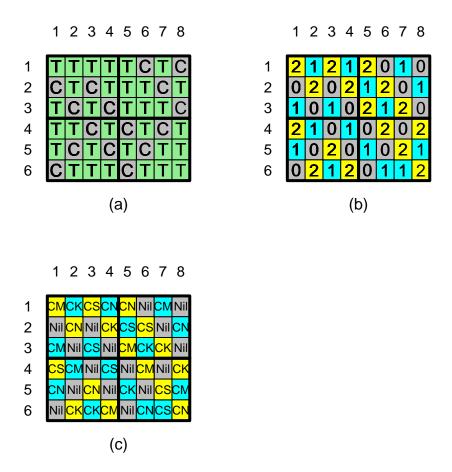


Figure 5.2: Sequential allocation: (a) Control, (b) Level within Control and (c) Fumigant within Control:Level.

allocated treatments must be respected. At each phase the added treatment is used to define a group code to use with aType = "Agg" (Table 5.2. This optimises on comparisons between treatments with different levels of the last factor added.

Phase	Treatments in design	Levels in design	Group code basis
1	Control	2	N/A
2	Control:Level	3	Level
3	Control:Level:Fumigant	9	Fumigant

Table 5.2: Sequential allocation of treatments

Split-plot designs rely on settings of mainPlotSizes to define the nested main plot sizes in split-plot designs. After the split-plot search phases mainPlotSizes should be c(1,1). Consider a trial with a 3-level factor in main plots and a 5-level factor on experimental units. The block structure of this experiment is:

```
Design: [15 × 3]
Replicate: [15 × 1]
Main plot: [5 × 1]
Sub-plot: [1 × 1]
```

```
DF15 <- createFactorialDF(c(3,5))
sp3x5 <- facDiGGer(
  factorNames = c("F1", "F2"),
  rowsInDesign = 15, columnsInDesign = 3,
  rowsInRep = 15, columnsInRep = 1,
  mainPlotSizes = list(c(5,1), c(1,1)),
  treatDataFrame = DF15,
  treatRepColumn = "Repeats",
  maxInt=100000)</pre>
```

```
plot(sp3x5, trts=1:5, col=5, new=TRUE, label=FALSE)
plot(sp3x5, trts=6:10, col=7, new=FALSE, label=FALSE)
plot(sp3x5, trts=11:15, col=8, new=FALSE, label=FALSE)
desPlot(matrix(sp3x5$dlist$F2,15), new=FALSE)
```

	Final Design				
	1	2	3		
1	3	5	5		
2	5	5 3	4		
3	1	4	1		
4	2	1	2		
5	4	2			
6	3	2	3 4 3 5 2		
7	2 4 5	4	3		
Row 8	4	3	5		
9	5	1	2		
10	1	5	1		
11	1	5	1		
12	3	2	3		
13	3 2 5	5 5 2 3 4	3 4 2 5		
14	5	4	2		
15	4	1	5		

Figure 5.3: Split plot design for 3 main plot and 5 sub-plot treatments.

5.6 Strict 2D designs, r2dDiGGer

r2dDiGGer forces strict replication in two directions even when the number of replicates do not evenly divide the design dimensions.

The arguments to r2dDiGGer are:

- numberOfTreatments
- rowsInDesign
- columnsInDesign
- rowsInReplicate
- columnsInReplicate
- maxInterchanges, default 100000.
- searchIntensity, default 100. Percentage of possible interchanges to monitor when a detrimental interchange is accepted.
- aType, default "A++", compare all treatments.
- targetAValue, default 0. Search stops when A measure falls below this value
- runSearch, default TRUE.
- rngSeeds, default NULL.
- rngState, current state of the random number generator.
- treatName
- treatNumber
- treatRepPerRep
- treatGroup
- spatial, default TRUE, defines separable autoregressive processes for rows and columns, ("AR", 0.5), applied after the blocking search phases.
- rowColumn, default TRUE, defines random row and column blocks with variance ratio 1.0. Applied after blocking phases of the search.
- nuggetVar, default variance ratio 0.1 added for each plot in the final search phase.
- initialDesign, default NULL. Matrix of design numbers.
- initialSwap, default NULL. Dimension pair or full matrix of codes giving allowable swaps. Plots with the same code may have treatments interchanged.

Strict replication in two dimensions was requested to ensure that any single treatment was spread in well separated zones where rectangular replicates were not possible. The restrictions on randomisation imposed by replication

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in two directions are that treatments are divided into sets that:

- always occur together in blocks
- occur with other sets in one block
- never occur together in blocks.

The 20 treatment example looked at in Section 5.1 can be replicated in two directions using r2dDiGGer.

(d20aT) Non-rectangular replicates in two directions, d20a.

5.7 High frequency control replicated designs, nurseryDiGGer

The nurseryDiGGer wrapper function was written to distribute high frequency check treatments evenly across a design where all treatments are replicated. The initial case was a disease nursery where varieties of known susceptibility needed to be spread across the design to monitor the disease pressure across a trial. The principle used in creating the design was to begin with an unreplicated design using only the high frequency controls as replicated treatments. The high frequency controls would be spread across the design to maximise the information about the remaining plots. The second phase of the search keeps the controls in fixed positions and distributes the remaining treatments around them. In some cases there are complete block replicates which need to be respected. Blocking sequences can be used in distributing the extra treatments across the design.

The arguments to nurseryDiGGer are:

- numberOfTreatments
- rowsInDesign
- columnsInDesign
- rowsInReplicate

	Range				
	1	2	3		
1	16	5	10		
2	2 8	15	12		
3	8	9	19		
4	6	18	4		
5	1	17 3	13		
6	14	3	7		
7	11	20	14		
8	12	4	17		
9	13 15	8	16		
Ø 10 ₩ 11	15	19	6		
ĭ 11	10	2 7	9		
12	20	7	1		
13	5	11	3 5		
14	18	1	5		
15	7	10	18		
16	17	6	2		
17	9	13	20		
18	4	14	15		
19	3	12	8		
20	19	16	11		

Figure 5.4: (d20aT)

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- columnsInReplicate
- blockSequence
- betweenRowCorrModel
- betweenRowCorr
- betweenColumnCorrModel
- betweenColumnCorr
- treatName
- treatNumber
- treatRepPerRep
- treatGroup
- checkGroup
- maxInterchanges
- rngSeeds

A small design for 10 treatments in a $[6 \times 9]$ design with $[6 \times 3]$ replicates illustrates the method. In each replicate two treatments have five replicates and the remaining 8 treatments have no repeats in a replicate.

```
ny1 <- nurseryDiGGer(
   numberOfTreatments = 10,
   rowsInDesign = 6, columnsInDesign = 9,
   rowsInRep = 6, columnsInRep = 3,
   blockSeq = list(c(6,1), c(3,1)),
   treatRep = rep(c(5,1),c(2,8)),
   treatGroup = rep(c(2,1), c(2,8)),
   checkGroup = 2, rngSeeds = c(4964, 17712))</pre>
```

The block sequence first blocks to $[6 \times 1]$ columns followed by $[3 \times 1]$ sub-columns which also induce $[3 \times 9]$ blocks.

Consider an example where the controls do not split neatly into replicates. A $[90 \times 12]$ design has 233 entries with 3 replicates, 4 entries with 76 replicates and one entry with 77 replicates. The blocking sequence should include $[30 \times 12]$ or $[90 \times 4]$ to hold replicates of the 3 replicate entries. By specifying $[30 \times 4]$ blocks both the 3 replicate blocks would be induced. Depending on

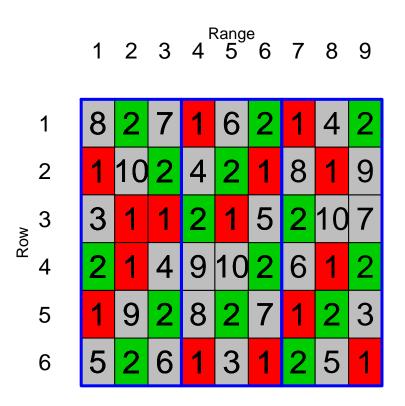


Figure 5.5: Nursery design with defined replicates.

5.7. HIGH FREQUENCY CONTROL REPLICATED DESIGNS, NURSERYDIGGER55

plot shape it may be sensible to include $[15 \times 1]$ blocks which give 72 small blocks nearly corresponding to the maximum replication levels.

```
ny238 <- nurseryDiGGer(</pre>
  numberOfTreatments = 238,
  rowsInDesign = 90, columnsInDesign = 12,
  rowsInRep = 90, columnsInRep = 12,
  treatRep = rep(c(3,76,77),c(233,4,1)),
  treatGroup = rep(c(1,2),c(233,5)),
  blockSequence = list(c(30,4), c(15,1)),
  checkGroup = 2, rngSeeds = c(4660, 21436))
    plot(ny238, trts=1:5 + 233, col = 2)
desTab(getDesign(ny238), 30,12)
##
                B2
                     ВЗ
            B1
           139 142 141
## freq 1
## freq 2
                41
            44
                     43
## freq 3
             2
                  3
                      2
                  3
## freq 25
             3
                      3
              2
                  2
                      2
## freq 26
desTab(getDesign(ny238), 90,4)
##
                B2
            B1
                     В3
## freq 1
           133 134 133
            50
## freq 2
                 48
                     50
## freq 3
             0
                  1
                      0
                  3
## freq 25
             3
                      3
             2
                  2
                      2
## freq 26
```

The tables show that the higher replication treatments have been evenly distributed to the proposed replicate blocks in each direction. The three replicate treatments have not. The search can be continued with a call to corDiGGer. The final search when nurseryDiGGer is run begins with the high replicate treatments in fixed positions. ny238\$iswap has swap codes that keep these treatments fixed but has no restriction on swaps between the three replicate entries. The relative importance of blocks in an objective can be controlled with the blockVarianceRatio parameters. setBlock is used to change the default interaction block variance component from 0.10 to 0.01.

The first phase maximum interchanges is changed to 200000.

```
ny238a <- corDiGGer(
  238, 90, 12, 90, 12,
 treatRep = rep(c(3, 76, 77), c(233, 4, 1)),
 treatGroup = rep(c(1, 2), c(233, 5)),
 blockSequence = list(c(30, 4), c(15, 1)),
 rngState = ny238\$.rng,
  initialDesign = getDesign(ny238),
  initialSwap = ny238$iswap, runSearch = FALSE)
setBlock(ny238a, phaseNo = 1, objectiveNo = 1, blockNo = 3,
         rowsInBlock = 30, columnsInBlock = 4,
         blockVarianceRatio = 0.01)
setMaxInterchanges(ny238a, phaseNo = 1, maxInt = 200000)
ny238a < run(ny238a)
desTab(getDesign(ny238a),30,12)
            B1 B2 B3
          233 233 233
## freq 1
                     3
## freq 25
             3
                 3
## freq 26
             2
                 2
                     2
desTab(getDesign(ny238a),90,4)
##
            B1 B2 B3
          233 233 233
## freq 1
## freq 25
             3
                 3
                     3
                 2
                     2
             2
## freq_26
desTab(getDesign(ny238a),30,4)
##
         B1 B2 B3 B4 B5 B6 B7 B8 B9
## freq 1 77 77 79 78 78 77 78 78 77
## freq 8 2 2 4
                   3
                      3
                         2
                            3
                                3
## freq_9 3 3 1
                      2
                    2
                         3 2
                                2
                                  3
```

The 3 replicate treatments are now replicated in two directions.

Chapter 6

Miscellaneous examples

In this section example designs illustrate some flexible features of the DiGGer search program.

6.1 Missing plots

Designs with missing plots can be handled in corDiGGer using initial designs with the missing plots coded as 0. Designs with missing plots must have:

- replicate dimensions equivalent to design dimensions
- correlation block dimensions equivalent to design dimensions.

6.1.1 Missing plots in a completely randomised design

Johnstone (2003) describes an experiment in a $[16 \times 11]$ design where the preparation of some internal plots failed and rows of the design had a gradation of dampness and shade which left some lower boundary plots unusable. The available plots are given as non-zero entries in an initial design matrix id0.

```
pl0 <- matrix(1,16,11)
pl0[c(2,10,15,22,44,48,64,80,92,93,94,95,96,104,111,112,
120,127,128,132,135,142,143,144,146,158,159,160,
169,174,175,176)] <- 0
```

```
# initial reps in row order
pl0 <- t(pl0)
id0 <- pl0
id0[pl0==1] \leftarrow c(sample(8), sample(8), sample(8),
                  sample(8),sample(8),sample(8),
                  sample(8),sample(8),sample(8),
                  sample(8),sample(8),sample(8),
                  sample(8),sample(8),sample(8),
                  sample(8),sample(8),sample(8))
pl0 <- t(pl0)
id0 \leftarrow t(id0)
zcol <- rainbow(8)</pre>
par(mfrow = c(1,2), mar = c(2,1,3,1)+0.1)
desPlot(pl0, 0, col = 8, new = TRUE,
        label = FALSE, border = FALSE,
        cstr = "", rstr = "")
desPlot(pl0, 1, col = 7, new = FALSE,
        label = FALSE, lwd = 3)
mtext('(a)', side = 1)
desPlot(id0,0,col=8,new=TRUE,
        label = FALSE, border=FALSE, cstr="", rstr="")
for (i in seq(8)){
  desPlot(id0,i,col=zcol[i],new=FALSE)
}
desPlot(id0, new=FALSE, label=FALSE, bdef=cbind(4,3), bwd=8)
```

Figure 6.1 shows the available plots and the locations of missing plots. The allocation of initial treatments was done row-wise but swaps were allowed across the full design. Blocks of $[4 \times 3]$ were used to spread treatments across the design. Row and column blocks were specified by c(1,1) in the block sequence. This results in multiple objectives in the final search phase:

desPlot(id0,new=FALSE,label=FALSE,bdef=cbind(4,3),bwd=4,bcol=7)

• random rows and columns with objective weight 0.8

mtext('(b)', side = 1)

• autoregressive processes with parameter 0.5 between rows and between columns and objective weight 0.2.

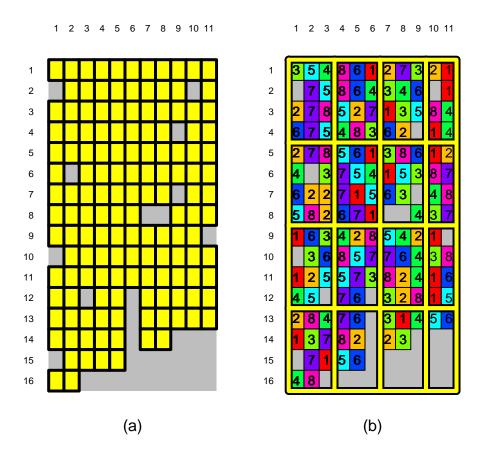


Figure 6.1: Design layout showing: (a) available plots and (b) an initial design showing proposed blocks.

```
mp1 <- corDiGGer(
   numberOfTreatments = 8,
   rowsInDesign = 16, columnsInDesign = 11,
   blockSeq = list(c(4, 3), c(1, 1)),
   initialDesign = id0,
   rngSeeds = c(4548, 9319))</pre>
```

Tables of the resulting design show that treatments have been spread across the design.

```
desTab(getDesign(mp1), 4, 11)
##
         B1 B2 B3 B4
## freq 2
          0
             0
                0
                  7
## freq_3
          1 0 0
## freq_4 0 1 1 0
## freq_5
          7 8 8 0
          1 0 0 0
## freq 6
## freq 21 0 0 0 1
desTab(getDesign(mp1), 16, 3)
         B1 B2 B3 B4
##
## freq_3
          0
             0
               0
                   8
## freq 4
         0 0
                3
                   0
## freq_5 6 7 5 0
## freq 6 3 1 0
                  0
## freq 7 0 1 0 0
            0
## freq 8
          0
               0
                   1
## freq 11 0 0 1
                   0
desTab(getDesign(mp1), 1, 11)
##
         B1 B2 B3 B4 B5 B6 B7 B8 B9 B10 B11 B12 B13 B14 B15 B16
            7
                  7
                    5
                       7
                          7
                             7
                               7
                                   7
                                       5
                                           7
                                               7
                                                  7
                                                         2
## freq 1 5
               5
## freq_2 3
            2
               3
                  2
                    3
                       2
                          2
                             2
                                2
                                   2
                                       3
                                           2
                                              2
                                                  0
                                                      0
                                                         0
               0 0 0 0 0 0
                                                         0
## freq 4 0 0
                                   0
                                       0
                                           0
                                              0
                                                  1
                                                      0
            0 0
                  0 0
                       0 0 0 0
                                   0
                                       0
                                           0
                                              0
                                                  0
                                                      1
                                                         0
## freq_7 0
## freq 9 0 0 0 0 0 0 0 0
                                   0
                                       0
                                           0
                                              0
                                                  0
                                                      0
                                                         1
```

```
desTab(getDesign(mp1), 16, 1)
##
           B1 B2 B3 B4 B5 B6 B7 B8 B9 B10 B11
                   2
                      2
                          2
                                       5
## freq 1
            3
                             5
                                3
                                   3
                                           4
                                                4
## freq 2 5
               7
                  7
                      7
                         7
                             3
                                5
                                   5
                                       3
                                                4
                                           4
## freq 3 1
               0
                   0
                      0
                         0
                             0
                                1
                                   1
                                       0
                                           0
                                                0
## freq 4 0
                  0
                                0
                                   0
               0
                      0
                         0
                             0
                                       0
                                           1
                                                1
## freq 5 0
               0
                   0
                      0
                         0
                                0
                                   0
                                           0
                                                0
                             1
                                       1
desTab(getDesign(mp1), 4, 3)
##
           B1 B2 B3 B4 B5 B6 B7 B8 B9 B10 B11 B12 B13 B14 B15 B16
## freq 1
               6
                                                                      2
            6
                   6
                      6
                         4
                             4
                                6
                                   6
                                       6
                                           7
                                                4
                                                    5
                                                         8
                                                             8
                                                                  8
## freq 2 3
               3
                   3
                      3
                         4
                             4
                                3
                                   0
                                       3
                                                4
                                                    0
                                                             0
                                                                  0
                                                                      0
                                           1
                                                         0
## freq 3 0
                                0
                                                                      0
               0
                   0
                      0
                         0
                             0
                                   0
                                       0
                                           1
                                                0
                                                    0
                                                         0
                                                             0
                                                                  0
## freq 6
               0
                   0
                      0
                         0
                             0
                                0
                                       0
                                           0
                                                0
                                                    0
                                                         0
                                                             0
                                                                  0
                                                                      1
            0
                                   1
## freq 7 0
               0
                  0
                      0
                         0
                                0
                                           0
                                                0
                                                    1
                                                         0
                                                             0
                                                                  0
                                                                      0
```

The final design is shown in Figure 6.2.

6.1.2 Missing plots in a replicated complete block design

Another example that requires missing plots is the situation where 17 treatments with 3 replicates are to fit in a $[6 \times 9]$ design. Two options could be considered:

- three identical $[6 \times 3]$ blocks with 1 missing plot
- interlocking replicates with the last 3 plots missing

In the code that follows swap matrices are created and initial allocations of 17 treatments are formed from them.

```
s17a <- matrix(rep(c(1,0,2,0,3,0), c(17,1,17,1,17,1)), 6)
m17a <- s17a
s17b <- matrix(rep(c(1,2,3,0), c(17,17,17,3)),6)
m17b <- s17b
for (i in seq(3)){
    m17a[s17a == i] <- sample(17)</pre>
```

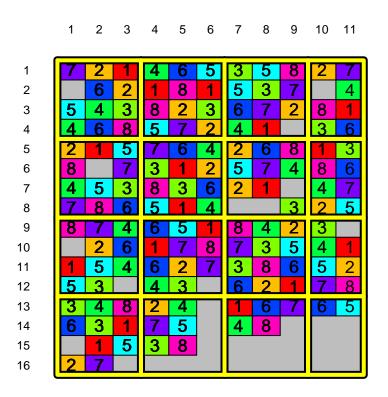


Figure 6.2: Final design with blocks and missing plots.

```
m17b[s17b == i] <- sample(17)
}
```

Searches can now be run restricting swaps using initialSwap acting on initial designs provided by initialDesign.

```
mp2a <- corDiGGer(
    numberOfTreatments = 17,
    rowsInDesign = 6, columnsInDesign = 9,
    blockSequence = list(c(2,3)),
    initialDesign = m17a,
    initialSwap = s17a)

mp2b <- corDiGGer(
    numberOfTreatments = 17,
    rowsInDesign = 6, columnsInDesign = 9,
    blockSequence = list(c(2,3)),
    initialDesign = m17b,
    initialSwap = s17b)</pre>
```

The first search phase splits the design into $[2 \times 3]$ blocks which will have unequal numbers of treatments. The final search phase has the standard objective of spatial plus random rows and columns.

The final designs are shown in Figure 6.3.

6.1.3 Missing plots in a factorial design

A design for 41 treatments was required for 4 varieties by 10 treatments with added control. The control treatment was to be included 4 times in each replicate. The design was $[15 \times 12]$ with replicates $[15 \times 3]$ with one missing plot per replicate.

With factorial designs a design template can be used to specify the location of the missing plots. The template may also include replicate codes. Where replicate codes are used the repeats in the treatment dataframe are repeats per replicate.

```
DF31 <- createFactorialDF(c(2,5,11))
indf <- DF31$F1 == 1 | DF31$F2 == 1 | DF31$F3 == 1</pre>
```

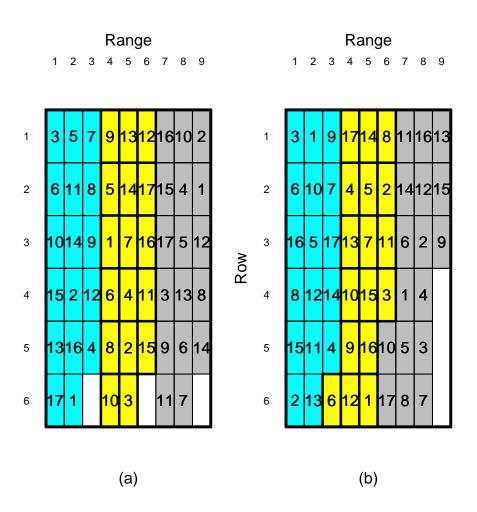


Figure 6.3: Alternative layouts with missing plots.

```
indf[1] <- FALSE
DF31 <- DF31[!indf,]
DF31$Repeats[1] <- 4
template44 <- findblks(15,12, 15,3)
template44[cbind(c(15,15,15,15),c(1,6,7,12))] <- 0</pre>
```

The template is shown in Figure 6.4 together with the design obtained with the following code.

```
f31 <- facDiGGer(
   factorNames = c("F1", "F2", "F3"),
   rowsInDesign =15, columnsInDesign =12,
   blockSeq = list(c(5, 3)),
   designLayoutTemplate = template44,
   treatDataFrame = DF31, rngSeeds = c(8871, 6732))</pre>
```

A quick indication of how overall treatments and factor levels are spread across $[5 \times 12]$ blocks can be found using desTab with groupCode} set for the factor of interest.

```
desTab(getDesign(f31), 5,12)
         B1 B2 B3
##
## freq_1 25 26 29
## freq 2 15 14 11
## freq 4 0 0 1
## freq 5 1 0 1
## freq 6 0 1 0
desTab(getDesign(f31), 5,12, groupCode = DF31$F2)
##
          B1 B2 B3
## freq_4
           0 0 1
## freq 12 1 0
## freq 13 0 1 0
## freq_14 1 2 1
## freq 15 1 0 0
## freq 17 0 1 1
## freq 18 1 0 0
```

desTab(getDesign(f31), 5,12, groupCode = DF31\$F3)

```
##
          B1 B2 B3
## freq_4
           0
              0
                 1
## freq_5
           4
              6
                 8
## freq 6
           5
              3 1
## freq_9
                 1
           1
              0
## freq_10 0
              1
                 0
```

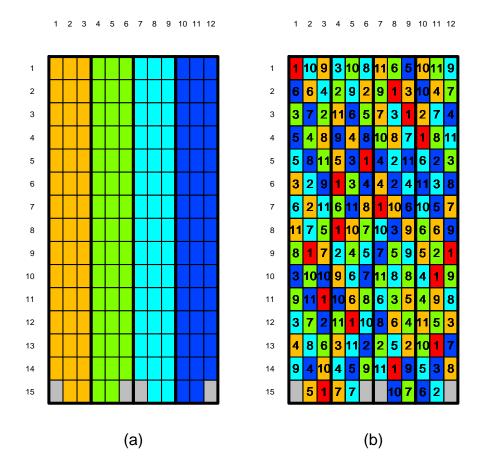


Figure 6.4: Design template (a) and final design (b) for the replicated factorial experiment with missing plots.

6.2 Restricting randomisation, a design with conditions

An initial design and an intitial swap matrix may be used to restrict randomisations to meet a researchers requirements. Consider the case where there are: - all entries included in the first $[12 \times 10]$ block of a $[24 \times 10]$ design - 39 entries with 4 replicates - 32 entries with two replicates in each block - 7 entries with one occurrence in the first block and 3 replicates in the second block - 35 entries with 2 replicates, one in each block - 14 entries with 1 occurrence in the first block only.

The first 39 entries may be split 32:7 randomly and the appropriate replications added to each $[12 \times 10]$ block.

With only 14 unreplicated entries and the restriction on randomisation corDiGGer can be used to produce an appropriate design. The initial design is supplied using initialDesign and swaps are restricted to $[12 \times 10]$ using initialSwap. Blocking using $[6 \times 5]$ blocks spread the unreplicated entries across the first major block. These are coded using blockSequence.

```
pr88 <- corDiGGer(
   numberOfTreatments = 88,
   rowsInDesign = 24, columnsInDesign = 10,
   blockSequence = list(c(6,5)),
   treatRepPerRep = c(table(idsgn)),
   initialDesign = idsgn, initialSwap=c(12,10))</pre>
```

```
desTab(getDesign(pr88), 24, 5)
```

```
##
          B1 B2
## freq 1 41 44
## freq 2 38 38
## freq_3 1 0
desTab(getDesign(pr88), 12, 10)
##
         B1 B2
## freq 1 56 35
## freq 2 32 32
## freq 3 0 7
desTab(getDesign(pr88), 6, 10)
##
          B1 B2 B3 B4
## freq 1 60 60 52 54
## freq 2 0 0 4
```

6.3 Multi-site p-rep designs

Consider an example where entries from several families are to be allocated across multiple sites. corDiGGer may be used to allocate entries to sites before each site is optimised separately. An example in Feoktistov, Pietravalle, and Heslot (2017) describes a design where 3 replicates of 400 entries from 3 families are allocated across 5 sites. The families have 14, 187 and 189 entries respectively with 240 entries to be allocated to each site. The full layout is specified as $[240 \times 5]$ and columns represent the sites. Designating replicates as $[80 \times 5]$ avoids the problem of too many possible swaps if an initial completely randomised design is used. Column blocks are specified using blockSequence and the spatial plus row-column optimisation phase is not applied. treatGroup has codes for the families and aType=Agg optimises comparisons between entries from different families.

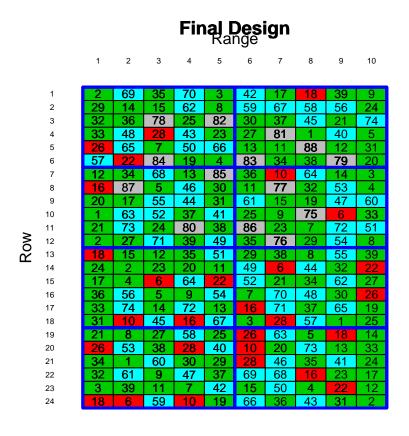


Figure 6.5: Partially replicated design with conditions.

```
maxInt=20000, rngSeeds = c(10207, 1084))
```

Tabulation is used to check family distribution to sites.

```
##
                         B4
            B1
                 B2
                     ВЗ
                              B5
## freq 1 240 240 240 240 240
##
             B1 B2 B3 B4 B5
                  0
## freq 8
               1
                     0
## freq 9
              0
                  1
                     1
                         0
                            0
## freq 112
                  1
              0
                     1
                         1
                            1
## freq 113
              1
                  0
                     0
                        0
                            0
## freq 119
              1
                  1
                     1
                         0
                            0
## freq 120
              0
                  0
                     0
                         1
                            1
```

The occurrences of each line at each site split for families is tabulated.

```
##
##
                F1 F2 F3
     0.0.1.1.1 0 19 21
##
##
     0.1.0.1.1
                 2 20 18
     0.1.1.0.1
                 1 18 21
##
     0.1.1.1.0
##
                 3 17 20
     1.0.0.1.1
##
                 2 20 18
     1.0.1.0.1
##
                 2 18 20
##
     1.0.1.1.0
                 1 18 21
                 1 17 22
##
     1.1.0.0.1
##
     1.1.0.1.0
                 0 18 22
     1.1.1.0.0
                 2 22 16
##
```

The optimisation of families within a single site is illustrated with an example from Feoktistov, Pietravalle, and Heslot (2017). Family 1 has a check variety with 9 replicates and 39 unreplicated lines. Family 2 has a check variety with 8 replicates and 39 unreplicated lines. Family 3 has a check variety with 8 replicates and 41 unreplicated lines. The $[12 \times 12]$ design can be split into 9 $[4 \times 4]$ blocks nearly corresponding to the replication levels of the check varieties. The AR1 correlation parameters are reduced to 0.1 to allow for correlation between plots but to discourage self-diagonals in the checks.

The pr122 design does not use family information to distribute the unreplicated across the design. The check entries may be held fixed while the family group codes of unreplicated lines are used in an optimisation.

```
iswap122s <- getDesign(pr122)</pre>
iswap122s[iswap122s > 3] <- 4
d122g3 <- corDiGGer(
    122, 12, 12,
   treatRep = rep(c(9,8,8,1), c(1,1,1,119)),
    treatGroup = rep(c(1,2,3,1,2,3), c(1,1,1,39,39,41)),
   blockSeq = list(c(4,4), c(4,1)),
    initialDesign = getDesign(pr122),
    initialSwap = iswap122s, rngState = pr122$.rng)
desPlot(getDesign(d122g3), trts=4:42, new=TRUE, label=FALSE,
        col='lightcyan1')
desPlot(getDesign(d122g3), trts=43:81, new=FALSE, label=FALSE,
        col='orchid1')
desPlot(getDesign(d122g3), trts=82:122, new=FALSE, label=FALSE,
        col='khaki1')
desPlot(getDesign(d122g3), trts=1, new=FALSE, label=TRUE, col=5)
desPlot(getDesign(d122g3), trts=2, new=FALSE, label=TRUE, col=6)
desPlot(getDesign(d122g3), trts=3, new=FALSE, label=TRUE, col=7,
        bdef=cbind(12,12), bcol=4, bwd=4)
```

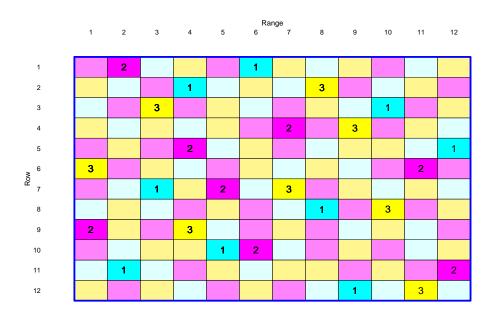


Figure 6.6: Partially replicated design showing family groups.

Chapter 7

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