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# Augmenting supersaturated designs with Bayesian *D*-optimality

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ABSTRACT

A methodology is developed to add runs to existing supersaturated designs. The technique uses information from the analysis of the initial experiment to choose the best possible follow-up runs. After analysis of the initial data, factors are classified into one of three groups: primary, secondary, and potential. Runs are added to maximize a Bayesian *D*-optimality criterion to increase the information gained about those factors. Simulation results show the method can outperform existing supersaturated design augmentation strategies that add runs without analyzing the initial response variables.



## 1. Introduction

Screening designs are used in the early stages of industrial and computer experiments to discover which input factors have major effects on a system's output. A screening experiment is intended to remove the negligible, or inactive, factors from further experiments, allowing the investigator to focus on the important, or active, factors. In a large set of factors, relatively few are likely to be active, a concept called effect sparsity (Box and Meyer, 1986). Traditional screening methods for $k$ factors, like two-level $2^{k-p}$ fractional factorial (Box et al., 2005) or Plackett–Burman designs (Plackett and Burman, 1946), require at least $k+1$ experimental runs to separate the few active factors from the many inactive. But, when $k$ is large or experimental runs are prohibitively expensive, the experimenter requires alternative designs that can screen $k$ factors in $n < k+1$ runs. Supersaturated designs (SSDs) are one such technique.

SSDs were introduced by Satterthwaite (1959) and Booth and Cox (1962) but did not receive considerable attention until Lin (1993) and Wu (1993) renewed interest in the field, which continues today. The focus of an SSD is on identifying the active main effects in a linear model. Consider an experiment with $k$ factors and $n$ runs. The underlying linear main-effect

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model is represented as:

$$\mathbf{y} = \beta_0\mathbf{1} + \beta_1\mathbf{x}_1 + \cdots + \beta_k\mathbf{x}_k + \boldsymbol{\epsilon} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}; \tag{1}$$

where $\mathbf{y}$ is the response vector, $\boldsymbol{\beta} = (\beta_0, \ldots, \beta_k)'$ is the $p \times 1$ vector of unknown model parameters ($p = k + 1$), and $\boldsymbol{\epsilon} \sim N(0, \sigma^2\mathbf{I}_n)$ is the error term. The model matrix $\mathbf{X}$ equals $(\mathbf{1}|\mathbf{S})$, where $\mathbf{1}$ is an $n \times 1$ column of 1's and $\mathbf{S} = (\mathbf{x}_1|\cdots|\mathbf{x}_k)$ is the design matrix. The rows of $\mathbf{S}$ contain the $k$ factor level settings for the $n$ experimental runs. For clarity, we adopt the notation in Gupta et al. (2010) and let SSD$(n, k) = \mathbf{S}$ represent an SSD with $n$ runs and $k$ factors.

An SSD$(n, k)$ with model matrix $\mathbf{X}$ is typically constructed to optimize a criterion that minimizes the bias of the parameter estimates. For two-level designs, in which factor levels are coded as $\pm 1$, the most popular criterion is $E(s^2)$. Denote the $(i, j)$th element of $\mathbf{X}'\mathbf{X}$ as $s_{ij}$. $E(s^2)$ is defined as $E(s^2) = \sum_{i<j} s_{ij}^2/(p(p-1)/2)$. A small $E(s^2)$ implies the average correlations between factor columns are as small as possible (see Nguyen (1996), Bulutoglu and Cheng (2004) and Suen and Das (2010), and references therein for more on $E(s^2)$-optimal designs). Another popular construction technique is based on the Bayesian $D$-optimality criterion by Jones et al. (2008), discussed in Sections 2 and 3. An overview of other design criteria for SSDs, including criteria for designs with more than two levels, can be found in Lin (2003).

Regardless of the construction method, the analysis of SSDs is rather challenging. Since $n < k+1$, $\mathbf{X}'\mathbf{X}$ is singular and the ordinary least squares estimates, $\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$, cannot be calculated. Due to effect sparsity, most of the $\beta_i$ terms in (1) are assumed to be zero, but choosing which factors to remove from the model is difficult. We refer the reader to Gupta and Kohli (2008) and Georgiou (2012) for reviews of proposed analysis methods, but we note that no method is infallible. There is a tradeoff between the economy of a design and the information gained from the experiment. The experimenter risks classifying an inactive factor as active (a Type I error), or worse, classifying an active factor as inactive (a Type II error). For this reason, screening designs are not intended to be utilized for an "all-encompassing" experiment, but rather as the first stage in a sequence of experiments (Box, 1992). This is especially pertinent with SSDs because the original analysis results are not always definitive, a consequence of the inability to simultaneously estimate all main-effects.

Adding follow-up runs to a design is a useful way to clarify or confirm initial results and guide the next phase of experimentation. The notion of sequential experimentation is a well-established approach in experimental design: Box (1992) provided general guidelines to consider, and traditional augmentation strategies like fold-over designs and the addition of center points are described in most experimental design textbooks (e.g. Montgomery (2009) and Wu and Hamada (2000)). However, the idea of augmenting SSDs has only recently been explored. Consider the following.

Suppose after running an SSD$(n_1, k)$, the experimenter can afford $n_2$ more runs to resolve ambiguities. What is the best way to augment the original design to reduce uncertainty and get the most information out of the final SSD$(n_1 + n_2, k)$? This is a relatively new research area. Two papers by Gupta et al. (2010, 2012) describe methods to add rows to two-level and $s$-level designs, respectively. With Gupta et al.'s method, $E(s^2)$-optimal designs are augmented with additional runs to create a new class of "extended $E(s^2)$-optimal" designs. Suen and Das (2010) used a similar approach to add or remove one row from an existing $E(s^2)$-optimal design to make a new $E(s^2)$-optimal design. However, in the current methods, there is no effort to analyze the initial results before adding runs. After running an SSD$(n_1, k)$, an experimenter should have *some* useful information about the process. Indeed, that is the motivation for running the experiment in the first place.

The focus of this paper is to present an alternative approach to the extended-$E(s^2)$ augmentation technique presented in Gupta et al. (2010). Our goal is to take the information gained from the initial design, SSD$(n_1, k)$, identify and classify factors of interest, and prioritize the additional $n_2$ runs to get the most information from the final design, SSD$(n_1 + n_2, k)$. Specifically, we propose an SSD augmentation strategy using the Bayesian $D$-optimality criterion from DuMouchel and Jones (1994) and Jones et al. (2008). Our approach has several benefits over current methods:

1. It uses information from the first $n_1$ runs to strategically plan the $n_2$ follow-up runs;
2. It can augment any SSD built from any construction method or optimality criterion;
3. It can add any number of runs; and
4. It uses the Coordinate-Exchange Algorithm (Meyer and Nachtsheim, 1995), a polynomial-time algorithm.

Like Gupta et al. (2010), we assume additional runs become available *after* the first experiment and that $n_2$ is provided by a decision maker. This is inherently different than a two-stage design where an experimenter purposefully partitions the allotted screening budget into two parts. SSDs are used when resources are heavily constrained, so had all the runs been available in the screening budget from the beginning, the experimenter would likely have chosen a design to accommodate all runs.

The next section reviews the relevant background of three key concepts: Bayesian $D$-optimality, the Coordinate-Exchange Algorithm, and algorithmic augmentation strategies for standard designs. Section 3 presents our approach to augment SSDs using information from the initial runs. Section 4 compares the performance of Bayesian $D$-optimal augmented designs with extended $E(s^2)$-optimal designs by highlighting examples where using information from the first runs leads to better recommendations than adding runs to maintain $E(s^2)$-optimality. We conclude with a discussion in Section 5.

## 2. Preliminaries

### 2.1. Bayesian D-optimality

$D$-optimality is a popular design criterion for traditional designs with an assumed $n \times k$ model matrix $\mathbf{X}$ with $n > k$. The goal of $D$-optimality is to reduce the error variances of the least squares estimates, given by $\sigma^2(\mathbf{X}'\mathbf{X})^{-1}$. This is accomplished

by maximizing the determinant of $\mathbf{X}'\mathbf{X}$, denoted $|\mathbf{X}'\mathbf{X}|$ (see Kiefer and Wolfowitz (1959) and Pukelsheim (1993) for more on *D*-optimality). Unfortunately, *D*-optimality is not always model-robust because the design may be 'optimal' to the wrong model. To reduce dependency on one model, researchers have proposed alternative optimality criteria under the Bayesian paradigm. A Bayesian design for a linear model is constructed to maximize the posterior information about the model parameters, which are conditional on prior information. In Bayesian design theory, the counterpart to *D*-optimality is Bayesian *D*-optimality. We refer the reader to Chaloner and Verdinelli (1995) and Atkinson et al. (2007, Chapter 18) for a detailed description and history of Bayesian design theory and Bayesian *D*-optimal methods. In this paper, we focus on the Bayesian *D*-optimality criterion as presented in DuMouchel and Jones (1994).

Consider the linear model $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$. Assume $\boldsymbol{\epsilon} \sim N(0, \sigma^2\mathbf{I}_n)$. Let the prior distribution of the parameters be $\boldsymbol{\beta}|\sigma^2 \sim N(\boldsymbol{\beta}_0, \sigma^2\mathbf{R}^{-1})$, where $\mathbf{R}$ is a prior covariance matrix, and the conditional distribution of $\mathbf{y}$ given $\boldsymbol{\beta}$ be $\mathbf{y}|\boldsymbol{\beta}, \sigma^2 \sim N(\mathbf{X}\boldsymbol{\beta}, \sigma^2\mathbf{I})$. The posterior distribution for $\boldsymbol{\beta}$ given $\mathbf{y}$ is then $\boldsymbol{\beta}|\mathbf{y} \sim N(\mathbf{b}, \sigma^2(\mathbf{X}'\mathbf{X} + \mathbf{R})^{-1})$, where $\mathbf{b} = (\mathbf{X}'\mathbf{X} + \mathbf{R})^{-1}(\mathbf{X}'\mathbf{y} + \mathbf{R}\boldsymbol{\beta}_0)$. As noted, *D*-optimal designs maximize $|\mathbf{X}'\mathbf{X}|$ to reduce the error variances of the parameter estimates. Similarly, Bayesian *D*-optimal designs aim to reduce the error variances of the parameter estimates, but the addition of prior information has changed the variance to $\mathrm{Var}(\mathbf{b}) = \sigma^2(\mathbf{X}'\mathbf{X} + \mathbf{R})^{-1}$. Therefore, Bayesian *D*-optimal designs are constructed to maximize $|\mathbf{X}'\mathbf{X} + \mathbf{R}|$.

The matrix $\mathbf{R}$ reflects the prior information assigned to each of the $p$ terms in the model matrix, $\mathbf{X}$. DuMouchel and Jones (1994) incorporate prior information and model uncertainty into the regression parameters by splitting models terms into two sets: primary terms and potential terms. Primary terms are assumed to be active (i.e. a nonzero $\beta_i$), whereas potential terms may or may not be active. Using this information, the $p_1$ primary terms are given a diffuse prior distribution with an arbitrary prior mean and prior variance tending towards infinity. The arbitrary mean reflects no knowledge of the direction of the effect of the primary term, and the "infinite" variance implies the effect is likely to be much different than zero. The $p_2 = p - p_1$ potential terms, on the contrary, are not expected to have large effects and are given a prior mean zero and finite variance $\sigma^2\tau^2$, where $\tau$ represents the expected effect of a factor relative to residual standard error (DuMouchel and Jones, 1994). The matrix, $\mathbf{R}$, is consequently set to $\mathbf{R} = \mathbf{K}/\tau^2$, where

$$\mathbf{K} = \begin{pmatrix} \mathbf{0}_{p_1\times p_1} & \mathbf{0}_{p_1\times p_2} \\ \mathbf{0}_{p_2\times p_1} & \mathbf{I}_{p_2\times p_2} \end{pmatrix}.$$

The posterior distribution for $\boldsymbol{\beta}$ given $\mathbf{y}$ is then

$$\boldsymbol{\beta}|\mathbf{y} \sim N\left[\left(\mathbf{X}'\mathbf{X} + \frac{\mathbf{K}}{\tau^2}\right)^{-1}\left(\mathbf{X}'\mathbf{y} + \frac{\mathbf{K}}{\tau^2}\boldsymbol{\beta}_0\right), \sigma^2\left(\mathbf{X}'\mathbf{X} + \frac{\mathbf{K}}{\tau^2}\right)^{-1}\right]; \tag{2}$$

and the Bayesian *D*-optimal design objective function becomes $|\mathbf{X}'\mathbf{X} + \mathbf{K}/\tau^2|$. The $p_1$ primary terms consist of those terms assumed to be in the true model, whereas higher-order effects make up the $p_2$ potential terms. The methodology allows the total number of model terms, $p = p_1 + p_2$, to be greater than the number of runs, $n$, because the addition of the prior information in $\mathbf{K}/\tau^2$ makes the information matrix invertible. As such, the designs can estimate all $p_1$ primary terms and detect some of the $p_2$ potential terms.

This method was adapted to create SSDs in Jones et al. (2008). In an SSD($n$, $k$), prior information is usually not available for any of the $k$ control factors, so all are classified as potential terms; the intercept is the only primary term. If information is available to suggest $p_1 > 1$ factors are active, the Bayesian *D*-optimality criterion can create such a design, provided $p_1 < n$. Incorporating this prior information makes the technique more dynamic than a naive regularization of the information matrix.

Jones et al. set $\tau^2 = 5$ and used the Coordinate-Exchange Algorithm to create the designs. For two-level designs, the Coordinate-Exchange Algorithm can be summarized with the following steps: Generate a uniform random number from $[-1, 1]$ for each $x_{i,j}$ in $\mathbf{X}$. Then, iterate through each entry in $\mathbf{X}$, replacing the random number with the entry from $\{-1, +1\}$ that results in the largest value of the objective function. Because the resulting design is likely only locally optimal, the algorithm is repeated many times with different random starting values for the $x_{i,j}$ entries. After many random starts, e.g. 100, the design with the largest determinant is approximately the Bayesian *D*-optimal design.

### 2.2. Augmenting designs

Augmenting a design with additional runs is the natural way to get more information about the system under study. One criterion used to add runs to traditional designs with $n < k$ is *D*-optimality. Suppose after an initial experiment, the investigator wishes to add specific terms to the assumed model matrix (e.g. two-factor interactions or quadratic effects). The model is specified *a priori* and runs are added to the original model matrix to create a *D*-optimal design for the full, updated model. The overall goal is to maximize the information gained from the combined design. For a step-by-step example, see Goos and Jones (2011, pp. 60–65).

Let $\mathbf{X}_1$ be a model matrix corresponding to the first $n_1$ runs of an experiment, and let $\mathbf{X}_2$ be the additional $n_2$ rows. To optimize the final design, we need to maximize $|\mathbf{X}'\mathbf{X}|$ of the final model matrix $\mathbf{X}$, where $\mathbf{X} = \begin{pmatrix}\mathbf{X}_1 \\ \mathbf{X}_2\end{pmatrix}$.

To find $|\mathbf{X}'\mathbf{X}|$, first note that

$$\begin{aligned}\mathbf{X}'\mathbf{X} &= \begin{pmatrix}\mathbf{X}_1\\ \mathbf{X}_2\end{pmatrix}' \begin{pmatrix}\mathbf{X}_1\\ \mathbf{X}_2\end{pmatrix}\\ &= \begin{pmatrix}\mathbf{X}_1'\mathbf{X}_2'\end{pmatrix} \begin{pmatrix}\mathbf{X}_1\\ \mathbf{X}_2\end{pmatrix}\\ &= \mathbf{X}_1'\mathbf{X}_1 + \mathbf{X}_2'\mathbf{X}_2. \end{aligned} \tag{3}$$

The Coordinate-Exchange Algorithm can be used to construct the appropriate $\mathbf{X}_2$ matrix to maximize $|\mathbf{X}_1'\mathbf{X}_1 + \mathbf{X}_2'\mathbf{X}_2|$ and create an augmented *D*-optimal design. Other algorithms and strategies for *D*-optimal augmentation can be found in Atkinson et al. (2007).

Follow-up runs to traditional designs can also be added with Bayesian techniques. Meyer et al. (1996) augmented designs with a Bayesian model-discrimination criterion to resolve ambiguities between many plausible models in the presence of observed data. Jones and Dumouchel (1996), in a discussion of Meyer et al.'s method, suggested an *F*-criterion based on Fisher's information matrix. Neff (1996) and Ruggoo and Vandebroek (2004) proposed a two-stage, sequential Bayesian *D*–*D* optimal method based on the Bayesian *D*-optimality criterion in Dumouchel and Jones. In the two-stage Bayesian *D*–*D* optimal method, a first stage design is constructing to support an assumed model with primary and potential terms. After the first stage, data are analyzed via Box and Meyer (1993)'s model-discrimination method of calculating posterior probabilities of possible models. A second stage design is then added to maximize a weighted *D*-optimality criterion to support and discriminate the many competing models.

In the next section, we extend the aforementioned work and develop the methodology to add runs to SSDs. It is important to mention several unique aspects to augmenting SSDs. First, we are typically not interested in adding interactions or quadratic effects to the assumed main-effect model; with the limited number of runs, detecting the active main effects is the top priority. Second, the large number of factors and small number of runs in SSDs means many models explain the data well. As such, it is difficult to pick which model or models to build upon in the follow-up runs. Therefore, instead of adding runs based on a model-discrimination criterion like in Ruggoo and Vandebroek (2004), we add runs based on a categorization of factors. A model-dependent augmentation strategy is computationally expensive. For example, it took 7 h to search for all 6 factor models in a 124 factor, 24 run design (Edwards and Mee, 2011). Calculating larger models with a model-discrimination criterion would be impractical. Categorizing factors into groups is more efficient. Further, categorization makes the augmentation method adaptable because it is not tied to a specific analysis method. The experimenter can analyze the initial data with several methods to search for active factors.

## 3. Augmenting supersaturated designs with Bayesian *D*-optimality

Suppose an experimenter ran an SSD($n_1$, $k$) and can afford to add $n_2$ more runs. Our objective is to create the best possible augmented design, SSD($n_1 + n_2$, $k$), given the information from the initial $n_1$ runs. To do this, we adopt the linear model assumptions used to create Bayesian *D*-optimal SSDs and adapt them to add $n_2$ runs to the design matrix. Let $\mathbf{X}_1$ be the original main-effect model matrix with response vector $\mathbf{y}_1$. Assume the prior distribution of $\boldsymbol{\beta}$ is $\boldsymbol{\beta}|\sigma^2 \sim N(\boldsymbol{\beta}_0, \sigma^2\mathbf{R}^{-1})$ for a prior covariance matrix, $\mathbf{R}$. Let the $n_2 \times 1$ vector of new observations, $\mathbf{y}_2$, have the conditional distribution $\mathbf{y}_2|\boldsymbol{\beta}, \sigma^2 \sim N(\mathbf{X}_2\boldsymbol{\beta}, \sigma^2\mathbf{I}_{n_2\times n_2})$, where $\mathbf{X}_2$ is the additional run matrix in model form. Then, as shown in Ruggoo and Vandebroek (2004), the posterior distribution for $\boldsymbol{\beta}$ given $\mathbf{y} = \begin{pmatrix}\mathbf{y}_1\\ \mathbf{y}_2\end{pmatrix}$ is

$$\boldsymbol{\beta}|\mathbf{y} \sim N\left[\mathbf{b}, \sigma^2\left(\mathbf{X}_1'\mathbf{X}_1 + \mathbf{X}_2'\mathbf{X}_2 + \mathbf{R}\right)^{-1}\right]; \tag{4}$$

where $\mathbf{b} = \left(\mathbf{X}_1'\mathbf{X}_1 + \mathbf{X}_2'\mathbf{X}_2 + \mathbf{R}\right)^{-1}\left(\mathbf{X}_1'\mathbf{y}_1 + \mathbf{X}_2'\mathbf{y}_2 + \mathbf{R}\boldsymbol{\beta}_0\right)$. To create a Bayesian *D*-optimal augmented SSD, $\mathbf{X}_2$ is chosen to maximize $|\mathbf{X}_1'\mathbf{X}_1 + \mathbf{X}_2'\mathbf{X}_2 + \mathbf{R}|$. Because runs are added to an existing design, the prior information for the $n_2$ follow-up runs comes from the analysis of the original SSD($n_1$, $k$) with response vector $\mathbf{y}_1$. Like DuMouchel and Jones (1994), prior information is incorporated into the design process through the choice in $\mathbf{R}$ by classifying factors as primary or potential terms. We also introduce a category of *secondary* terms.

After the first $n_1$ runs, the experimenter can likely identify factors that appear to be the most active. For instance, some factor or factor set may be detected in many different analysis methods. If evidence suggests the factor is in the true model, the experimenter can classify it as a primary term. If there is an indication the factor may be active, but it is not a predominant as the primary terms, the factor can be classified as a secondary term. Any factor that does not appear active can be classified as a potential term (Section 3.1 expounds on classifying factors). Using this classification, the augmented design SSD($n_1+n_2$, $k$) is constructed to reduce the error variances of the parameter estimates under the Bayesian paradigm.

Let $p_1$ denote the number of primary terms, $p_2$ denote the number of secondary terms, and $p_3$ be the number of potential terms, where $p_1 + p_2 + p_3 = k + 1 = p$. The $p_1$ primary terms are the most likely to be active, so their effects, denoted $\boldsymbol{\beta}_{\text{pri}}$, are given a diffuse prior. The $p_2$ secondary terms with effects $\boldsymbol{\beta}_{\text{sec}}$ are given a prior mean of zero and a finite variance $\sigma^2\gamma^2$, while the $p_3$ potential terms with effects $\boldsymbol{\beta}_{\text{pot}}$ are assigned a prior mean of zero and a finite variance $\sigma^2\tau^2$, where $\tau < \gamma$.

Larger scaling factors for $\sigma^2$ represent stronger beliefs that certain factors are active (Ruggoo and Vandebroek, 2004). Using this information, $\mathbf{R} = \mathbf{J}/\gamma^2 + \mathbf{K}/\tau^2$, where

$$\mathbf{J} = \begin{pmatrix} 0 & & & \\ & j_{1,1} & & \mathbf{0} \\ & & j_{2,2} & \\ & \mathbf{0} & & \ddots \\ & & & j_{k,k} \end{pmatrix} \quad \text{and} \quad \mathbf{K} = \begin{pmatrix} 0 & & & \\ & k_{1,1} & & \mathbf{0} \\ & & k_{2,2} & \\ & \mathbf{0} & & \ddots \\ & & & k_{k,k} \end{pmatrix}. \tag{5}$$

For each $i = 1, 2, \ldots, k$, we set $j_{i,i} = 1$ if $\mathbf{x}_i$ is a secondary term, 0 otherwise, and $\sum_{i=1}^{k} j_{i,i} = p_2$. Similarly, $k_{i,i} = 1$ if $\mathbf{x}_i$ is a potential term, 0 otherwise, and $\sum_{i=1}^{k} k_{i,i} = p_3$.

The posterior distribution for $\boldsymbol{\beta}$ in (4) can be rewritten as

$$\boldsymbol{\beta}|\mathbf{y} \sim N\left[\mathbf{b}, \sigma^2\left(\mathbf{X}_1'\mathbf{X}_1 + \mathbf{X}_2'\mathbf{X}_2 + \frac{\mathbf{J}}{\gamma^2} + \frac{\mathbf{K}}{\tau^2}\right)^{-1}\right]; \tag{6}$$

where $\mathbf{b} = \left(\mathbf{X}_1'\mathbf{X}_1 + \mathbf{X}_2'\mathbf{X}_2 + \mathbf{J}/\gamma^2 + \mathbf{K}/\tau^2\right)^{-1}\left(\mathbf{X}_1'\mathbf{y}_1 + \mathbf{X}_2'\mathbf{y}_2 + (\mathbf{J}/\gamma^2 + \mathbf{K}/\tau^2)\boldsymbol{\beta}_0\right)$. Therefore, a Bayesian $D$-optimal augmented SSD$(n_1 + n_2, k)$ with model matrix $\mathbf{X} = \begin{pmatrix}\mathbf{X}_1 \\ \mathbf{X}_2\end{pmatrix}$ is constructed by choosing $\mathbf{X}_2$ to maximize

$$\left|\mathbf{X}_1'\mathbf{X}_1 + \mathbf{X}_2'\mathbf{X}_2 + \frac{\mathbf{J}}{\gamma^2} + \frac{\mathbf{K}}{\tau^2}\right|. \tag{7}$$

Note that $p_1 < n_1 + n_2$ is a necessary condition to make the determinant calculation in (7) nonzero. The Coordinate Exchange Algorithm is used to construct $\mathbf{X}_2$ to optimize the objective function in (7).

### 3.1. Classifying factors

Getting information from the original SSD$(n_1, k)$ is not trivial, hence the motivation for additional runs. However, the objective function in (7) is dependent on the experimenter using *some* information from the initial runs in order to classify the $k$ factors into groups. Analysis methods for SSDs range from basic regression techniques (e.g. stepwise and all-subsets regression, as in Abraham et al. (1999)) to more sophisticated methods, like a cluster analysis strategy (Li et al., 2010) and a combination of singular value decomposition (SVD), principle components analysis (PCA), and regression (Georgiou, 2008). Different analysis techniques may identify different sets of active factors, so it is useful to consider the results of several analysis methods (Lin, 1995). Regardless of which techniques are implemented, we suggest the following guidelines when assigning the $k$ factors in the primary, secondary, or potential groups.

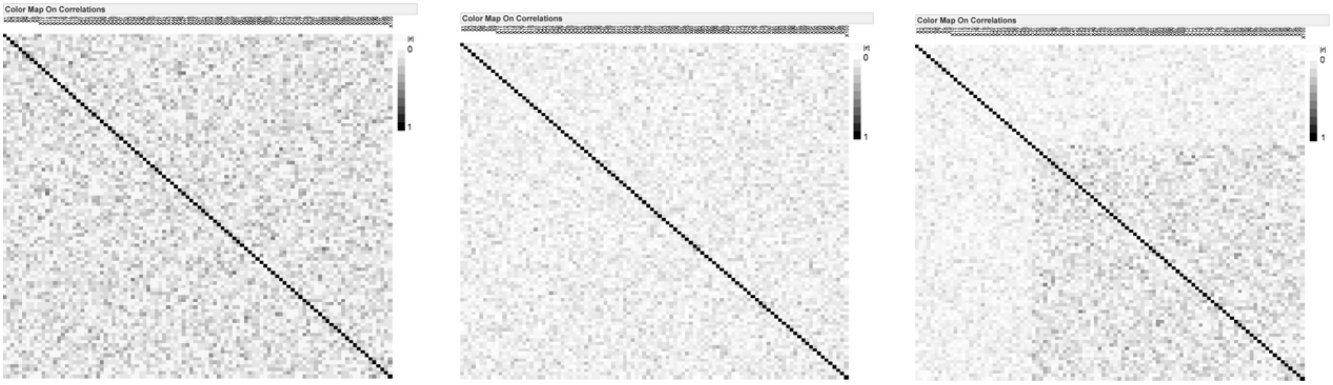
1. The intercept is always a primary term.
2. If an experimenter must add runs but is not comfortable classifying the factors, we suggest specifying all factors as potential terms to mimic the construction of Bayesian $D$-optimal SSDs.
3. If an analysis method (or many methods) highlight a group of less than $n_1 + n_2$ key factors, specify the terms as primary.
4. If the number of factors of interest is larger than $n_1 + n_2$ runs, specify the terms as secondary.
5. Terms with little evidence to suggest they are active should be classified as potential.

Secondary terms let the experimenter differentiate between terms when more than $n_1 + n_2$ factors are of interest. After running an SSD$(n_1, k)$, an experimenter may identify a group of $s$ key factors, where $s > n_1 + n_2$. Therefore, not all $s$ factors can be classified as the $p_1$ primary terms, as $p_1 < n_1 + n_2$ is required. To differentiate between the $s$ key factors and the remaining $k - s$, the experimenter can classify all $s$ factors as the $p_2$ secondary terms. Secondary terms are given a larger prior variance to suggest they are likely more active than the $k - p_2$ potential terms. The augmentation criterion then selects runs to discriminate between the two groups. An example is given in Section 4.2.

### 3.2. Example augmentation

To visually compare how prior information influences the final SSD matrix, we created a Bayesian $D$-optimal SSD$(25, 100)$ with the JMP statistical software and added 25 runs to the original design. Using the Bayesian $D$-optimal augmentation strategy, we created two augmented designs. For the first design, SSD$(50, 100)_1$, every factor was classified as a potential term prior to adding the 25 runs. For the second design, SSD$(50, 100)_2$, factors $\mathbf{x}_1 - \mathbf{x}_{30}$ were listed as primary and all others potential. Fig. 1 shows the grayscale maps of the correlations between the factors. All examples in this paper use $\gamma^2 = 100$ and $\tau^2 = 5$; see Jones et al. (2008).

In the grayscale correlation maps, white represents a small correlation between factors (in absolute value), while black represents a perfect correlation. Maximizing the criterion in (7) has the byproduct of de-aliasing factors by reducing the




(a) SSD(25, 100). (b) SSD(50, 100)$_1$. (c) SSD(50, 100)$_2$.

**Fig. 1.** Correlation grayscale maps of supersaturated designs: SSD(25, 100) ($L$), SSD(50, 100)$_1$ with all potential terms ($M$), and SSD(50, 100)$_2$ with 30 primary terms ($R$).

**Table 1**
Average correlations of factors in augmented SSD(50, 100).

| Correlations | $\overline{\lvert r_{\text{pri}\times\text{pri}}\rvert}$ | $\overline{\lvert r_{\text{pri}\times\text{pot}}\rvert}$ | $\overline{\lvert r_{\text{pot}\times\text{pot}}\rvert}$ | $\overline{\lvert r\rvert}$ |
|---|---|---|---|---|
| SSD(25, 100) | 0.150 | 0.143 | 0.145 | 0.145 |
| SSD(50, 100)$_1$ | 0.078 | 0.083 | 0.089 | 0.086 |
| SSD(50, 100)$_2$ | 0.064 | 0.068 | 0.128 | 0.097 |

correlations between factors. Comparing SSD(25, 100) to SSD(50, 100)$_1$, it is not surprising the color has lightened; the additional runs reduced the correlations between the 100 factors in the model, thereby increasing the likelihood an active factor will be identified. The difference between SSD(50, 100)$_1$ (Fig. 1(b)) and SSD(50, 100)$_2$ (Fig. 1(c)) shows how classifying factors in the primary group reduces the pairwise correlations between those factors. Analyzing the correlation values makes this relationship clearer.

The average absolution correlation between a group of factors is defined as

$$\overline{|r|} = \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} |r_{i,j}|/(k(k-1)/2);$$

where $r_{i,j}$ is the correlation between factors $\mathbf{x}_i$ and $\mathbf{x}_j$. Smaller values $\overline{|r|}$ are preferred. Table 1 compares the designs' absolute average correlations between primary terms, primary terms and potential terms, and potential terms, denoted by $\overline{|r_{\text{pri}\times\text{pri}}|}$, $\overline{|r_{\text{pri}\times\text{pot}}|}$, and $\overline{|r_{\text{pot}\times\text{pot}}|}$, respectively. First, note that only SSD(50, 100)$_2$ differentiates between primary and potential terms, but Table 1 contains values for each group vs. group calculation to highlight how prior information reduces correlations between factors of interest.

SSD(25, 100) has the highest correlation in all groups because it has the least number of runs. Comparing $\overline{|r_{\text{pri}\times\text{pri}}|}$ and $\overline{|r_{\text{pri}\times\text{pot}}|}$ for SSD(50, 100)$_1$ and SSD(50, 100)$_2$ reveals that identifying factors as primary terms reduces the correlation between those factors. The average absolute correlations between factors $\mathbf{x}_1, \ldots, \mathbf{x}_{30}$ are lower in SSD(50, 100)$_2$ (0.064) than in SSD(50, 100)$_1$ (0.078) because we specified the terms *a priori* as primary factors of interest and the design criterion in (7) forces the additional runs to reduce the correlations between those factors. Note, however, that the reduced correlations of $\overline{|r_{\text{pri}\times\text{pri}}|}$ and $\overline{|r_{\text{pri}\times\text{pot}}|}$ for SSD(50, 100)$_2$ were offset by a higher $\overline{|r_{\text{pot}\times\text{pot}}|}$.

To compare the designs further, define the maximum absolute correlation of factors in a group

$$|r|^{\max} = \max_{i\neq j} |r_{i,j}|.$$

Smaller values are also preferred here. Let $|r_{\text{pri}\times\text{pri}}|^{\max}$, $|r_{\text{pri}\times\text{pot}}|^{\max}$, and $|r_{\text{pot}\times\text{pot}}|^{\max}$ denote the maximum absolute correlations of factors in the primary, primary and potential, and potential groups, respectively. Table 2 shows the augmented designs have smaller values than the original SSD(25, 100), as expected. Further, classifying factors as primary reduces the maximum absolute correlation between those factors in SSD(50, 100)$_2$ compared to SSD(50, 100)$_1$.

## 4. Comparisons

In this section, we compare the performance of Bayesian $D$-optimal SSDs to extended $E(s^2)$-optimal designs. Gupta et al. (2010) added runs to two $E(s^2)$-optimal designs, SSD(8, 13) and SSD(7, 15). For SSD(8, 13), Gupta et al. listed the best $n_2 = 1, 2, 3$, and 4 run(s) to add to the original design to minimize $E(s^2)$. For SSD(7, 15), they listed the best $n_2 = 3$

**Table 2**
Maximum correlations of factors in augmented SSD(50, 100).

| Correlations | $\lvert r_{\text{pri}\times\text{pri}}\rvert^{\max}$ | $\lvert r_{\text{pri}\times\text{pot}}\rvert^{\max}$ | $\lvert r_{\text{pot}\times\text{pot}}\rvert^{\max}$ | $\lvert r\rvert^{\max}$ |
|---|---|---|---|---|
| SSD(25, 100) | 0.603 | 0.603 | 0.603 | 0.603 |
| $\text{SSD}(50, 100)_1$ | 0.281 | 0.414 | 0.361 | 0.414 |
| $\text{SSD}(50, 100)_2$ | 0.250 | 0.327 | 0.560 | 0.560 |

**Table 3**
$E(s^2)$-optimal SSD(8, 13) and additional 1, 2, 3, & 4 runs to create extended $E(s^2)$-optimal designs, as presented in Gupta et al. (2010).

| Run | $\mathbf{x}_1$ | $\mathbf{x}_2$ | $\mathbf{x}_3$ | $\mathbf{x}_4$ | $\mathbf{x}_5$ | $\mathbf{x}_6$ | $\mathbf{x}_7$ | $\mathbf{x}_8$ | $\mathbf{x}_9$ | $\mathbf{x}_{10}$ | $\mathbf{x}_{11}$ | $\mathbf{x}_{12}$ | $\mathbf{x}_{13}$ | $\mathbf{y}_1$ | $\mathbf{y}_2$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 15.320 | −6.433 |
| 2 | 1 | 1 | 1 | −1 | −1 | 1 | −1 | −1 | −1 | 1 | −1 | −1 | 1 | 3.588 | −11.122 |
| 3 | 1 | −1 | −1 | −1 | 1 | −1 | 1 | −1 | 1 | −1 | −1 | 1 | 1 | −3.159 | 19.684 |
| 4 | 1 | −1 | 1 | 1 | 1 | −1 | −1 | −1 | −1 | −1 | 1 | −1 | −1 | 14.380 | 12.237 |
| 5 | −1 | 1 | −1 | 1 | −1 | −1 | −1 | 1 | 1 | −1 | −1 | −1 | 1 | 1.696 | −22.798 |
| 6 | −1 | 1 | −1 | −1 | 1 | −1 | −1 | 1 | −1 | 1 | 1 | 1 | −1 | −20.391 | 8.646 |
| 7 | −1 | −1 | 1 | −1 | −1 | 1 | 1 | 1 | 1 | −1 | 1 | −1 | −1 | −12.956 | 21.218 |
| 8 | −1 | −1 | −1 | 1 | −1 | 1 | 1 | −1 | −1 | 1 | −1 | 1 | −1 | 0.306 | −20.313 |
| 9 | 1 | 1 | 1 | 1 | −1 | −1 | 1 | 1 | −1 | −1 | −1 | 1 | −1 | 20.707 | −12.700 |
| 9 | 1 | 1 | 1 | 1 | −1 | −1 | 1 | 1 | −1 | −1 | −1 | 1 | −1 | 18.236 | −11.398 |
| 10 | −1 | −1 | −1 | −1 | 1 | 1 | −1 | −1 | 1 | 1 | 1 | −1 | 1 | −19.953 | 12.007 |
| 9 | −1 | −1 | −1 | 1 | 1 | 1 | −1 | −1 | 1 | 1 | 1 | −1 | 1 | −4.712 | −9.609 |
| 10 | 1 | 1 | −1 | −1 | 1 | 1 | 1 | 1 | −1 | −1 | −1 | −1 | −1 | −3.304 | 47.024 |
| 11 | 1 | −1 | 1 | −1 | −1 | −1 | −1 | 1 | 1 | 1 | −1 | 1 | −1 | 6.918 | −13.521 |
| 9 | 1 | 1 | 1 | 1 | −1 | −1 | 1 | 1 | −1 | −1 | −1 | 1 | −1 | 21.600 | −11.596 |
| 10 | 1 | −1 | −1 | 1 | 1 | 1 | −1 | 1 | 1 | 1 | −1 | −1 | −1 | 14.120 | 4.539 |
| 11 | −1 | 1 | −1 | −1 | 1 | 1 | 1 | −1 | −1 | −1 | 1 | −1 | 1 | −20.515 | 33.206 |
| 12 | −1 | −1 | 1 | −1 | −1 | −1 | −1 | −1 | 1 | 1 | 1 | 1 | 1 | −13.339 | −25.110 |

additional runs. We highlight these examples because, to date, they are the only two-level augmented SSDs in the literature. The additional runs suggested in Gupta et al. are optimal with respect to $E(s^2)$, but the runs are independent of the initial data. Hence, for a given SSD($n_1$, $k$) and number of new runs, $n_2$, the same additional runs are suggested. In contrast, the Bayesian $D$-optimal augmentation method uses information from the first $n_1$ runs to improve the selection of the additional $n_2$ runs.

We perform a side-by-side comparison of the proposed methods with the following methodology: First, we randomly created two main-effect models to study for both SSD(8, 13) and SSD(7, 15). Each model was randomly chosen to have 3–5 active factors with effect sizes drawn uniformly between −15 and 15. The location of the active factors was also random. All responses were generated from the models with random noise, $\epsilon \sim N(0, 1)$. Next, we added the extended $E(s^2)$-optimal runs prescribed in Gupta et al. and recorded the new response(s). For the Bayesian $D$-optimal approach, the initial design and response variables were analyzed. Then, we classified factors into their appropriate groups, added the required number of runs by maximizing the objective function in (7), and recorded the new responses. Finally, we analyzed the screening results of the final full Bayesian $D$-optimal augmented SSDs and Gupta et al.'s final extended $E(s^2)$-optimal SSDs to see which strategy provides a better recovery of the underlying model.

The SSDs in this section are analyzed with basic regression methods and screening techniques: forward and all-subsets regression (for up to 5 factors) and Half Normal plots, which visually identify factors whose effects seem larger than random noise (Daniel, 1959). All analysis results were calculated using the JMP software, though similar analyses can be made in any statistical software package. For forward regression, terms were added based on a $p$-value to enter of 0.05. The combined results of forward regression, all-subsets regression, and Half Normal plots will guide the classification of each factor into either the primary, secondary, or potential group. While traditional regression methods do not always work well when used for the analysis of SSDs (Edwards and Mee, 2011), the supposition is that if augmentation works well for the traditional methods, it will work well for more sophisticated techniques.

### 4.1. Adding runs to an $E(s^2)$-optimal SSD(8, 13)

Consider the $E(s^2)$-optimal SSD(8, 13) in Table 3 (Runs 1–8) with responses generated from the equations

1. $\mathbf{y}_1 = 10\mathbf{x}_3 + 8\mathbf{x}_4 + 6\mathbf{x}_5 - 9\mathbf{x}_{11} + \boldsymbol{\epsilon}$, $\boldsymbol{\epsilon} \sim N(\mathbf{0}, \mathbf{I}_8)$; and
2. $\mathbf{y}_2 = -10\mathbf{x}_4 + 12\mathbf{x}_5 + 7\mathbf{x}_6 - 11\mathbf{x}_{10} - 6\mathbf{x}_{13} + \boldsymbol{\epsilon}$, $\boldsymbol{\epsilon} \sim N(\mathbf{0}, \mathbf{I}_8)$.

**Table 4**
Analysis of initial SSD(8, 13) data and classification of factors. Active factors are identified with a •.

| Analysis | Results | $\mathbf{x}_1$ | $\mathbf{x}_2$ | $\mathbf{x}_3$ | $\mathbf{x}_4$ | $\mathbf{x}_5$ | $\mathbf{x}_6$ | $\mathbf{x}_7$ | $\mathbf{x}_8$ | $\mathbf{x}_9$ | $\mathbf{x}_{10}$ | $\mathbf{x}_{11}$ | $\mathbf{x}_{12}$ | $\mathbf{x}_{13}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Model 1 | Half Normal | | | | | | | | | | | | | |
| | Forward | • | | | • | • | | | | | | • | | |
| | All subsets | • | | • | • | • | | | | | | | | |
| | Classification | $\beta_{pri}$ | $\beta_{pot}$ | $\beta_{pri}$ | $\beta_{pri}$ | $\beta_{pri}$ | $\beta_{pot}$ | $\beta_{pot}$ | $\beta_{pot}$ | $\beta_{pot}$ | $\beta_{pot}$ | $\beta_{pri}$ | $\beta_{pot}$ | $\beta_{pot}$ |
| Model 2 | Half Normal | | | | | | | | | | | | | |
| | Forward | | • | | • | • | | | | | • | • | | |
| | All subsets | | | | • | • | • | | | | • | | | • |
| | Classification | $\beta_{pot}$ | $\beta_{pri}$ | $\beta_{pot}$ | $\beta_{pri}$ | $\beta_{pri}$ | $\beta_{pri}$ | $\beta_{pot}$ | $\beta_{pot}$ | $\beta_{pot}$ | $\beta_{pri}$ | $\beta_{pri}$ | $\beta_{pot}$ | $\beta_{pri}$ |

**Table 5**
Additional 1, 2, 3, & 4 Bayesian *D*-optimal runs for SSD(8, 13). Runs $9_i^*$–$(9+j)_i^*$ are Bayesian *D*-optimal for responses $\mathbf{y}_i$.

| | Run | $\mathbf{x}_1$ | $\mathbf{x}_2$ | $\mathbf{x}_3$ | $\mathbf{x}_4$ | $\mathbf{x}_5$ | $\mathbf{x}_6$ | $\mathbf{x}_7$ | $\mathbf{x}_8$ | $\mathbf{x}_9$ | $\mathbf{x}_{10}$ | $\mathbf{x}_{11}$ | $\mathbf{x}_{12}$ | $\mathbf{x}_{13}$ | $\mathbf{y}_1$ | $\mathbf{y}_2$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 Run | $9_1{}^*$ | −1 | 1 | 1 | 1 | 1 | 1 | 1 | −1 | −1 | −1 | −1 | −1 | 1 | 32.764 | |
| | $9_2{}^*$ | 1 | 1 | 1 | 1 | 1 | 1 | −1 | −1 | 1 | −1 | −1 | −1 | −1 | | 25.358 |
| 2 Runs | $9_1{}^*$ | 1 | −1 | −1 | 1 | −1 | −1 | 1 | 1 | −1 | 1 | 1 | −1 | 1 | −17.549 | |
| | $10_1{}^*$ | −1 | −1 | 1 | 1 | 1 | −1 | 1 | 1 | −1 | 1 | −1 | −1 | 1 | 34.161 | |
| | $9_2{}^*$ | 1 | 1 | −1 | −1 | −1 | −1 | 1 | −1 | −1 | −1 | 1 | 1 | 1 | | −5.498 |
| | $10_2{}^*$ | 1 | 1 | −1 | −1 | 1 | 1 | 1 | −1 | −1 | −1 | −1 | 1 | −1 | | 46.855 |
| 3 Runs | $9_1{}^*$ | −1 | −1 | 1 | 1 | 1 | 1 | −1 | 1 | −1 | −1 | −1 | 1 | 1 | 30.908 | |
| | $10_1{}^*$ | −1 | −1 | −1 | −1 | 1 | 1 | −1 | −1 | 1 | 1 | 1 | −1 | 1 | −20.592 | |
| | $11_1{}^*$ | 1 | −1 | −1 | 1 | −1 | 1 | −1 | 1 | −1 | −1 | 1 | 1 | 1 | −17.837 | |
| | $9_2{}^*$ | 1 | 1 | 1 | −1 | 1 | −1 | 1 | 1 | 1 | 1 | −1 | −1 | −1 | | 11.525 |
| | $10_2{}^*$ | 1 | −1 | 1 | −1 | −1 | −1 | 1 | 1 | 1 | 1 | 1 | −1 | 1 | | −23.607 |
| | $11_2{}^*$ | −1 | −1 | 1 | 1 | 1 | 1 | −1 | 1 | −1 | 1 | −1 | −1 | 1 | | −7.140 |
| 4 Runs | $9_1{}^*$ | −1 | −1 | 1 | −1 | −1 | −1 | −1 | −1 | 1 | 1 | 1 | 1 | 1 | −13.432 | |
| | $10_1{}^*$ | −1 | 1 | −1 | 1 | 1 | 1 | 1 | −1 | −1 | −1 | 1 | −1 | 1 | −6.887 | |
| | $11_1{}^*$ | 1 | −1 | −1 | −1 | −1 | 1 | −1 | 1 | −1 | −1 | 1 | 1 | −1 | −34.060 | |
| | $12_1{}^*$ | −1 | −1 | 1 | −1 | 1 | 1 | −1 | 1 | −1 | −1 | −1 | 1 | 1 | 16.459 | |
| | $9_2{}^*$ | 1 | 1 | 1 | −1 | −1 | −1 | 1 | 1 | 1 | 1 | −1 | 1 | −1 | | −14.887 |
| | $10_2{}^*$ | −1 | 1 | 1 | −1 | 1 | 1 | 1 | −1 | −1 | −1 | −1 | −1 | −1 | | 45.149 |
| | $11_2{}^*$ | −1 | −1 | 1 | −1 | 1 | −1 | 1 | 1 | −1 | 1 | −1 | −1 | 1 | | 1.230 |
| | $12_2{}^*$ | −1 | 1 | 1 | −1 | −1 | −1 | 1 | −1 | −1 | −1 | 1 | 1 | 1 | | −3.211 |

Table 3 also contains the $n_2 = 1, 2, 3$, and 4 runs to add suggested by Gupta et al. to create SSD$(8+n_2, 13)$ $E(s^2)$-optimal designs along with the appropriate responses. Again, we emphasize that extended $E(s^2)$-optimality recommends the same runs for each model, whereas the runs added via the Bayesian *D*-optimal approach will be different for each model.

Using Half Normal Plots, forward regression, and all-subsets regression, we analyzed the response variables from SSD(8, 13) and classified factors as primary, secondary, or potential. Table 4 summarizes the initial analysis results. For example, the Half Normal Plot failed to indicate any factor as significantly greater than experimental noise for either model. However, forward regression on $\mathbf{y}_1$ selected factors $\mathbf{x}_4$, $\mathbf{x}_1$, $\mathbf{x}_5$, $\mathbf{x}_{11}$ as the top four "active" factors. Further analysis on the first 8 runs with all-subsets regression indicated factors $\mathbf{x}_1$, $\mathbf{x}_3$, $\mathbf{x}_4$, and $\mathbf{x}_5$ are of particular interest, as the top models contain only those four factors. Coupled with the results from forward regression, five factors are likely to be active: $\mathbf{x}_1$, $\mathbf{x}_3$, $\mathbf{x}_4$, $\mathbf{x}_5$, and $\mathbf{x}_{11}$. If the analysis stopped here, all true active factors would be identified – $\mathbf{x}_3$, $\mathbf{x}_4$, $\mathbf{x}_5$, and $\mathbf{x}_{11}$ – but a false effect would remain, $\mathbf{x}_1$. Augmenting the design with additional runs may help resolve this issue. Based on the initial results, these five factors of interest were classified as primary terms, as indicated by $\boldsymbol{\beta}_{pri}$ in Table 4. All other terms were classified as potential because there was no indication any other factor was likely active.

A similar approach was carried out to analyze $\mathbf{y}_2$. Forward regression identified $\mathbf{x}_2$, $\mathbf{x}_4$, $\mathbf{x}_5$, $\mathbf{x}_{10}$, and $\mathbf{x}_{11}$ as potentially active, whereas the best five-term model selected with all-subsets regression contained $\mathbf{x}_4$, $\mathbf{x}_5$, $\mathbf{x}_6$, $\mathbf{x}_{10}$, and $\mathbf{x}_{13}$. The union of terms were placed in the primary group; all others were classified as potential. Next, runs were added to SSD(8, 13) to get more information out of the respective models. The suggested $n_2 = 1, 2, 3$, or 4 Bayesian *D*-optimal runs to add for each model are listed in Table 5.

Table 6 compares the final analysis results of $\mathbf{y}_1$ on SSD(9, 13), SSD(10, 13), SSD(11, 13), and SSD(12, 13). The true underlying model contained the active factors $\mathbf{x}_3$, $\mathbf{x}_4$, $\mathbf{x}_5$, and $\mathbf{x}_{11}$. These factors, and only these factors, were identified by at least one analysis method in each of the Bayesian *D*-optimal designs. In all extended $E(s^2)$-optimal designs, $\mathbf{x}_1$ was incorrectly selected as an active factor, a Type I error. Moreover, all three analysis methods correctly identified all active factors for the 11-run and 12-run Bayesian *D*-optimal designs. The results suggest using information from the initial design can improve the selection of additional runs and ultimately improve screening results. This example also highlights that having a false effect, $\mathbf{x}_1$, labeled as a primary factor after the first 8 runs is helpful because the new runs will test to see if it is

**Table 6**
Final analysis of $\mathbf{y}_1$ on SSD($8 + n_2$, 13): comparing extended $E(s^2)$-optimal SSDs and augmented Bayesian $D$-optimal SSDs. Active factors are identified with a •.

| Factors | | $\mathbf{x}_1$ | $\mathbf{x}_2$ | $\mathbf{x}_3$ | $\mathbf{x}_4$ | $\mathbf{x}_5$ | $\mathbf{x}_6$ | $\mathbf{x}_7$ | $\mathbf{x}_8$ | $\mathbf{x}_9$ | $\mathbf{x}_{10}$ | $\mathbf{x}_{11}$ | $\mathbf{x}_{12}$ | $\mathbf{x}_{13}$ | Correct? |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | True model | | | • | • | • | | | | | | • | | | |
| 9 Run $E(s^2)$ | Half Normal | • | | | • | • | | | | | | • | | | |
| | Forward | • | | | • | • | | | • | | | • | | | |
| | All subsets | • | | • | • | • | | | | | | | | | |
| 9 Run Bayes $D$ | Half Normal | | | | | | | | | | | | | | |
| | Forward | | | • | • | • | | | • | | | • | | | |
| | All subsets | | | • | • | • | | | | | | • | | | • |
| 10 Run $E(s^2)$ | Half Normal | • | | • | • | | | | | | | | | | |
| | Forward | • | | • | • | • | | | | | | | | • | |
| | All subsets | • | | • | • | • | | | | | | | | | |
| 10 Run Bayes $D$ | Half Normal | | | • | • | • | | | • | | | • | | | |
| | Forward | | | • | • | • | | | • | | | • | | | |
| | All subsets | | | • | • | • | | | | | | • | | | • |
| 11 Run $E(s^2)$ | Half Normal | • | | • | • | • | | | | | | | | | |
| | Forward | • | | | • | • | | | | | | • | | | |
| | All subsets | • | | • | • | • | | | | | | | | | |
| 11 Run Bayes $D$ | Half Normal | | | • | • | • | | | | | | • | | | • |
| | Forward | | | • | • | • | | | | | | • | | | • |
| | All subsets | | | • | • | • | | | | | | • | | | • |
| 12 Run $E(s^2)$ | Half Normal | • | • | | • | • | | | | | | • | | | |
| | Forward | • | | | • | • | | | • | | | • | | | |
| | All subsets | • | | | • | • | | | | | | • | | | |
| 12 Run Bayes $D$ | Half Normal | | | • | • | • | | | | | | • | | | • |
| | Forward | | | • | • | • | | | | | | • | | | • |
| | All subsets | | | • | • | • | | | | | | • | | | • |

truly active. Table 7 compares the final analysis results of the data generated from the second model. Analysis of $\mathbf{y}_2$ is more consistent between the $E(s^2)$ and Bayesian $D$-optimal SSDs than for $\mathbf{y}_1$, but note for the 9 and 10-run designs, the Bayesian design performed better with respect to forward regression.

### 4.2. Adding runs to an $E(s^2)$-optimal SSD(7, 15)

Consider the $E(s^2)$-optimal SSD(7, 15) in Table 8 (Runs 1–7) with responses generated from the equations

1. $\mathbf{y}_1 = -8\mathbf{x}_5 - 3\mathbf{x}_{10} + 11\mathbf{x}_{14} + \boldsymbol{\epsilon}, \boldsymbol{\epsilon} \sim N(\mathbf{0}, \mathbf{I}_7)$.
2. $\mathbf{y}_2 = -10\mathbf{x}_2 + 6\mathbf{x}_4 + 3\mathbf{x}_7 + 11\mathbf{x}_9 + 5\mathbf{x}_{13} + \boldsymbol{\epsilon}, \boldsymbol{\epsilon} \sim N(\mathbf{0}, \mathbf{I}_7)$.

In this example, we can afford to add three more runs to the design. Table 8 contains the three runs suggested by Gupta et al. (Runs 8–10), as well as the three runs created with the Bayesian $D$-optimal method. Note again that the new runs under the Bayesian approach are different for each model. The runs were added based on the classification presented in Table 9.

An initial analysis of $\mathbf{y}_1$ on SSD(7, 15) correctly identified the true active factors. To confirm the results, $\mathbf{x}_5$, $\mathbf{x}_{10}$, and $\mathbf{x}_{14}$ were placed in the primary group while all others were classified as potential terms. For $\mathbf{y}_2$, the analysis of SSD(7, 15) was more challenging. A Half Normal Plot did not indicate any factors were substantially larger than experimental noise. Forward regression, on the other hand, selected $\mathbf{x}_1$, $\mathbf{x}_9$, $\mathbf{x}_5$, $\mathbf{x}_{10}$, $\mathbf{x}_4$ as the five most important factors. All-subsets regression presented conflicting results because the best five-factor model only contained one factor in the best four-factor model. Factors $\mathbf{x}_2$, $\mathbf{x}_3$, $\mathbf{x}_4$, $\mathbf{x}_7$, $\mathbf{x}_8$, $\mathbf{x}_{10}$, $\mathbf{x}_{12}$, and $\mathbf{x}_{13}$ were all flagged in either the best four-factor or five-factor model in all-subsets regression. Coupled with the factors from forward regression, this creates 11 factors of interest.

Because 11 factors are of interest and the final design will only have 10 runs, all factors cannot be listed as primary terms. Moreover, there is not substantial evidence to suggest some of the 11 factors are more active than the others, but evidence does suggest these 11 factors are likely more important than the four factors not detected by any analysis method. Therefore, we classified these 11 factors as secondary and classified the remaining four as potential terms.

The final analysis of both models is presented in Table 10. For the first model, both the $E(s^2)$ and Bayesian $D$ designs performed well. For the second model, however, the Bayesian design performed better. In the Half Normal Plot, factors $\mathbf{x}_1$, $\mathbf{x}_9$, $\mathbf{x}_5$, and $\mathbf{x}_2$ were deemed active using the method proposed by Gupta et al., but only factors $\mathbf{x}_2$ and $\mathbf{x}_9$ are truly active. Further, factors $\mathbf{x}_4$, $\mathbf{x}_7$, and $\mathbf{x}_{13}$ were not detected, even though they are active. In contrast, the Half Normal Plot

**Table 7**
Final analysis of $\mathbf{y}_2$ on SSD($8 + n_2$, 13): comparing extended $E(s^2)$-optimal SSDs and augmented Bayesian $D$-optimal SSDs.

| Factors | | $\mathbf{x}_1$ | $\mathbf{x}_2$ | $\mathbf{x}_3$ | $\mathbf{x}_4$ | $\mathbf{x}_5$ | $\mathbf{x}_6$ | $\mathbf{x}_7$ | $\mathbf{x}_8$ | $\mathbf{x}_9$ | $\mathbf{x}_{10}$ | $\mathbf{x}_{11}$ | $\mathbf{x}_{12}$ | $\mathbf{x}_{13}$ | Correct? |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | True model | | | | • | • | • | | | | • | | | • | |
| 9 Run $E(s^2)$ | Half Normal | | | | | | | | | | | | | | |
| | Forward | | | | • | | | | • | | • | • | • | | |
| | All subsets | | | | • | • | • | | | | • | | | • | • |
| 9 Run Bayes $D$ | Half Normal | | | | | | | | | | | | | | |
| | Forward | | | | • | • | • | | | | • | | | • | • |
| | All subsets | | | | • | • | • | | | | • | | | • | • |
| 10 Run $E(s^2)$ | Half Normal | | | • | | | | | | | | | | | |
| | Forward | | | | • | | | | | | • | • | | | |
| | All subsets | | | | • | • | • | | | | • | | | • | • |
| 10 Run Bayes $D$ | Half Normal | | | | | | | | | | | | | | |
| | Forward | | | | • | • | • | | | | • | | | • | • |
| | All subsets | | | | • | • | • | | | | • | | | • | • |
| 11 Run $E(s^2)$ | Half Normal | | | | | | | | | | | | | | |
| | Forward | | | | • | • | • | | | | • | | | • | • |
| | All subsets | | | | • | • | • | | | | • | | | • | • |
| 11 Run Bayes $D$ | Half Normal | | | | • | • | | | | | • | | | | |
| | Forward | | | | • | • | • | | | | • | | | • | • |
| | All subsets | | | | • | • | • | | | | • | | | • | • |
| 12 Run $E(s^2)$ | Half Normal | | | | | | | | | | | | | | |
| | Forward | | | | • | • | • | | | | • | | | • | • |
| | All subsets | | | | • | • | • | | | | • | | | • | • |
| 12 Run Bayes $D$ | Half Normal | | | | • | • | • | | | | • | | | • | • |
| | Forward | | | | • | • | • | | | | • | | | • | • |
| | All subsets | | | | • | • | • | | | | • | | | • | • |

**Table 8**
Adding 3 runs to an $E(s^2)$-optimal SSD(7, 15): Runs 8–10 are extended $E(s^2)$-optimal from Gupta et al.; Runs $8_i^*$–$10_i^*$ are Bayesian $D$-optimal for responses $\mathbf{y}_i$.

| Run | $\mathbf{x}_1$ | $\mathbf{x}_2$ | $\mathbf{x}_3$ | $\mathbf{x}_4$ | $\mathbf{x}_5$ | $\mathbf{x}_6$ | $\mathbf{x}_7$ | $\mathbf{x}_8$ | $\mathbf{x}_9$ | $\mathbf{x}_{10}$ | $\mathbf{x}_{11}$ | $\mathbf{x}_{12}$ | $\mathbf{x}_{13}$ | $\mathbf{x}_{14}$ | $\mathbf{x}_{15}$ | $\mathbf{y}_1$ | $\mathbf{y}_2$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | −1 | 1 | −1 | −1 | −1 | −1 | 1 | 1 | 1 | −1 | −1 | 1 | 1 | −1 | −1 | −0.700 | 3.381 |
| 2 | −1 | −1 | −1 | −1 | 1 | −1 | −1 | 1 | −1 | −1 | −1 | −1 | −1 | 1 | 1 | 4.847 | −16.135 |
| 3 | −1 | 1 | 1 | −1 | 1 | 1 | −1 | 1 | −1 | 1 | 1 | 1 | 1 | 1 | −1 | 0.429 | −25.445 |
| 4 | 1 | −1 | −1 | 1 | −1 | −1 | −1 | −1 | −1 | 1 | −1 | 1 | 1 | 1 | −1 | 16.358 | 8.879 |
| 5 | 1 | −1 | −1 | −1 | 1 | 1 | 1 | −1 | 1 | 1 | 1 | 1 | −1 | −1 | 1 | −20.882 | 13.271 |
| 6 | −1 | 1 | 1 | 1 | −1 | −1 | −1 | −1 | 1 | 1 | 1 | −1 | −1 | −1 | 1 | −6.671 | −0.594 |
| 7 | 1 | −1 | 1 | 1 | −1 | 1 | 1 | 1 | 1 | −1 | 1 | −1 | 1 | 1 | 1 | 21.237 | 33.838 |
| 8 | 1 | 1 | 1 | −1 | 1 | −1 | 1 | −1 | 1 | 1 | −1 | −1 | 1 | 1 | 1 | 0.547 | 3.185 |
| 9 | 1 | −1 | 1 | 1 | 1 | −1 | −1 | 1 | 1 | −1 | 1 | 1 | −1 | −1 | −1 | −16.836 | 18.931 |
| 10 | −1 | 1 | −1 | 1 | −1 | 1 | 1 | −1 | −1 | −1 | 1 | 1 | −1 | 1 | 1 | 22.934 | −13.361 |
| $8_1*$ | 1 | 1 | 1 | 1 | 1 | −1 | 1 | −1 | 1 | −1 | −1 | 1 | −1 | 1 | −1 | 2.962 | |
| $9_1*$ | 1 | 1 | −1 | 1 | 1 | 1 | −1 | −1 | −1 | −1 | 1 | 1 | 1 | −1 | −1 | −15.616 | |
| $10_1*$ | 1 | −1 | 1 | 1 | 1 | −1 | 1 | 1 | −1 | 1 | −1 | −1 | 1 | −1 | −1 | −21.181 | |
| $8_2*$ | 1 | 1 | −1 | 1 | 1 | 1 | −1 | 1 | 1 | −1 | −1 | 1 | 1 | −1 | −1 | | 8.842 |
| $9_2*$ | 1 | 1 | 1 | −1 | −1 | 1 | −1 | −1 | −1 | −1 | 1 | −1 | −1 | −1 | 1 | | −34.834 |
| $10_2*$ | −1 | 1 | −1 | 1 | 1 | 1 | 1 | −1 | −1 | −1 | 1 | −1 | −1 | 1 | 1 | | −18.872 |

**Table 9**
Analysis of initial SSD(7, 15) data and classification of factors.

| Analysis | Results | $\mathbf{x}_1$ | $\mathbf{x}_2$ | $\mathbf{x}_3$ | $\mathbf{x}_4$ | $\mathbf{x}_5$ | $\mathbf{x}_6$ | $\mathbf{x}_7$ | $\mathbf{x}_8$ | $\mathbf{x}_9$ | $\mathbf{x}_{10}$ | $\mathbf{x}_{11}$ | $\mathbf{x}_{12}$ | $\mathbf{x}_{13}$ | $\mathbf{x}_{14}$ | $\mathbf{x}_{15}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Model 1 | Half Normal | | | | | • | | | | | • | | | | • | |
| | Forward | | | | | • | | | | | • | | | | • | |
| | All subsets | | | | | • | | | | | • | | | | • | |
| | Classification | $\beta_{pot}$ | $\beta_{pot}$ | $\beta_{pot}$ | $\beta_{pot}$ | $\beta_{pri}$ | $\beta_{pot}$ | $\beta_{pot}$ | $\beta_{pot}$ | $\beta_{pot}$ | $\beta_{pri}$ | $\beta_{pot}$ | $\beta_{pot}$ | $\beta_{pot}$ | $\beta_{pri}$ | $\beta_{pot}$ |
| Model 2 | Half Normal | • | | | | | | | | | | | | | | |
| | Forward | • | | | • | • | | | | • | • | | | | | |
| | All subsets | | • | • | • | | | • | • | | • | | • | • | | |
| | Classification | $\beta_{sec}$ | $\beta_{sec}$ | $\beta_{sec}$ | $\beta_{sec}$ | $\beta_{sec}$ | $\beta_{pot}$ | $\beta_{sec}$ | $\beta_{sec}$ | $\beta_{sec}$ | $\beta_{sec}$ | $\beta_{pot}$ | $\beta_{sec}$ | $\beta_{sec}$ | $\beta_{pot}$ | $\beta_{pot}$ |

**Table 10**
Final analysis of $\mathbf{y}_1$ and $\mathbf{y}_2$ on SSD(10, 15): comparing extended $E(s^2)$-optimal SSDs and augmented Bayesian $D$-optimal SSDs.

| Factors | | $\mathbf{x}_1$ | $\mathbf{x}_2$ | $\mathbf{x}_3$ | $\mathbf{x}_4$ | $\mathbf{x}_5$ | $\mathbf{x}_6$ | $\mathbf{x}_7$ | $\mathbf{x}_8$ | $\mathbf{x}_9$ | $\mathbf{x}_{10}$ | $\mathbf{x}_{11}$ | $\mathbf{x}_{12}$ | $\mathbf{x}_{13}$ | $\mathbf{x}_{14}$ | $\mathbf{x}_{15}$ | Correct? |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Model 1 | True model | | | | | • | | | | | • | | | | • | | |
| 10 Run $E(s^2)$ | Half Normal | | | | | • | | | | | • | • | | | • | | |
| | Forward | | | | | • | | | | | • | | | | • | | • |
| | All subsets | | | | | • | | | | | • | | | | • | | • |
| 10 Run Bayes $D$ | Half Normal | | | | | • | | | | | • | | | | • | | • |
| | Forward | | | | | • | | | | | • | | | | • | | • |
| | All subsets | | | | | • | | | | | • | | | | • | | • |
| Model 2 | True model | | • | | • | | | • | | • | | | | • | | | |
| 10 Run $E(s^2)$ | Half Normal | • | • | | | • | | | | • | | | | | | | |
| | Forward | • | • | | | • | | | • | • | | | | | | | |
| | All subsets | • | | | | • | | | • | | | | | | • | • | |
| 10 Run Bayes $D$ | Half Normal | | • | | • | | | • | | • | | | | • | | | • |
| | Forward | | • | | • | | | • | | • | | | | • | | | • |
| | All subsets | | • | | • | | | • | | • | | | | • | | | • |

for the Bayesian $D$-optimal SSD(10, 15) correctly identified only the five important factors. Forward regression and all-subsets regression also indicate the Bayesian $D$-optimal method is favorable, as forward regression on the extended $E(s^2)$-optimal SSD(10, 15) detected $\mathbf{x}_1, \mathbf{x}_9, \mathbf{x}_5, \mathbf{x}_2, \mathbf{x}_8$ as important, whereas forward regression on the extended Bayesian $D$-optimal SSD(10, 15) identified all active factors: $\mathbf{x}_9, \mathbf{x}_2, \mathbf{x}_4, \mathbf{x}_{13}, \mathbf{x}_7$.

## 5. Discussion and conclusions

We adapted Bayesian $D$-optimality to add runs to existing supersaturated designs by using information from the initial experiment. After running and analyzing an SSD($n_1, k$), an experimenter can classify factors as primary, secondary, or potential depending on how active they appear to be. Using this prior information, $n_2$ runs are added to form a Bayesian $D$-optimal augmented SSD($n_1 + n_2, k$). The comparison study in Section 4 indicates the augmentation strategy performs well against previous methods where designs are augmented to maintain $E(s^2)$-optimality independently of the data.

Our goal with this paper is to introduce the method, but several points deserve explanation. Additional runs are chosen to maximize the Bayesian $D$-optimality criterion, which is dependent on a classification of factors. The initial classification can play a role in the reliability of the method, but misclassification is not always troubling. In Section 4.1, an inactive factor, $\mathbf{x}_1$, was listed as a primary term because the complicated confounding pattern in the SSD(8, 13) inflated its initial parameter estimate. The additional runs reduced the bias from the true active factors, so in the final design, the parameter estimate for $\mathbf{x}_1$ was no longer artificially inflated. The misclassification was not detrimental to the screening process. We have seen some models where an incorrect initial classification led to more Type I or Type II errors than the extended $E(s^2)$-optimal designs, but this is not a surprising result. Regardless of the optimality criterion used to add runs, both the initial design and augmented design are still supersaturated with complicated aliasing structures. As such, there is always a risk of not finding the true active factors. Our methodology, however, is more general than the extended $E(s^2)$-optimality approach, as it can augment any SSD with any number of designed runs, whereas extended $E(s^2)$-optimal designs are only known for certain combinations of $n_1$, $n_2$, and $k$. Moreover, our technique can easily extend to SSDs with more than two levels, and while we employed the Coordinate Exchange Algorithm, different design algorithms could be applied if desired.

Another important issue, suggested by one referee, is the determination of $n_2$ if the decision maker asked for a recommendation. In other words, given $n_1$, what will be an ideal $n_2$? This is a sensible issue; we hope that we will be able to report some findings in the near future. In a perfect world, $n_2$ would be as large as possible while keeping within the screening budget. The results in Section 4.1 provide evidence to this because the simulation results improved as more runs were added. Of course, all SSDs take place in a constrained environment. If the budget was highly constrained, an experimenter is already taking on a certain amount of risk. Some research suggests SSDs work best when $k$ is no more than $2n$ (Marley and Woods, 2010). Thus, an initial suggestion to a decision maker on $n_2$ may be to add at least $n_2$ runs to make $n_1 + n_2 > .5k$. With that said, the presented method can still augment an existing SSD with any number of runs.

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