

Comparison of the Optimal Design: Split-Plot Experiments

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Abstract

Over the past decade, there have been rapid advances in the development of methods for the design and analysis of optimal split-plot experiment. Industrial experimentation involving optimality criteria has not been fully exhausted. In this study, we present a literature review on the development of optimal design of split-plot experiments. Split-plot designs, optimality criteria are discussed. Recent developments of optimal split-plot designs is evaluated and compared.

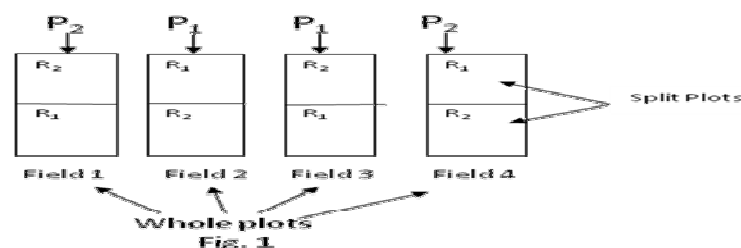
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1.0 Introduction

Split-Plot experiments were introduced by Fisher (1925) and their importance in industrial experimentation had been discussed by Yates (1935).

A split – plot experiment is regarded as a blocked experiment, where the blocks themselves serve as experimental units for a subset of the levels of experimental units, the blocks are regarded as whole plots, while the experimental units within blocks are called split plots, split unit, or sub plots.

Split Plot Agricultural layout (Factor P is the whole –plot factor and factor R is the split – plot factor) is shown below



Corresponding to the two levels of experimental units are two levels of randomizations. One randomization is conducted to determine the assignment of block –level treatments to whole plots. Then, as changes in a blocked experiment a randomization of treatments to split – plot experimental units occurs within each block or whole plot. This restricted randomization of the experimental run results is a split-plot Design (SPD).

A factor whose level varies within each plot is called a split-plot factor. A lot of industrial and agricultural experiments involve two types of factors, some with levels that are hard or costly to change and others with levels that are relatively easy to change. Those factors which are expensive or time –consuming to change are regarded as hard-to-change factors. Hard-to-change factors consist of mechanical setups, environmental factors etc. It is in the practitioner’s best interest when hard –to-change factors exist, to minimize the number of times the levels of these factors are change.

A split –plot experiment is performed by fixing the levels of the hard –to-change factors and then running all or some of the combinations of the easy –to-change factor levels then, a new setting in the hard-to-change factors are selected and the process is repeated.

The hard-to-change factors are called whole plot factors and the easy – to-change factors are called the subplot

factors.

The works by Anbari and Lucas (1994), Ganju and Lucas (1997, 1999, 2005), Ju and Lucas (2002) Webb et al. (2004) has revealed that a lot of industrial experiments previously thought to be completely randomized experiments also exhibit split-plot structures.

Split-plot designs are considered for experimentation when a completely randomized design is structurally impossible, expensive or inconvenient.

1.1 Exact and Continuous Designs

The reason why we study the optimal design theory is to enable us to determine the value of the explanatory variable x each time an experimental observation is made. If the linear model

$$E(y) = F\beta \quad 1.1$$

The equation 1.1 represents an experiment in which there exist m factors, where y is the $N \times 1$ vector of responses, β is a vector of p unknown parameters to be calculated by least squares and F is the $N \times p$ extended design matrix. $f^T(x_i)$ is a known function of the m explanatory variables which is the i th row of F . It can take values in the design region χ .

For the second-order model with interaction

$$E(y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 \quad 1.2$$

$$\text{where } f^T(x_i) = (1 \ x_1 \ x_2 \ x_1^2 \ x_2^2 \ x_1 x_2) \quad 1.2.1$$

Two known approaches can be used in estimating the optimal design. In the first approach, the requirement that the number of observations at a certain point must be an integer is replaced by assigning weights to the design point. This method gives rise to continuous, approximate or asymptotic designs. The measure ξ , is used in representing the continuous designs on the region χ .

Given that the design has observations at h distinct points $x_i \in \chi$, we have

$$\mathcal{E} = \begin{Bmatrix} x_1 & x_2 & \dots & x_h \\ w_1 & w_2 & \dots & w_h \end{Bmatrix} \quad 1.3$$

In 1.3, the first row shows the levels of the experimental factor in each design. The weight associated with each design point is shown by the second row. Also, $\int_{\chi} \xi(dx) = 1$ and $0 \leq w_i \leq 1$ for all i . The information matrix for a continuous design is defined as

$$M(\xi) = \sum_{i=1}^h w_i f(x_i) f^T(x_i) \quad 1.4$$

where T stands for transpose and the standardized prediction variance is defined as

$$d(x, \xi) = f^T(x) [M(\xi)]^{-1} f(x) \quad 1.5$$

We represent an exact or discrete design with n observations as

$$\mathcal{E}_n = \begin{Bmatrix} x_1 & x_2 & \dots & x_h \\ n_1 & n_2 & \dots & n_h \end{Bmatrix} \quad 1.6$$

Where n_i shows the number of observations at design point x_i and

$$\sum_{i=1}^h n_i = n$$

For a discrete design, the information matrix is defined as

$$M = \sigma_{\epsilon}^{-2} \sum_{i=1}^h n_i f(x_i) f^T(x_i) \quad 1.7$$

and the standardized prediction variance is defined as

$$\begin{aligned} (x, \xi) &= n\sigma_{\epsilon}^{-2} f^T(x_i) M^{-1} f(x_i) \\ &= n\sigma_{\epsilon}^{-2} \text{var} \left\{ \hat{y}(x) \right\} \end{aligned} \quad 1.8$$

- It should be noted that all designs are discrete in practice. By multiplying the weights w_i of the optimal continuous design by n and having this product rounded to the nearest integer results in discrete designs.

2.0 Literature Review

Experimenters often think of a split-plot experiment as running every sub-plot combination in every whole plot. However, Kempthorne (1952) described split-plot design that does not satisfy this restriction.

The optimal design theory was put forward by Kiefer (1959). Alkinson and Donev (1992) provided a concise introduction to the central theory of the general equivalence theorem.

An excellent overview of Kiefer's work was given by Fedorov (1972), which was extended to optimum experimental design.

The concepts of split-plotting, and bi-randomization are used in industrial experimentation. Cornell (1988) and Kowalski, et al (2002) pointed out that mixture experiments containing process of variables are of the split-plot type.

Box and Jones (1992) described an experiment in which a packed-foods manufacturer wished to develop an optimal formulation of a cake mix. Because cake mixes are made in large batches, the ingredient factors (flour, shortening and egg powder) are hard-to-change.

The risks of improperly analyzing a split-plot experiment are pointed out by Box and Jones (1992). Letsinger et al (1996) refers to split-plot as bi-randomization designs.

Huang et al (1998) and Bingham and Sitter (1999) also use split-plot design when not all the sub-plot combinations occur in each plot.

Letsinger et al (1996), Ganju and Lucas (1999) and Lucas and Ju (2002) described how split-plot designs (SPDs) are obtained by not resetting the factor levels for the consecutive runs of an experiment.

Bisgaard (2000) described an experiment involving four prototype combustion engine designs and two grade of gasoline. The engineers preferred to make up the four motor designs and test both of the gasoline types while a particular motor was on a test stand. Here the hard-to-change factor is motor type and the easy-to-change factor is gasoline grade.

Many packages of cake mix are produced from each batch, and the individual packages of cake mix can be baked using different baking times and baking temperatures. Here the easy-to-change, split-plot factors are time and temperature. Bingham and Sitter (2001) described an experiment in which a company wished to study the effect of various factor on the swelling of a wood product after it has been saturated with water and allowed to dry. A batch is characterized by the type and size of a wood being tested, the level of moisture saturation. Batches can later be subdivided for processing, which is characterized by three easy-to-change factors, i.e., process time, pressure and material density.

Trinca and Gilmour (2001) compute a split-plot design for a protein extraction experiment.

Kowalski and Vining (2001) gave an overview of the current literature on the use of split-plot experiments in industry.

Goos and Vandebroek (2001) developed a design construction algorithm that computes the optimal number of whole plots and the whole plot sizes with respect to D-optimality criterion.

Box et al (2005) described a prototypical Split-plot experiment with one easy-to-change factor and one hard-to-change factor. The experiment was design to study the corrosion resistance of steel bars treated with four coatings, C_1 , C_2 , C_3 and C_4 , at these furnace temperatures, 360°C , 370°C , and 380°C . Furnace temperature is the hard-to-change factor because of the time it takes to reset the furnace and reach a new equilibrium temperature.

A candidate set-free algorithm for generating D-optimal split-plot designs was developed by Jones and Goos (2007).

We note in particular, the development of optimal split-plot designs by Jones and Goos (2007 and 2009). Jones and Nachtsheim (2009) are also known for their contributions to the advancement of split-plot experiments.

3.0 Statistical Model and Analysis

The regression model for a split-spot experiment with b whole plots of k runs is:

$$Y_{ij} = f(x_{ij}) \beta + \gamma_i + \varepsilon_{ij} \quad 3.1$$

Where Y_{ij} represent the response measured at the j th run in the i th whole plot, x_{ij} is a vector that contains the levels of all the experimental factors at the j th run in the i th whole plot, $f(x_{ij})$ is its model expansion, and β contains the intercept and all the factor effects that are in the model. γ_i represents the random effect of the i th whole plot and ε_{ij} is the error associated with the j th run in the whole plot i th. The dimension of $f(x_{ij})$ and β is denoted by p .

In a split-spot experiment two factors are involved and we denote the N_w hard-to-change factors with the symbol w_1, \dots, w_{n_w} or w , while the N_s easy-to-change factors are represented by the symbol S_1, \dots, S_{n_s} or S .

This gives the split-spot model as

$$Y_{ij} = f'(w_i, s_{ij}) \beta + \gamma_i + \varepsilon_{ij} \quad 3.2$$

Such that W_i represents the settings of the hard-to-change factors in the i th whole plot and S_{ij} shows the setting of the easy-to-change factors at the j th run within the whole plot.

In matrix notation a split-plot experiment with sample size of n and b whole plots, the model is:

$$Y = X\beta + Z\gamma + \varepsilon, \quad 3.3$$

Where Y is the vector of responses, X represents the $n \times p$ model matrix containing the setting of both the whole-plot factors w and the sub-plot factors and their model expansions, β is the P -dimensional vector containing the P fixed effects in the model, Z is an $n \times b$ matrix of zeroes and ones assigning the n runs to the b whole plots. The term γ is the b -dimensional vector containing the random effects of the b whole plots and ε is the n -dimensional vector containing the random errors. It is assumed that:

$$E(\varepsilon) = O_n \text{ and } \text{cov}(\varepsilon) = \sigma_\varepsilon^2 I_n, \quad 3.4$$

$$E(\gamma) = O_b \text{ and } \text{cov}(\gamma) = \sigma_\gamma^2 I_b, \quad 3.5$$

$$\text{Cov}(\gamma, \varepsilon) = O_{b \times n} \quad 3.6$$

Using these assumptions, the covariance matrix of the responses, $\text{Var}(\gamma)$, is

$$V = \sigma_\varepsilon^2 I_n + \sigma_\gamma^2 Z Z' \quad 3.7$$

If the entries of γ are arranged per whole plot, then

$$V = \text{diag}(V^*, \dots, V^*), \quad 3.8$$

$$V^* = \sigma_\varepsilon^2 I_k + \sigma_\gamma^2 1_k 1_k' = \sigma_\varepsilon^2 (I_k + \eta 1_k 1_k'), \quad 3.9$$

k is the number of runs in each whole plot and the variance ratio $\eta = \sigma_\gamma^2 / \sigma_\varepsilon^2$ is a measure for the extent to which response from runs within the same whole plot are correlated. The larger η , the more the responses within one whole plot are correlated.

4.0 Optimality Criteria

Optimality criterion can be regarded as a single number or value that summarizes how good a design is and it is maximized or minimized by an optimal design. It can also be regarded as a number which provides a measure of the fit of the data to a given hypothesis. The optimality criteria are all functions Ψ of the information matrix M . The class of generalized optimality criteria includes the A-, D- and E- optimality criteria which were introduced by Kiefer (1975). Furthermore, a detailed work in this area was done by Cheng (1978). The optimal design ξ^* with respect to a given criterion is the design that optimizes the given criterion values over the space Ξ of all feasible designs. Mathematically

$$[M(\xi)] = \xi \in \Xi \Psi[M(\xi)] \quad 4.1$$

4.1 D- Optimality

This optimality design minimizes the variance of the parameter estimators. This is achieved by maximizing the determinant of the information matrix or, equivalently by minimizing the determinant of the variance-covariance matrix of the parameter estimators. We obtain the D-optimal design by maximizing the determinant

$$|X'X| \quad 4.2$$

Where $\lambda_1, \lambda_2, \dots, \lambda_p$ represent the p eigenvalues of the information matrix. Using these eigenvalues, the D-criterion is equivalent to minimizing.

$$\prod_{i=1}^p \lambda_i \quad 4.3$$

4.2 Optimal Split – Plot Designs

Given any number of observations, an optimal design can be constructed. It also accommodates any possible restriction on the setting of the experimental variable. For any combination of quantitative and mixture variables, efficient design can be constructed for any given experimental situation by the optimum design theory (see Kiefer, 1959).

Optimal designs for split-plot experiments were first proposed by Goos and Vandebroek (2001).

The general approach is as follows:

1. Specify the number of whole plots n_w
2. Specify the number of split-plots per whole plot, n_s
3. Specify the response model, $f^T(w, s)$.
4. Specify a prior estimate of the variance ratio, η .
5. Use computer software to construct the design for steps 1 through 4 that maximizes the D – optimality criterion $C_D(X, Z, V) = |X'V^{-1}X|$
6. Study the sensitivity of the optimal design to small changes in d , n_w and n_s .

The algorithm given by Goos and Vandebroek (2001) also requires that the user specify a candidate set of possible design points. Meyer and Nachtsheim (1995) developed an alternative algorithm based on the coordinate exchange algorithm. An alternative algorithm, which does not require candidate sets, was later developed by Jones and Goos (2007).

5.0 Benefits of Split-Plot Designs

In this work, we advocate greater consideration of split-plot experiments for three reasons: cost, efficiency, and validity. These benefits are explained below:

5.1 Cost

Generally, it cost less to run a set of treatments in split-plot order than when the same experiment is completely randomized. As noted by Ganju and Lucas (1997, 1998, 2005), a properly implemented completely randomized design (CRD) requires that all factors must be independently reset with each run. If a factor level does not change from one run to the next and the factor level is not reset, inadvertent split plotting occurs. Such designs, termed random run order (RRO) designs by Ganju and Lucas (1997) are widely used and always analyzed inappropriately. The cost of a split-plot experiment can be significantly less since much of the cost of running a split-plot experiment is tied to changes in the hard-to-change factors. If the cost of setting a hard-to-change factor is C_w and the cost of setting an easy-to-change factor is C_s , and if there are n_w whole plots and n_s split plots, the CRD cost is $n_s(C_w + C_s)$, whereas the SPD cost is $n_w C_w + n_s C_s$, so that the additional cost for the CRD is $(n_s - n_w) C_w$. Split-plot designs are useful precisely because this additional cost can be substantial. Anbari and Lucas (1994, 2008) contrast the costs of CRDs and SPDs for various design scenarios. Bisgaard (2000) also discussed cost functions.

5.2 Efficiency

Split-plot experiments apart from being less expensive to run than completely randomized experiments; they are often more efficient statistically. Ju and Lucas (2002) show that, with a single hard-to-change factor or a single easy-to-change factor, use of a split-plot layout leads to increased precision in the estimates for all factor effects except for whole-plot main effects. Anbari and Lucas (1994) and Goos and Vandebroek (2004) considered the overall measures of design efficiency. Goos and Vandebroek (2001, 2004) demonstrated that the determinant of a D-optimal split-plot design frequently exceeds that of the corresponding D-optimal completely randomized design. The results above indicate that running split-plot designs can represent less cost with greater overall precision. Hence, many researchers recommend the routine use of split-plot layouts, even when a CRD is a feasible alternative.

5.3 Validity

In the industry, completely randomized designs are prescribed, but are typically not run as such in the presences of hard-to-change factors. In order to saving time or money, the experimenter may take one of two shortcuts.

1. A random-run-order (RRO) design also referred to as a random-not-reset (RNR) design- is utilized. Here, the order of treatment is randomized, but the factor level is not reset with each run of the

experiment, or perhaps all the hard-to-change factors are reset. Not resetting the level of the hard-to-change leads to a correlation between adjacent runs. Statistical tests that do not consider these correlations will be biased (Ganju and Lucas (1997))

2. Here, the experimenter may decide to resort the treatment order to minimize the order of changes of the hard –to-change factor. This leads to a split-plot design but the results are typically analyzed as if the design had been fielded as a completely randomized experiment.

6.0 Evaluation of the D-Optimal Split-Plot Algorithms

Here, comparison is made in terms of ease of use, quality of the design produced and computing time of the candidate-set-free algorithm with alternative methods for constructing D -optimal designs.

6.1 Ease of use

The candidate-set-free algorithm does not require the user to specify a candidate set. This is its main benefit. For simple design problems, such problems involves unconstrained continuous factors only and a cuboidal experimental region, good candidate sets for first- and second-order models are given by the points of two- or three-level factorial designs respectively. For other design problems, involving constrained continuous and/or mixture variables, constructing a good candidate set may be difficult and time consuming. The construction of good candidate sets for such problems requires experience and is, for spherical design regions, even a matter of on-going research (see Mee (2007)). Since running design construction algorithms using poor candidate sets leads to inefficient designs, the fact that the candidate-set-free algorithm does not require a candidate set is an important practical advantage over the algorithm of Goos and Vandebroek (2003) and sequential algorithmic approaches like that in Trinca and Gilmour (2001). The fact that the construction of a good candidate set often takes more time than running a classical algorithm for computing an optimal design is not captured by the timing study. Obviating the need for the construction of a candidate set, however, is a major contribution of the candidate-set-free algorithm.

6.2 Design efficiency

D -optimal designs for various design problems have been computed (see Jones and Goos (2007)), including the examples in Goos and Vandebroek (2003), using the candidate-set-free algorithm, the algorithm of Goos and Vandebroek (2003) and two sequential approaches. In the sequential approaches, one of which was proposed by Trinca and Gilmour (2001). The designs for the whole-plot factors and the subplot factors are constructed sequentially. Compared with the algorithm of Goos and Vandebroek (2003), the sequential approaches offer the advantage that two smaller candidate sets can be used instead of one large candidate set when the design problem involves a large number of factors. Though, from a computational point of view this is attractive but, unfortunately, the sequential approaches to constructing D -optimal split-plot designs do not always lead to highly efficient designs, even when the designs for the whole-plot factors and the subplot factors are both constructed by using the D -optimality criterion. The sequential approaches yield designs that are more than 10% less efficient than the design that is produced by the candidate-set-free algorithm. When the goal is to construct D -optimal split-plot designs, we would therefore not recommend a sequential approach in general.

The candidate-set-free algorithm and the algorithm of Goos and Vandebroek (2003) are close competitors in terms of efficiency of the designs generated provided that the latter algorithm is run with a good candidate set. For first-order models in the absence of constraints on the factor levels, the two algorithms produce equivalent designs. For second-order models and for design problems involving constraints on the factor levels, applying the candidate-set-free algorithm for a given computing time leads to designs that perform up to 0.5% better in terms of D -optimality than the algorithm of Goos and Vandebroek (2003). These small gains in efficiency are due to the nearly continuous optimization that can be performed with the candidate-set-free algorithm.

6.3 Computing time

The use of a candidate set and exchange and interchange steps by Goos and Vandebroek (2003) makes it computationally more intensive than the candidate-set-free algorithm. The candidate set grows exponentially with the number of factors in an experiment. Considering all exchanges between rows of the candidate set and rows of the design makes such an algorithm run in exponential time in the number of factors. The candidate-set-free algorithm runs in polynomial time in the number of factors and the number of levels considered for each factor. For a fixed number of factors, the candidate-set-free algorithm can allow for a much finer discretization of the range of each factor for the same computational cost as an algorithm using a candidate set, leading to the small efficiency improvements.

8.0 Theoretical example

8.1 Two whole-plot factors and five subplot factor of 24 runs.

Here, there are resources for 24 runs to be performed in eight whole plots of three runs each. All the factors have two levels.

Table 1 shows a globally optimal design using the candidate-set-free algorithm construct for estimating a main effects model. Note that the values of the two whole-plot factors over the eight whole plots are a replicated 2^2 factorial design. Within each whole plot the sum of the values of each subplot factor is always either -1 or 1 ; in addition, the inner product of any pair of columns is 0. So, the design is as balanced as it possibly can be given that each whole plot is only three runs instead of four.

Table 1
 Optimal 24-run split-plot design in eight whole plots of size 3

Whole plot	W ₁	W ₂	S ₁	S ₂	S ₃	S ₄	S ₅
1	1	1	-1	-1	-1	-1	-1
1	1	1	-1	1	1	-1	1
2	-1	1	1	-1	1	-1	-1
2	-1	1	-1	1	1	-1	1
2	-1	1	1	1	-1	1	-1
3	1	-1	1	-1	-1	1	1
3	1	-1	1	1	-1	-1	-1
3	1	-1	-1	-1	1	-1	-1
4	-1	-1	-1	-1	1	1	-1
4	-1	-1	-1	-1	-1	1	-1
4	-1	-1	1	1	1	-1	1
5	1	1	-1	1	-1	-1	-1
5	1	1	-1	1	-1	1	1
5	1	1	1	-1	1	1	-1
6	-1	1	1	1	1	1	-1
6	-1	1	1	-1	-1	-1	1
6	-1	1	-1	-1	-1	1	1
7	1	-1	1	1	1	1	1
7	1	-1	1	-1	-1	-1	1
7	1	-1	-1	1	1	1	-1
8	-1	-1	-1	-1	1	-1	1
8	-1	-1	1	1	-1	-1	-1
8	-1	-1	-1	1	-1	1	1

Table1 shows the information matrix of the design, assuming that the ratio of the whole-plot variance to the error variance (η) and σ_{ϵ}^2 are both 1. The matrix is diagonal therefore estimates of the model coefficients are uncorrelated. Here, the diagonal elements that are associated with the intercept and whole-plot factor effects are 6. However, the elements that are associated with the subplot effects are 22. These values could be viewed as the effective sample sizes for estimating these effects. The individual variances of the coefficients are proportional to the reciprocals of the diagonal elements of the matrix. The variances of the whole-plot factor effects (and intercept) are thus much larger than the variances of the subplot factor effects. This is a direct result of the split-plot structure. If we assume that η and σ_{ϵ}^2 are 1 and that completely randomized designs were run, then the values on the diagonal of the information matrix would be 12. Hence, this variance ratio, the split-plot design estimates, the main effects of the two whole-plot factors will be twice the variance of a completely randomized design but those of the five subplot factors with only 6/11ths the variance. The split-plot design is more efficient.

Table 2

Diagonal information matrix for the split-plot design in Table 1

I	W ₁	W ₂	S ₁	S ₂	S ₃	S ₄	S ₅
6	0	0	0	0	0	0	0
0	6	0	0	0	0	0	0
0	0	6	0	0	0	0	0
0	0	0	22	0	0	0	0
0	0	0	0	22	0	0	0
0	0	0	0	0	22	0	0
0	0	0	0	0	0	22	0
0	0	0	0	0	0	0	22

9.0 Conclusion

In this work, we have presented a detailed literature review on the development of optimal design of split-plot experiments. Split-plot designs, optimality criteria were discussed. The benefits of split-plot designs were presented. The comparison of the candidate-set-free algorithm and other existing algorithms was done.

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