Supersaturated Split-Plot Designs

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Abstract

In this work, we develop a new general methodology for designing and analysing informative experiments that feature both restricted randomisation and large numbers of factors. The application of such methods o ers the potential for economic savings in industrial quality improvement experiments and in the development of new products and processes. We adopt and extend methodology from both the design of split-plot and supersaturated experiments, and propose a Bayesian optimality criterion for design construction. For model selection, we combine ideas from Bayesian inference, REML and shrinkage regression to identify important factorial e ects. We study the performance of our approach using various practical examples, and investigate its properties in a simulation study.

Keywords: Bayesian optimal design; D-optimality; multi-stratum design; restricted randomisation

1. Introduction

In this work, we combine features of two common classes of design: split-plot designs and supersaturated designs. Split-plot designs incorporate restrictions to the randomisation of an experiment that result from incorporating hard-to-change factors or two-stage processes to reduce cost. Supersaturated designs are screening designs for large numbers of factors, with the number of runs less than the number of factors. The advantage of supersaturated designs is that they dramatically reduce the experimental cost but their crucial disadvantage is the introduction of complex partial aliasing between factorial e ects, resulting in the requirement for more sophisticated statistical analysis. The goal of this work is to combine features of split-plot and supersaturated designs to give the exibility to experimenters to use cost-e ective screening designs under the restricted randomisation situations that appear very often in industrial experimentation. The combination of these two well-known classes of designs is a relatively unexplored research area. General construction and analysis methods for supersaturated split-plot designs will allow experiments that can extract the maximum information from the data with minimum time and cost.

A supersaturated design with m factors and n runs has $n \leq m$. The model typically used in screening experiments is $\boldsymbol{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$ where $\boldsymbol{Y}$ is an n-dimensional vector of responses, $\mathbf{X}$ is an $n \times p$ model matrix, where $\boldsymbol{Y}$ is an n-dimensional vector of responses, $\boldsymbol{\beta}$ is a p-dimensional vector containing the p xed model parameters, and $\boldsymbol{\varepsilon}$ is the $n \times 1$ vector containing the random errors for each of the n measured response. The elements of $\boldsymbol{\varepsilon}$ are assumed to be mutually independently normally distributed with zero mean and variance σ_ε^2. The aim of factor screening will be to identify those factors which have substantive non-zero e ects. Georgiou (2014) provides an extensive literature review on construction and analysis methods for supersaturated designs.

Supersaturated experiments are usually designed assuming the treatments (combinations of factor levels) are completely randomised to the experimental units. However, just as with any designed experiment, there may be some structure in the experimental units, or uncontrolled covariates that vary between batches, that should be accounted for via blocking. In addition, some sets of units may have to have treatments with the same levels of some factors; for example, if the treatments are run sequentially, some factors may only be able to be changed less frequently than every run (e.g. factors whose levels are hard or costly to change). This necessitates the use of multi-stratum designs, which provide a more economic alternative to fully randomised designs. Generally, each level of hardness-to-set in factors taken account of in the design defines a stratum, as does each level of blocking. The split-plot design is the simplest case of a multi-stratum design with two strata, whole plots and subplots. Split-plot designs were originally utilized in agricultural experiments, where large plots of land were subdivided into relatively large portions (whole plots). Each of the possible levels of the whole-plot factors were then randomly assigned to these plots. Whole plots were further divided into smaller portions (subplots) to which levels of the subplot factors were applied. Thus, whole-plot factor levels vary from whole plot to whole plot while sub-plot factor levels vary from subplot to subplot. In industrial experimentation, hard-to-change factors act as whole-plot factors, whereas the easy-to-change factors act as subplot factors. These designs are very popular for experimentation in industry, which led to a large body of published research on the subject (e.g., Bingham & Sitter 1999, Goos & Vandebroek 2004, Jones & Goos 2009, Goos & Donev 2007, Vining, Kowalski & Montgomery 2005). The usual form of analysis of these designs is to fit the linear mixed model

$$\boldsymbol{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\varepsilon}, \tag{1}$$

where in addition to the previous model, $\mathbf{Z}$ is an $n \times b$ matrix of zeros and ones whose (i, j)th element is one when the ith observation is obtained in whole plot j, $\boldsymbol{\gamma}$ is the $b \times 1$ vector containing the random effects γ_i describing the whole-plot-to-whole-plot variation in the responses, and $\boldsymbol{\varepsilon}$ is the $n \times 1$ vector containing the random errors ε_{ij} for each of the n measured responses. The elements of $\boldsymbol{\gamma}$ and $\boldsymbol{\varepsilon}$ are assumed to be mutually independently normally distributed with zero mean and variances σ^2_γ and σ^2_ε, respectively. Key to successful screening using a supersaturated design is the principle of effect sparsity (Box and Meyer, 1986), that states that only a small proportion of the $p - 1$ effects will have a substantive effect on the response.

A state-of-the-art method for estimating model (1) is generalized least squares (GLS) for the fixed model effects, combined with restricted maximum likelihood (REML) estimation of the variances of the random effects, the variance components (Letsinger, Myers & Lentner 1996, Gilmour & Trinca 2000, Goos, Langhans & Vandebroek 2006). Mylona, Goos and Jones (2014) proposed a new Bayesian optimal design criterion to construct designs for efficient estimation of both the fixed effects and the variance components. The criterion is suitable for blocked and split-plot response surface experiments. However, it cannot be directly applied to the experiments considered in this work, because of their supersaturated nature.

A limited class of supersaturated split-plot designs was described by Koh, Eskridge & Hanna (2013) and applied by Lee, Eskridge, Koh & Hanna (2009). These authors constructed supersaturated split-plot designs based on Plackett-Burman designs, and they used stepwise regression methods to analyse the data. The disadvantage of these designs is that they exist only for certain cases, as they demand orthogonality between certain factors in order to make the analysis simpler. The authors recognised, however, that the cost of requiring this orthogonality is that fewer factors can be screened. In addition, Marley and Woods (2010) provided evidence that stepwise methods do not perform well when used to analyse data from supersaturated experiments. The goal here is to provide a general methodology, including construction methods that can be used in many experimental situations. These designs can be of great practical value as both restricted randomisation situations and a large number of variables appear very often in experiments from industry and science.

2. Motivating example

Tribocorrosion is the study of degradation or alteration of materials through the combined action of corrosion and wear. An experiment is proposed to optimise diamond-like carbon coatings for use in orthopaedic implants. The tests explore the effects of seven factors; six factors with hard-to-change levels including coating structure, interlayer and substrate and one easy-to-change factor (immersion time). Interactions are also of interest. Three replicates of each treatment are needed to perform all the tests and the water bath used for immersion can hold at most 30 samples at a time. In this situation, not only is there no efficient design available but the notion of an efficient design in this context has not even been defined in a meaningful manner. In addition, novel methodology will be needed to analyse the data in order to draw the correct conclusions. There is no guidance for practitioners on how to plan and to analyse such an experiment, potentially slowing down the scientific progress in application areas.

3. Bayesian optimal design for supersaturated split-plot designs

A Bayesian optimal design criterion is proposed which focuses on efficiency of estimation of both fixed effects and variance components.

Perhaps the most commonly used optimality criterion for selecting experimental designs is the D-optimality criterion (Atkinson, Donev and Tobias, 2007), which seeks designs that maximize the determinant of the information matrix for $\boldsymbol{\beta}$. For a blocked experiment and a split-plot experiment, a D-optimal design therefore maximizes

$$|\mathbf{M}| = |\mathbf{X}^{'}\mathbf{V}^{-1}\mathbf{X}|, \tag{2}$$

when the GLS estimator is used and the variance components are known. Here, $\mathbf{V}$ is the $n \times n$ variance-covariance matrix for the response vector $\boldsymbol{Y}$. This criterion minimises the generalized variance of the estimators of the fixed effects. In Mylona et al. (2014) a composite Bayesian D-optimality criterion, for split-plot designs, that incorporates prior information about the variance components, assuming that they are estimated using REML, was proposed. Also, a Bayesian optimality criterion for supersaturated designs has been proposed by Jones, Lin and Nachtsheim (2008).

The proposed new criterion extends the criterion in Mylona et al. (2014), addressing the supersaturated nature of the designs through regularisation using an informative prior distribution for $\boldsymbol{\beta}$. Assume the following prior distributions for $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$:

$$\pi(\boldsymbol{\beta}) \sim N(\boldsymbol{\beta}_0, \mathbf{R}^{-1}) \quad \pi(\mathbf{y}|\boldsymbol{\beta},\boldsymbol{\gamma}) \sim N(\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma}, \mathbf{R}) \text{ and } \quad \pi(\boldsymbol{\gamma}|\mathbf{D}) \sim N(0, \mathbf{D})\,.$$

Then the proposed Bayesian composite design maximises

$$D_B = \int_0^{+\infty} (\eta) \cdot \pi_1(\eta) \cdot d\eta, \tag{3}$$

where $= \frac{\alpha}{p} \log|\mathbf{X}^{'}\mathbf{V}^{-1}\mathbf{X} + \mathbf{R}| + \frac{1-\alpha}{2} \log|\mathbf{N}|$, $\pi_1(\eta)$ is a prior distribution for the variance ratio $\eta = \sigma^2_{\gamma}/\sigma^2_{\varepsilon}$, and α, $0 < \alpha < 1$, represents the weight attached to the fixed effects estimation and $1-\alpha$ is the weight attached to the variance component estimation. $\mathbf{N}$ is the REML information matrix for the variance components, given in our case by

$$\mathbf{N} = \frac{1}{2}\begin{bmatrix} \text{tr}\{(\mathbf{PZZ}')^2\} & \text{tr}(\mathbf{P}^2\mathbf{ZZ}') \\ \text{tr}(\mathbf{P}^2\mathbf{ZZ}') & \text{tr}(\mathbf{P}^2) \end{bmatrix},$$

where

$$\mathbf{P} = \mathbf{V}^{-1} - \mathbf{V}^{-1}\mathbf{X}(\mathbf{X}^{'}\mathbf{V}^{-1}\mathbf{X} + \mathbf{R})^{-1}\mathbf{X}^{'}\mathbf{V}^{-1}.$$

4. Results

The Bayesian D-optimal design for the tribocorrosion experiment is give in Table 1. The design was constructed via a coordinate exchange algorithm, by assuming a log-normal distribution for η and $\alpha = 1/2$.

5. Conclusions

We develop methodology for the optimal design of supersaturated split-plot experiments for estimating fixed effects as well as variance components in linear mixed models. This new methodology takes the form of mathematical criteria for the selection of efficient designs, and their implementation in computer code. We study the performance of our approach using a motivated example and various models, and investigate its properties in a simulation study.

There has been little research into how to analyse data for mixed effects models with more parameters than available observations. A two-stage approach is studied in this work via simulation. The first stage includes empirical Bayes methods for the estimation of the variance components. The second stage includes the penalized least squares method (Fan and Li, 2001) that has been used in the literature for supersaturated experiments, adapted to incorporate restricted randomisation schemes. When effect sparsity holds, this method as been shown to be effective in the literature on analysing data from supersaturated designs.

Table 1: Bayesian D-optimal design for a supersaturated split-plot experiment with 6 whole-plot factors ($w1$-$w6$), 1 subplot factor ($s1$), and 10 whole plots of size 3.

WP	$w1$	$w2$	$w3$	$w4$	$w5$	$w6$	$s1$
1	1	-1	1	-1	1	-1	1
	1	-1	1	-1	1	-1	1
	1	-1	1	-1	1	-1	-1
2	-1	-1	1	-1	-1	1	-1
	-1	-1	1	-1	-1	1	1
	-1	-1	1	-1	-1	1	-1
3	-1	-1	1	1	-1	-1	-1
	-1	-1	1	1	-1	-1	-1
	-1	-1	1	1	-1	-1	1
4	-1	-1	-1	-1	1	1	1
	-1	-1	-1	-1	1	1	-1
	-1	-1	-1	-1	1	1	-1
5	-1	1	1	1	1	1	-1
	-1	1	1	1	1	1	-1
	-1	1	1	1	1	1	1
6	-1	1	-1	-1	-1	-1	-1
	-1	1	-1	-1	-1	-1	1
	-1	1	-1	-1	-1	-1	-1
7	-1	-1	-1	1	1	-1	-1
	-1	-1	-1	1	1	-1	-1
	-1	-1	-1	1	1	-1	1
8	-1	1	-1	-1	-1	-1	-1
	-1	1	-1	-1	-1	-1	1
	-1	1	-1	-1	-1	-1	-1
9	1	-1	-1	1	-1	1	-1
	1	-1	-1	1	-1	1	1
	1	-1	-1	1	-1	1	1
10	1	-1	1	-1	1	-1	1
	1	-1	1	-1	1	-1	-1
	1	-1	1	-1	1	-1	1

In addition, these methods simultaneously select the regressors to be included in the model and estimate the model coe cients, and as a result they are less computationally intensive than the traditional methods.

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