Computers and Electronics in Agriculture 133 (2017) 37–45

Contents lists available at ScienceDirect

Computers and Electronics in Agriculture

journal homepage: www.elsevier.com/locate/compag

Application note

On the generation of cost effective response surface designs

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ARTICLE INFO

Article history:
Received 7 September 2016
Accepted 25 November 2016

Keywords:
Randomization
Run order
Response surface design
Minimum change
Cost effective

ABSTRACT

Run order consideration for mixed factorial, fractional factorial and confounded factorial have been studied by several authors in depth, but is lacking for Response Surface Designs (RSDs) except the results obtained by Quinlan and Lin (2015) for Plackett-Burman Design, a commonly used first order response surface design for screening purpose. Second Order Response Surface Designs (SORDs) are used to explore relationship between the response variable and the input variables and to find out the optimum input combinations to achieve a desired response. In this paper, we aim to find out optimal run orders with respect to minimizing level changes using a computer programme. Minimizing the level changes implies the minimization of experimental cost. Generation of four classes of designs viz., Plackett-Burman Design, Cost-effective Central Composite Design (CCD) with full factorial as well as fractional factorial points and Cost-effective Box Behnken Design (BBD) have been described through Macros developed using SAS IML.
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1. Introduction

Response Surface Designs (RSDs) are commonly used in agricultural/industrial experiments for exploring relationship between the response variable and the input variables. RSDs are used in situations where several input variables influence some performance measure or quality characteristic of a process. First order RSDs are mainly used for the screening experiments and Second order RSDs are used for optimization studies. For details on RSDs, one can refer to Khuri and Cornell (1996), Montgomery et al. (2006) and Myers et al. (2009). The procedure of randomization of the run sequences is a technique commonly employed while implementing RSD to avoid bias which may lead to misinterpretation of the result. But this can induce a large number of changes in factor levels and thus make experimentation expensive, time-consuming and difficult.

Here our focus is on the run order consideration of RSDs. The number of level changes is of serious concern to experimenters in many agricultural, post-harvest and processing, engineering and industrial experiments as in such experiments one may come across some situations where it is physically very difficult to change levels of some factors. An example from laboratory experiment conducted in the division of Post-Harvest Technology, Indian Agricultural Research Institute (IARI), New Delhi to study the effect of Viscozyme L. in enhancing the extraction of Juice yield and recovery of total anthocyanins (ACNs) from black carrot mash. The input variables were enzyme concentration, incubation temperature and extraction time each at three levels. Here, it is very difficult to randomize the level of incubation temperature as it requires time to change the temperature from its higher level to lower level.

The criteria for the number of level changes for factors are possibly one of the most important elements to consider when taking on an experimentation process, as this can have a significant impact on effort and costs necessary to carry out the experimentation. This is due to the existence of factors that are difficult to change. Thus, experiments where changing of input factor levels are very difficult/costly, instead of using the standard form of run sequences, response surface design with less factor level changes in run sequences should be used.

Run order consideration for mixed factorial, fractional factorial and confounded factorial have been studied by several authors in depth (Draper and Stoneman, 1968; Dickinson, 1974; Cheng and Jacroux, 1988; Coster and Cheng, 1988; Wang, 1991; Cheng et al., 1998; De León et al., 2005; Correa et al., 2009, 2012; Bhowmik et al., 2015, 2016), but is lacking for Response Surface Designs (RSDs) except by the results obtained by Quinlan and Lin (2015) for Plackett-Burman Design, a commonly used first order response surface design for screening purpose and Varghese et al. (2016) for SORDs.

In this paper, our aim is to find out optimal run orders with respect to minimizing level changes in SORDs using (Varghese et al., 2016, in press) and also to develop some software solution/macros for generation of cost-effective SORDs for easy accessibility and quick reference as developed by Taksande et al. (2012), Sharma et al. (2013) and Jaggi et al. (2015). The subsequent

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http://dx.doi.org/10.1016/j.compag.2016.11.020
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discussions have been summarized in 5 sections. In first four sections, methods of constructing the cost-effective response surface designs have been discussed and in the last section, SAS Macro (SAS Institute Inc., Cary, NC, USA.) for the generation of four classes of designs viz., Placket-Burman Designs, cost-effective Central Composite Design (CCD) with full factorial as well as fractional factorial points and cost-effective Box Behnken Design (BBD) have been given.

2. Plackett-Burman Designs

Plackett and Burman (1946) proposed a class of two-level factorial designs which only require N = 4t, where N is the number of runs. Thus, these designs are often used for screening purposes when there are a large number of factors. For example, a Placket-Burman design with 16 nuns can be used to study 15 factors assuming the interaction among the factors to be negligible. It was shown by Quinlan and Lin (2015) that the total number of changes for a Plackett-Burman design is constant. Hence, the cost effective Plackett-Burman design is the Plackett-Burman design itself.

Plackett-Burman designs have a cyclic structure. Therefore, to construct Plackett-Burman design we only need to give the first row. Then rotate each value one position to the right (or left) and move the furthest value to the other side. Repeat the process until there are N − 1 rows. Finally add a row of '−1' (lower level) to the design.

	A 8 run Plackett-Burman Design						
Run	X_1	X_2	X_3	X_4	X_5	X_6	X_7
1	+1	+1	+1	+1	−1	−1	−1
2	−1	+1	+1	+1	+1	−1	−1
3	−1	−1	+1	+1	+1	+1	−1
4	−1	−1	−1	+1	+1	+1	+1
5	+1	−1	−1	−1	+1	+1	+1
6	+1	+1	−1	−1	−1	+1	+1
7	+1	+1	+1	−1	−1	−1	+1
8	−1	−1	−1	−1	−1	−1	−1
Changes	3	3	3	1	2	2	2

The total number of changes in the run sequence here is 16. This 16 will be same for Plackett-Burman design generated from any initial row and same has been ensured by generating all possible run sequences of 8! = 40,320 designs. It can also be seen that the number level changes for the factor which is coming in the middle is 1 and for each of (k − 1)/2 factors which are coming after the middle factor, the number of level changes is 2 and for each of (k − 1)/2 factors which are coming before the middle factor the number of level changes is 3. General expression for total change is $\frac{5(k-1)}{2} + 1$ (where k is the number of input factors)

3. Cost-effective CCD

CCD is very commonly used rotatable designs in agricultural experiments especially processing and engineering experiments with an objective of optimizing the input factors to produce a desired output. It consists of three parts viz., (i) 2^k factorial points, (ii) 2k axial points and (iii) $n_0 \cong 4\sqrt{2^k} + 4 - 2k$ centre points, where k is the number of input factors.

Let k = 2 (represented by A and B), then a usual CCD can be constructed by taking (i) 2^2 factorial points, (ii) 4 axial points and (iii) 8 centre points as shown below.

A	B	
-1	-1	Factorial Points
-1	1	
1	-1	
1	1	
α	0	Axial Points
-α	0	
0	α	
0	-α	
0	0	Centre Points
0	0	
0	0	
0	0	
0	0	
0	0	
0	0	
0	0	

Here, the number of changes for Factor A = 4 and for Factor B = 7 and the total number of changes is 11. This will increase as the number of factors increase. Hence, a method has been devised to generate CCD with minimum level changes for any given number of factors. It is very clear from the design that the number of changes is mainly depending on the factorial portion. Hence, a method for obtaining CCD with minimum level changes in the run sequences should be based on the method of constructing minimally changed run sequence for the 2 level factorial experiments. Hence, the method developed by Bhowmik et al. (2015) is used for obtaining 2 level factorial experiments with minimum level changes in the run sequences. Then, merging the factorial points with axial points and centre points in the following fashion will result in a CCD with minimum level changes in the run sequences.

Minimal CCD	
A	B
−1	−1
−1	1
1	1
1	−1
α	0
−α	0
0	0
0	0
0	0
0	0
0	0
0	0
0	0
0	0
0	α
0	−α

General expression for total change is 2k + 4k − 3 (where k is the number of input factors) and it is true for every CCD and this is the lower limit for total number of changes in the design. For the above design, the number of changes for Factor A = 4 and for Factor B = 5 and the total number of changes is 9.

The value of α should be so chosen that the design possess the property of rotatability and it can be obtained as $\alpha = (2^k)^{1/4}$ and number of centre points will be approximately equal to $4\sqrt{2^k} - 2k + 4$. Here, the value of α = 1.414 and the number of centre points are approximately equal to 8.

It may be noted here that increasing the number of centre points will not make any difference in the factor-wise level changes as well as the total level changes.

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