Improved Split-Plot and Multi-Stratum Designs

Journal:	*Technometrics*
Manuscript ID:	TCH-12-043
Manuscript Type:	Original Article
Keywords:	A-optimality, D-optimality, hard-to-change factor, hard-to-set factor, mixed model, prediction variance

Improved Split-Plot and Multi-Stratum Designs

Abstract

Many industrial experiments involve some factors whose levels are harder to set than others. The best way to deal with these is to plan the experiment carefully as a split-plot, or more generally a multi-stratum, design. Several different approaches for constructing split-plot type response surface designs have been proposed in the literature in the last 10 years or so, which has allowed experimenters to make better use of their resources by using more efficient designs than the classical balanced ones. One of these approaches, the stratum-by-stratum strategy, has been shown to produce designs that are less efficient than locally D-optimal designs. An improved stratum-by-stratum algorithm is given, which, though more computationally intensive than the old one, makes most use of the advantages of this approach, i.e. it can be used for any structure and does not depend on prior estimates of the variance components. This is shown to be almost as good as the locally optimal designs in terms of their own criteria and more robust across a range of criteria.

Keywords: A-optimality; D-optimality; hard-to-change factor; hard-to-set factor; mixed model; prediction variance; response surface.

1 Introduction

Fractional factorial and response surface designs are widely used in industrial and laboratory based experiments. It has been increasingly recognized in recent years that many, perhaps most, industrial experiments and many laboratory experiments involve some factors whose levels are harder to set than others. It is clear that the best way to deal with such situations is to take account in a structured way, when designing the experiment, of the hard-to-set factors by ensuring that their levels do not have to be set for each run, but only less frequently. If there are only hard-to-set and easy-to-set factors, this leads to a (usually nonorthogonal) split-plot structure. If there are very-hard-to-set (VHS), fairly-hard-to-set (HS) and easy-to-set (ES) factors, we have a split-split-plot structure. Generally, each level of hardness-to-set in factors which is taken account of in the design defines a *stratum*, as does each level of blocking, and, following Trinca and Gilmour (2001), we refer to designs with factors in at least two strata as *multi-stratum* designs.

The restricted randomization in multi-stratum designs introduces additional random effects into the model. We will assume that there are s strata, with stratum i having n_i units within each unit at stratum $(i-1)$, stratum 0 being defined as the entire experiment ($n_0 = 1$). The model can then be written as

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \sum_{i=1}^{s} \mathbf{Z}_i \boldsymbol{\epsilon}_i,$$

where $\mathbf{y}$ is the $n \times 1$ vector of responses, assumed to be a realization of the random variable $\mathbf{Y}$, $\mathbf{X}$ is the $n \times p$ design matrix for the p-parameter treatment model, $\boldsymbol{\beta}$ is a $p \times 1$ vector of fixed treatment parameters, $\mathbf{Z}_i$ is an $n \times m_i$ indicator matrix for the units in stratum i, $m_i = \prod_{j=1}^{i} n_j$, $\boldsymbol{\epsilon}_i \sim N(\mathbf{0}, \sigma_i^2 \mathbf{I}_{m_i})$ is an $m_i \times 1$ vector of random effects and all random effects are uncorrelated. The main aim is usually to estimate the treatment parameters $\boldsymbol{\beta}$ but, in order to estimate their standard errors, it is also necessary to estimate the variance components $\sigma_i^2,\ i = 1, \ldots, s$.

Following Huang, Chen and Voelkel (1998) and Bingham and Sitter (1999), there is a large body of work on regular (mainly two-level) fractional factorial designs in multi-stratum structures - see Cheng and Tsai (2009) for recent comprehensive results. This work extends the concepts of resolution and aberration to orthogonal multi-stratum structures. The orthogonality means that all information on each effect appears in a single stratum and the parameters and their standard errors can be estimated by least squares using any standard analysis of variance program which deals with orthogonal multi-stratum structures.

Irregular fractional factorial and response surface designs require different procedures for the analysis of data, due to the nonorthogonality, which means that information on some parameters appears in more than one stratum. Letsinger, Myers and Lentner (1996) recommended analyzing the data using residual maximum likelihood (REML) to estimate the variance components and generalized least squares (GLS) to estimate the fixed (treatment) effects. This has become accepted as the standard analysis method, although Gilmour and Goos (2009) showed that it can be unreliable when there are small numbers of units in the higher strata.

Letsinger, Myers and Lentner (1996) and Draper and John (1998) studied the properties of standard response surface designs when they are run in split-plot structures, but the treatment designs were not specifically chosen to take account of the split-plot structure. The first paper to recommend choosing designs with a specific split-plot or other multi-stratum structure in mind was by Trinca and Gilmour (2001). They suggested a stratum-by-stratum strategy for building designs and then combining the designs from the different strata to optimize particular criteria for each step in the procedure.

Trinca and Gilmour (2001) also outlined the possibility of finding a globally D- or A-optimum design using a modified exchange algorithm. They preferred the stratum-by-stratum construction because the globally optimum designs are only optimal for specific values of the ratios of variance components, whereas the stratum-by-stratum method is optimal in the most challenging situation in which $\sigma_i^2/\sigma_j^2 \to \infty$, for all $1 \le i < j \le s$, and because it can be implemented using only standard designs and interchange algorithms, which are computationally less expensive than exchange algorithms.

Other authors followed up the suggestion of finding globally optimum designs for point prior estimates of the variance components in specific types of structure. In particular, Goos (2002), Goos and Vandebroek (2003), Goos and Donev (2007) and Jones and Goos (2007, 2009) developed efficient exchange algorithms for split-plot response surface and mixtures designs and split-split-plot response surface designs. They found designs which, even though the search procedures depend on point prior estimates of the variance components, convincingly outperform the designs of Trinca and Gilmour (2001) even in situations where the latter were claimed to be better.

A different approach to split-plot response surface design, motivated by the equivalent-estimation (E-E) property, has being considered by Vining and co-authors. An equivalent-estimation design is one in which the GLS estimator of the fixed effects gives the same estimates as the ordinary least squares (OLS) estimator. Vining, Kowalski and Montgomery (2005) showed how to accommodate the treatments of central composite designs (CCDs) and Box-Benhken designs in the split-plot framework such that E-E is satisfied. Parker, Kowalski and Vining (2007) proposed strategies for systematically constructing E-E designs. However, in general, such construction methods result in very inefficient designs with respect to the usual design criteria. In their search for globally D-optimum designs, Goos and co-authors noted many D-efficient designs also satisfy the E-E property. Macharia and Goos (2010) presented an algorithm to select among D-efficient split-plot designs those satisfying the E-E property and produced better designs than the original E-E ones.

The aim of the present paper is to re-examine the stratum-by-stratum strategy of Trinca and Gilmour (2001) for design construction, to introduce a modification which is a considerable improvement and to compare designs resulting from the existing approaches with respect to popular design criteria. For a range of design criteria see Atkinson, Donev and Tobias (2007).

The relative advantages of stratum-by-stratum and global construction methods are described in Section 2. The new algorithm is described in Section 3 and examples of response surface designs are given in Section 4. Some general recommendations are made in Section 5.

2 Methods for Construction of Multi-Stratum Designs

In a GLS analysis, assuming that the ratios of variance components are known, the covariance matrix of the estimated fixed effects is given by $\mathbf{V}(\hat{\boldsymbol{\beta}}|\boldsymbol{\eta}) = \sigma^2(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}$, where $\mathbf{V} = \sum_{i=1}^{s} \eta_i \mathbf{Z}_i\mathbf{Z}_i'$, $\boldsymbol{\eta}' = [\eta_1, \ldots, \eta_s]$, $\eta_i = \sigma_i^2/\sigma^2$ and $\sigma^2 = \sigma_s^2$. In practice, the variance components have to be estimated and the covariance matrix of the fixed effects is usually estimated by $\widehat{\mathbf{V}(\hat{\boldsymbol{\beta}})} = \hat{\sigma}^2(\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-1}$, where $\hat{\mathbf{V}} = \sum_{i=1}^{s} \hat{\eta}_i \mathbf{Z}_i\mathbf{Z}_i'$, $\hat{\eta}_i = \hat{\sigma}_i^2/\hat{\sigma}^2$ and $\hat{\sigma}_i^2$ is usually the REML estimator of σ_i^2.

Two difficulties arise when experiments are being designed. First, neither η_i nor $\hat{\eta}_i$ are known, so we do not know $\mathbf{V}(\hat{\boldsymbol{\beta}})$ or $\widehat{\mathbf{V}(\hat{\boldsymbol{\beta}})}$ even up to the constant σ^2. Secondly, $\widehat{\mathbf{V}(\hat{\boldsymbol{\beta}})}$ is only an estimate of $\mathbf{V}(\hat{\boldsymbol{\beta}})$, can be a very poor one, especially when there are few units in some strata, and can be better for some designs than for others. The global optimization and stratum-by-stratum algorithms deal with these difficulties in different ways.

The global optimization algorithms optimize some scalar function $\phi(\mathbf{X}|\boldsymbol{\eta})$ of $\mathbf{V}(\hat{\boldsymbol{\beta}}|\boldsymbol{\eta})$, such as the determinant (for D-optimality) or the trace (for A-optimality), for some point prior estimate of the ratios of variance components $\boldsymbol{\eta}$. The authors of these algorithms typically search for optimal designs for a few different values of $\boldsymbol{\eta}$ and then examine ϕ as a function of $\boldsymbol{\eta}$ for the different optimal designs found. They then choose one which is optimal across a wide range of values of $\boldsymbol{\eta}$ in the expectation that this design will perform well. Conceptually, it would be a small step to use a prior distribution for $\boldsymbol{\eta}$ and find a design which is optimal integrated across this prior. However, this is computationally very expensive and not usually regarded as being worthwhile.

The stratum-by-stratum algorithm, on the other hand, takes a minimax approach and aims to optimize the information in stratum i when $\sigma_{i-1}^2/\sigma_i^2 \to \infty$. The justification for this approach is that we are ensuring that the design is optimal in the most difficult situation in which the higher order variance components are large. This is easiest to see in a two-stratum, i.e. split-plot, structure. If η_1 is large, the variances of parameters estimated in the whole plots stratum will be very large compared with the variances of the parameters estimated in the subplots stratum; the variances of the parameters estimated in the subplots stratum will be essentially identical to those obtained by treating the whole plots as fixed block effects. If η_1 is small, on the other hand, the variances of the parameters estimated in the whole plots stratum will be much smaller, typically only slightly bigger than the variances of the parameters estimated in the subplots stratum. The philosophy of stratum-by-stratum construction is that it is better to ensure that we get variances as small as possible in the case that they are very large and accept that, when they are small, it might have been possible to make them smaller.

3 An Improved Stratum-By-Stratum Method

The algorithm of Trinca and Gilmour (2001) did not implement the stratum-by-stratum construction in the simplest or most effective way. Motivated by computational efficiency, they chose the treatment combinations in each stratum separately, usually based on central composite or other classical designs, and then arranged them in blocks using interchange algorithms. A second interchange algorithm was then used to match the designs from neighboring strata and then a third to adjust the design for even higher strata. By using only interchange, rather than exchange, algorithms, the method was very fast and could deal with very large problems where other methods struggled. However, Goos and his co-workers have shown that the designs obtained are often quite inefficient. In this section, we describe an improved procedure, which makes use of exchange algorithms. Given the increased computing power in the last fifteen years, it is now possible to easily realize the full benefits of the stratum-by-stratum approach.

Consider the general multi-stratum unit structure with s strata, where there may or may not be treatment factors applied in any particular stratum. We construct designs from the highest stratum to the lowest. For the highest stratum i ($i \in \{1,\ 2,\ \ldots,\ s\}$) for which there are factors to be applied, proceed as follow:

1. If $i = 1$ choose the treatment design for the factors to be applied to the units in stratum i considering the efficiency for estimating the model parameters involving the factors in this stratum only. Otherwise treat the units in stratum $i-1$ as blocks with fixed effects. Choose the treatment for the factors to be applied in this stratum and their blocking arrangement considering the efficiency for estimating the model parameters involving the factors in this stratum only.

2. Set $i = i + 1$. Maintaining the design chosen in the last step, treat the units in $i - 1$ as blocks with fixed effects. Choose the treatment combinations and their arrangement in the units in stratum i considering the efficiency for estimating the model parameters involving the factors in this stratum and the interactions between the factors in this stratum and the factors in higher strata.

3. If $i > 2$ rearrange the blocks within the units in stratum $i - 2$ such that the efficiency is maximized when we treat these units as blocks. Repeat this step for the units in strata $i - 3, \ldots, 1$.

4. If $i = s$ stop; otherwise repeat 2 and 3, always considering efficiency for estimating parameters in stratum i and interactions between the factors in the current stratum and all higher strata.

The main modification of this method from that of Trinca and Gilmour (2001) is that the treatment set at each stage is not chosen independently of the structures formed in the previous stage. Thus we use a candidate treatment set for each stratum. The treatments that are actually chosen in each stratum are optimized by an exchange algorithm rather than an interchange algorithm. Simultaneous optimization of treatments and their blocking arrangement is performed. The method can be used for any design criteria based on the variance matrix for blocked designs with fixed number and sizes of blocks. Any algorithm for blocked designs can be used with slight modification of construction of the model matrix in each step. We will refer to this method as the MSS (modified stratum-by-stratum) approach.

In the illustrations in the next section we used D_S- and A_S-optimality criteria, the intercept and block effects being considered as nuisance parameters. For second order models we used A_S on a scale such that the relative weights are 1/4 for each quadratic effect and 1 for other effects, whenever the design region is a hypercube. An unblocked design will be needed only when there are factors to be applied to the units in stratum 1. Let $\boldsymbol{\beta}_i$ be the model parameter vector ($p_i - 1$ parameters, excluding the intercept) to be estimated in stratum i. Let $\mathbf{X}_i$ be the $m_i \times (p_i - 1)$ associated model matrix where m_i is the number of units in this stratum. The partition of interest of the variance covariance matrix of $\hat{\boldsymbol{\beta}}_i$ is $(\mathbf{M}_i^{-1})_{22} = (\mathbf{X}_i'\mathbf{Q}_i\mathbf{X}_i)^{-1}$. For unblocked structures, $\mathbf{Q}_i = \mathbf{I} - \frac{1}{m_i}\mathbf{1}\mathbf{1}'$ while for blocked structures $\mathbf{Q}_i = \mathbf{I} - \mathbf{B}_i(\mathbf{B}_i'\mathbf{B}_i)^{-1}\mathbf{B}_i'$ with $\mathbf{B}_i$ being a $m_i \times n_{i-1}$ indicator matrix for blocks in stratum i. Thus for D_S we minimise $|(\mathbf{M}_i^{-1})_{22}|$ and for A_S-optimality we minimise $trace\{\mathbf{W}_i(\mathbf{M}_i^{-1})_{22}\}$ where $\mathbf{W}_i$ is a diagonal matrix with the weights scaled so that $trace(\mathbf{W}_i) = 1$.

4 Examples

In this section we present several illustrations comparing designs constructed by the MSS approach and other existing methods. For constructing the designs, for each stratum, in general, the candidate treatment set was the full 3-level factorial or 2-level factorial, depending on the underlying model. In some cases, the designs are compared with respect to properties of the expected variance-covariance matrix of the GLS estimator, $\hat{\boldsymbol{\beta}}$, $(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}$ for a range of $\boldsymbol{\eta}$ values. A_S values are calculated as $trace[\mathbf{W}\{(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\}_{22}]$ in which $\mathbf{W}$ is a diagonal matrix of weights as in Section 3 re-scaled such that $trace(\mathbf{W}) = 1$. D_S values are calculated as $|\{(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\}_{22}|^{\frac{1}{p-1}}$ (eliminating the row and column relating to the intercept). We find it useful to show differences between designs on a variance scale, rather than a relative efficiency scale, since it is variances which are important in practice. One design might be only 50% efficient with respect to another, but if they both give very small variances, this is unimportant; conversely, one design might have only slightly less than 100% efficiency relative to another, but if they both give very high variances, the difference could still be important in practice. However, for the sake of quick comparisons we also show the efficiencies of alternative designs calculated with respect to the globally D-optimal design, as best known from the literature, which is used as a baseline. The efficiency of one particular design is defined as the ratio between the criterion value (as defined above) of the baseline design and the particular design, the larger the ratio the more efficient the design is compared with the baseline.

We also compare the designs with respect to their prediction performances. The prediction performance is evaluated by the average or integrated variance of estimated mean response, the I_V-efficiency, sometimes called I-, V- or IV-efficiency, and by the integrated variances of estimated differences of responses, across the design region. For a multi-stratum design involving a total of q factors, the average variance (I_V) is proportional to

$$I_V \propto \frac{\int_{\mathbf{x}\in\mathcal{X}} \mathbf{f}'(\mathbf{x})(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{f}(\mathbf{x})d\mathbf{x}}{\int_{\mathbf{x}\in\mathcal{X}} d\mathbf{x}}, \quad (1)$$

where $\mathcal{X} \subset \mathbb{R}^q$ is the experimental region of interest and $\mathbf{f}(\mathbf{x})$ is the model expansion of $\mathbf{x}$, the combination of the levels of the q factors. The numerator of (1) can be simplified to $trace\{\mathcal{M}(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\}$ where $\mathcal{M} = \int_{\mathbf{x}\in\mathcal{X}} \mathbf{f}(\mathbf{x})\mathbf{f}'(\mathbf{x})d\mathbf{x}$ is the region moment matrix of the region of interest. For spherical and cuboidal regions the calculations of the integrals are exact (Hardin and Sloane, 1993).

Difference variance dispersion graphs were suggested by Trinca and Gilmour (1999) based on the argument that often differences in response from some particular point, such as the expected position of the optimum or standard operating conditions, are more important than the response itself. Here we apply the concept of integrated variance for the difference between the estimated mean response in the design region and the mean response estimated at the centre of the region. The I_{DV} criterion function is given by

$$I_{DV} = \frac{\int_{\mathbf{x}\in\mathcal{X}} var(\hat{y}(\mathbf{x}) - \hat{y}(\mathbf{0}))}{\int_{\mathbf{x}\in\mathcal{X}} d\mathbf{x}},$$

that is proportional to

$$I_{DV} \propto \frac{\int_{\mathbf{x}\in\mathcal{X}}[\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{0})]'(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}[\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{0})]}{\int_{\mathbf{x}\in\mathcal{X}} d\mathbf{x}} = \frac{trace\{\mathcal{M}_0(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\}}{\int_{\mathbf{x}\in\mathcal{X}} d\mathbf{x}}, \quad (2)$$

where $\mathcal{M}_0 = \int_{\mathbf{x}\in\mathcal{X}}[\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{0})][\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{0})]'d\mathbf{x}$ and $\mathbf{f}(\mathbf{0})$ is the vector whose first element is one and all others are zero.

4.1 Example 1 (1 HS and 4 ES factors, 21 whole plots with 2 subplots each)

This example was described in Trinca and Gilmour (2001) and served as motivation for some other publications. Five factors were to be investigated in an experiment on protein extraction from a mixture of two types of proteins and other components. The runs were to be executed sequentially and one of the factors, the feed position for the inflow of the mixture, was hard to set (HS). Fixing it for a day, two runs could be done per day and 21 days experimentation were considered reasonable. The primary model proposed was the second order polynomial. Here we compare four designs, two of them previously proposed, one by Trinca and Gilmour (2001), the design being referred to here as SS, and the other by Goos (2002), referred to as D, a D-optimum design for $1 \leq \eta \leq 10$. The two other designs were constructed by the approach proposed in this paper, MSS_A (using A_S) and MSS_D (using D_S). For these the treatment set for the whole-plots stratum is the same as that used in Trinca and Gilmour (2001), i.e. three equally replicated levels, which is D_S- and A_S-optimal. The new designs are shown in Table 1.

Properties of the designs, such as A_S and D_S values and efficiencies, for several values of η, are plotted in Figures 1 and 2. Figure 2 shows that, for very small η values design D has the best and design SS the worst performance, in terms of A_S efficiency. As η increases design D becomes less efficient. The newer designs (MSS_A and MSS_D) become more efficient for η larger than about 1.7. In terms of the determinant, designs D, MSS_A and MSS_D have similar performances, design D being better for the range of η studied with the efficiencies of the new designs ranging from about 94.0% to 98.7%. Table 2 shows the square root of the mean of expected variances for the model parameter estimators averaged according to the type of effects. We note that using an exchange algorithm in stratum 2 improves considerably the design compared with the SS approach that fixed the treatment set to be a CCD. The D-optimal design penalizes the quadratic effects of HS factors, but gives very good estimation of the corresponding linear effects, as usual. In terms of predicting the responses, the new designs are clearly better than the D-optimal design and, for larger values of the whole plot variance component, are also better than the original design obtained by the old SS algorithm. For estimating differences in response, the new designs are clearly the best. We also note that the MSS algorithm which uses A_S is better than that which uses D_S.

Table 1: Designs for Example 1 (21 whole plots with 2 subplots each) using the MSS approach, A_S and D_S criterion

MSS$_A$										MSS$_D$									
w_1	x_1	x_2	x_3	x_4	w_1	x_1	x_2	x_3	x_4	w_1	x_1	x_2	x_3	x_4	w_1	x_1	x_2	x_3	x_4
-1	-1	-1	-1	1	0	1	1	0	1	-1	-1	-1	-1	1	0	1	0	0	1
-1	1	-1	1	-1	0	-1	1	1	-1	-1	-1	1	1	-1	0	0	-1	-1	0
-1	0	1	-1	1	0	1	-1	0	1	-1	1	-1	-1	1	0	1	0	-1	1
-1	-1	-1	-1	-1	0	0	0	-1	-1	-1	-1	-1	1	-1	0	-1	1	-1	-1
-1	0	1	1	0	0	1	1	-1	0	-1	0	0	-1	-1	0	0	1	0	1
-1	-1	1	-1	1	0	-1	0	0	1	-1	1	-1	1	-1	0	-1	0	-1	0
-1	-1	1	0	-1	1	1	0	-1	1	-1	1	1	1	1	1	1	1	1	-1
-1	0	-1	1	1	1	1	-1	1	0	-1	1	-1	-1	-1	1	-1	1	-1	1
-1	-1	1	1	1	1	1	1	1	-1	-1	1	-1	1	1	1	1	1	1	1
-1	1	-1	-1	1	1	1	-1	1	1	-1	-1	1	-1	1	1	-1	-1	1	-1
-1	1	0	1	1	1	-1	1	1	1	-1	-1	1	1	1	1	1	1	-1	0
-1	0	-1	0	-1	1	1	0	0	-1	-1	1	1	-1	-1	1	1	-1	1	1
-1	-1	-1	1	-1	1	-1	-1	0	0	-1	1	1	1	0	1	-1	1	1	-1
-1	1	0	-1	-1	1	1	-1	-1	-1	-1	-1	-1	1	1	1	1	-1	-1	-1
0	-1	0	1	0	1	-1	1	-1	0	0	0	0	1	-1	1	1	-1	-1	1
0	0	1	1	-1	1	-1	-1	1	-1	0	-1	-1	0	0	1	-1	1	1	1
0	0	0	-1	0	1	-1	1	0	-1	0	-1	-1	-1	-1	1	-1	-1	1	1
0	1	1	-1	-1	1	-1	-1	-1	1	0	0	0	0	0	1	-1	1	-1	-1
0	1	1	1	1	1	-1	-1	-1	-1	0	1	1	-1	-1	1	1	-1	1	0
0	-1	-1	1	1	1	1	0	1	1	0	-1	-1	0	-1	1	-1	-1	-1	1
0	-1	1	-1	-1						0	1	1	-1	1					
0	1	-1	-1	0						0	1	0	0	-1					

Table 2: Square root of mean of expected variances of parameter estimators and prediction performances for alternative designs for Example 1 (21 whole plots of 2 subplots)

η	Design	Linear(HS)	Quad.(HS)	Linear(ES)	Quad.(ES)	Int.(HS×ES)	Int.(ES)	I_V	I_{DV}
1	SS	.3438	.6196	.2342	.5440	.3256	.2767	.5105	.4433
1	D	.2932	.8264	.1950	.5370	.2016	.2305	.6551	.4148
1	MSS$_A$	.3467	.6165	.2063	.4812	.2431	.2400	.5582	.3959
1	MSS$_D$	.3346	.7131	.1984	.5701	.2251	.2259	.5850	.3964
10	SS	.8745	1.5291	.2756	.6191	.3947	.3581	1.6909	1.2000
10	D	.7658	2.0525	.2102	.5812	.2176	.2823	2.6157	1.3498
10	MSS$_A$	.8740	1.5237	.2263	.5306	.2632	.2719	1.6648	1.0566
10	MSS$_D$	.8694	1.5706	.2170	.6055	.2459	.2658	1.7084	1.0584
100	SS	2.6823	4.6512	.2875	.6380	.4156	.3911	12.0312	7.2564
100	D	2.3636	6.2629	.2134	.5919	.2211	.2979	21.3090	10.0358
100	MSS$_A$	2.6819	4.6486	.2304	.5411	.2674	.2785	11.9670	7.0696
100	MSS$_D$	2.6804	4.6648	.2211	.6136	.2505	.2752	12.0178	7.0737

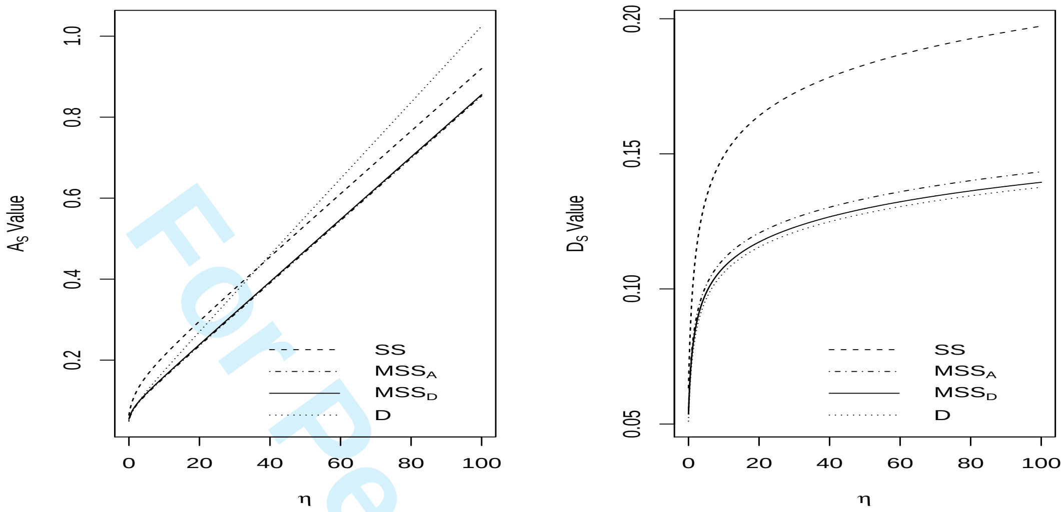

Figure 1: Expected A_S and D_S values, as functions of η, for alternative designs for Example 1.

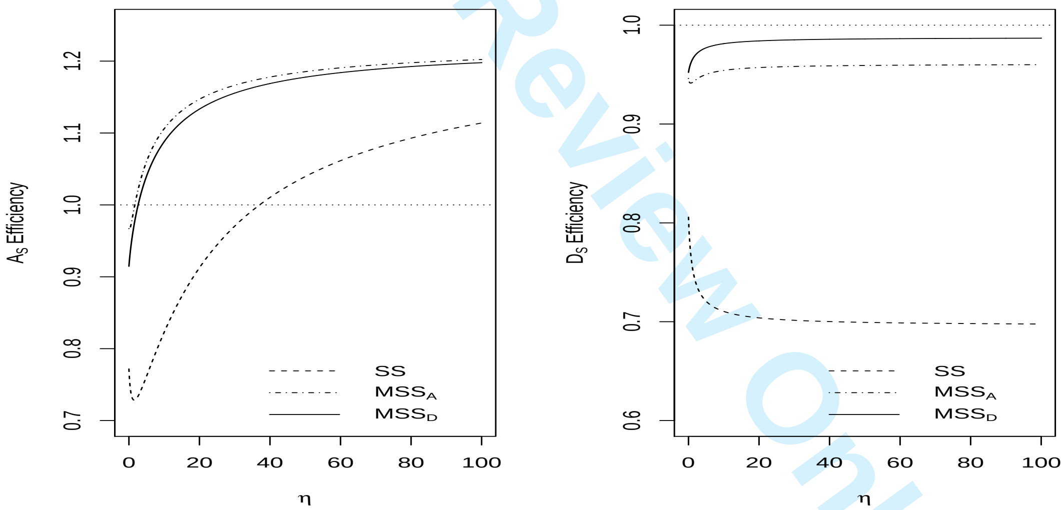

Figure 2: Expected A_S and D_S efficiencies, relative to design D, as functions of η, for alternative designs for Example 1.

4.2 Example 2 (7 HS and 4 ES factors, 20 whole plots with 5 subplots each)

The second example compares alternative designs for the polypropylene experiment described in Jones and Goos (2007). There are 7 two-level HS and 4 ES factors, 3 continuous and 1 a three-level qualitative factor. The model includes linear main effects for all factors, quadratic effects for the 3 ES continuous factors and 50 two-factor interactions (only one of the HS factors, W_1, is expected to interact with the others). There was a constraint among two of the HS factors, W_3 and W_4, which were not allowed to both appear at the highest level, and this was taken into account when specifying the candidate set for the exchange algorithm. Jones and Goos (2007) compared two designs for these factors in 20 whole plots of 5 subplots each, one constructed by the SS approach (D criterion in each phase) and the other by the global D-optimum approach ($\eta = 1$). We found two other designs for this experiment, MSS_A and MSS_D designs, which are shown in Tables 3 and 4. We compare the designs in Figures 3 and 4 and in Table 5. The new designs are better than the older ones with respect to the A_S criterion and even the old SS design is better for $\eta > 10$. We note that even for $\eta = 1$ design MSS_D outperforms design D. As can happen, especially for such a large experiment, the optimization procedure failed to find the globally D-optimum design.

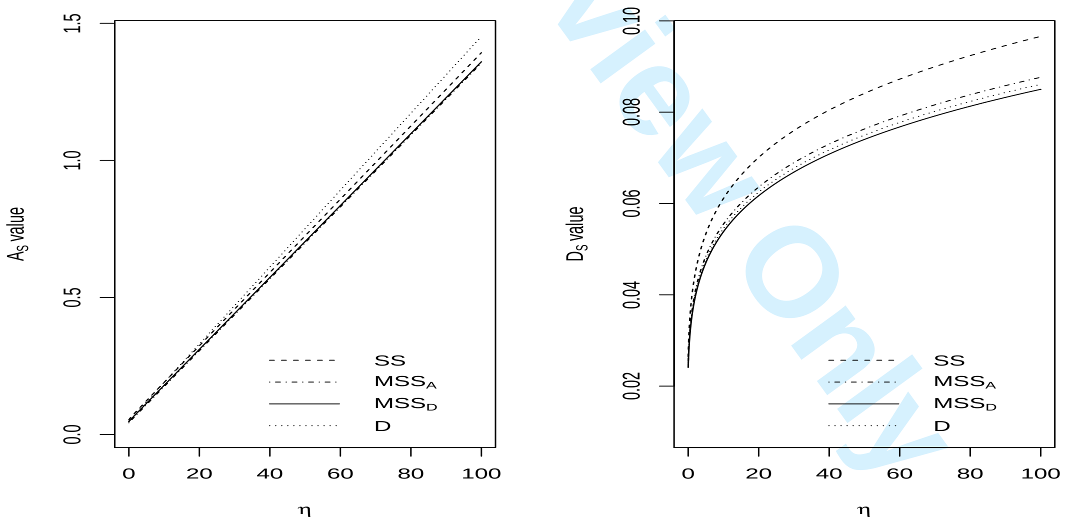

Figure 3: Expected A_S and D_S values as functions of η for alternative designs for Example 2.

Table 3: Design for Example 2 (20 whole plots with 5 subplots each) using the MSS approach and the A_S criterion

MSS$_A$																					
W_1	W_2	W_3	W_4	W_5	W_6	W_7	X_1	X_2	X_3	X_4	W_1	W_2	W_3	W_4	W_5	W_6	W_7	X_1	X_2	X_3	X_4
−1	−1	−1	−1	−1	1	−1	−1	0	0	B	−1	−1	−1	1	1	1	1	1	1	0	C
−1	−1	−1	−1	−1	1	−1	−1	−1	−1	C	−1	−1	−1	1	1	1	1	−1	1	−1	B
−1	−1	−1	−1	−1	1	−1	0	−1	1	A	−1	−1	−1	1	1	1	1	1	−1	1	B
−1	−1	−1	−1	−1	1	−1	1	1	−1	B	−1	−1	−1	1	1	1	1	−1	−1	−1	C
−1	−1	−1	−1	−1	1	−1	1	1	1	C	−1	−1	−1	1	1	1	1	−1	0	1	A
−1	−1	−1	−1	1	−1	1	−1	1	−1	A	−1	1	−1	−1	1	1	−1	1	1	1	A
−1	−1	−1	−1	1	−1	1	1	1	1	C	−1	1	−1	−1	1	1	−1	−1	−1	−1	A
−1	−1	−1	−1	1	−1	1	−1	0	1	B	−1	1	−1	−1	1	1	−1	−1	1	1	C
−1	−1	−1	−1	1	−1	1	1	0	1	A	−1	1	−1	−1	1	1	−1	1	−1	1	B
−1	−1	−1	−1	1	−1	1	−1	−1	0	C	−1	1	−1	−1	1	1	−1	1	−1	−1	C
−1	−1	−1	1	1	−1	−1	−1	−1	−1	B	1	−1	−1	−1	−1	1	1	1	1	−1	C
−1	−1	−1	1	1	−1	−1	0	1	1	B	1	−1	−1	−1	−1	1	1	−1	1	−1	A
−1	−1	−1	1	1	−1	−1	−1	0	1	C	1	−1	−1	−1	−1	1	1	0	−1	1	C
−1	−1	−1	1	1	−1	−1	1	0	−1	C	1	−1	−1	−1	−1	1	1	1	−1	−1	B
−1	−1	−1	1	1	−1	−1	1	−1	1	A	1	−1	−1	−1	−1	1	1	1	−1	1	B
−1	−1	1	−1	−1	−1	−1	0	1	−1	C	1	−1	−1	−1	1	1	−1	1	1	1	B
−1	−1	1	−1	−1	−1	−1	0	−1	1	C	1	−1	−1	−1	1	1	−1	−1	1	−1	C
−1	−1	1	−1	−1	−1	−1	1	0	0	B	1	−1	−1	−1	1	1	−1	−1	−1	0	B
−1	−1	1	−1	−1	−1	−1	1	1	−1	A	1	−1	−1	−1	1	1	−1	1	1	−1	A
−1	−1	1	−1	−1	−1	−1	−1	−1	−1	A	1	−1	−1	−1	1	1	−1	1	−1	1	C
−1	−1	1	−1	−1	1	1	1	1	−1	C	1	−1	−1	1	1	−1	1	1	0	0	B
−1	−1	1	−1	−1	1	1	1	1	1	B	1	−1	−1	1	1	−1	1	1	1	−1	A
−1	−1	1	−1	−1	1	1	−1	1	1	A	1	−1	−1	1	1	−1	1	−1	1	−1	C
−1	−1	1	−1	−1	1	1	−1	−1	1	C	1	−1	−1	1	1	−1	1	−1	−1	−1	A
−1	−1	1	−1	−1	1	1	0	−1	−1	A	1	−1	−1	1	1	−1	1	1	−1	1	C
−1	1	−1	−1	−1	−1	1	−1	−1	1	A	1	−1	1	−1	−1	−1	−1	1	−1	−1	C
−1	1	−1	−1	−1	−1	1	1	1	1	B	1	−1	1	−1	−1	−1	−1	−1	1	1	C
−1	1	−1	−1	−1	−1	1	−1	1	−1	C	1	−1	1	−1	−1	−1	−1	−1	1	−1	B
−1	1	−1	−1	−1	−1	1	1	−1	0	C	1	−1	1	−1	−1	−1	−1	0	0	1	A
−1	1	−1	−1	−1	−1	1	0	−1	−1	B	1	−1	1	−1	−1	−1	−1	−1	−1	1	B
−1	1	−1	1	−1	1	−1	1	0	1	B	1	1	−1	−1	−1	−1	1	0	0	1	C
−1	1	−1	1	−1	1	−1	−1	1	−1	A	1	1	−1	−1	−1	−1	1	−1	−1	−1	C
−1	1	−1	1	−1	1	−1	1	−1	0	A	1	1	−1	−1	−1	−1	1	1	−1	1	B
−1	1	−1	1	−1	1	−1	0	−1	1	C	1	1	−1	−1	−1	−1	1	1	0	−1	A
−1	1	−1	1	−1	1	−1	0	1	−1	C	1	1	−1	−1	−1	−1	1	−1	1	0	B
−1	1	−1	1	−1	−1	1	1	−1	−1	C	1	1	−1	−1	1	−1	−1	1	−1	−1	A
−1	1	−1	1	−1	−1	1	−1	1	1	C	1	1	−1	−1	1	−1	−1	−1	−1	1	C
−1	1	−1	1	−1	−1	1	1	1	−1	B	1	1	−1	−1	1	−1	−1	−1	0	−1	B
−1	1	−1	1	−1	−1	1	−1	−1	0	B	1	1	−1	−1	1	−1	−1	1	1	−1	C
−1	1	−1	1	−1	−1	1	0	1	1	A	1	1	−1	−1	1	−1	−1	−1	1	1	A
−1	1	1	−1	1	−1	−1	−1	−1	−1	C	1	1	−1	1	−1	1	−1	−1	−1	0	C
−1	1	1	−1	1	−1	−1	−1	−1	1	A	1	1	−1	1	−1	1	−1	−1	−1	1	A
−1	1	1	−1	1	−1	−1	1	−1	−1	B	1	1	−1	1	−1	1	−1	1	1	1	C
−1	1	1	−1	1	−1	−1	1	1	1	C	1	1	−1	1	−1	1	−1	−1	1	1	B
−1	1	1	−1	1	−1	−1	−1	1	1	B	1	1	−1	1	−1	1	−1	1	−1	−1	B
−1	1	1	−1	1	1	1	−1	1	−1	C	1	1	1	−1	1	1	1	1	−1	1	A
−1	1	1	−1	1	1	1	1	1	−1	B	1	1	1	−1	1	1	1	−1	1	1	C
−1	1	1	−1	1	1	1	1	0	−1	A	1	1	1	−1	1	1	1	0	0	1	B
−1	1	1	−1	1	1	1	−1	−1	−1	B	1	1	1	−1	1	1	1	−1	1	−1	A
−1	1	1	−1	1	1	1	1	−1	1	C	1	1	1	−1	1	1	1	1	−1	−1	C

Table 4: Design for Example 2 (20 whole plots with 5 subplots each) using the MSS approach and the D_S criterion

MSS$_D$

W_1	W_2	W_3	W_4	W_5	W_6	W_7	X_1	X_2	X_3	X_4	W_1	W_2	W_3	W_4	W_5	W_6	W_7	X_1	X_2	X_3	X_4
−1	−1	−1	−1	−1	1	−1	1	−1	0	C	−1	1	−1	1	−1	−1	1	−1	−1	0	A
−1	−1	−1	−1	−1	1	−1	1	1	−1	A	−1	1	−1	1	−1	−1	1	−1	−1	1	C
−1	−1	−1	−1	−1	1	−1	1	1	1	B	−1	1	−1	1	−1	−1	1	1	1	−1	A
−1	−1	−1	−1	−1	1	−1	−1	0	−1	B	−1	1	−1	1	−1	−1	1	1	1	1	B
−1	−1	−1	−1	−1	1	−1	−1	−1	1	A	−1	1	−1	1	−1	−1	1	1	−1	−1	C
−1	−1	−1	−1	1	−1	1	−1	1	0	B	−1	1	1	−1	1	1	1	1	−1	1	B
−1	−1	−1	−1	1	−1	1	−1	−1	1	C	−1	1	1	−1	1	1	1	−1	−1	−1	C
−1	−1	−1	−1	1	−1	1	1	1	−1	C	−1	1	1	−1	1	1	1	1	1	−1	B
−1	−1	−1	−1	1	−1	1	1	−1	1	B	−1	1	1	−1	1	1	1	−1	1	1	C
−1	−1	−1	−1	1	−1	1	−1	−1	−1	A	−1	1	1	−1	1	1	1	0	−1	1	A
−1	−1	−1	1	1	−1	−1	−1	0	1	A	1	−1	−1	−1	−1	−1	−1	1	−1	1	C
−1	−1	−1	1	1	−1	−1	1	1	1	C	1	−1	−1	−1	−1	−1	−1	0	0	0	A
−1	−1	−1	1	1	−1	−1	−1	−1	1	B	1	−1	−1	−1	−1	−1	−1	1	1	−1	C
−1	−1	−1	1	1	−1	−1	1	−1	−1	A	1	−1	−1	−1	−1	−1	−1	−1	1	1	B
−1	−1	−1	1	1	−1	−1	−1	1	−1	C	1	−1	−1	−1	−1	−1	−1	−1	−1	−1	B
−1	−1	−1	1	1	1	1	−1	1	−1	C	1	−1	−1	−1	−1	1	1	1	0	1	A
−1	−1	−1	1	1	1	1	1	−1	1	C	1	−1	−1	−1	−1	1	1	−1	1	1	C
−1	−1	−1	1	1	1	1	1	1	0	A	1	−1	−1	−1	−1	1	1	1	1	−1	B
−1	−1	−1	1	1	1	1	1	−1	−1	B	1	−1	−1	−1	−1	1	1	−1	−1	−1	C
−1	−1	−1	1	1	1	1	−1	1	1	B	1	−1	−1	−1	−1	1	1	0	−1	1	B
−1	−1	1	−1	−1	−1	−1	−1	−1	−1	A	1	−1	−1	1	1	1	−1	−1	−1	−1	A
−1	−1	1	−1	−1	−1	−1	−1	1	1	C	1	−1	−1	1	1	1	−1	1	1	1	A
−1	−1	1	−1	−1	−1	−1	1	1	1	A	1	−1	−1	1	1	1	−1	−1	0	1	C
−1	−1	1	−1	−1	−1	−1	1	1	−1	B	1	−1	−1	1	1	1	−1	1	1	−1	B
−1	−1	1	−1	−1	−1	−1	1	−1	1	B	1	−1	−1	1	1	1	−1	1	−1	−1	C
−1	−1	1	−1	−1	1	1	−1	1	0	A	1	−1	1	−1	1	−1	1	0	1	−1	A
−1	−1	1	−1	−1	1	1	1	−1	−1	A	1	−1	1	−1	1	−1	1	1	1	1	B
−1	−1	1	−1	−1	1	1	1	1	1	C	1	−1	1	−1	1	−1	1	−1	−1	−1	B
−1	−1	1	−1	−1	1	1	0	−1	−1	C	1	−1	1	−1	1	−1	1	1	−1	0	C
−1	−1	1	−1	−1	1	1	−1	−1	1	B	1	−1	1	−1	1	−1	1	−1	−1	1	A
−1	1	−1	−1	−1	−1	1	1	1	1	A	1	1	−1	1	−1	−1	1	1	−1	−1	A
−1	1	−1	−1	−1	−1	1	1	−1	1	C	1	1	−1	1	−1	−1	1	1	1	0	C
−1	1	−1	−1	−1	−1	1	1	−1	−1	B	1	1	−1	1	−1	−1	1	1	−1	1	B
−1	1	−1	−1	−1	−1	1	−1	−1	1	B	1	1	−1	1	−1	−1	1	−1	1	1	A
−1	1	−1	−1	−1	−1	1	−1	1	−1	C	1	1	−1	1	−1	−1	1	−1	1	−1	B
−1	1	−1	−1	1	1	−1	−1	1	1	A	1	1	−1	−1	1	−1	−1	1	−1	1	A
−1	1	−1	−1	1	1	−1	1	−1	−1	A	1	1	−1	−1	1	−1	−1	−1	1	0	A
−1	1	−1	−1	1	1	−1	−1	−1	0	C	1	1	−1	−1	1	−1	−1	0	1	1	C
−1	1	−1	−1	1	1	−1	1	0	1	B	1	1	−1	−1	1	−1	−1	−1	−1	−1	C
−1	1	−1	−1	1	1	−1	−1	1	−1	B	1	1	−1	−1	1	−1	−1	1	1	−1	B
−1	1	−1	1	−1	1	−1	−1	−1	−1	B	1	1	−1	−1	1	1	1	1	−1	1	C
−1	1	−1	1	−1	1	−1	−1	1	1	C	1	1	−1	−1	1	1	1	−1	−1	1	B
−1	1	−1	1	−1	1	−1	1	−1	1	A	1	1	−1	−1	1	1	1	1	1	1	A
−1	1	−1	1	−1	1	−1	0	1	−1	A	1	1	−1	−1	1	1	1	−1	0	−1	A
−1	1	−1	1	−1	1	−1	1	0	−1	C	1	1	−1	−1	1	1	1	0	1	−1	C
−1	1	1	−1	1	−1	−1	1	−1	1	C	1	1	1	−1	−1	1	−1	1	−1	−1	B
−1	1	1	−1	1	−1	−1	0	−1	−1	B	1	1	1	−1	−1	1	−1	−1	−1	1	C
−1	1	1	−1	1	−1	−1	1	1	−1	C	1	1	1	−1	−1	1	−1	−1	1	−1	C
−1	1	1	−1	1	−1	−1	−1	0	−1	A	1	1	1	−1	−1	1	−1	−1	1	1	B
−1	1	1	−1	1	−1	−1	−1	1	1	B	1	1	1	−1	−1	1	−1	1	1	1	A

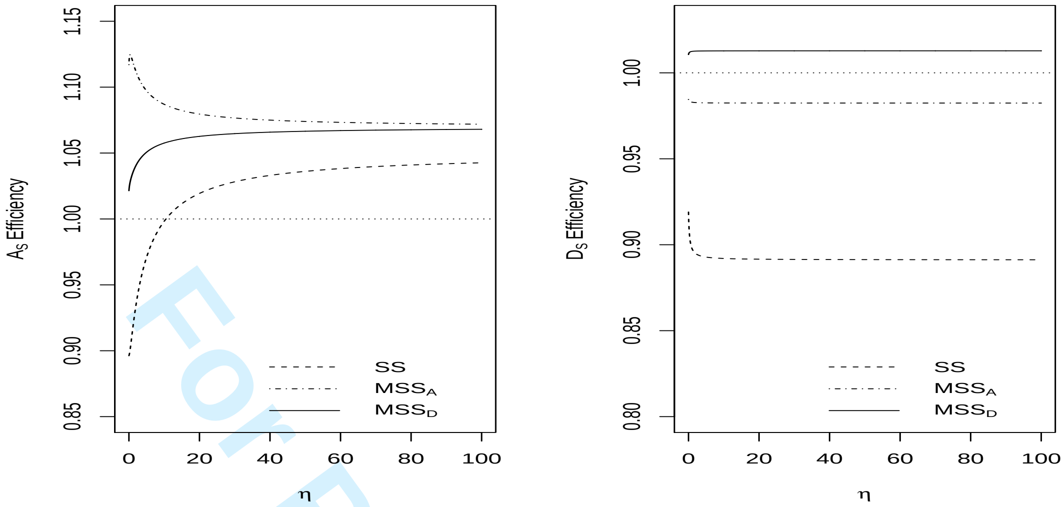

Figure 4: Expected A_S and D_S efficiencies, relative to design D, as functions of η for alternative designs for Example 2.

Table 5: Square root of mean of expected variances of parameter estimators and prediction performances for alternative designs for Example 2

η	Design	Linear(HS)	Int.(HS)	Linear(ES)	Quad.(ES)	Int.(HS×ES)	Int.(ES)	I_V	I_{DV}
1	SS	.3402	.2981	.2771	.3470	.2291	.2402	.8915	.8113
1	D	.3398	.2877	.2711	.4198	.2085	.2231	1.1102	.8038
1	MSS$_A$	.3135	.2760	.2667	.3794	.1957	.2111	.8571	.7099
1	MSS$_D$	.3296	.2736	.2904	.4136	.2021	.2188	1.0897	.7863
10	SS	.8400	.8121	.2789	.3486	.2307	.2422	3.4585	2.5742
10	D	.8555	.8272	.2724	.4227	.2093	.2239	3.6603	2.6481
10	MSS$_A$	.8292	.7894	.2669	.3815	.1960	.2116	3.5463	2.4518
10	MSS$_D$	.8355	.7885	.2916	.4147	.2024	.2198	3.6777	2.5299
100	SS	2.5687	2.5224	.2791	.3488	.2309	.2425	28.0430	20.1273
100	D	2.6254	2.5884	.2726	.4231	.2095	.2240	29.0780	21.0343
100	MSS$_A$	2.5652	2.4682	.2669	.3818	.1960	.2117	29.3804	19.8479
100	MSS$_D$	2.5673	2.4679	.2917	.4149	.2024	.2200	29.5116	19.9263

Table 5 shows expected precisions for each type of effects as η increases. On average the new designs are better to estimate almost all types of effects. Conversely, the new designs are not so impressive in terms of I_V-efficiency, although their advantage is clearer with respect to the difference-based prediction criterion.

4.3 Example 3 (2 HS and 2 ES factors, 12 whole plots with 4 subplots each)

Vining, Kowalski and Montgomery (2005) gave a second-order equivalent-estimation design (EE) for 2 HS and 2 ES factors in 12 whole plots of size 4, based on the Box-Behnken treatment set. Jones and Nachtsheim (2009) constructed a D optimum design (D) for the same problem. We constructed the MSS_A and MSS_D designs shown in Table 6.

The performances of the four designs are presented in Figures 5 and 6 and in Table 7. Designs MSS_A and MSS_D show very similar performances and are barely distinguishable in the graphs. The graphs highlight the inefficiency of the equivalent-estimation design. The other three designs have similar performances with some loss of efficiency of design D, with respect to the A_S criterion, for $\eta > 0.7$. The newer designs are slightly more efficient than the D-optimum design in terms of variances and almost as efficient in terms of the determinant. Table 7 shows the low precision for estimating all effects of the EE design, except quadratic effects of the HS factors. Again we find that the new designs outperform all others in terms of predicting differences in response and are competitive in terms of predicting the response.

4.4 Example 4 (3 HS and 3 ES factors, 12 whole plots with 4 subplots each)

Macharia and Goos (2010) found that some D-optimum designs also satisfy the equivalent-estimation property and that for a given structure there can be many equivalent-estimation designs, some of them with high efficiency in terms of the D criterion. They compared D-optimal designs (considering $\eta = 1$) and D-efficient equivalent-estimation designs (EE_D) for several structures including the situation with 3 HS and 3 ES factors in 12 whole plots with 4 subplots each. Here we compare their designs and A_S and D_S optimal designs obtained by the MSS approach. The

Table 6: Designs for Example 3 (2 HS and 2 ES factors, 12 whole plots with 4 subplots each) using the MSS approach, A_S and D_S criteria

MSS_A								MSS_D							
W_1	W_2	X_1	X_2	W_1	W_2	X_1	X_2	W_1	W_2	X_1	X_2	W_1	W_2	X_1	X_2
−1	−1	−1	−1	0	0	−1	0	−1	−1	−1	−1	0	0	−1	0
−1	−1	−1	1	0	0	0	0	−1	−1	−1	1	0	0	0	0
−1	−1	1	−1	0	0	0	1	−1	−1	0	−1	0	0	0	1
−1	−1	1	1	0	0	1	−1	−1	−1	1	0	0	0	1	−1
−1	−1	−1	0	0	1	−1	−1	−1	−1	−1	−1	0	1	−1	−1
−1	−1	0	1	0	1	−1	1	−1	−1	−1	1	0	1	−1	1
−1	−1	1	1	0	1	0	0	−1	−1	1	−1	0	1	0	0
−1	−1	1	−1	0	1	1	1	−1	−1	1	1	0	1	1	1
−1	0	−1	−1	1	−1	−1	−1	−1	0	−1	0	1	−1	−1	−1
−1	0	0	0	1	−1	−1	1	−1	0	1	−1	1	−1	−1	1
−1	0	1	−1	1	−1	1	−1	−1	0	1	1	1	−1	1	−1
−1	0	1	1	1	−1	1	1	−1	0	0	1	1	−1	1	1
−1	1	−1	−1	1	0	−1	−1	−1	1	−1	−1	1	0	−1	0
−1	1	−1	1	1	0	−1	1	−1	1	−1	1	1	0	1	−1
−1	1	1	−1	1	0	0	−1	−1	1	1	−1	1	0	0	1
−1	1	1	1	1	0	1	0	−1	1	1	1	1	0	1	1
−1	1	−1	−1	1	1	−1	−1	−1	1	−1	−1	1	1	−1	−1
−1	1	−1	1	1	1	−1	1	−1	1	1	−1	1	1	−1	1
−1	1	0	−1	1	1	1	−1	−1	1	−1	1	1	1	0	−1
−1	1	1	0	1	1	1	1	−1	1	1	1	1	1	1	0
0	−1	−1	−1	1	1	−1	0	0	−1	−1	−1	1	1	−1	−1
0	−1	−1	1	1	1	0	1	0	−1	−1	1	1	1	−1	1
0	−1	0	−1	1	1	1	−1	0	−1	0	0	1	1	1	−1
0	−1	1	0	1	1	1	1	0	−1	1	1	1	1	1	1

Table 7: Square root of mean of expected variances of parameter estimators and prediction performances for alternative designs for Example 3

η	Design	Linear(HS)	Quad.(HS)	Int.(HS)	Linear(ES)	Quad.(ES)	Int.(HS×ES)	Int.(ES)	I_V	I_{DV}
1	EE	.4564	.6972	.5590	.2887	.5833	.5000	.5000	.7079	.7773
1	D	.3539	.8912	.3963	.1619	.4062	.1758	.1735	1.1825	.5363
1	MSS_A	.3849	.7627	.4384	.1650	.3983	.1848	.1764	.7208	.4161
1	MSS_D	.3845	.7653	.4392	.1636	.4272	.1810	.1709	.7235	.4190
10	EE	1.3070	1.9965	1.6008	.2887	1.5298	.5000	.5000	4.3245	4.8940
10	D	1.0125	2.5336	1.1323	.1626	.4091	.1760	.1737	8.9095	3.7627
10	MSS_A	1.0998	2.1629	1.2528	.1654	.4004	.1852	.1767	5.2606	2.8264
10	MSS_D	1.0997	2.1638	1.2531	.1638	.4286	.1814	.1711	5.2630	2.8290
100	EE	4.0876	6.2439	5.0062	.2887	4.7266	.5000	.5000	40.4912	46.0607
100	D	3.1663	7.9164	3.5401	.1627	.4095	.1760	.1737	86.1598	36.0129
100	MSS_A	3.4387	6.7558	3.9170	.1654	.4006	.1852	.1768	50.6486	26.9215
100	MSS_D	3.4386	6.7561	3.9171	.1639	.4288	.1815	.1712	50.6510	26.9241

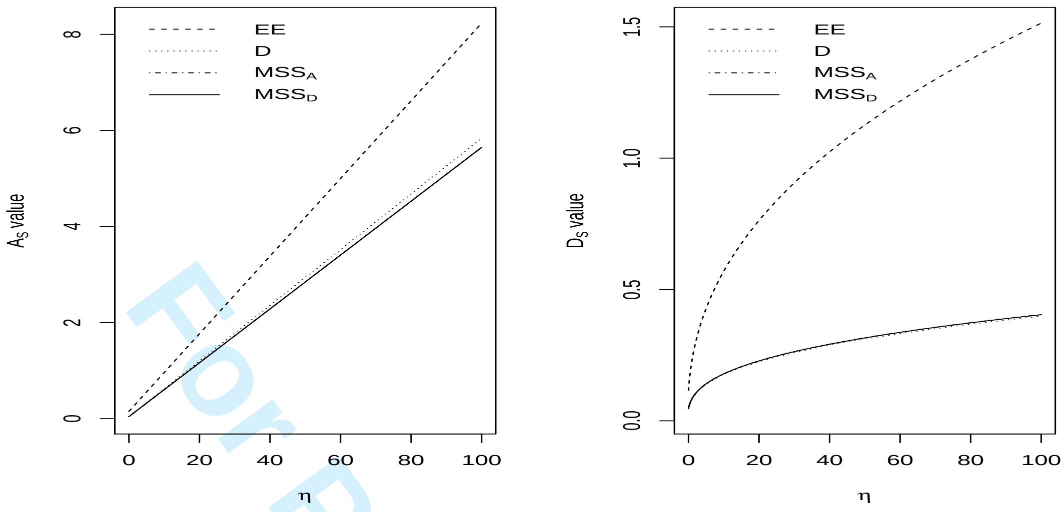

Figure 5: Expected A_S and D_S values as functions of η for alternative designs for Example 3.

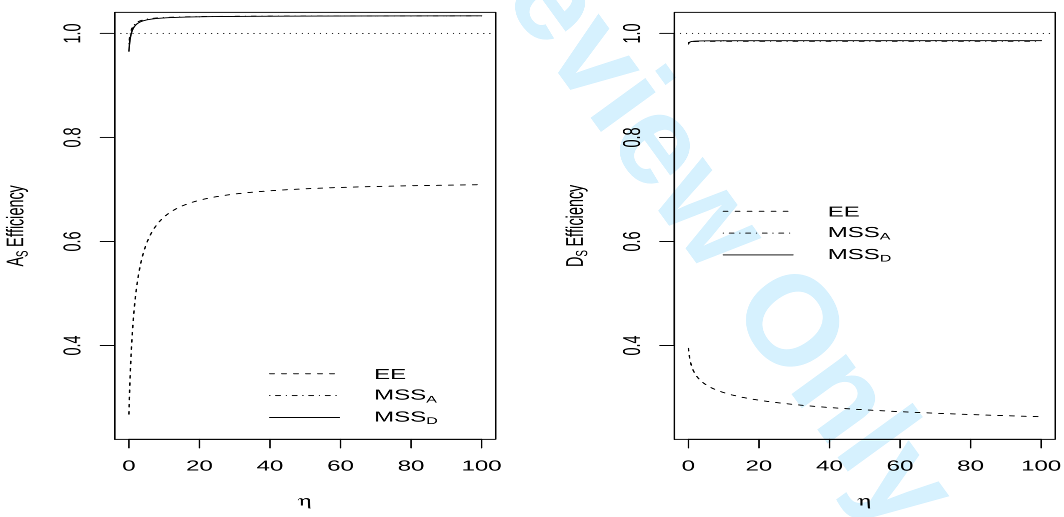

Figure 6: Expected A_S and D_S efficiencies, relative to design D, as functions of η for alternative designs for Example 3.

new designs are given in Table 8 and Figures 7 and 8 compare the performances of the designs. In terms of A_S values designs D, MSS_A and MSS_D have almost the same performance, though for very small η the D-optimum design is slightly more efficient. In terms of D_S values, both MSS_A and MSS_D designs also perform very similarly to design D and do somewhat better in terms of prediction criteria - see Table 9. The D-efficient equivalent-estimation design (EE_D) is clearly poor in terms of both A_S and D_S values, as well as the prediction criteria.

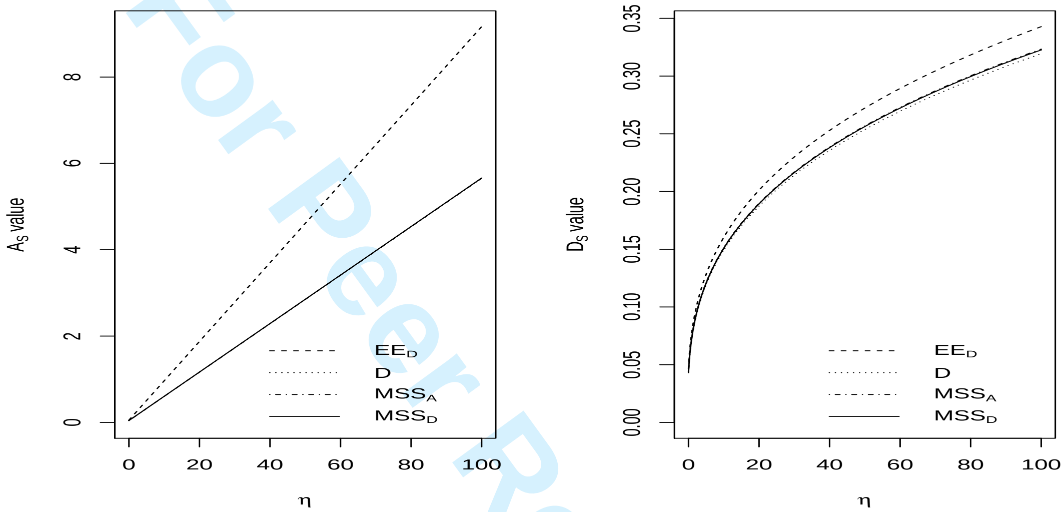

Figure 7: Expected A_S and D_S values as functions of η for alternative designs for Example 4.

4.5 Example 5 (2 VHS, 1 HS and 3 ES factors, 8 whole plots with 2 subplots each, each with 2 sub-subplots each)

In this example we consider the design problem with three strata presented in Jones and Goos (2009). The model has linear main effects and two-factor interactions with 2 VHS, 1 HS and 3 ES factors. The unit structure is 8 whole plots, each with 2 subplots with 2 sub-subplots each. Jones and Goos (2009) constructed a D-optimum design fixing $\eta_1 = \eta_2 = 1$. As the number of in each stratum is a power of 2 and the model is supported by a two-level factorial, they also presented an alternative design constructed by fractionating and aliasing high order terms. In this case our approach resulted in the same design for A and D criteria (Table 10).

Table 8: Designs for Example 4 (3 HS and 3 ES factors, 12 whole plots with 4 subplots each) using the MSS approach, A_S and D_S criteria

MSS$_A$						MSS$_D$					
W_1	W_2	W_3	X_1	X_2	X_3	W_1	W_2	W_3	X_1	X_2	X_3
−1	−1	−1	−1	−1	1	−1	−1	−1	−1	−1	−1
−1	−1	−1	−1	1	−1	−1	−1	−1	−1	1	1
−1	−1	−1	1	−1	−1	−1	−1	−1	1	−1	1
−1	−1	−1	1	1	1	−1	−1	−1	1	1	−1
−1	−1	1	−1	1	0	−1	−1	1	−1	0	1
−1	−1	1	0	−1	−1	−1	−1	1	0	1	−1
−1	−1	1	1	−1	1	−1	−1	1	1	−1	0
−1	−1	1	1	0	−1	−1	−1	1	1	1	1
−1	0	1	−1	0	−1	−1	0	0	−1	−1	0
−1	0	1	−1	0	1	−1	0	0	−1	1	0
−1	0	1	0	−1	0	−1	0	0	0	0	1
−1	0	1	1	1	0	−1	0	0	1	−1	−1
−1	1	−1	−1	−1	1	−1	1	−1	−1	−1	1
−1	1	−1	−1	1	−1	−1	1	−1	−1	1	−1
−1	1	−1	1	−1	−1	−1	1	−1	1	−1	−1
−1	1	−1	1	1	1	−1	1	−1	1	1	1
−1	1	1	−1	−1	−1	−1	1	1	−1	−1	−1
−1	1	1	−1	1	1	−1	1	1	−1	1	1
−1	1	1	1	−1	1	−1	1	1	1	−1	1
−1	1	1	1	1	−1	−1	1	1	1	1	−1
0	0	−1	−1	−1	−1	0	−1	0	−1	−1	1
0	0	−1	−1	1	1	0	−1	0	−1	1	−1
0	0	−1	0	1	0	0	−1	0	0	−1	−1
0	0	−1	1	0	0	0	−1	0	1	0	0
0	−1	0	−1	−1	0	0	0	−1	−1	1	1
0	−1	0	1	−1	0	0	0	−1	0	0	0
0	−1	0	1	1	−1	0	0	−1	1	−1	1
0	−1	0	0	0	1	0	0	−1	1	1	−1
1	−1	−1	−1	1	1	0	0	1	−1	0	−1
1	−1	−1	0	0	−1	0	0	1	0	−1	1
1	−1	−1	1	−1	1	0	0	1	0	1	0
1	−1	−1	1	1	−1	0	0	1	1	0	−1
1	−1	1	−1	−1	1	1	−1	−1	−1	−1	−1
1	−1	1	−1	1	−1	1	−1	−1	−1	1	1
1	−1	1	1	−1	−1	1	−1	−1	1	−1	1
1	−1	1	1	1	1	1	−1	−1	1	1	−1
1	0	0	−1	−1	−1	1	−1	1	−1	−1	1
1	0	0	−1	1	1	1	−1	1	−1	1	−1
1	0	0	0	−1	1	1	−1	1	1	−1	−1
1	0	0	1	0	0	1	−1	1	1	1	1
1	1	−1	−1	0	0	1	1	−1	1	−1	−1
1	1	−1	0	−1	−1	1	1	−1	1	1	1
1	1	−1	1	−1	1	1	1	−1	−1	1	−1
1	1	−1	1	1	−1	1	1	−1	−1	−1	1
1	1	1	−1	−1	1	1	1	1	−1	1	1
1	1	1	−1	1	−1	1	1	1	1	−1	1
1	1	1	1	−1	−1	1	1	1	−1	−1	−1
1	1	1	1	1	1	1	1	1	1	1	−1

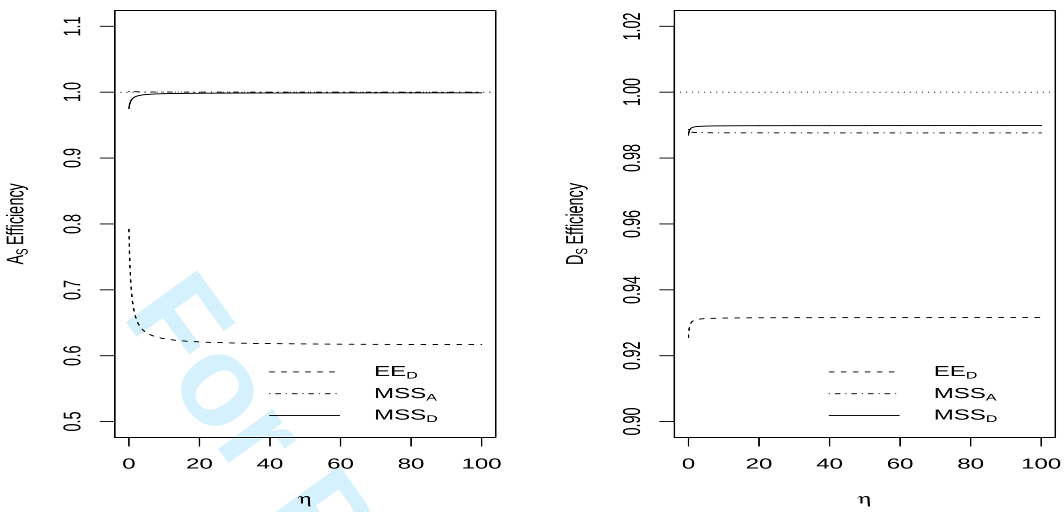

Figure 8: Expected A_S and D_S efficiencies, relative to design D, as functions of η for alternative designs for Example 4.

Table 9: Square root of mean of expected variances of parameter estimators and prediction performances for alternative designs for Example 4

η	Design	Linear(HS)	Quad.(HS)	Int.(HS)	Linear(ES)	Quad.(ES)	Int.(HS×ES)	Int.(ES)	I_V	I_{DV}
1	EE_D	.5142	1.1202	.5387	.1609	.4920	.1793	.1713	1.4241	1.0722
1	D	.3813	.9650	.3941	.1571	.5019	.1724	.1654	1.1718	.7790
1	MSS_A	.3811	.9674	.3960	.1634	.4416	.1774	.1763	1.0839	.7511
1	MSS_B	.3835	.9621	.3966	.1579	.5150	.1737	.1655	1.0711	.7479
10	EE_D	1.4627	3.1803	1.5338	.1609	.4920	.1793	.1713	9.8491	7.4816
10	D	1.0869	2.7418	1.1232	.1573	.5033	.1725	.1655	7.4467	5.0279
10	MSS_A	1.0868	2.7426	1.1239	.1635	.4424	.1776	.1765	7.3569	4.9986
10	MSS_D	1.0941	2.7193	1.1324	.1581	.5158	.1738	.1655	6.9721	4.8672
100	EE_D	4.5705	9.9352	4.7935	.1609	.4920	.1793	.1713	94.0991	71.5753
100	D	3.3972	8.5660	3.5106	.1573	.5034	.1725	.1655	70.1658	47.4961
100	MSS_A	3.3971	8.5663	3.5108	.1635	.4425	.1776	.1766	70.0758	47.4674
100	MSS_D	3.4201	8.4901	3.5401	.1581	.5159	.1738	.1655	65.9723	46.0547

Table 10: Design for Example 5 (2 VHS, 1 HS and 3 ES factors, 8 whole plots with 2 subplots with 2 sub-subplots each) using the MSS approach, A_S and D_S criteria

MSS$_A$ and MSS$_D$											
W_1	W_2	S_1	X_1	X_2	X_3	W_1	W_2	S_1	X_1	X_2	X_3
−1	−1	−1	−1	1	1	1	−1	−1	−1	−1	1
−1	−1	−1	1	−1	1	1	−1	−1	1	1	1
−1	−1	1	−1	−1	−1	1	−1	1	−1	1	−1
−1	−1	1	1	1	−1	1	−1	1	1	−1	−1
−1	−1	−1	−1	−1	1	1	−1	−1	−1	−1	−1
−1	−1	−1	1	−1	−1	1	−1	−1	1	−1	1
−1	−1	1	−1	1	−1	1	−1	1	−1	1	1
−1	−1	1	1	1	1	1	−1	1	1	1	−1
−1	1	−1	−1	−1	1	1	1	−1	1	−1	1
−1	1	−1	−1	1	−1	1	1	−1	1	1	−1
−1	1	1	1	−1	1	1	1	1	−1	−1	−1
−1	1	1	1	1	−1	1	1	1	1	1	1
−1	1	−1	−1	−1	−1	1	1	−1	−1	1	1
−1	1	−1	1	1	1	1	1	−1	1	−1	−1
−1	1	1	−1	1	1	1	1	1	−1	−1	1
−1	1	1	1	−1	−1	1	1	1	−1	1	−1

Table 11: Square root of mean of expected variances of parameter estimators (L: linear effects; I: two-factor interactions) and prediction performances for alternative designs for Example 5

η_1	η_2	Design	L(VHS)	I(VHS)	L(HS)	I(VHS×HS)	L(ES)	I(VHS×ES)	I(HS×ES)	I(ES)	I_V	I_{DV}
1	1	D	.4677	.4677	.3062	.3062	.1863	.1863	.1846	.2829	.5369	.3181
1	1	MSS	.4732	.4711	.3345	.3305	.2064	.2042	.2214	.2512	.5691	.3432
1	10	D	.8839	.8839	.8101	.8101	.1998	.1998	.1858	.5407	1.9290	1.1478
1	10	MSS	.8870	.8858	.8213	.8202	.2146	.2170	.2286	.3145	1.9028	1.1139
1	100	D	2.5311	2.5311	2.5062	2.5062	.2036	.2036	.1863	1.4751	15.6844	9.2781
1	100	MSS	2.5322	2.5317	2.5099	2.5096	.2163	.2206	.2305	.3355	15.0347	8.6207
100	1	D	3.5488	3.5488	.3062	.3062	.1863	.1863	.1863	.2955	22.5395	9.9458
100	1	MSS	3.5495	3.5492	.3345	.3309	.2072	.2050	.2245	.2577	22.5716	9.9705
100	10	D	3.6272	3.6272	.8101	.8101	.1998	.1998	.1863	.5443	23.9304	10.7741
100	10	MSS	3.6279	3.6276	.8213	.8203	.2148	.2173	.2296	.3177	23.9039	10.7399
100	100	D	4.3337	4.3337	2.5062	2.5062	.2036	.2036	.1863	1.4752	37.6846	18.9033
100	100	MSS	4.3344	4.3341	2.5099	2.5096	.2163	.2207	.2306	.3358	37.0348	18.2458

The efficiencies of the MSS design relative to the globally D optimum design of Jones and Goos (2009), design D, are shown in Figure 9. In the plots, σ^2 (the third stratum variance) is fixed to be 1 and σ_2^2 (the second stratum variance component) and σ_1^2 (the first stratum variance component) are varied. For very small values of the variance ratios the new design is less efficient than design D but it becomes more efficient as the ratios increase. We note that, with respect to D efficiencies, both designs (the globally D-optimum and the MSS design) are robust to changes in σ_1^2, especially when σ_2^2 is large. Jones and Goos (2009) also noted the robustness of D-optimum designs for changes in σ_1^2. Although the two designs show similar performances in terms of efficiencies, design D has one interaction term between the ES factors that is fully estimated in stratum 2. Our design distributed the loss of information among all terms and thus none of the terms is sacrificed as shown in Table 11. It should be noted that the alternative design of Jones and Goos (2009), constructed by fractionating and aliasing terms, has two interactions of ES factors fully estimated in stratum 2 and one in stratum 1. Our new design also improves on the old one in terms of prediction variances, except when the ratios of variance components are small.

4.6 Example 6 (2 HS and 2 ES factors, 5 blocks with 3 whole plots each, each with 3 subplots)

In this last example we re-design the experiment for the blocked split-plot structure presented in Trinca and Gilmour (2001). This is aimed at a response surface model for 2 HS and 2 ES factors. In the first stratum there are 5 units (blocks) to which no factors are applied. In the second stratum each block has 3 whole plots and 2 HS factors are to be applied. In the third stratum each whole plot is divided into three subplots and the 2 ES factors are to be applied. In this case the design to start with is a blocked design for the whole plots and this example is aimed at showing the flexibility of our methodology. The designs we constructed are shown in Table 12. Note that although in the third stratum the number of units would allow 5 replicates of the 3^2, it is not that treatment set that comes out of the search, no matter which criterion is used.

The D_S-efficiency based on the previous design (Figure 10) shows that the new designs are more efficient for a wide range of variance component values with the gain being up to around 10%. Very similar plots are obtained for MSS$_A$. Table 13 shows that very little information comes from the highest stratum (inter-block information) no matter what are the sizes of the variance

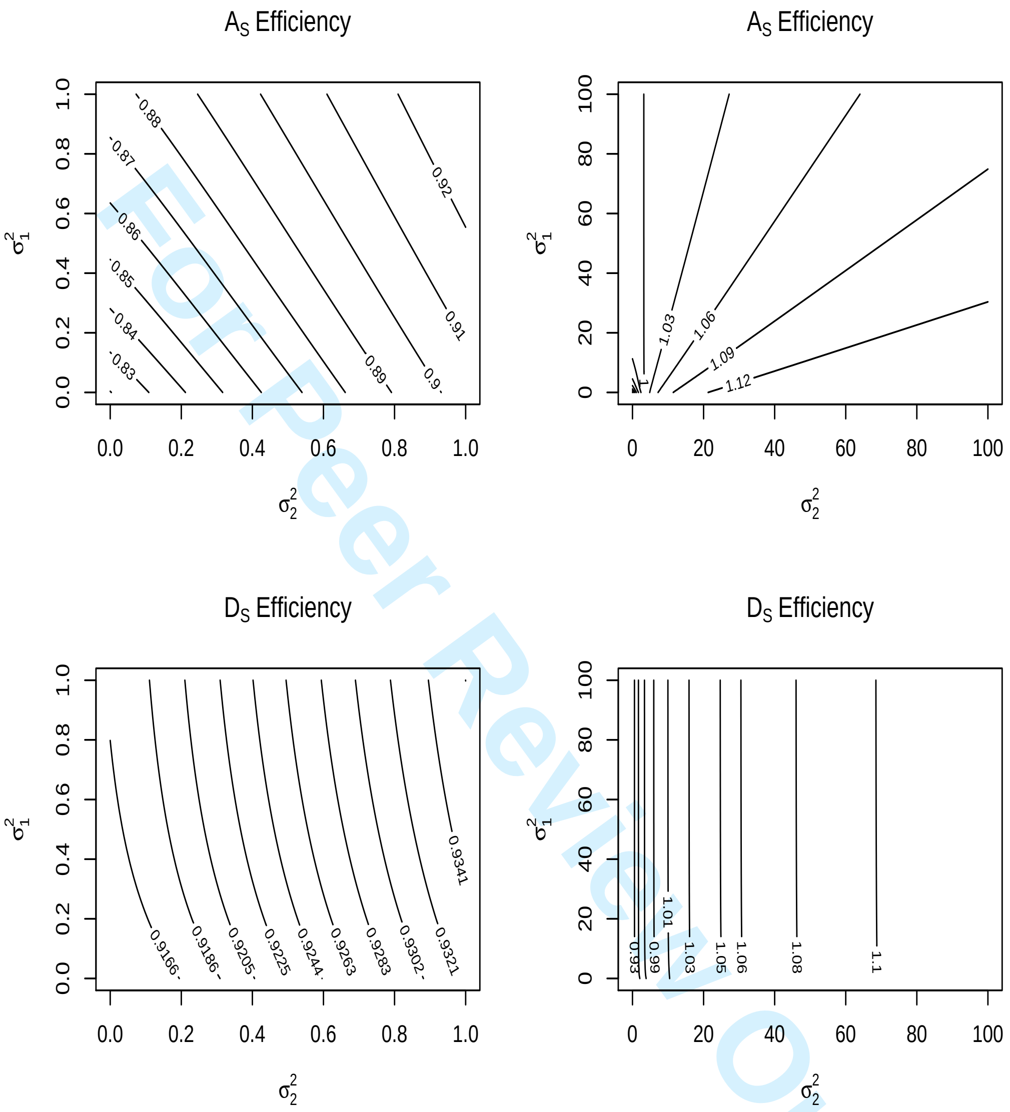

Figure 9: Expected A_S and D_S efficiencies, relative to design D, of design MSS (A and D criterion) for Example 5, as functions of σ_1^2 and σ_2^2 (fixing $\sigma^2 = 1$).

Table 12: Designs for Example 6 (2 HS and 2 ES factors, 5 blocks with 3 whole plots each, each with 3 subplots) using the MSS approach, A_S and D_S criteria

MSS$_A$								MSS$_D$							
W_1	W_2	X_1	X_2	W_1	W_2	X_1	X_2	W_1	W_2	X_1	X_2	W_1	W_2	X_1	X_2
−1	0	−1	1	−1	1	−1	−1	−1	−1	−1	−1	−1	0	−1	−1
−1	0	0	−1	−1	1	0	1	−1	−1	−1	1	−1	0	0	0
−1	0	1	0	−1	1	1	−1	−1	−1	1	0	−1	0	1	1
0	−1	−1	−1	0	0	−1	1	−1	1	−1	−1	1	−1	−1	0
0	−1	0	1	0	0	0	0	−1	1	−1	1	1	−1	1	−1
0	−1	1	−1	0	0	1	1	−1	1	1	0	1	−1	1	1
1	1	−1	−1	1	1	−1	−1	0	0	0	0	1	1	−1	−1
1	1	0	1	1	1	−1	1	0	0	1	−1	1	1	−1	1
1	1	1	−1	1	1	1	0	0	0	1	1	1	1	1	0
−1	−1	−1	−1	−1	0	−1	0	−1	−1	−1	−1	−1	0	−1	0
−1	−1	−1	1	−1	0	0	−1	−1	−1	0	1	−1	0	0	1
−1	−1	1	0	−1	0	1	1	−1	−1	1	−1	−1	0	1	−1
−1	1	−1	0	0	1	−1	1	0	1	−1	0	0	1	−1	0
−1	1	1	−1	0	1	0	−1	0	1	0	1	0	1	0	−1
−1	1	1	1	0	1	1	0	0	1	1	−1	0	1	1	1
1	0	−1	−1	1	−1	−1	1	1	0	−1	1	1	−1	−1	−1
1	0	0	1	1	−1	0	−1	1	0	0	−1	1	−1	−1	1
1	0	1	−1	1	−1	1	1	1	0	1	1	1	−1	1	0
−1	−1	−1	−1					−1	1	−1	1				
−1	−1	0	1					−1	1	0	−1				
−1	−1	1	−1					−1	1	1	1				
0	1	−1	0					0	−1	−1	1				
0	1	0	−1					0	−1	0	−1				
0	1	1	1					0	−1	1	1				
1	−1	−1	0					1	1	−1	−1				
1	−1	1	−1					1	1	0	1				
1	−1	1	1					1	1	1	−1				

components. In the original design (SS) that was also true for most of the effects, but not the interaction between the HS factors.

5 Discussion

We have modified the stratum-stratum method of construction of multi-stratum response surface designs and compared it with several other approaches from the literature. The procedure produces efficient designs that are competitive with other popular designs. The step-by-step design construction makes the method quite attractive due to its direct application to designing experiments for any number of strata. The same program code can be run sequentially, once for each stratum, as long as the entries are correctly specified. The step-by-step approach does not experience the problems with storage of large candidate treatment sets and thus the usual point

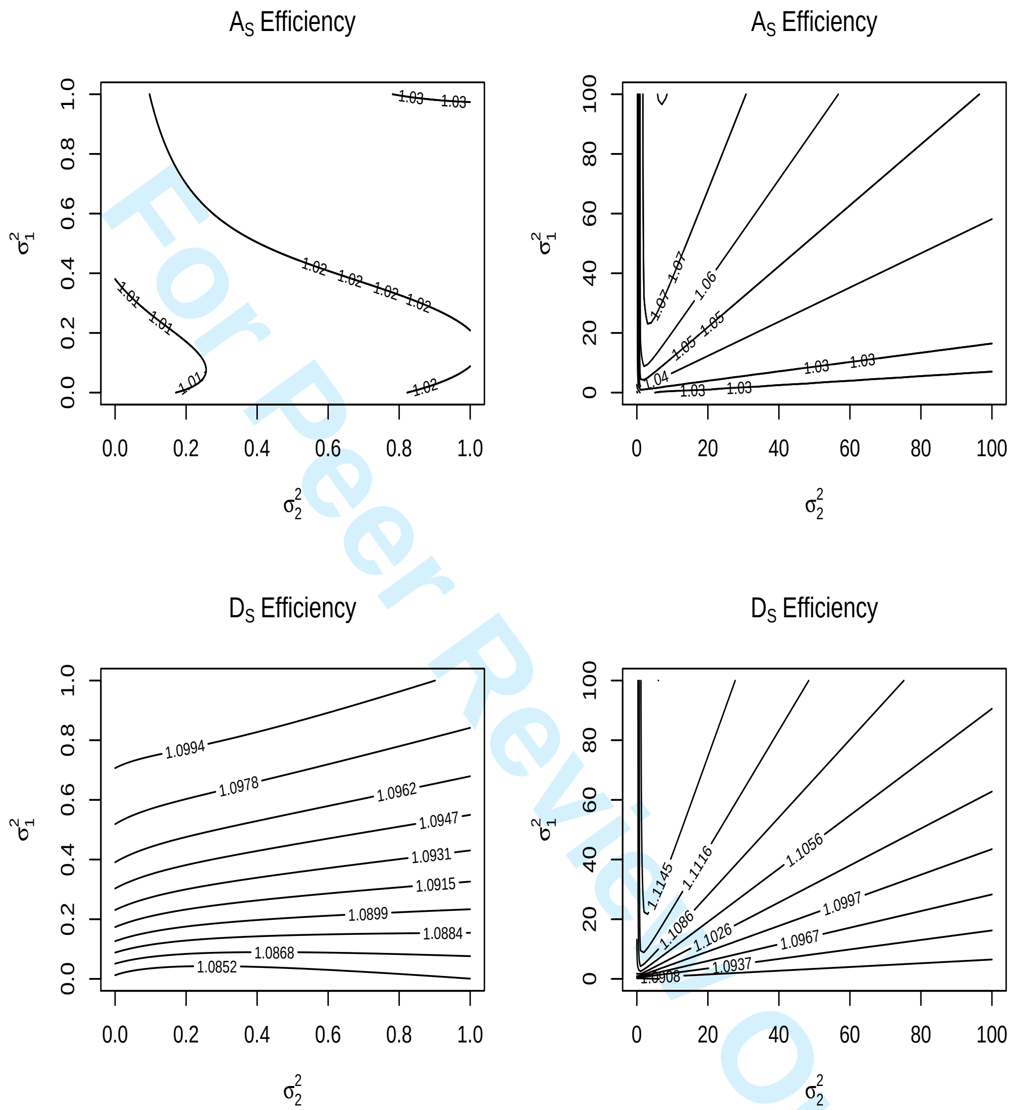

Figure 10: Expected A_S and D_S efficiencies, relative to design presented in Trinca and Gilmour (2001), of design MSS_D for Example 6, as functions of σ_1^2 and σ_2^2 (fixing $\sigma^2 = 1$).

Table 13: Square root of mean of expected variances of parameter estimators and prediction performances for alternative designs for Example 6

η_1	η_2	Design	L(HS)	Q(HS)	I(HS)	L(ES)	Q(ES)	I(HS×ES)	I(ES)	I_V	I_{DV}
1	1	SS	.3651	.6967	.5288	.1826	.3162	.2247	.2886	.7161	.3637
1	1	MSS$_A$	.3666	.7082	.4224	.1751	.3871	.1999	.2007	.8806	.4028
1	1	MSS$_D$	.3659	.7093	.4218	.1752	.3839	.2002	.2002	.8746	.3992
1	10	SS	1.0165	1.9239	1.2194	.1826	.3162	.2247	.3120	3.4806	2.0996
1	10	MSS$_A$	.9922	1.9165	1.1480	.1758	.3913	.2004	.2017	3.5659	2.3707
1	10	MSS$_B$	.9919	1.9170	1.1478	.1759	.3884	.2008	.2017	4.5410	2.3672
1	100	SS	3.1675	5.9870	3.5718	.1826	.3162	.2247	.3158	31.0190	19.3523
1	100	MSS$_A$	3.0623	5.9133	3.5459	.1760	.3920	.2005	.2018	41.0772	21.8088
1	100	MSS$_B$	3.0622	5.9134	3.5459	.1760	.3891	.2009	.2020	41.0727	21.8054
100	1	SS	.3651	.6968	.6308	.1826	.3162	.2247	.2895	20.5393	.3769
100	1	MSS$_A$	.3730	.7202	.4281	.1752	.3875	.2000	.2008	20.6939	.4087
100	1	MSS$_D$	.3722	.7212	.4274	.1753	.3844	.2003	.2004	20.6879	.4157
100	10	SS	1.0165	1.9239	1.7211	.1826	.3162	.2247	.3123	23.4496	2.2636
100	10	MSS$_A$	1.0314	1.9923	1.1859	.1759	.3914	.2004	.2017	24.5935	2.5327
100	10	MSS$_B$	1.0311	1.9926	1.1857	.1760	.3885	.2008	.2018	24.5945	2.5291
100	100	SS	3.1675	5.9870	4.7204	.1826	.3162	.2247	.3158	51.8772	20.4105
100	100	MSS$_A$	3.1723	6.1296	3.6577	.1760	.3920	.2005	.2018	62.8964	23.2342
100	100	MSS$_B$	3.1722	6.1298	3.6576	.1761	.3891	.2009	.2020	62.9371	23.2307

exchange algorithm is used. However the approach can also be used with the coordinate exchange algorithm of Jones and Goos (2007). As the construction basis is a blocked design in each stratum, the updating formulae of Cook and Nachtsheim (1989) can be used to speed the search. Another important practical advantage is that it does not require prior estimates of variance component ratios.

Although the examples show that globally optimum designs for fixed η are quite robust to the variance component ratios, this method does not share the generality of the stratum-by-stratum approach. Typically, a new algorithm is needed for each different multi-stratum structure (split-plot, split-split plot, split-plot with blocks, etc.). The advantages of designs constructed using the modified stratum-by-stratum approach for prediction properties was not anticipated and is not immediately easy to explain. The I_V criterion concentrates on estimating the intercept and therefore, in completely randomized structures, concentrates points near the centre of the design. Consequently, designs with many points near the centre, such as those obtained from classical designs using the original SS approach, tend to do well in terms of this criterion. However, it is not obvious that the MSS approach gives any more points near the centre than the single stage D-optimal designs have. A possible explanation is that prediction at every point, whether of the response or differences in response, depends on all parameters and therefore those estimated in higher strata have more impact, especially when the variance components are large. In contrast, in the D criterion (and more obviously in the A criterion), the poor estimation of a few effects in high strata are swamped by good estimation of many effects in low strata. For prediction, therefore, by far the most important thing is precise estimation in the higher strata. By optimizing this first, the MSS algorithm achieves exactly what is needed.

We believe that, along with other algorithms, the stratum-by-stratum approach deserves a place in the experimental designer's toolbox and should be seriously considered for producing designs for any experiment which involves factors which are hard to set.

References

Atkinson, A. C., Donev, A. N. and Tobias, R. D. (2007). *Optimum Experimental Designs, with SAS*. Oxford: Oxford University Press.

Bingham, D. and Sitter, R. R. (1999). Minimum-aberration two-level fractional factorial split-plot designs. *Technometrics*, **41**, 62–70.

Cheng, C.-S. and Tsai, P.-W. (2009). Optimal two-level regular fractional factorial block and split-plot designs. *Biometrika*, **96**, 83–93.

Cook, R. D. and Nachtsheim, C. J. (1989). Computer-aided blocking of factorial and response surface designs. *Technometrics*, **31**, 339–46.

Draper, N. R. and John, J. A. (1998). Response surface designs where levels of some factors are difficult to change. *Australian and New Zealand Journal of Statistics*, **40**, 487–495.

Gilmour, S. G. and Goos, P. (2009). Analysis of data from nonorthogonal multi-stratum designs in industrial experiments. *Applied Statistics*, **58**, 467–484.

Goos, P. (2002). *The Optimal Design of Blocked and Split-Plot Experiments*. New York: Springer.

Goos, P. and Donev, A. N. (2007). Tailor-made split-plot designs with mixture and process variables. *Journal of Quality Technology*, **39**, 326–339.

Goos, P. and Vandebroek, M. (2003). D-optimal split-plot designs with given numbers and sizes of whole plots. *Technometrics*, **45**, 235–245.

Hardin, R. H. and Sloane, N. J. A. (1993) A new approach to the construction of optimal designs. *Journal of Statistical Planning and Inference*, **37**, 339–369.

Huang, P., Chen, D. and Voelkel, J. O. (1998). Minimum-aberration two-level split-plot designs. *Technometrics*, **40**, 314–326.

Jones, B. and Goos, P. (2007). A candidate-set-free algorithm for generating D-optimal split-plot designs. *Applied Statistics*, **56**, 347–364.

Jones, B. and Goos, P. (2009). D-optimal design of split-split-plot experiments. *Biometrika*, **96**, 67–82.

Jones, B. and Nachtsheim, C. (2009). Split-plot designs: what, why, and how. *Journal of Quality Technology*, **41**, 340–361.

Letsinger, J. D., Myers, R. H. and Lentner, M. (1996). Response surface methods for bi-randomization structures. *Journal of Quality Technology*, **28**, 381–397.

Macharia, H. and Goos, P. (2010). D-optimal and D-efficient equivalent-estimation second-order split-plot designs. *Journal of Quality Technology*, **42**, 358–372.

Parker, P. A., Kowalski, S. M. and Vining, G. G. (2007). Construction of balanced equivalent estimation second-order split-plot designs. *Technometrics*, **49**, 56–65.

Trinca, L. A. and Gilmour, S. G. (1999). Difference variance dispersion graphs for comparing response surface designs with applications in food technology. *Applied Statistics*, **48**, 441–455.

Trinca, L. A. and Gilmour, S. G. (2001). Multi-stratum response surface designs. *Technometrics*, **43**, 25–33.

Vining, G. G., Kowalski, S. M. and Montgomery, D. C. (2005) Response surface designs within a split-plot structure. *Journal of Quality Technology*, **37**, 115–129.