EFFICIENT RESPONSE-SURFACE DESIGNS WITH UNKNOWN BLOCK SIZES

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Summary: This paper focuses on the construction of D- and D_s-optimal designs for a second-order response surface model when the block sizes are not fixed. Overviews of the Procedure OPTEX in SAS for the construction of these designs are given. With the BLOCK statement this procedure can produce optimal designs when the block sizes are fixed but for unknown block sizes it requires additional programming to generate the optimal designs for a given number of runs and number of blocks (see Atkinson, Donev and Tobias, 2007). An example about a pastry dough experiment (Goos and Jones, 2011) is used to demonstrate how to generate designs in such situations.

1. Preliminaries

1.1. Introduction

Response surface methodology (RSM) comprises a group of statistical techniques for empirical model building and model exploitation. By careful design and analysis of experiments, it seeks to relate a response variable to the levels of a number of predictors or factors that affect it (Box and Draper, 1987). One of the main goals of RSM is to find the levels of input variables that optimize a response or set of responses. This optimization is done by fitting data collected from an experiment and selecting the operating conditions that meet specifications or goals for each response. The basic theory of RSM is well established and is presented in a number of texts such as those by Box and Draper (1987), Box, Hunter and Hunter (2005), Khuri (2006) and Myers, Montgomery and Anderson-Cook (2009). The focus of this paper is on optimal designs related to second-order polynomial models.

1.2. Model and Designs

Let k denote the number of independent variables or factors or treatments $x_1, x_2, \ldots, x_k$, i.e. k is the dimension of the experimental region. Let the true functional relationship between the response variable y and the set of the k independent variables be approximated by the second-order, or quadratic model

$$y_j = \beta_0 + \sum_{i=1}^{k} \beta_i x_{ji} + \sum_{i=1}^{k} \beta_{ii} x_{ji}^2 + \sum\sum_{h<i} \beta_{hi} x_{jh} x_{ji} + \varepsilon_j,\ j = 1, \ldots, N \tag{1}$$

where β_0 denotes the intercept, β_i is the main effect of the ith factor, β_{ii} is the quadratic effect of the ith factor, β_{hi} is the effect of the interaction involving the hth and ith factors, N is the total number of experimental runs, and ε_j is IID $N(0, \sigma^2)$. In matrix form model (1) can be written as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon} \tag{2}$$

with $E(\boldsymbol{\varepsilon}) = \mathbf{0}$ and $Var(\boldsymbol{\varepsilon}) = \sigma^2\mathbf{I}$ where $\boldsymbol{\beta}$ is the parameter vector and $\mathbf{X}$ is the design matrix. In response surface designs the factors could naturally have different ranges or they could be measured on different scales; by convention all the factor levels or settings are coded to -1 as the lowest level for the factor and $+1$ for the highest level.
Assuming that $\mathbf{X}$ is of full rank, that is $\mathbf{X}'\mathbf{X}$ is nonsingular, the least squares estimate of $\boldsymbol{\beta}$ is given by $\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$ with the variance-covariance matrix $\sigma^2\,(\mathbf{X}'\mathbf{X})^{-1}$. In order to support estimation of the coefficients of the second-order, an experimental design must include at least three distinct values for each input variable. A number of classes of designs have been developed to fit this type of response surface, such as Central Composite designs, CCD (Box and Wilson, 1951), Box-Behnken designs (Box and Behnken, 1960), Augmented pairs designs (Morris, 2000), and Complete three-level factorial designs (Morris, 2011).

2. Computer-generated optimal designs

The standard response surface designs, such as CCD and the Box-Behnken designs, have been developed to accommodate common situations observed in practice and hence may not be appropriate in certain situations, for example when the experimental region is not a cube or a sphere, when there is prior knowledge that the experimental process should be represented by a nonstandard model and when the experimental runs are extremely expensive or time consuming and hence the number of experimental runs required by the standard response surface design should be reduced. In such cases, computer-generated optimal designs, i.e. designs that are best with respect to some optimality criterion, are alternatives to consider. Since optimal designs are the solution to optimization problems for which the number of experimental runs can be specified to be any integer value, the selection of designs need not be restricted to the values that are convenient for any particular standard designs (Morris, 2011, page 301). There are several optimality criteria but in this paper we use D- and D_s-optimality criteria; where a D-optimal design maximizes $|\mathbf{X}'\mathbf{X}|$ or, equivalently, minimizes $|(\mathbf{X}'\mathbf{X})^{-1}|$, i.e. it minimizes the generalized variance of $\hat{\boldsymbol{\beta}}$. Geometrically, this is equivalent to maximizing the volume spanned by the columns of $\mathbf{X}'\mathbf{X}$, which is inversely proportional to the size of the confidence ellipsoid for the parameters of a linear model. In contrast, a D_s optimal design is appropriate when the interest is in estimating a subset of the s parameters in the model as precisely as possible. This will be discussed in the following section.
A computer-based algorithm is required to compute these designs. Procedure OPTEX in conjunction with procedure PLAN in SAS can be used to generate these designs. In this paper we will illustrate

how these procedures can be used to generate blocked response-surface designs with desirable properties.

3. Blocking in response surface design

When using a response surface design, if it is possible to group the experimental runs in such a way that runs in each group are more like each other than they are like runs in a different group, then statistically it is more efficient to make grouping explicit (Goos and Jones, 2011). It is ideal to make the blocking factor orthogonal to the other factors. A response surface design is said to be orthogonally blocked, if it is divided into blocks such that the block effects do not affect the parameter estimates of the response surface model. However, in some experimental situations the constraints on block sizes and the total number of runs available can make the orthogonal blocking impossible. In such cases, an optimal blocking is a useful alternative.

Suppose that the block effects are fixed. By extending the linear model (2) to accommodate the fixed block effects, the model for a blocked response surface design can be given by

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{B}\boldsymbol{\alpha} + \boldsymbol{\varepsilon} = \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\varepsilon}, \tag{3}$$

where $\mathbf{B}$ is a matrix whose columns are indicators of the blocks, $\boldsymbol{\alpha}$ is the vector of block effects, $\mathbf{Z} = [\mathbf{X}\,\mathbf{B}]$, $\boldsymbol{\gamma} = [\boldsymbol{\beta}\ \boldsymbol{\alpha}]$ and the other terms are as defined in (2). The most commonly used design criterion when vector $\boldsymbol{\beta}$ in (3) is the only parameter of interest is D_s-optimality. A D_s-optimal design minimizes the variance-covariance matrix of the least squares estimator of $\boldsymbol{\beta}$ or equivalently maximizes the determinant of the information matrix of $\boldsymbol{\beta}$, $\mathbf{X}'\mathbf{G}\mathbf{X}$ where $\mathbf{G} = \mathbf{I} - \mathbf{B}(\mathbf{B}'\mathbf{B})^{-1}\mathbf{B}'$. Or equivalently a D_s-optimal design maximizes

$$|\mathbf{M}_{\beta}(\xi_N)| = \frac{|\mathbf{Z}'\mathbf{Z}|}{|\mathbf{B}'\mathbf{B}|} = |\mathbf{X}'\mathbf{X} - \mathbf{X}'\mathbf{B}(\mathbf{B}'\mathbf{B})^{-1}\mathbf{B}'\mathbf{X}|$$

where ξ_N is an exact or discrete design (Atkinson et al., 2007, page 139). Observe that if the block sizes are fixed, the determinant $|\mathbf{B}'\mathbf{B}|$ is constant. Therefore, maximizing $|\mathbf{M}_{\beta}(\xi_N)|$ is equivalent to maximizing $|\mathbf{Z}'\mathbf{Z}|$ and hence the D-optimum designs of model (2) and D_s-optimum designs are the same for fixed block sizes. However, in general this result does not hold when the block sizes are not fixed and possibly differ from block to block. Note that designs where blocks are orthogonal to the treatment effects, i.e. $\mathbf{X}'\mathbf{B} = \mathbf{0}$, or $\mathbf{X}'\mathbf{G}\mathbf{X} = \mathbf{X}'\mathbf{X}$ are 100% D_s efficient.

The optimum block designs for fixed block sizes, i.e. D_s-optimum designs, can be calculated using the OPTEX procedure with a BLOCK statement. However, when block sizes are not fixed and need to be optimally allocated, for a given number of experimental runs and number of blocks, the OPTEX procedure needs additional programming to calculate the efficient designs; for example the OPTEX procedure can be combined with the SAS macro of Atkinson et al. (2007, pages 219–220). For the example that is discussed in the following section we have used the OPTEX procedure and this macro, but other alternative methods are also available in the literature, e.g. Meyer and Nachtsheim (1995).

Table 1: Factors and factor levels used in the pastry dough mixing experiment

Flow rate (kg/h)[1]	Moisture content (%)	Screw speed (rpm)
30.0	18	300
37.5	21	350
45.0	24	400

4. The Pastry Dough Experiment

The example used in this section is discussed in Chapter 7 of Goos and Jones (2011). The experiment is about the baking of pastry dough. There are three continuous factors, namely the initial moisture content of the dough (Moisture), the screw speed of the mixer (Screw), and the feed flow rate of water being added to the mix (Flow). Since the researchers expected a curvature in the responses that they were going to measure and wanted to fit a second-order response surface model, they decided to consider three levels for each of the factors (see Table 1). They scheduled the laboratory for seven days in two weeks and planned to do four runs a day. Therefore, the experiment has 28 runs and 7 blocks of size 4. The standard design, e.g. the central composite design, does not accommodate their plan. Assuming the day effect is fixed we generated the D-optimal designs which are also D_s-optimal because the block sizes are equal. The designs generated (Table 3) have efficiency values which are greater than 0% implying that the three main effects, the three first-order interactions and the three quadratic effects are estimable.

The SAS code shown in Table 2 illustrates the use of Proc PLAN and Proc OPTEX. The Proc PLAN is used to create the full $3 \times 3 \times 3$ factorial and stores it in the file Table74. In the Proc OPTEX, the model statement specifies a quadratic model in the three factors, Flow, Moisture and Screw. The **block** and the **generate** statements specify that a design with all 28 treatment combinations be created, that is blocked into 7 blocks of size 4. When this code is run, Proc OPTEX calculates a D_s-optimal design for estimating all the effects listed in the **model** statement. In this code we have used **chain** to select candidate points in the order in which they occur in the original data set (i.e. Table74) and **noexchange** to force only interchange steps, making sure the final design is a reordering of the 27 candidates. The **method** option specifies the procedure used to search for the optimal design. The **examine** statement displays the characteristics, such as information and variance-covariance matrices, of a selected design (SAS Institute Inc., 2010). The option **orthcan** is used to make the efficiency measures more interpretable.

The exact D_s-optimal designs in Table 3 are obtained using the default search algorithm that uses the simple exchange method of Mitchell and Miller (1970), starting with a completely random design. The default size of the design is the number of parameters in the model plus 10 and OPTEX searches for a D-optimum design 10 times with different random initial designs and displays the efficiencies of the resulting designs in a table.

However, besides those used in Table 2, different options available in the OPTEX procedure include the size of the design, type of initial designs, optimality criterion and search algorithm that can be fixed by the practitioner. Atkinson et al. (2007) advise almost always using the options CODING = ORTHCAN in order to make the efficiency measures more interpretable and METHOD =

Table 2: SAS code to calculate a D_s optimal block design

```
proc plan;
  factors Flow = 3 Moisture = 3 Screw=3 ordered;
  output out = Table74 Flow nvals = (30.0, 37.5, 45.0)
        Moisture nvals = (18, 21, 24)
        Screw nvals = (300, 350, 400);
run;

proc optex data=Table74 coding=orthcan seed=12345;
  model Flow|Moisture|Screw@2 Flow*Flow Moisture*Moisture Screw*Screw;
  block structure = (7)4 init = chain noexchange;
  generate initdesign = Table74 method = M_FEDOROV criterion = D;
  examine design information variance;
  output out = DesignMF;
run;
```

M_FEDOROV, i.e. the Modified Fedorov algorithm of Cook and Nachtsheim (1980), in order to use a more reliable search algorithm than the default one. They have found that the Modified Fedorov algorithm of Cook and Nachtsheim (1980) is the most reliable and takes less time to compute an optimum design.

The variances of the factor-effect estimates can be calculated using the inverse of the information matrix of the D_s-optimal design, i.e. the variances are the diagonal elements of the variance-covariance matrix $(\mathbf{X}'\mathbf{X})^{-1}$, where $\mathbf{X}$ is the design matrix of D_s-optimal design. The variances of the factor-effect estimates using the fixed block or day effects are presented in Table 4 and they are obtained using the statement **examine** with **variance** option in Proc OPTEX.

Suppose that the researchers have budget to conduct either 24 or 25 or 26 runs, but on each day they will be able to do not more than four runs and not less than two runs. As the block sizes are not fixed and can vary among the days the BLOCK option in Procedure OPTEX was combined with the SAS macro of Atkinson et al. (2007) to generate the optimal designs. The block sizes for the seven days that yield the D_s-optimum designs are listed in Table 5. The days with 3 or 4 runs occurring do not affect the optimality of the designs as long as the factor levels generated by the program are not swapped.

For brevity we have not discussed in this paper the efficiency measures of optimal designs. However, we would like to remind readers that the formula used to calculate the efficiency measures, e.g. D_s-efficiency reported in Section 4, by Proc OPTEX are different from those given in the optimal designs literature. We therefore advise that the efficiency measures from the procedure OPTEX should be used to compare one design to another for the same situation or to use the SAS macro that is discussed in Chapter 13 of Atkinson et al. (2007). In the example, although we have generated the designs using fixed block effect, for the analysis Goos and Jones (2011) treated block (i.e. day) as a random effect because the responses on any given day are more alike than responses from different days and hence they may introduce correlation in the model for the data.

Table 3: Exact D_s-optimal designs with seven blocks of size four using the factor levels

	Factor levels		
Day (Block)	Flow rate (kg/h)	Moisture content (%)	Screw speed (rpm)
1	30.0	18	300
	45.0	18	400
	37.5	21	350
	45.0	24	300
2	30.0	21	400
	45.0	24	400
	45.0	18	350
	37.5	24	300
3	30.0	18	350
	37.5	24	400
	30.0	24	300
	45.0	21	300
4	45.0	18	300
	30.0	18	400
	30.0	24	300
	37.5	21	350
5	30.0	18	300
	35.0	18	400
	45.0	24	300
	30.0	24	400
6	45.0	24	350
	30.0	24	400
	30.0	21	300
	37.5	18	400
7	30.0	18	400
	30.0	24	350
	37.5	18	300
	45.0	21	400

Table 4: Variances of the factor effect estimates

Factor effect	Variances
Flow rate	0.0332
Moisture content	0.0342
Screw speed	0.0342
Flow rate × Moisture content	0.0269
Flow rate × Screw speed	0.0269
Moisture content × Screw speed	0.0260
Flow rate × Flow rate	0.0507
Moisture content × Moisture content	0.0507
Screw speed × Screw speed	0.0507

Table 5: Block sizes for the seven days, $n_i, i = 1, 2, \ldots, 7$ that yield the D_s-optimum designs

		Block sizes					
Runs	n_1	n_2	n_3	n_4	n_5	n_6	n_7
24	4	4	4	3	3	3	3
25	4	4	4	4	3	3	3
26	4	4	4	4	4	3	3

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