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Evaluation of Optimal Split-Plot Designs

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Abstract: The study introduced an algorithm for generating optimal split-plot designs. The designs were considered as optimal because they were capable and efficient in estimating the fixed effects of the statistical model that is appropriate given the split-plot design structure. Here, we introduced I-optimal design of split-plot experiments. The algorithm used in this research does not require the prior specification of a candidate set. Therefore, making the design of split-plot experiments computationally feasible in situations where the candidate set is too large to be tractable. Flexible choice of the sample size, inclusion of both continuous and categorical factors were allowed by this method. We show through an example the substantial benefits of this method.

Key words: I-optimal; Categorical data; Tractable; Sample size; Split-plot; Algorithm

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1. INTRODUCTION

Due to cost constraints and logistic problems, complete randomization of designs for industrial experiments may be difficult. A reasonable alternative to complete randomization is the split-spot design, which involves a restricted randomization. The presence of factors whose level are hard-to-change, in addition to factors whose level are easy to change is the main reason why a lot of experiments avoid complete randomization.

In the past few years, increasing attention has been given to the prediction-oriented optimal design criterion. That is, the I-optimality criterion (also known as V-optimality), IV-optimality or Q-optimality due to its usefulness.

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

In Haines (1987), Meyer and Nachtsheim (1988, 1995) and Hardin and Sloane (1993) the generation of I-optimal completely randomized designs (which minimizes the average prediction variance) is discussed. Hardin and Sloane (1993) demonstrated that D-optimal response surface designs perform poorly in terms of the I-optimality criterion while I-optimal designs perform reasonably well with respect to the D-optimality criterion, when the experimental region in cuboidal. Completely randomized response surface experiment involving three-level categorical factors, where the performance of the I-optimal design in terms of the D-optimality criterion is much better than the performance of the D-optimal design in terms of the I-optimality criterion was reported in Goos and Jones (2011). The reasons stated above is responsible for why we prefer to minimize the average variance of prediction and focus on I-optimal split-spot designs. The model used for data from split-spot experiments is described in this work. The model estimation is discussed. The D-optimality criterion and the I-optimality criterion are defined. We therefore indicate how to qualify the relative performance of two designs using D- or I-efficiency.

2. STATISTICAL MODEL AND ANALYSIS

To analyze data from a split-spot experiment with b whole plots of k runs the model used is:

$$Y_{ij} = f'(x_{ij})\beta + \gamma_i + \varepsilon_{ij} \tag{2.1}$$

Where Y_{ij} represent the response measured at the jth run in the ith whole plot, x_{ij} is a vector that contains the levels of all the experimental factors at the jth run in the ith 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 ith whole plot and ε_{ij} is the error associated with the jth run in the whole plot ith. 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 $w_1, ..., w_{nw}$ or w, while the N_s easy-to-change factors are represented by the symbol $S_1, ..., S_{ns}$ or S.

This gives the split-spot model as

$$Y_{ij} = f'(w_i, s_{ij})\beta + \gamma_i + \varepsilon_{ij} \tag{2.2}$$

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

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

$$Y = X\beta + z\gamma + \varepsilon, \tag{2.3}$$

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

$$E(\varepsilon) = O_n \quad and \quad cov(\varepsilon) = \sigma_\varepsilon^2 I_n, \tag{2.4}$$

$$E(\gamma) = O_b \quad and \quad cov(\gamma) = \sigma_\gamma^2 I_b, \tag{2.5}$$

$$Cov(\gamma, \varepsilon) = O_{bxn} \tag{2.6}$$

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

$$V = \sigma_\varepsilon^2 I_n + \sigma_\gamma^2 ZZ', \tag{2.7}$$

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

$$V = diag(V^*, \ldots\ldots, V^*), \tag{2.8}$$

$$V^* = \sigma_\varepsilon^2 I_k + \sigma_\gamma^2 l_k l_k', = \sigma_\varepsilon^2 (I_k + \eta' l_k l_k'), \tag{2.9}$$

k is the number of runs in each whole plot and the variance ratio $\eta = \sigma_r^2/\sigma_\varepsilon^2$ 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.

When the random error terms as well as the whole-plot effects are normally distributed, the maximum likelihood estimate of the unknown model parameter vector β is generalized least square estimator

$$\beta = (x'v^{-1}x)^{-1} x'v^{-1} Y, \tag{2.10}$$

With covariance matrix

$$Var(\beta) = (x'V^{-1}X)^{-1} \tag{2.11}$$

The information matrix for the parameter vector β is given by

$$M = x'v^{-1}x \tag{2.12}$$

3. OPTIMALITY CRITERIA

3.1. D-Optimality Criterion

The D-optimality criterion is the most popularly used criterion to select experimental designs. It maximizes the determinant of the information matrix,

$$|M| = |X'V^{-1}X| \tag{3.0}$$

D-efficiency is used in comparing the quality of two designs with information matrices M_1 and M_2. The D-efficiency of any given design with M_1 as information matrix relative to a design with information matrix M_2 is:

$$D - efficiency = \left(\frac{|M_1|}{|M_2|}\right)^{1/p} \tag{3.1}$$

When the value of D-efficiency is larger than 1, it indicates that design 1 is better than design 2 in terms of the D-optimality criterion. Split-plot designs were constructed using D-optimality criterion by Goos and Vandebroek (2001, 2003, 2004), Jones and Goos (2007), Macharia and Goos (2010) and Schoen, Jones and Goos (2011).

Generally, the D-optimality design depends on the variance ratio η through the covariance matrix V of the responses, as does the D-efficiency of one design relative to another.

3.2. I-Optimality Criterion

The I-optimality split-plot design minimizes the average prediction variance.

$$Average\ variance = \int_{\chi} f'(x)(X'V^{-1}X)^{-1}f(x)dx \tag{3.2}$$

Over the design region χ. The above expression for an arbitrary model is not difficult to calculate. For N quantitative experimental variables, while the experiment region is $[-1,+1]^n$, the volume of the experimental design in the denominator is 2^N. $f'(x)(X'V^{-1}X)^{-1}f(x)$, the variance of prediction is a scalar, such that

$$f'(x)(X'V^{-1}X)^{-1}f(x) = tr\left[f'(x)(X'V^{-1}X)^{-1}f(x)\right] \tag{3.2.1}$$

When evaluating the trace of a matrix product, we can cyclically permit the matrices. Hence,

$$tr\left[f'(x)(X'V^{-1}X)^{-1}f(x)\right] = tr\left[(X'V^{-1}X)^{-1}f(x)f'(x)\right] \tag{3.2.2}$$

$$\int_{\chi} tr\left[f'(x)(X'V^{-1}X)^{-1}f(x)\right]dx = tr\left[\int_{\chi}(X'V^{-1}X)^{-1}f(x)f'(x)dx\right] \tag{3.2.3}$$

It should be noted that since the factor level setting are fixed, the matrix X, and hence $(x'v^{-1}x)^{-1}$, is constant as far as this integration is concerned. Hence,

$$\int_{\chi} f'(x)(X'V^{-1}X)^{-1}f(x)dx = tr\left[(X'V^{-1}X)^{-1}\int_{\chi} f(x)f'(x)dx\right] \tag{3.4}$$

Therefore the average prediction variance can be rewritten as:

$$Average\ variance = 2^{-N}tr\left[(X'V^{-1}X)^{-1}\int_{\chi} f(x)f'(x)dx\right] \tag{3.5}$$

Therefore the average prediction variance can be rewritten as:

$$Average\ variance = 2^{-N}tr\left[(X'V^{-1}X)^{-1}\int_{\chi} f(x)f'(x)dx\right]$$

The integral in Equation 3.2 is applied to a matrix of one-term monomials. This notation is to be interpreted as the matrix of integrals of these monomials.

If $\chi = [-1, +1]^N$ is the experimental region, then the integral becomes quite easy to manipulate. If

$$B = \int_{\chi=[-1,+1]^N} f(x)f'(x)dx \tag{3.5.1}$$

Then,

$$Average\ variance = 2^{-N} tr\left[(X'V^{-1}X)^{-1}B\right] \tag{3.5.2}$$

B is called the moment's matrix. B has a very specific structure for full quadric model as pointed out by Hardin and Sloane (1991). That is:

$$B = 2^N \begin{bmatrix} 1 & O'_N & O'_N* & \frac{1}{3}1'_N \\ O_N & \frac{1}{3}1_N & O_{N\times N*} & O_{N\times N} \\ O_{N*} & O_{N*\times N} & \frac{1}{9}1_{N*} & O_{N*\times N} \\ \frac{1}{3}1_N & O_{N\times N} & O_{N\times N*} & \frac{1}{45}(4I_N + 5J_N) \end{bmatrix} \tag{3.5.3}$$

Such that $N = N_w + N_s$ is the number of factors and $N* = N(N-1)/2$ is the number of two factor interaction effects. Given that P_1 is the average variance of prediction of one design and P_2 is the average variance of prediction of a second design, the I-efficiency of the former design compared to the latter is

$$I - efficiency = P_2/P_1$$

Note that, I-efficiency larger than 1 indicates that design 1 is better than design 2 in terms of the average prediction variance. I-optimal design and the I-efficiency of one design relative to another depend on the variance ration η through the covariance matrix V.

4. THE VARIANCE COMPONENTS

The shortcoming with determining the D- or I-optimal split-plot design is that the matrix V and the D- and I-optimality criteria depends on the unknown variances σ_y^2 and σ_ε^2.

An educated guess of the variance ratio is good enough in order to generate an optimal design, since a design that is optimal for one variance ratio is also optimal for a broad range of variance ratios around the specified one.

At times, different variance ratios lead to different designs, however the quality of these designs in almost the same. Goos (2002) recommended a variance ratio of one for finding optimal split-plot designs in the absence of detailed prior information about the design is at available.

5. ALGORITHM

This algorithm avoids the need for the explicit construction of a candidate set. A rough general description of our candidate-set-free algorithm for generating I-optimal split-plot designs is presented here. This work is actually an extension of the candidate-set-free algorithm for generating D-optimal designs by Goos and Jones (2007). The pseudo code of the algorithm is provided below.

The algorithm requires the prior specification of the following:

i. For each factor whether it is continuous, categorical or a mixture ingredient
ii. Designation of the factors that are hard to change
iii. Any additional constraints on factor combinations
iv. The number b and size of the whole plots (which yields the sample size)
v. The ratio n of the whole plot to the error variance
vi. The a priori model and
vii. The number of starting designs or tries t to be considered.

With the above information in place, the algorithm is in two parts. Part 1 of the algorithm deals with the creation of a starting design. Part 11 deals with the iterative improvement of this design until no further improvement are possible. Improvement is determine by the decrease in the objective function $2^{-N}tr[(X'V^{-1}X)^{-1}B]$. These two parts of the algorithm are performed t times.

The value of I_c that is computed in the current iterate is compared with the minimum value of I_c from all the previous iterates. If the current value of I is lower, then it becomes the new minimum and the current design is stored.

We form the starting design column by column. We choose randomly the values for each row for the subplot factor columns. The b random numbers are chose for the whole-plot factor columns. All the rows in a given whole plot have the same value. The desired split-plot structure for the starting design is obtained through this procedure. The starting design can be improved upon by considering changes in the design element by element. This depends on whether that element is in a subplot factor column or a whole-plot factor column.

Where, an element is in a subplot factor column, the objective function is evaluated over a discrete number of values spanning the range of that factor. If the minimal value of the objective function is smaller than the current minimum, then the current minimum is replace and the current element in the design is replaced by the factor setting corresponding to the minimal value.

For an element in a whole-plot factor column the procedure is more involved. If this element changes then, all the elements in the same whole plot for that column must also change. Here, we consider a discrete number of values for that whole-plot value taken. Also, if the minimal value of the objective function is smaller than the current minimum, then the current minimum is replaced and all the rows in that whole plot are replaced by the factor setting corresponding to the minimal value.

We continue this element-by-element procedure until a complete cycle through the entire design has been completed. Then, another complete cycle through the design is performed noting whether any element changes in the current pass. This continues until no changes are made in a whole pass or until a specified maximum number of passes have been executed.

5.1. Algorithm: Pseudo Code (I-Optimality Criterion)

It is assumed that all whole-plot sizes in the design are equal to k and that all factors are continuous. It is also assumed that the values of m_w whole-plot factors have been arranged in the first m_w columns of the design matrix and the m_s subplot factors have been arranged in the columns from $m_w + 1$ to $m_w + m_s$.

The current best I-criterion value found by the algorithm is denoted by I_{opt}. The current I-criterion value during a try denoted by I_c. We assume that an appropriate discretization of the range for each continuous factor has been generated. The number of values for the discretized factor i is denoted by L_i and the set of values by $F_i = \{\int_{ij}, ..., \int_{iL_i}\}$. Conclusively, we represent the number of tries by t and the number of current try by t_c.

Step 1: set $I_{opt} = 0$ and $t_c = 1$.

Step 2: generate the starting design.

a) Randomly generate values for the m_w whole-plot factor.

i. Set $i = 1$.

ii. Set $j = 1$.

iii. Randomly generate a value for whole-plot factor j in whole plot i.

iv. Assign that value to rows $k(i-1)+1$ to k_i of column j of the factor settings matrix.

v. If $j < m_w$, then set $j = j+1$ and go back to step 2, part (a) (iii).

vi. If $i < b$, then set $i = i+1$ and go back to step 2, (a) (ii).

b) Randomly generate levels for the m_s subplot factors.

i. Set $i = 1$.

ii. Set $j = 1$.

iii. Randomly generate a value for subplot factor j in run i.

iv. Assign that value to cell $(i, m_w + j)$ of the design matrix.

v. If $j < m$, then set $j = j+1$ and go back to step 2, part (b) (iii).

vi. If $i < n$, then set $i = i+1$ and go back to step 2, part (b) (ii).

Step 3: compute the I-criterion value I of the starting design.

Step 4: improve the current design.

a) Set $k = 0$.

b) Set $i = 1$.

c) Improve whole-plot factor levels in whole plot i.

i. Set $j = 1$.

ii. Set $\delta = 0$.

iii. $\forall f_{ij} \in F_i$:

A. Replace the value of whole-plot factor j with $f_j\iota$ in rows $k(i-1)+1$ to k_i of the factor setting matrix;

B. Compute the I-criterion value I_ι of the modified design;

C. If $I_1 > I$, then set $k = 1, \delta = 1, I = I_\iota$ and $\iota_{max} = \iota$.

iv. If $\delta = 1$, then replace the value of whole-plot factor j with the ι_{max}th element of F_1 in rows $k(i-1)+1$ to k_i of the factor settings matrix.

v. If $j < m_w$ then set $j = j+1$ and go back to step 4, part (c) (ii).

d) Improve subplot factor level for all k runs in whole plot i.

i. Set $r = 1$.

ii. Set $j = 1$.

iii. Set $\delta = 0$.

iv. $\forall f_{m_w+j,\iota} \in F_{m+j}$.

A. Replace the value of subplot factor j with $\forall f_{m+j,\iota}$, in cell $(k(i-1)+r, m_w+j)$ of the factor settings matrix;

B. Compute the D-criterion value D_ι of the modified design;

C. If $I_\iota > I$, then set $k = 1, \delta = 1, I = I_\iota$ and $\iota_{mw} = \iota$.

v. If $\delta = 1$, then replace the value of subplot factor j with $f_{m+j,\iota_{max}}$ in cell $(k(i-1)+r, m_w+j)$ of the factor settings matrix.

vi. If $j < m_s$, then set $j = j+1$ and go back to step 4, part (d)(iii).

vii. If $r < k$, then set $r+1$ and go back to step 4, part (d)(ii).

Step 5: if $\iota < b$, then set $i = i+1$ and go back to step 4, part (c).

Step 6: if $k = 1$, then go back to step 4, part (a).

Step 7: if $I > I_{opt}$, then set $I_{opt} = I$ and store the current design.

Step 8: if $t_c < t$, then $t_c = t_c + 1$ and go to step 2: otherwise stop.

5.2. Implementation of I-Optimal Criterion for Split-Plot Designs

There is presently expanding literature on the design of split-plot experiments, after many years of comparative neglect. Goos (2002) published a book on the treatment of blocked and split-plot experiments. Goos and Vandebroek (2004) allow for the different costs of changing the levels of two kinds of factor. Jones and Nachtsheim (2009) discussed split-plot: what, why and how.

If logistic reasons make changing the level of the first factor very difficult so that it is necessary to divide the 20 runs in a given experiment into four whole plots of five runs such that within each group of runs, the first factor level remains the same, this leads to a split-plot structure for the design.

Table 1
I-Optimal 20-Runs Split-Plot Designs in Four Whole Plots of Size Five for Estimating a Full Quadratic Model in One Whole Plot Factor W and One Sub-Plot Factor S

	I - optimal	
Whole plot	**w**	**s**
1	-1	-1
1	-1	-1
1	-1	0
1	-1	1
1	-1	1
2	0	-1
2	0	0
2	0	0
2	0	0
2	0	1
3	0	-1
3	0	0
3	0	0
3	0	0
3	0	1
4	1	-1
4	1	-1
4	1	0
4	1	1
4	1	1

Table 2
Relative Variances of Factor-Effect Estimates Obtained from I-Optimal Split-Plot Designs in Table 1

	$\eta = \mathbf{0.1}$	$\eta = \mathbf{1}$	$\eta = \mathbf{10}$
Effect	I-opt	I-opt	I-opt
Intercept	0.190	0.640	5.140
w	0.150	0.600	5.100
s	0.083	0.083	0.083
ws	0.125	0.125	0.125
w^2	0.340	1.240	10.240
s^2	0.250	0.250	0.250
Average (incl. intercept)	0.190	0.490	3.490
Average (excl. intercept)	0.190	0.460	3.160

6. CONCLUSION

In this work, the model used for data is obtained from split-plot experiments. The model estimation was described. The D-optimality criterion as well as the I-optimality criterion was defined and evaluated. A new algorithm for generating I-optimal split-plot designs was developed. A theoretical example was used in testing the feasibility of this algorithm.

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