# Designing comparative experiments using R (Chris Brien and Sam Rogers)

III. Multiphase and partially replicated (*p*-rep) designs

#### **Outline**

- 1. Multiphase designs.
- 2. Partially replicated designs.
- 3. Summary.

### 1. Multiphase designs

- Brien (2017) gives a review, including published applications.
- Three introductory papers are Brien and Bailey (2006), Brien et al. (2011) and Brien (2019).
- "Normal" two-phase experiments (Brien et al., 2011, Section 4) involve a single-randomization in each phase.
  - > This implies that a design is required for each phase.
  - The object of the second phase is to evaluate material produced in the first phase and one or more response variables are measured in the second phase.
  - > There may also be response variables from the first-phase.
  - The phase is the period of time during which a set of units are engaged in producing their outcome: material and/or response variables.
  - One phase might overlap another phase.



### 1.1 A simple two-phase athlete training experiment

Brien, Harch, Correll, Bailey (2011)

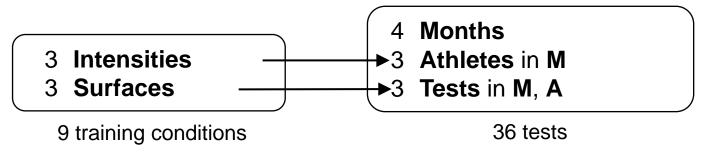
- Suppose in a simple two-phase athlete training experiment:
  - > in addition to heart rate taken immediately upon completion of a test,
  - the free haemoglobin is to be measured using blood specimens taken from the athletes after each test, which are to be transported to the lab for analysis.
- The experiment consists of a test phase and a laboratory phase:
  - > Test phase: 36 tests involving 3 athletes in each of 4 months; heart rate is measured and a blood specimen taken.
    - The unit is a test taken by an athlete.
    - The outcomes are the heart rate, a response variable, and a blood sample, material for the second phase.
  - Laboratory phase: each month 3 blood samples are taken to the laboratory for analysis.
    - The unit is a blood specimen.
    - The outcome is the free haemoglobin in the blood specimen, a response variable.



### First phase: athlete testing

Brien, Harch, Correll, Bailey (2011)

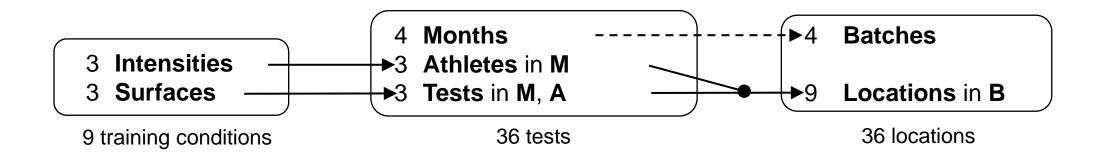
- Recall from the standard athlete training experiment in Session 1 that 9 training conditions are to be investigated:
  - > combinations of 3 surfaces and 3 intensities of training.
- In each of the 4 Months of testing:
  - > 3 endurance athletes are recruited.
  - ➤ Each athlete undergoes 3 tests, separated by 7 days, under 3 different training conditions.
- A split-unit design was employed to allocate Intensities and Surfaces.



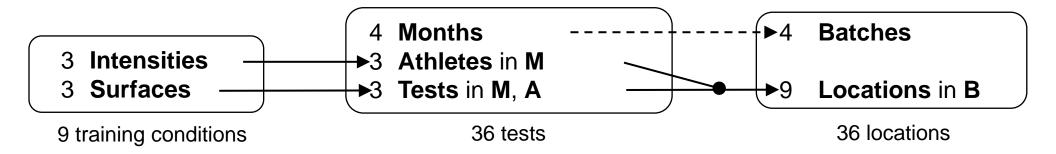
For the second phase the 36 tests need to be allocated for analysis in the laboratory.

### **Second laboratory phase**

- A restriction in the second phase:
  - > The blood specimens from the first phase need to be processed as soon as possible (not held for 4 months).
  - > Thus, the 9 specimens collected each month are to be processed together.
- Suppose that it is decided to process them in a random order,
  - That is, it is assumed that there is no systematic trend across the processing of the 9 samples so that a nested second-phase design is required.

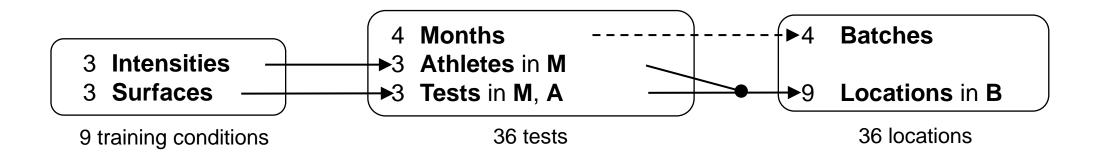


### A simple two-phase athlete training experiment (cont'd)



- It is two-phase with three sets of objects:
  - > training conditions, tests and locations:
    - training conditions are allocated in the first-phase and the second-phase i.e. only ever allocated.
    - tests are recipients factors in the second phase and are allocated factors in the second phase i.e. different roles in the two phases.
    - locations are recipient factors in the second phase i.e. only ever recipient.

### A simple two-phase athlete training experiment (cont'd)

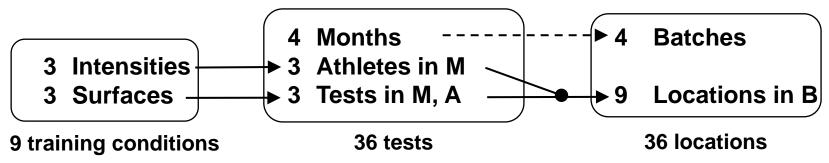


- It is described as involving two composed allocations, one of two types of allocations in a chain:
  - > Training conditions are allocated to tests and tests to locations;
- Here, the second phase begins during the first phase.
- Have not allowed for an overall, processing-order effect.
  - More about that soon.

### Randomization in the second phase

- Principle 7 (Allocate all and randomize in laboratory) (Brien et al, 2011):
  - > The laboratory-phase design should *always* allocate *all* the first-phase unit factors, as well as any laboratory treatments, to the laboratory units, using randomization wherever possible.
- As is the case for any randomization, randomizing the lab phase:
  - Guards against unanticipated systematic effects.
  - > Justifies the form of the variance matrix used for the experiment.
  - > Required for a valid estimate of error.
- Additionally, for a second (lab) phase, randomizing
  - > compensates for unfortunate randomizations in the first phase.
- However, have seen that practical problems can limit randomization.
- But, are there other reasons for not randomizing the second phase?
  - Does it make it difficult to estimate first-phase phenomena?
  - > For example, spatial correlation, linear trends, unequal variances?

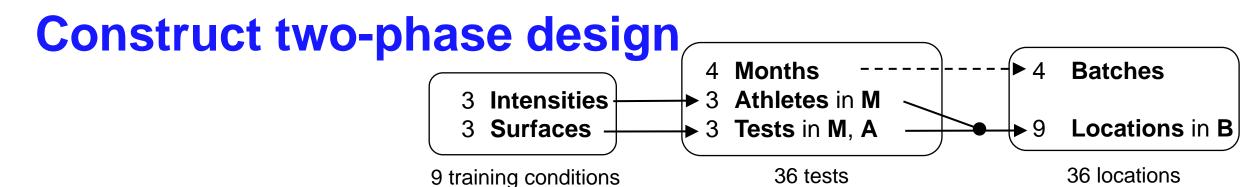
### The design species for a normal two-phase design



- The four design species for allocating sets of objects when there is an allocation in each of the two phases (Brien, 2019):
  - First-phase design: allocated and recipient objects from the first phase
     (training conditions and tests);
  - Second-phase design: first- and second-phase recipient objects
     (tests and locations);
  - Cross-phase design: first-phase allocated objects and second-phase recipient objects
    - (training conditions and locations);
  - > Two-phase or combined design: all three sets of objects.
- designTwophaseAnatomies produces the four anatomies for them,

#### The anatomy for the first phase design (from Session 1)

```
> split.canon <- designAnatomy(formulae = list(tests = ~Months/Athletes/Tests,</pre>
                                                      = ~Intensities*Surfaces),
                                                cond
+
                             data
                                         = split.lay)
+
                                                                  Formulae for recipient
 summary(split.canon, which.criteria="none")
                                                                  and allocated.
                                                              Layout is in split.lay.
Summary table of the decomposition for tests & cond
                           df1 Source.cond
 Source.tests
                                                       df2
Months
                             3
                                Intensities
Athletes[Months]
                                Residual
                                                          6
 Tests[Months:Athletes]
                            24 Surfaces
                                Intensities#Surfaces
                               Residual
                                                         18
```



Have to randomize tests (and training conditions) to locations

```
> eg1.lay <- designRandomize(allocated</pre>
                                                                = split.lay,
                                       recipient
                                                                = list(Batches = 4, Locations = 9),
                                       nested.recipients = list(Locations = "Batches");
                                                                = "Batches",
                                       except
                                       seed = 71230)
                                                                Randomized Intensities-Surfaces combinations
                                                                     C.3
                                                                                   C,1
                                                                                                  B,1
                                                                                                                B.3
                                                                     B,2
                                                                                    A,2
                                                                                                  A,2
                                                                                                                B,1
                                                                     C.1
                                                                                    B.3
                                                                                                  C.1
                                                                                                                A.3
                                                             Locations 9
                                                                     A,1
                                                                                    B,2
                                                                                                  C,3
                                                                                                                A,2
                                                                                                                          Athletes
                                                                     A,2
                                                                                    C,3
                                                                                                  C.2
                                                                                                                A.1
                                                                     B.3
                                                                                    A,3
                                                                                                  A,1
                                                                                                                C.1
                                                                     C,2
                                                                                    A,1
                                                                                                  A,3
                                                                                                                B,2
                                                                     B,1
                                                                                    C,2
                                                                                                  B,3
                                                                                                                C,3
                                                                     A,3
                                                                                                                C,2
                                                                                    B,1
                                                                                                  B,2
```

12

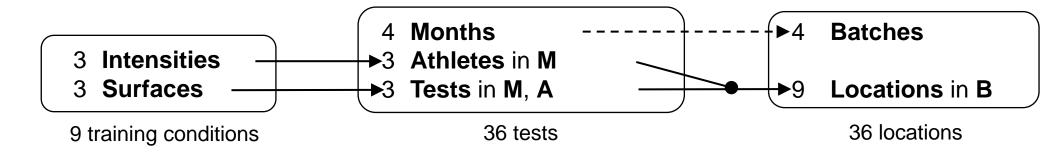
Batches (Months)

### Check properties of the multiphase design

```
eg1.canon <- designAnatomy(formulae = list(locs = ~ Batches/Locations,
                                                  test = ~ Months/Athletes/Tests,
+
                                                  cond = ~ Intensities*Surfaces),
                                data
                                          = eq1.lay)
                                                                  Three formulae reflecting the
  summary(eg1.canon, which.criteria=c("aeff", "order"))
                                                                  factor-allocation diagram
Summary table of the decomposition for locs, test & cond
                                                                  (no limit on the number).
Source.locs
                                              df2 Source.cond
                                                                        df3 aefficiency order
                   df1 Source.test
Batches
                                                                                 1,0000
                      3 Months
Locations[Batches]
                     32 Athletes[Months]
                                                 8 Intensities
                                                                                 1.0000
                                                   Residual
                                                                                 1.0000
                        Tests[Months:Athletes]
                                                24 Surfaces
                                                                                 1.0000
                                                   Intensities#Surfaces
                                                                                 1.0000
                                                   Residual
                                                                         18
                                                                                 1.0000
```

- All sources are orthogonal and all, except Months, are confounded with Locations[Batches].
- Note also that there are no residuals for Batches or Locations[Batches].
  - > They are exhaustively confounded, which will always be the case when the numbers of objects are equal for two consecutive tiers.
- Question that remains: what mixed model to fit?

#### Initial allocation model



- Initial allocation model (like the anatomy, reflects the factor allocation diagram):
  - Intensities + Surfaces + Intensities:Surfaces | Months + Months:Athletes + Months:Athletes:Tests + Batches + Batches:Locations.
- However, this model will not fit because of confounding between tests and locations.

#### **Prior allocation model**

Summary table of the decomposition for locs, test & cond

Source.locs	df1	Source.test	df2	Source.cond	df3	aefficiency	order
Batches	3	Months	3			1.0000	1
Locations[Batches]	32	Athletes[Months]	8	Intensities	2	1.0000	1
				Residual	6	1.0000	1
		Tests[Months:Athletes]	24	Surfaces	2	1.0000	1
				Intensities#Surfaces	4	1.0000	1
				Residual	18	1.0000	1

- Need to remove
  - One of Months and Batches, and make the retained term fixed:
  - Locations:Batches or both Months:Athletes and Months:Athletes:Tests.
- Must retain Months:Athletes, otherwise it would be pooled, either into Months:Athletes:Tests or Batches:Locations.
- The prior allocation model is the model for the first phase and is a model of convenience:
  - Months + Intensities + Surfaces + Intensities:Surfaces | Months:Athletes + Months:Athletes:Tests.
- The very important point is that, while they are not in the model, the lab terms contribute to those that are e.g. Months is not just due to Months differences, but is also due to Batches variance.

### 1.2 Allowing for lab order in the athletic experiment

Brien (2017)

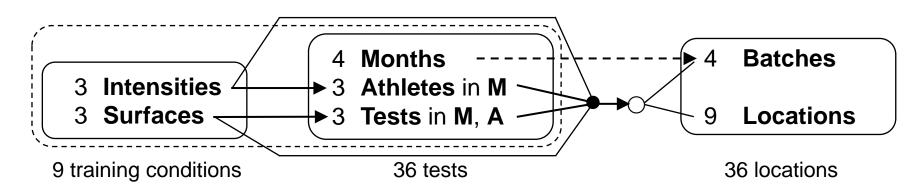
- If it is expected that there will be consistent differences between locations across the months, then the initial allocation model would be:
  - ➤ Intensities + Surfaces + Intensities:Surfaces |

    Months + Months:Athletes + Months:Athletes:Tests + The Locations term has been added.
  - > That is, Batches and Locations are now crossed (similar to RCBD versus LSD).
  - > A row-column design is required for the crossed, second phase.

### **Design considerations**

- To produce a good two-phase design, the allocation of the first phase to locations cannot ignore Intensities and Surfaces: a good cross-phase design is needed.
  - In the previous design, they could be ignored because everything within Months was being randomized to Locations within Batches.
- In addition, the second-phase design cannot be ignored because the split-unit nature of the first-phase design must be taken into account.
  - Because of the time constraints Months must be associated with Batches.
  - Within a month, assigning Athletes to triples of consecutive Locations is consistent with the use of a split-unit design in the first-phase.
  - > Tests can then be assigned to the locations within a triple.
- Thus the cross-phase design must efficiently assign Intensities to Location triples and Surfaces to the Locations within a triple.

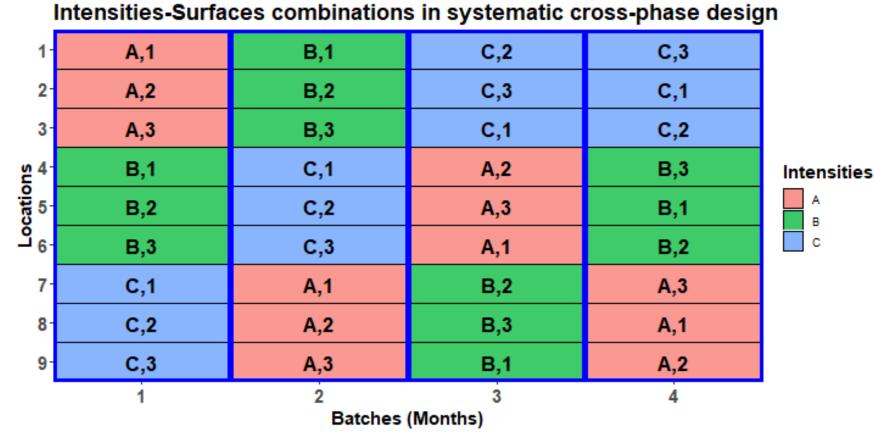
The factor allocation diagram





## Systematic cross-phase design

 A balanced factorial design (Hinkelmann & Kempthorne, 2005, section 12.5).



- A 3 × 4 extended Latin square (LS + column of repeats) is used to allocate Intensities to the triples (colours & letters);
- A  $3 \times 4$  extended Latin square is used for a Locations triple  $\times$  Batches; the same extended Latin square is used for all 3 triples.
- To ensure no repeat Intensities-Surfaces combinations for a Location, the repeated columns for the two ELSs must be associated with different Batches.
- The Intensities and Surfaces are arranged in a split-unit pattern.

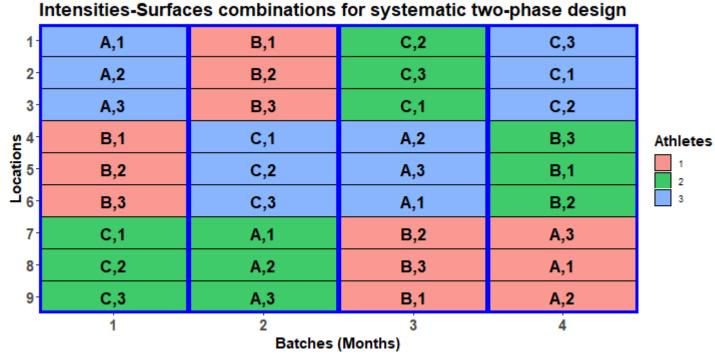


Construct a systematic second-phase design and randomize it

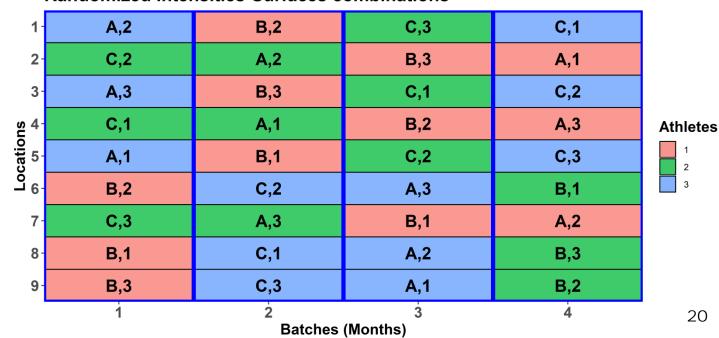
```
> #'## Generate a systematic cross-phase design for Intensities and Surfaces
> eg2.phx.sys <- cbind(fac.gen(list(Batches = 4, Locations = 9)),</pre>
                       data.frame(Intensities = factor(rep(c(designLatinSqrSys(3), c(3,2,1))),
                                                             each = 3), labels = LETTERS[1:3]),
                                   Surfaces
                                                = factor(c(rep(1:3, times = 3),
                                                            rep(1:3, times = 3),
                                                                                             An ELSD
                                                            rep(c(2,3,1), times = 3),
                                                            rep(c(3,1,2), times = 3)))))
> #'## Generate a systematic two-phase design by bringing in first-phase recipient factors
> eg2.phx.sys$Months <- eg2.phx.sys$Batches</pre>
> eg2.sys <- merge(split.lay, eg2.phx.sys) #merge on commmon factors Months, Intensities & Surfaces
> eg2.sys <- with(eg2.sys, eg2.sys[order(Batches,Locations),])</pre>
> #'## Allocate the second phase
> eg2.lay <- designRandomize(allocated = eg2.sys[c("Months", "Athletes", "Tests",</pre>
                                                    "Intensities", "Surfaces")],
                             recipient = eg2.sys[c("Batches", "Locations")],
                             except
                                        = "Batches"
                              seed
                                        = 243526)
                                                                         Don't randomize Batches.
```

### **Systematic** versus randomized designs

- The randomized design is obtained from the systematic design by permuting:
  - its rows (Locations),
  - but not its columns (Batches).



#### Randomized Intensities-Surfaces combinations



### Anatomy of the two-phase design allowing for lab processing order

Summary table of the decomposition for locs, test & cond (based on adjusted quantities)

Source.locs	df1	Source.test	df2	Source.cond	df3	aefficiency	order
Batches	3	Months	3			1.0000	1
Locations	8	Athletes[Months]	2	Intensities	2	0.0625	1
		<pre>Tests[Months:Athletes]</pre>	6	Surfaces	2	0.0625	1
				Intensities#Surfaces	4	0.2500	1
Batches#Locations	24	Athletes[Months]	6	Intensities	2	0.9375	1
				Residual	4	1.0000	1
		Tests[Months:Athletes]	18	Surfaces	2	0.9375	1
				Intensities#Surfaces	4	0.7500	1
				Residual	12	1.0000	1

The design is not orthogonal

Most of the information about Intensities and Surfaces is confounded with Batches#Locations.

The Residual for Intensities has been reduced from 6 to 4 df.

The design is balanced

#### **Prior allocation model**

Summary table of the decomposition for locs, test & cond (based on adjusted quantities)

Source.locs	df1	Source.test	df2	Source.cond	df3	aefficiency	order
Batches	3	Months	3			1.0000	1
Locations	8	Athletes[Months]	2	Intensities	2	0.0625	1
		Tests[Months:Athletes]	6	Surfaces	2	0.0625	1
				Intensities#Surfaces	4	0.2500	1
Batches#Locations	24	Athletes[Months]	6	Intensities	2	0.9375	1
				Residual	4	1.0000	1
		Tests[Months:Athletes]	18	Surfaces	2	0.9375	1
				Intensities#Surfaces	4	0.7500	1
				Residual	12	1.0000	1

- Same exhaustive confounding issues as for the nested second-phase design.
- Must retain Locations and Months: Athletes to prevent undesirable pooling.
- One possible prior allocation model is the model for the first phase plus Locations:
  - Months + Intensities + Surfaces + Intensities:Surfaces | Months:Athletes + Months:Athletes:Tests + Locations.
- Again this is a model of convenience and does not portray all the sources of variation affecting the response variables for this experiment

### Using od to construct a design

- Split-plot designs
  - > involve a two-step process to optimize:
    - i. optimize the main-unit factors;
    - ii. optimize the sub-unit factors, given the main-unit optimization;
  - Only optimizes main effects.

### Optimizing the main-unit, cross-phase design

Hash table size 4

Final A-value after 50 tabu iterations: 0.533333

> eg2.main.des <- eg2.main.od\$design</pre>

```
> #'## Optimize the main-unit, cross-phase design, based on assigning Intensities to Locations tripletss
> #'### Set up a randomized starting design
                                                                                            Set up an
> eg2.main.ini <- cbind(fac.gen(list(Batches = 4, Triplets = 3)),</pre>
                                                                                            RCBD for
                        fac.gen(list(Intensities = LETTERS[1:3]), times = 4))
+
                                                                                            Intensities
> eg2.main.ini <- designRandomize(allocated</pre>
                                                    = eg2.main.ini[c("Intensities")],
                                  recipient
                                                    = eg2.main.ini[c("Batches", "Triplets")], as a starting
+
                                  nested.recipients = list(Triplets = "Batches"),
+
                                                                                            design.
                                                    = 61461)
                                  seed
> #'### Use od to optimize the main-unit design
> eg2.main.od <- od(fixed = ~ Batches + Triplets + Intensities,</pre>
                                                                            Use swap to
                   permute = ~ Intensities, swap = ~ Batches,
+
                                                                            keep the design
                   maxit
                           = maxit, search = "tabu",
                                                                            resolved for
                    data
                            = eg2.main.ini)
                                                                            Batches.
Mon Oct 7 15:00:29 2019
Initial A-value = 0.727273 (3 A-equations; rank C 2)
A-value after tabu loop 1 is 0.533333
A-value after tabu loop 2 is 0.533333
A-value after tabu loop 50 is 0.533333
```

### Optimizing the sub-unit, cross-phase design

```
> #'## Optimize the sub-unit, cross-phase design, based on assigning Surfaces to Locations within triplets
> #'### Set up a randomized starting design
                                                                            A starting-design design
> eg2.ini <- cbind(fac.gen(list(Surfaces = 3), times = 12),</pre>
                                                                            with Surfaces randomized
                  fac.gen(list(Batches = 4, Triplets = 3, Locations = 3)))
+
                                                                            Within Batches-Triplets.
> eg2.ini <- designRandomize(allocated = eg2.ini["Surfaces"],</pre>
                            recipient
                                              = eg2.ini[c("Batches", "Triplets", "Locations")],
                            nested.recipients = list(Locations = c("Batches", "Triplets")),
                                              = c("Batches", "Triplets"),
                             except
                             seed
                                              = 65435)
                                                                                    Add the main-unit
> eg2.ini$Locations <- with(eg2.ini, fac.combine(list(Triplets, Locations)))</pre>
                                                                                    design.
> eg2.ini <- merge(eg2.ini, eg2.main.des[c("Batches", "Triplets", "Intensities")])</pre>
> #'### Use od to optimize the sub-unit design
> eg2.od <- od(fixed = ~ Batches*Triplets + Locations + Surfaces,</pre>
                                                                          Use swap to only
              permute = ~ Surfaces, swap = ~ Batches:Triplets,
+
                                                                          interchange within
              maxit = maxit, search = search,
                                                                          Batches-Triplets,
                      = eq2.ini)
              data
                                                                          so keeping main-unit
Mon Oct 7 15:02:14 2019
Initial A-value = 0.191781 (3 A-equations; rank C 2)
                                                                          design.
A-value after tabu loop 1 is 0.177778
```

A-value after tabu loop 50 is 0.177778

A-value after tabu loop 2 is 0.177778

Final A-value after 50 iterations: 0.177778

### Produce the two-phase design based on the od designs

```
Combine cross-phase
> eg2.des <- eg2.od$design</pre>
                                                                      and first-phase designs.
> split.lay$Batches <- split.lay$Months</pre>
> eg2.lay <- merge(eg2.des, split.lay)</pre>
> eg2.lay <- with(eg2.lay, eg2.lay[order(Batches, Locations),])</pre>
> eg2.lay <- designRandomize(allocated = eg2.lay[c("Months","Athletes","Tests",</pre>
                                                                                     Randomize the first-
                                                    "Intensities", "Surfaces")],
                                                                                     phase design to the
                             recipient = eg2.lay[c("Batches","Locations")],
                                        = "Batches",
                             except
                                                                                     second-phase units.
                                        = 87620)
                             seed
> #'## Check properties of the design
> eg2.canon <- designAnatomy(formulae = list(locs = ~ Batches*Locations,
                                              test = ~ Months/Athletes/Tests,
                                              cond = ~ Intensities*Surfaces),
                                                                                   The interaction and
                             data
                                       = eg2.lay)
                                                                                   Surfaces main effects
Warning messages:
                                                                                   are not orthogonal.
1: In projs.2canon(CombinedSets$Q[[ntiers]], struct[[ktier]]$Q):
  Intensities#Surfaces and Surfaces are partially aliased in Locations&Tests[Months:Athletes]
2: In projs.2canon(CombinedSets$Q[[ntiers]], struct[[ktier]]$Q):
  Intensities#Surfaces and Surfaces are partially aliased in Batches#Locations&Tests[Months:Athletes]
```

### Properties of the od-based two-phase design

Summary table of the decomposition for locs, test & cond (based on adjusted quantities)

Source.locs	df1	Source.test	df2	Source.cond	df3	aefficiency	order
Batches	3	Months	3			1.0000	1
Locations	8	Athletes[Months]	2	Intensities	2	0.0625	1
		Tests[Months:Athletes]	6	Surfaces	2	0.0625	1
				Intensities#Surfaces	3	0.1121	3
				Residual	1	1.0000	1
Batches#Locations	24	Athletes[Months]	6	Intensities	2	0.9375	1
				Residual	4	1.0000	1
		Tests[Months:Athletes]	18	Surfaces	2	0.9375	1
				Intensities#Surfaces	4	0.6559	4
				Residual	12	1.0000	1

Table of (partial) aliasing between sources derived from the same formula

Source	df	Alias	In	aefficiency	order
Intensities#Surfaces	3	Surfaces	Locations&Tests[Months:Athletes]	0.1121	3
Intensities#Surfaces	4	Surfaces	<pre>Batches#Locations&amp;Tests[Months:Athletes]</pre>	0.6559	4

The design is not orthogonal

The design is unbalanced and the interaction efficiency is low (cf 0.75 for manual construction).

### Properties of the four species of od-based designs

- Used designTwophaseAnatomies to output the 4 species of designs for a two-phase design.
  - > The anatomy of the two-phase design has been presented.
  - > The second-phase anatomy is:

Summary table of the decomposition for locs & test

Source.locs	df1	Source.test	df2	aefficiency	eefficiency	order
Batches	3	Months	3	1.0000	1.0000	1
Locations	8	Athletes[Months]	2	1.0000	1.0000	1
		<pre>Tests[Months:Athletes]</pre>	6	1.0000	1.0000	1
Batches#Locations	24	Athletes[Months]	6	1.0000	1.0000	1
		Tests[Months:Athletes]	18	1.0000	1.0000	1

- ➤ It shows that the allocation of second-phase units (tests) to first-phase units (locations) is orthogonal.
- > This is desirable because it means that the variance matrix is relatively straightforward.

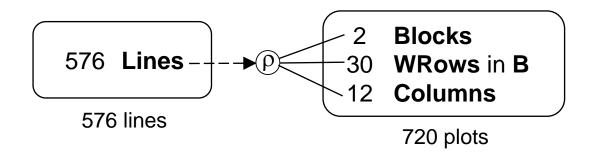
### 2. Partially replicated (p-rep) designs

- These designs were introduced by Cullis et al. (2006)
- They are a variation of the augmented designs, introduced by Federer in 1956.
- An augmented design is one in which a design is used to allocate replicated treatments and these are then augmented with unreplicated treatments.
- The particular features of a *p*-rep design are:
  - Both the unreplicated and replicated treatments are new genotypes; in augmented designs, the unreplicated treatments are usually controls or check varieties;
  - > The *p*-rep designs are spatially-optimized.

### 2.1 A field experiment — a single-phase p-rep

■ 576 Lines on 60 rows x 12 columns.

(Cullis, Smith & Coombes, 2006)



Dashed line because Lines are allocated to the plots factors, but not using classic randomization.

- 144 Lines are to be duplicated p = 0.25.
- Local spatial correlation is expected and a spatial design is needed.
- The initial allocation model is:
  - Lines | Blocks + Blocks:WRows + Columns + Blocks:Columns + Blocks:WRows:Columns).
- The prior allocation model is:
  - Blocks | Lines + Blocks:WRows + Columns + nugget variance Blocks:Columns + units + ar1(Blocks:WRows):ar1(Columns).

- Lines and Blocks interchanged between fixed-random model;
- Autocorrelation for Rows and Columns is added;
- units is added for nugget variance.

### A field p-rep — variance parameters

- The prior allocation model:
  - Blocks | Lines + Blocks:WRows + Columns + Blocks:Columns + units + ar1(Blocks:WRows):ar1(Columns).
- To search for a spatially-optimized design using od need to specify values for the variance parameters.
- The general way to do this is to
  - i. set the residual (or identity) term component to 1:  $\phi_{BRC} = 1$ ;
  - ii. Use  $\gamma$  to denote the ratio of each component to the residual:  $\gamma_i = \phi_i / \phi_{BRC}$ .
- Suppose past experience tells us that the following are reasonable values (Smith et al, 2006, p.405):
  - $ho_{L} = 1$ ,  $\gamma_{BR} = 0.5$ ,  $\gamma_{C} = 0.1$ ,  $\gamma_{BC} = 0.05$ ,  $\gamma_{U} = 0.5$ ,  $\phi_{BRC} = 1$ ,  $\rho_{BR} = 0.6$ ,  $\rho_{C} = 0.4$ .
  - The magnitude of  $\phi_L$  equals that of  $\phi_{BRC}$ ;  $\gamma_u$  is the nugget variance; the  $\rho$ s are the first-order autocorrelation parameters.

### A field p-rep — setting up

```
> #'## 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>
> n <- r*c # no. Plots
>
> #'## Set up variance parameters
                                               > #'## Set od options
> g.L <- 1
                                               > maxit <- 50
> g.BR < - 0.5
                                               > search <- "tabu+rw"</pre>
> q.C <- 0.1
                                               > od.options(P = 0.10, localSearch = 10000, tabuStop = 100)
> q.BC < - 0.05
> g.u < - 0.5
> g.BRC <- 1.0
> \text{rho.R} < - 0.6
> rho.C <- 0.4
> params <- c(g.L, g.BR, g.C, g.BC, g.u, g.BRC, rho.R, rho.C)</pre>
> names(params) <- c("g.L", "g.BR", "g.C", "g.BC", "g.u", "g.BRC", "rho.R", "rho.C")</pre>
```

## A field *p*-rep — initial design

```
#'## Generate a simple lattice for Lines 1:144
> #' 1:144 are replicated twice 145:g are replicate
> latt.mat <- matrix(1:ndup, nrow = 12, ncol = 12)</pre>
> blk1.lines <- sample((ndup+1):g, (g-ndup)/2)</pre>
> latt.lay <- fac.gen(list(Blocks = 2, WRows = 30,</pre>
> latt.lay <- within(latt.lay,</pre>
                        Lines <- factor(c(latt.mat</pre>
                                          t(latt.ma
 #'## Randomize the initial design
> latt.lay <- designRandomize(allocated</pre>
                              recipient
                              nested.recipients = :
                              seed
> latt.lay <- within(latt.lay,</pre>
                       Rows <- fac.combine(list(Blo))</pre>
                                                                              Columns
```

This is a resolved, augmented design – the replicates of the duplicated Lines are in different blocks and the unduplicated lines are added to the block design.

### A field p-rep — setting variance parameters in od

```
> #'## Use od to generate the p-rep starting with the simple lattice - with units and autocorrelation
> prepuar1.latt.od <- od(fixed</pre>
                                      = ~ Blocks,
                         random
                                       = ~ Lines + Rows + Columns/Blocks + units,
                         residual
                                      = ~ ar1(Rows):ar1(Columns),
                                                                         Note Rows used rather than
                         permute
                                      = ~ Lines, swap_= ~ Blocks,
                                                                         Blocks: Rows:
                         start.values = TRUE,
                                                                         ar1 requires a single factor;
                                       = latt.lay)
                         data
                                                                         the two terms are equivalent as
> vp.table <- prepuar1.latt.od$vparameters.table</pre>
                                                                         a random term.
> vp.table$Value <- params</pre>
> vp.table
                                                                         swap restricts interchanges to
                 Component Value
                     Lines
                            1.00
1
                                                                         be within Blocks and so
                      Rows
                            0.50
                                                                         ensures that the design remains
                   Columns
                            0.10
                                                                         resolved.
            Columns: Blocks
                            0.05
5
                     units
                           0.50
            Rows:Columns!R
6
                            1.00
     Rows:Columns!Rows!cor
                            0.60
8 Rows:Columns!Columns!cor
```

### A field p-rep — generating the design

```
> prepuar1.latt.od <- od(fixed</pre>
                                   = ~ Blocks,
                          random
                                   = ~ Lines + Rows + Co
                          residual = ~ ar1(Rows):ar1(Col
                                   = ~ Lines, swap = ~ I
                          permute
                          G.param
                                   = vp.table, R.param =
                          maxit
                                   = maxit, search = sea
                          data
                                   =l att.lay)
Fri Sep 6 16:52:46 2019
Initial A-value = 1.026048 (576 A-equations; rank C 576
A-value after tabu loop 1 is 1.016726
A-value after tabu loop 2 is 1.016552
A-value after tabu loop 49 is 1.016174
A-value after tabu loop 50 is 1.016174
Hash table size 2477
Final A-value after 50 iterations: 1.016174
> prepuar1.latt.lay <- prepuar1.latt.od$design</pre>
Note that all the border plots are duplicated
Lines: the same does not occur when an
RCBD is used as the starting design (in Prac).
                                                                                  Columns
```

### Canonical analysis of the design: investigating its anatomy

- Want to look at the relationships of the lines sources to the plots sources.
- The plots sources:
  - Blocks + Rows[Blocks] + Columns + Blocks#Columns +Rows#Columns[Blocks].
- The lines source:
  - Lines.
- Using dae:

- > A is the harmonic mean of the efficiency factors.
- M is the mean of the efficiency factors.
- E is the minimum of the efficiency factors.
- dforth is the number of efficiency factors equal to one.
- Order is the number of unique efficiency factors.

#### A field p-rep — anatomy

Summary table of the decomposition for plot & trt (based on adjusted quantities)

63

Source.plot	df1	Source.trt	df2	aefficiency	mefficiency	eefficiency	order	dforthog
Blocks	1	Lines	1	0.6000	0.6000	0.6000	1	0
Rows[Blocks]	58	Lines	58	0.7849	0.8000	0.4840	58	0
Columns	11	Lines	11	0.7713	0.7818	0.5731	11	0
Blocks#Columns	11	Lines	11	0.8126	0.8182	0.6727	11	0
Rows#Columns[Blocks]	638	Lines	575	0.4135	0.8877	0.0061	82	494

The design is not orthogonal

- All of the plots sources are orthogonal (no aliasing).
- A is the harmonic mean of the efficiency factors.
- M is the mean of the efficiency factors.
- > E is the minimum of the efficiency factors.
- > dforth is the number of efficiency factors equal to one.

Residual

Order is the number of unique efficiency factors.

- A lot of information about some Lines contrasts in other than Rows#Columns[Blocks] (plots).
- Not a unique decomposition, but Rows#Columns[Blocks] decomposition is.
- Concentrate on the last Lines source, where all 575 Lines df are partially confounded.

37

#### A field p-rep — anatomy

Summary table of the decomposition for plot & trt (based on adjusted quantities)

Source.plot	df1	Source.trt	df2	aefficiency	mefficiency	eefficiency	order	dforthog
Blocks	1	Lines	1	0.6000	0.6000	0.6000	1	0
Rows[Blocks]	58	Lines	58	0.7849	0.8000	0.4840	58	0
Columns	11	Lines	11	0.7713	0.7818	0.5731	11	0
Blocks#Columns	11	Lines	11	0.8126	0.8182	0.6727	11	0
Rows#Columns[Blocks]	638	Lines	575	0.4135	0.8877	0.0061	82	494

Residual 63

Lines efficiencies											
≤0.1	0.1-0.2	0.2-0.3	0.3-0.4	0.4-0.5	0.5-0.6		1				
23	21	17	12	7	1		494				

- A is the harmonic mean of the efficiency factors.
- M is the mean of the efficiency factors (the sum is the Fisher information for the design and is a component of (M,S optimality).
- dforth is the number of efficiency factors equal to one.

- A lot (86%) of orthogonal df in Plots.
- But, a lot of efficiencies close to 0 in Plots, which is to be expected for for *p*-rep designs
  - distorts A so M better?

## The effect on the anatomy of assuming that Blocks#Columns is zero

Summary table of the decomposition for plot & trt (based on adjusted quantities)

Source.plot	df1	Source.trt	df2	aefficiency	mefficiency	eefficiency	order	dforthog
Blocks	1	Lines	1	0.6000	0.6000	0.6000	1	0
Rows[Blocks]	58	Lines	58	0.7849	0.8000	0.4953	58	0
Columns	11	Lines	11	0.7729	0.7818	0.6024	11	0
Blocks#Rows#Columns	649	Lines	575	0.5168	0.9033	0.0119	71	505
		Residual	74					

The design is not orthogonal

- More lines information in Blocks#Rows#Columns and more Residual df.
- Still some information about Lines almost orthogonal to Blocks#Rows#Columns.
- AVPD =  $1.014\phi_{BRC}$ . (minor change was  $1.016\phi_{BRC}$ .)

# Calculating the A-measure (AVPD) using designAmeasures and mat. Vpredicts from dae

The model arguments of the od call

Corresponding designAmeasures call

- To calculate without Columns:Blocks, drop "/Blocks" and "g.BC".
- What happens if ar1 and nugget variance are dropped from od call? 40

### Comparing spatial and nonspatial designs

Design	Nonspatial A	Spatial A	aefficiency	mefficiency	eefficiency	dforthog
Nonspatial	0.988486	1.018665	0.5168	0.8877	0.0264	494
Spatial	0.988857	1.016151	0.4180	0.8877	0.0080	494

- Both designs are equally suitable for nonspatial data.
- The difference between the designs for spatial data is very small.
  - > The only differences are in aefficiency and eefficiency.
  - The nonspatial design is slightly better because the range of the efficiency factors is less.

# Comparing canonical analysis and A-measures (AVPD)

#### Canonical analysis

- Shows the anatomy of the design: where the information is in the design and the nonorthogonality that is present.
- Do not need to specify the variance parameter values and not dependent on them.
- > Does not account for spatial correlation and nonlinear trends.
- Limited relationship with AVPD
  - When target is fixed, variance-components-only model and equally replicated, aefficiency is directly related to AVPD, otherwise it is not.
- Only useful for characterizing a design, rather than searching for an optimal design.

#### AVPD

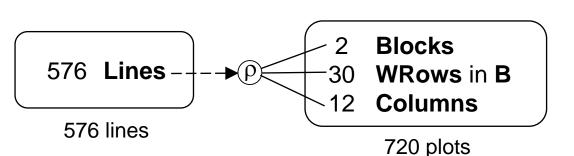
- ▶ Is a measure of the precision in the experiment that gives equal weight to all contrasts, and is used by od, but is not the same as PEV.
- > Need to specify the variance parameter values because depends on them.

#### 2.2 Partially replicated designs in two phases

- Smith et al. (2006) give examples of experiments that employ designs in which both phases employ partially replicated designs in both phases:
  - $\triangleright$  They are dubbed p/q-rep designs.
  - That is, p% of the lines are replicated in the first phase and q% of the plots with unreplicated lines are replicated in the second phase.
- We will produce a design for a an experiment with p = 0.25 and q = 0.10.
  - $\triangleright$  Previous example is a *p*-rep design for a field experiment, with p=0.25.
  - It will be extended to include a milling phase.

## The first phase design— a p-rep field experiment (Cullis, Smith &

■ 576 Lines on 60 rows x 12 columns.



Dashed line because Lines are allocated to the plots factors, but not using classic randomization.

Coombes, 2006)

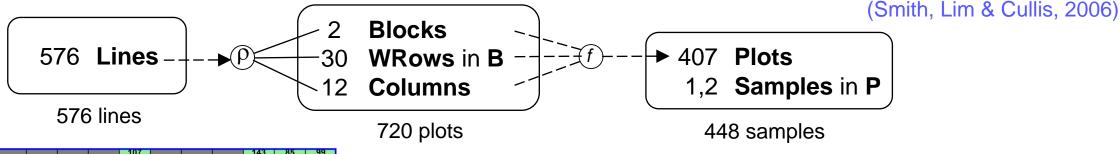
- 144 Lines are to be duplicated p = 0.25.
- A spatially optimized design was used to allocate lines to plots.
- Suppose that samples of grain from the field experiment are to be taken to the laboratory for milling and analysis in the laboratory.
  - After the field experiment 370 lines have been identified for processing in the milling phase.

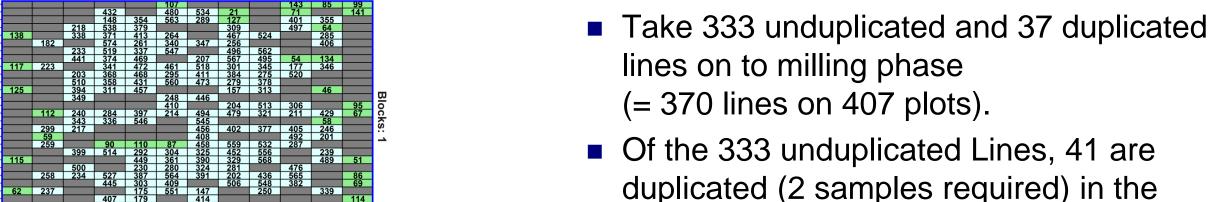


#### Sampling plots for the milling (second) phase

Replication

Columns





What will happen here as compared to previous design?

milling phase — q = 0.10 (of plots).

- Answer: Blocks, Rows and Columns will no longer be orthogonal — unit terms are partially aliased (cf. confounding).
- Also, Lines confounding will change.

### First-phase anatomy for the fraction

(without Blocks#Columns)

```
> summary(designAnatomy(formulae
                                   = list(plot = ~ ((Blocks/WRows)*Cols)/Samp,
                                          trt = ~ Lines).
+
                        keep.order = TRUE, data = layout),
+
         which.criteria = c("ae", "me", "ee", "dfor"))
+
Table of (partial) aliasing between sources derived from the same formula
           df Alias
                           {\tt In}
                               aefficiency mefficiency eefficiency dforthog
Source
Cols
           11 Blocks
                                    0.9992
                                               0.9992
                                                         0.9908
                           plot
                                                                     10
Cols
                                                         0.8374
           11 WRows[Blocks] plot
                                    0.9230
                                              0.9249
Blocks#Cols 22 WRows[Blocks] plot
                                    0.9210
                                              0.9240
                                                         0.8151
```

- The terms are fitted in the order Blocks, WRows[Blocks] and Columns (see next slide).
- Eleven df for Columns is aliased with Blocks and WRows[Blocks] but 92.3% of the information is retained.
- The analysis will depend on whether Columns is fitted first or not, but not greatly given the high aefficiency.

#### First-phase anatomy for the fraction

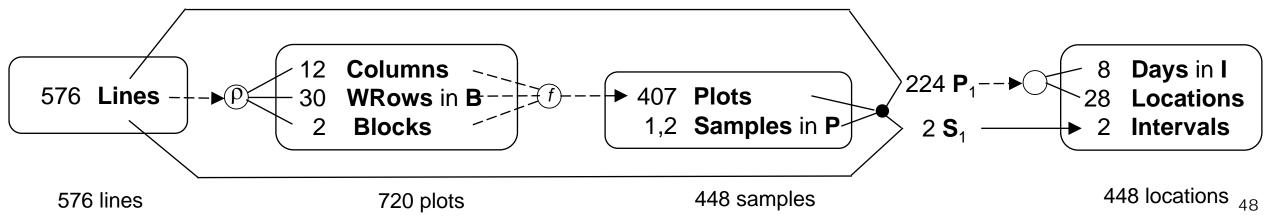
Source.plot	df1	Source.trt	df2	aefficiency	mefficiency	eefficiency	dforthog
Blocks	1	Lines	1	0.8348	0.8348	0.8348	0
WRows[Blocks]	58	Lines	58	0.7742	0.9013	0.0950	26
Cols	11	Lines	11	0.8347	0.8760	0.5187	0
Blocks#Cols	11	Lines	11	0.8231	0.8695	0.4784	0
WRows#Cols[Blocks]	325	Lines	325	0.4602	0.9129	0.0177	288

Samp[Blocks:WRows:Cols] 41

- Not unique, but the WRows#Cols[Blocks] strata is.
- Of the 369 Lines df, 325 are estimable in WROWS#Cols[Blocks], including 288 (78%) only there.
- There are 44 Lines df estimable elsewhere, with 26 of these orthogonally confounded with WRows[Blocks].
  - > Thus for Lines fixed, the design is disconnected for all plot terms fixed except the last two.
  - Would be connected if all plots terms (except Blocks) random (needed for od).
- The mefficiency for the 369 Lines df in wRows#Cols[Blocks] is 0.8040 (= 0.9129 x 325 / 369).
- Samp[Blocks:WRows:Cols] (Error) has full 41 df.

## Milling-phase allocation for the p/q-rep design

- There are 448 (407 + 41) samples and so 448 time-locations for milling required:
  - > Take 16 days divide them into 2 intervals.
  - > Each day there are 28 time-locations for milling.
- Samples are assigned to locations using two pseudofactors, S₁ and P₁:
  - ➤ The 448 samples are assigned to the 2 levels of S<sub>1</sub> so that milling duplicates have different levels and, as far as is possible, so do plots from different blocks;
  - ➤ The 224 plots in each level of S<sub>1</sub> are assigned to the 224 levels of the pseudofactor P<sub>1</sub> in Rows-Columns order:
    - The 224 plots are comprised of those (i) for the 41 lines that are milling-duplicated, (ii) from the same block for the 37 lines that are field duplicated, and (iii) for 183 lines that are from the same block as (ii) or rows nearby.
  - S<sub>1</sub> is randomized to Intervals and P<sub>1</sub> is systematically allocated to the Days-Locations combinations, the design being nonorthogonal



#### Check properties of the multiphase design

- Note three formulae supplied.
- Have used designTwophaseAnatomies and this will produce the four species of designs for a two-phase design:
  - > The first-phase design for the fraction is not used for the analysis of first-phase responses (e.g. grain yield).

#### Anatomy of the second-phase design

Summary table of the decomposition for lab & plot (based on adjusted quantities)

Source.lab	df1	Source.plot	df2	aefficiency	mefficiency	eefficiency	dforthog	A lot of
Int	1	Blocks	1	0.6386	0.6386	0.6386	0	Blocks
Days[Int]	14	Blocks	1	0.2827	0.2827	0.2827	0	confounded
		WRows[Blocks]	13	0.6963	0.7831	0.2458	0	here.
Locn	27	Blocks	1	0.0061	0.0061	0.0061	0	110101
		WRows[Blocks]	26	0.0130	0.0974	0.0023	0	
Int#Locn	27	Blocks	1	0.0037	0.0037	0.0037	0	
		WRows[Blocks]	26	0.0140	0.0903	0.0027	0	
Days#Locn[Int]	378	Blocks	1	0.0689	0.0689	0.0689	0	
		WRows[Blocks]	58	0.2760	0.7074	0.0234	0	
		Cols	11	0.8298	0.8336	0.7439	0	
	N/	Blocks#Cols	11	0.8251	0.8304	0.7058	Q	
		WRows#Cols[Blocks]	297	0.4358	0.8991	0.0142	256	
			R				NA 1 6-	

Blocks#Cols mainly confounded here.

The estimable df for Wrows#Cols[Blocks] has gone from 638 (first-phase) to 325 (fraction) to 297.

Much of WRows [Blocks] and Cols confounded here.

#### Anatomy of the two-phase design

Source.lab	df1	Source.plot	df2	Source.trt	df3	aefficiency	mefficiency	eefficiency	dforthog
Int	1	Blocks	1	Lines	1	0.6696	0.6696	0.6696	0
Days[Int]	14	Blocks	1	Lines	1	0.6679	0.6679	0.6679	0
		WRows[Blocks]	13	Lines	13	0.8261	0.8449	0.5362	0
Locn	27	Blocks	1	Lines	1	0.8062	0.8062	0.8062	0
		WRows[Blocks]	26	Lines	26	0.8135	0.8248	0.6160	0
Int#Locn	27	Blocks	1	Lines	1	0.8050	0.8050	0.8050	0
		WRows[Blocks]	26	Lines	26	0.8187	0.8279	0.6432	0
Days#Locn[Int]	378	Blocks	1	Lines	1	0.4723	0.4723	0.4723	0
		WRows[Blocks]	58	Lines	58	0.7908	0.8443	0.3224	0
		Cols	11	Lines	11	0.8309	0.8597	0.5507	0
		Blocks#Cols	11	Lines	11	0.8304	0.8587	0.5412	0
		WRows#Cols[Blocks]	297	Lines	297	0.2940	0.8207	0.0101	219

- Just 297 of the total 369 df for Lines is estimable from Wrows#Cols[Blocks].
- In all 66.1 % (0.8207 \* 297 / 369) of the Lines information is estimable here.
- A lot of Lines information is confounded with the variation from other field and milling phase sources of variation.

#### Substituting a linear Locations term

```
> #'## Look at the effect of substituting a linear Columns term for the Column variation term
                                                = list(lab = ~ Int:Days + xLocn
> ph2sys.lin.canon <- designAnatomy(formulae</pre>
                                                                                             Linear term for
                                                                Int:Days:Losn,
+
                                                                                             Locations.
                                                                 Rows (ols)/Samp
                                                             = ~ Lines),
                                                                                             Pool to simplify
                                     keep.order = TRUE, data = layout)
                                                                                             the analysis.
> print(summary(ph2sys.lin.canon, which.criteria = c("ae", "me", "ee", "dfor")))
Summary table of the decomposition for lab, plot & trt (based on adjusted quantities)
 Source.lab
                 df1 Source.plot
                                      df2 Source.trt df3 aefficiency mefficiency eefficiency dforthg
                                       15 Lines
                                                               0.7852
                                                                           0.8214
                                                                                        0.4469
 Int:Days
                  15 Rows
                                                      15
                                                                                                     0
                                        1 Lines
                                                               0.8095
                                                                           0.8095
                                                                                        0.8095
xLocn
                   1 Rows
                                                                                                     0
 (Int:Days)#Locn 431 Rows
                                       59 Lines
                                                               0.7021
                                                                           0.8452
                                                                                        0.0802
                                                      59
                                                                                                    13
                     Cols
                                       11 Lines
                                                               0.8257
                                                                           0.8659
                                                                                        0.5129
                                                      11
                                                                                                     0
                     Rows#Cols
                                      333 Lines
                                                                                        0.0066
                                                      333
                                                               0.3245
                                                                           0.8903
                                                                                                   283
                     Samp[Rows:Cols]
                                       28
                                                               1.0000
                                                                           1.0000
                                                                                        1.0000
                                                                                                    28
```

- Just 333 of the total 638 df for Rows#Cols and of the total 369 df for Lines is estimable here.
- Now 80.3% (0.8903 \* 333 / 369) of the Lines information is estimable here (cf. 66.1% & 0.8207 with R#C included).
- Also 28 of the 41 df for Samples[Rows:Cols] (Error df) is available.

#### **Summary**

- Here, dividing the factors based on allocation of factors results in three sets of factors: only ever allocated; allocated and recipient; and only ever recipient.
- For a two-phase experiment there are four species of design: first-phase; second-phase; cross-phase; two-phase.
- The same methods of design selection apply, but need to consider three designs and how they combine.
- Again, designRandomize can be used to randomize the experiment and designAnatomy can be used to check the properties of the design, irrespective of the nonorthogonality and the number of tiers e.g. p/q-rep designs.
  - > can be slow when the number of observations is large (several hundreds).

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