

Design and Analysis of Experiments 11 - Blocking

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"Science doesn't always go forwards. It's a bit like doing a Rubik's cube. You sometimes have to make more of a mess with a Rubik's cube before you can get it to go right."

> Jocelyn Bell Burnell 1943 -Irish astrophysicist



Blocking

Nuisance factors

In the completely randomized design (CRD) introduced in the last chapter, the observations are assigned - as the name implies -in a completely random manner.

Implicitly, we assume that the experimental conditions are homogeneous, i.e., that no other important effects are present besides those of the experimental factor.

In some situations, however, the experiment may present other factors that are not of immediate interest, but that can influence the response variable. This was already discussed when we introduced the concept of *pairing* in Chapter 7.

Blocking

Nuisance factors

The generalization of the *paired design* for an arbitrary number of factor levels is called *blocking*, which is an elegant way configure the data collection in order to enable the modeling and exclusion of the effects of nuisance factors.

In fact, it can be argued that the systematic use of blocking is beneficial even in the absence of known nuisance factors, as it

helps boosting statistical power by excluding the between-replicates variability from the residual term.

"Block what you can, randomize what you cannot."

George E.P. Box (1919–2013) British Statistician



Blocking

Blocking versus Randomizing

The idea behind randomization is trying to prevent unknown factors to bias our observations;

Blocking comes into play whenever we know from the beginning that certain factors can influence our response variable, but for some reason we are not interested in their effects^a, for instance:

- the effect of different batches of raw material when comparing the performance of chemical reactions;
- the effect of different benchmark problems when comparing the performance of computer algorithms.

^a If we're interested in their effects, they are no longer nuisance factors, but additional experimental factors. We'll deal with factorial designs in the next chapter.

Example: algorithm comparison

Problem definition

A Ph.D. student decides to compare a standard optimization algorithm with six modified versions for the solution of a certain family of Vehicle Routing Problems (VRPs). His intention is to verify whether any of the modified versions is systematically better than the standard one.

The algorithms are applied for the solution of 180 problem instances, divided in 36 groups of five homogeneous instances. The algorithms are run 30 times on each instance, and the cost value found after each run is recorded.

Example: algorithm comparison

Nuisance factor

Besides the effect of the experimental factor (*Algorithm*), we have a possible nuisance effect due to the variability between experimental units (instance groups).

If we employ a CRD, the residual term would contain all the between-instances variability, which would almost certainly mask any between-algorithms effect of interest.

Since we can control the allocation of algorithm runs within each instance, one possibility is to do it in a systematic way so that we can model the instance effects (in addition to the factor effect).

Example: algorithm comparison

Randomized complete block design

Within each *block*, the order of execution should in principle be randomized, so as to prevent other unknown factors from affecting our analysis^b.

This experimental setup is known as a *randomized complete block design* (RCBD) with one blocking factor.

^bFor this kind of computer experiment the within-block randomization is unnecessary. It is very important, however, when dealing with systems that are less controllable.

Randomized complete block design Assumptions

The RCBD assumes:

- one replicate per block^c;
- independent blocks;
- independent within-block randomization.

Failure to account for dependency structures (i.e., using blocks that are not independent) can result in pseudoreplication, i.e., the use of the incorrect number of degrees-of-freedom in the test statisticsm, which usually results in an inflation of the type-I error rate.

^CFor multiple within-block replicates the appropriate design is known as *Generalized randomized block design* (GRBD), which is analyzed using a factorial model.

Example: algorithm comparison RCBD

To comply with these requirements, we consider as our response variable the average performance of an algorithm on a particular *instance group*.

The performance of each algorithm will be averaged within each individual instance (mean of 30 runs), and then within each group (mean of 5 instances), so that each algorithm has 36 independent observations.

Statistical model

In the general case, we have a levels of the experimental factor, and b levels for the blocking factor. The statistical model is given as:

$$y_{ij} = \mu + \tau_i + \beta_j + \epsilon_{ij} \begin{cases} i = 1, \dots, a \\ j = 1, \dots, b \end{cases}$$
, assuming $\epsilon_{ij} \sim \mathcal{N}\left(0, \sigma^2\right)$

Similarly to the CRD we have, by construction:

$$\sum_{i=1}^{a} \tau_i = 0 \qquad \qquad \sum_{j=1}^{b} \beta_j = 0$$

Statistical model

In the RCBD, we are interested only on the effect of the experimental factor. Consequently, the test hypotheses refer only to its coefficients:

$$\begin{cases} H_0: \tau_i = 0, \ \forall i = 1, \dots, a \\ H_1: \exists \ \tau_i \neq 0 \end{cases}$$

The partition of the total sample variability is given by:

$$SS_{T} = \sum_{i=1}^{a} \sum_{j=1}^{b} (y_{ij} - \bar{y}_{..})^{2}$$

$$= b \sum_{i=1}^{a} (\bar{y}_{i.} - \bar{y}_{..})^{2} + a \sum_{j=1}^{b} (\bar{y}_{.j} - \bar{y}_{..})^{2} + \sum_{i=1}^{a} \sum_{j=1}^{b} (y_{ij} - \bar{y}_{i.} - \bar{y}_{.j} + \bar{y}_{..})^{2}$$

$$SS_{\text{levels}}$$

$$SS_{\text{blocks}}$$

$$SS_{\text{blocks}}$$

Statistical model

The mean squares are given by:

$$extit{MS}_{ ext{levels}} = rac{SS_{ ext{levels}}}{a-1} \hspace{0.5cm} extit{MS}_{ ext{blocks}} = rac{SS_{ ext{blocks}}}{b-1} \hspace{0.5cm} extit{MS}_{ extit{E}} = rac{SS_{ extit{E}}}{(a-1)(b-1)}$$

and their expected values are:

$$E[MS_{\text{levels}}] = \sigma^2 + \frac{b\sum_{i=1}^{a} \tau_i^2}{a-1}$$

$$E[MS_{\text{blocks}}] = \sigma^2 + \frac{a\sum_{j=1}^{b} \beta_j^2}{b-1}$$

$$E[MS_E] = \sigma^2$$

Statistical model

$$E[MS_{\text{levels}}] = \sigma^2 + \frac{b\sum_{i=1}^a \tau_i^2}{a-1}$$
 $E[MS_E] = \sigma^2$

Under the null hypotheses we have that the test statistic

$$F_0 = rac{\mathit{MS}_{\mathsf{levels}}}{\mathit{MS}_{\mathit{E}}}$$

is a distributed according to an F distribution with (a-1) numerator degrees-of-freedom and (a-1)(b-1) denominator DoFs.

The critical region for the test is therefore given by

$$f_0 > F_{\alpha;(a-1),(a-1)(b-1)}$$

Multiple blocking factors

If there is more than one factor that need to be blocked out of the analysis, it is possible to simply add new terms to the statistical model. The sum of squares for this new term is similar to the ones already shown for the single block case;

However, since we are not really interested in the block effects - all we want is to get them out of our residual term - we can use the *KISS* principle^d, merge the two (or more) blocking factors into a single one and proceed with the analysis as if only one blocking factor actually existed.

d"Keep It Simple, Stupid!", as introduced by American engineer C.L. "Kelly" Johnson in the 1970's. If one wants to be more polite, there is a quote attributed to Einstein that reads "Make everything as simple as possible, but not simpler", but the acronym MEASAPBNS is just not as catchy.

Blocking efficiency

After an experiment is performed and the ANOVA model is fit to the data, it is possible to calculate the *relative blocking efficiency* (E), which quantifies how much larger a CRD would have to be in order to attain the same power as the corresponding RCBD.

The relative efficiency can be calculated from the mean squares returned in the ANOVA table of the RCBD as:

$$E = \frac{(b-1)MS_{\text{Blocks}} + b(a-1)MS_{\text{E}}}{(ab-1)MS_{\text{E}}}$$

A value of 1.3, for instance, would indicate that the CRD would have required 30% more observations to achieve the same power.

Sample size calculations

The determination of the required sample size for an RCBD follows the same procedures as the CRD: the number of replicates calculated using the CRD formulas represent the number of blocks required (since we have one replicate per block).

The within-group variability term necessary for calculating the required sample size corresponds to the estimated residual variance, i.e., the unexplained variability after accounting for the experimental and blocking factors, which can be somewhat challenging to estimate without a information on previous studies (or a pilot experiment).

Multiple comparisons

For the post-hoc multiple comparison procedures, we also follow the same general guidelines used for the CRD, with some minor differences.

Paired t-tests are used for the pairwise comparisons, with $df_E = (a-1)(b-1)$ as the number of degrees of freedom used for the reference distributions;

As with the CRD, it may be convenient to use the post-hoc pairwise comparison procedures as the basis for sample size calculations, particularly in cases where the cost of observations is relatively low.

Bibliography

Required reading



Recommended reading



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