Bayesian Optimal Designs with High Prediction Efficiency

by

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Abstract

Design of experiments is a strategy used to identify the important factors which affect the response. A well-designed experiment plays a vital role in all disciplines of science since it can provide information to conduct time- and cost-efficient process. The ultimate goal of designing an experiment is to gain the maximum experimental outcome. Optimal designs are the designs that have best outcomes in pre-defined senses. Designs that are appropriate for one instance varies with another based on prior knowledge and available limited resources. Bayesian methods are ideal when prior information is available. Bayesian approach guides the experimenter to gain maximum outcome based on available prior information. It is well known that classical optimal designs depend on an assumed model which may not be a true model. To overcome this, Bayesian designs were introduced. For response surface experiments, the prediction of the response is an important task. Bayesian I-optimal design minimizes the average variance of prediction, thereby increases the prediction efficiency. Replication is an important technique in experimental designs. Since full replication is economically infeasible at most of the time, partial replication becomes an alternative to costly experiments. We introduce three new Bayesian optimality criteria for constructing partially replicated optimal designs that have high prediction efficiency and less dependence on an assumed model. Simulation studies are conducted to obtain optimal designs and to compare the

performance of newly introduced criteria with existing criteria using graphical methods and some efficiency measures.

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Dedication

To my parents, brother and love of my life Isuru,

Without whom none of my success would be possible.

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Chapter 1

Introduction

1.1 Design of experiments

Design of experiments plays a vital role in industry and also in many fields of scientific research including agriculture, medicine, psychology, biology and immunology. Before conducting an experiment we need to identify all aspects of the experiment such as treatments of interest, blocking factors, number of replications, sample size, control variables, etc. Motivation, prior-knowledge and available resources help to identify the important attributes regards to the specific problem of interest.

A well designed experiment means the correct decisions gained before conducting the experiment which eventually helps to conduct time and cost efficient process. A design that is appropriate for one property may not be good for another. Decisions might be based on prior knowledge and may be restricted by available limited resources. Bayesian methods are ideal when prior information is available. Thus Bayesian experimental design has gained a lot of attention in recent years.

1.2 Optimal designs

Optimal designs are the designs that are selected from a design space that has the best values in some pre-defined sense. This can be either a maximum value or a minimum value. There are number of pre-defined ways to choose optimal designs such as information based criteria, distance based criteria, compound criteria and other types.

Information matrix is the inverse matrix of variance-covariance matrix of least square estimates. As the name suggests information based criteria are directly related to information matrix of the design. G-, D- and I- are some of the examples to information based criteria. One of the first stated criterion was proposed by Smith (1918). She proposed to obtain the minimum value of maximum prediction variance over the design space. This was a response estimation criterion which was later named as global or G-optimality by Kiefer and Wolfowitz (1959).

D-optimality aims to minimize the variance of parameters. It is the most widely used criterion which was named as D-optimality by Kiefer and Wolfowitz (1959). It was introduced by Wald (1943), put the emphasis on quality of the parameter estimates. D-criterion maximises the determinant of information matrix.

I-optimality, which stands for integrated variance, minimizes the average prediction variance. In recent years I-optimality has become popular since prediction of response is vital in many scientific research. Jones and Goos (2012) compared the predictive capability of I- and D-optimality in split plot response surface designs and shows that I-optimality performs better than D-optimality in prediction as well as the precision of factor effect estimates. Lin (2018) proposed a compound criterion and utilized the coordinate-exchange 2-phase local search algorithm to select robust designs with high prediction efficiency.

Trinca and Gilmour (1999) pointed out that the pattern of the response is more interesting than the actual response and introduced the I_D criterion which minimize the average difference of prediction variance.

Screening designs are used to identify the important factors affecting the process. These are usually unreplicated, thus there is no way of estimating experimental error. Gilmour and Trinca (2012) showed how important it is to choose which estimate to use for the estimate of variance of experimental units. Even though, there is no assent among all researchers, they recommend that separating lack of fit from pure error and using pure error mean square for inference is better than using residual mean squared error from fitted model. Under this argument, it is necessary to conduct replicated experiments. Obviously, full replicated designs are the best solution to provide replicates but it usually leads to costly experiments.

Partially replicated designs becomes an promising alternative to costly time consuming full replicated designs. Partially replicated designs has gained considerable attention in recent studies. Based on hadamard matrices, Lupinacci and Pigeon (2008) developed a class of partially replicated designs which always produces a n/4 replicates. Ou et al. (2013) utilized semifoldover techniques to obtain partially replicated designs. Tsai and Liao (2014) proposed a compound criterion called extended minimum aberration to obtain partially replicated designs. Another method of constructing partially replicated designs is by utilizing standard exchange algorithms which proceed through optimizing a pre-defined optimal criterion. Draper and Smith (1998) found a proportional relationship among the volume of a confidence interval region for least square estimate with the correlation matrix of least square estimate and quantile of the F distribution. Based on this idea, Gilmour and Trinca (2012) introduced DP-optimality criterion, which combine the D-criterion with a quantile of the F distribution, and used standard candidate exchange algorithm to obtain partially replicated designs with high parameter estimation efficiency. de Oliveira et al. (2019) adopted the same idea and defined IP-optimality criterion. They constructed partially replicated designs with high prediction efficiency.

It is well known that traditional optimal designs such as D- and I- optimal designs depend on an assumed model. To overcome this, Bayesian designs were introduced (Chaloner and Verdinelli, 1995). DuMouchel and Jones (1994) introduced a notion to empirical models classifying the factor effects as primary or potential terms, where primary terms are those with active effects while potential terms may or may not be active. They combined this idea with Bayesian approach and introduced the Bayesian D-criterion to address the problem of bias caused by selecting an incorrect model. From this approach primary terms are precisely estimated while potential terms were able to provide some of the information.

By adopting the idea in Gilmour and Trinca (2012), Leonard and Edwards (2017) defined Bayesian DP-optimality criterion to obtain partially replicated designs. They compared seven-factor designs with various run sizes using various measures such as degrees of freedom of pure error, degrees of freedom of lack of fit, D-efficiency, DP-efficiency, etc. They have also considered the correlation structure of each obtained optimal design. Based on their results, they concluded that Bayesian DP-optimal designs perform well in constructing partially replicated designs when compared to traditional Bayesian D-optimal designs which rarely have replicate points and DP-optimal designs which tend to have excessive number of replicate runs. But they accept that the cost of implementing the Bayesian DP-optimal design may be high.

Bayesian I-optimality criterion has been in the literature for many years. However, to our knowledge, almost no work has been done for Bayesian I-optimal designs. In this thesis, we consider Bayesian I-optimal designs. We also introduce Bayesian I_D-optimality which minimizes the average difference variance of prediction. Moreover, we introduce Bayesian IP- and Bayesian I_DP-optimality criteria to obtain partially replicated designs with high prediction efficiency. We use the same notion proposed by DuMouchel and Jones (1994) to classify factor effects as primary and potential terms. For each of the newly defined criteria, we have searched optimal designs. For comparison purpose, we also searched optimal designs using I-, I_D-, IP-, I_DP-, D-, Bayesian D-, DP-, Bayesian DP-optimality criteria. A number of measures and graphical methods are used to make comparison. We include several illustrative examples to show how each of these criteria perform based on number of factors, number of factor levels and run size. We performed all our simulation studies and analysis using R statistical software version 1.3.1073.

1.3 Thesis organization

The thesis is organized as follows. In Chapter 2, we introduce optimality criteria, algorithm and our newly introduced optimality criteria. In Chapter 3, we construct two-level optimal designs using our newly proposed optimality criteria and some existing criteria. We use the first-order model for non-Bayesin designs and the first-order model with two-factor interactions for Bayesian designs. Two examples are provided. The first one is to select 18-run optimal designs with 6 factor; the second one is to select 24-run optimal designs with 7 factors. The comparison is made among the optimal designs. In Chapter 4, we compare optimal designs with three-factor levels utilizing the second order model for non-Bayesian designs and the second-order model with two-factor interactions for Bayesian designs. We consider two examples. The first one is to construct 12-run optimal designs with 3 factors; the second one is to construct 30-run optimal designs with 4 factors. Finally, we summarize our results and make our conclusion in Chapter 5.

Chapter 2

Optimality Criteria

To find optimal designs, different optimality criteria have been introduced in the literature. In this chapter, we will review some existing optimality criteria and introduce new optimality criteria. In section 2.1, some basic concepts such as the first-order model and the second-order model will be introduced. In section 2.2, we will review optimality criteria for parameter estimation and response prediction. In section 2.3, we will introduce some comparison measures which will be used to see the differences among designs. Section 2.4 introduces point exchange algorithm. We will define new Bayesian criteria for selecting optimal designs with high prediction efficiency in section 2.5.

2.1 Design matrix and model matrix

Consider a completely randomized design with n runs. The model is defined as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon},$$

where $\mathbf{y}$ is the column vector of random variables of dimension n, $\mathbf{X}$ is the $n \times p$ model matrix, $\boldsymbol{\beta}$ is the $p \times 1$ vector of unknown model parameters and $\boldsymbol{\epsilon} \sim N(\mathbf{0}, \sigma^2\mathbf{I})$ is the random error vector.

Example Consider a 12-run three-level I-optimal design with 3 factors given in Table 2.1.

Table 2.1: A 12-run I-optimal design with 3 factors

Run	X_1	X_2	X_3
1	0	0	0
2	0	0	0
3	0	0	0
4	0	0	0
5	0	1	1
6	0	-1	-1
7	1	1	0
8	1	-1	1
9	1	0	-1
10	-1	1	-1
11	-1	-1	0
12	-1	0	1

Assume that a model includes only main effects, such model is called *the first-order model*. In this case, the design matrix in Table 2.1 is also a model matrix.

If we are interested in a model that incorporates all main effects and all two-factor interactions. Then the model matrix is given in Table 2.2.

Table 2.2: The model matrix that includes main effects and two-factor interactions for the design in Table 2.1.

Run	X_1	X_2	X_3	X_1X_2	X_1X_3	X_2X_3
1	0	0	0	0	0	0
2	0	0	0	0	0	0
3	0	0	0	0	0	0
4	0	0	0	0	0	0
5	0	1	1	0	0	1
6	0	-1	-1	0	0	1
7	1	1	0	1	0	0
8	1	-1	1	-1	1	-1
9	1	0	-1	0	-1	0
10	-1	1	-1	-1	1	-1
11	-1	-1	0	1	0	0
12	-1	0	1	0	-1	0

Now let us consider the model that incorporates all main effects and the second-order effects. Then the model is called *the second-order model* or *a quadratic model*. If a model includes all main effects, the second-order effects, and all two-factor interactions, then the model is called *the full second-order model* or *a full quadratic model*, and the model matrix of the design in Table 2.1 is given in Table 2.3.

Table 2.3: The second-order model matrix for the design in Table 2.1.

Run	X_1	X_2	X_3	X_1X_2	X_1X_3	X_2X_3	X_1^2	X_2^2	X_3^2
1	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	0
5	0	1	1	0	0	1	0	1	1
6	0	-1	-1	0	0	1	0	1	1
7	1	1	0	1	0	0	1	1	0
8	1	-1	1	-1	1	-1	1	1	1
9	1	0	-1	0	-1	0	1	0	1
10	-1	1	-1	-1	1	-1	1	1	1
11	-1	-1	0	1	0	0	1	1	0
12	-1	0	1	0	-1	0	1	0	1

2.2 Optimality criteria

An optimality criterion is a computed value based on maximizing or minimizing a pre-defined function which is used to evaluate how good a design performs. Optimal designs are said to have the best value regard to the selected criteria. Different optimality criteria are available based on statistical inferences to be conducted. In this section, we will review some optimality criteria in the literature.

2.2.1 D-optimality criterion

D-criterion is the most widely used criterion which aims to minimize the variances of parameters, that is, to minimize the variance of the least square estimates $\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$. It is known that the variance-covariance matrix of $\hat{\boldsymbol{\beta}}$ is $Var(\hat{\boldsymbol{\beta}}) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}$. Thus, a D-optimal design maximizes $|\mathbf{X}'\mathbf{X}|$.

The D-efficiency of a design ξ is defined as

$$D_{eff} = \left(\frac{|\mathbf{X}(\xi)'\mathbf{X}(\xi)|}{|\mathbf{X}(\xi^*)'X(\xi^*)|}\right)^{(\frac{1}{p})},$$

where ξ^* is the D-optimal design.

2.2.2 I-optimality criterion

The I-optimality criterion aims to minimize the average variance of prediction over the experimental region χ. For any point $\mathbf{x} \in X$, the variance of $\hat{y}(\mathbf{x})$ is $\sigma^2\mathbf{f}(\mathbf{x})'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{f}(\mathbf{x})$. The average variance of prediction is defined as (Jones and Goos, 2012):

$$\begin{aligned}\text{Average prediction variance} &= \frac{\int_{\mathbf{x}\in\boldsymbol{\chi}} var(\hat{y}(\mathbf{x}))d\mathbf{x}}{\int_{\mathbf{x}\in\boldsymbol{\chi}} d\mathbf{x}} \\ &= \frac{\int_{\mathbf{x}\in\boldsymbol{\chi}} \mathbf{f}'(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{f}(\mathbf{x})d\mathbf{x}}{\int_{\mathbf{x}\in\boldsymbol{\chi}} d\mathbf{x}} \\ &\propto \int_{\mathbf{x}\in\boldsymbol{\chi}} \mathbf{f}'(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{f}(\mathbf{x})d\mathbf{x},\end{aligned}$$

where $\int_{\mathbf{x}\in\boldsymbol{\chi}} d\mathbf{x}$ is the volume of the region χ.

Since $\mathbf{f}'(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{f}(\mathbf{x})$ is a scalar,

$$\mathbf{f}'(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{f}(\mathbf{x}) = tr[\mathbf{f}'(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{f}(\mathbf{x})].$$

By cyclically permuting matrices,

$$tr[\mathbf{f'}(\mathbf{x})(\mathbf{X'X})^{-1}\mathbf{f}(\mathbf{x})] = tr[(\mathbf{X'X})^{-1}]\mathbf{f}(\mathbf{x})\mathbf{f'}(\mathbf{x}).$$

It follows that,

$$\begin{aligned}\int_{\mathbf{x}\in\boldsymbol{\chi}} tr[\mathbf{f'}(\mathbf{x})(\mathbf{X'X})^{-1}\mathbf{f}(\mathbf{x})]d\mathbf{x} &= \int_{\mathbf{x}\in\boldsymbol{\chi}} tr[(\mathbf{X'X})^{-1}\mathbf{f}(\mathbf{x})\mathbf{f'}(\mathbf{x})]d\mathbf{x} \\ &= tr[\int_{\mathbf{x}\in\boldsymbol{\chi}}(\mathbf{X'X})^{-1}\mathbf{f}(\mathbf{x})\mathbf{f'}(\mathbf{x})d\mathbf{x}].\end{aligned}$$

Since factor settings are fixed, $(\mathbf{X'X})^{-1}$ is a constant, thus,

$$\int_{\mathbf{x}\in\boldsymbol{\chi}} \mathbf{f'}(\mathbf{x})(\mathbf{X'X})^{-1}\mathbf{f}(\mathbf{x})d\mathbf{x} = tr[(\mathbf{X'X})^{-1}\int_{\mathbf{x}\in\boldsymbol{\chi}}\mathbf{f}(\mathbf{x})\mathbf{f'}(\mathbf{x})d\mathbf{x}].$$

If the experimental region $\chi = [-1\ ,\ +1]^N$, the volume of the experimental region is 2^N. So we can rewrite the formula for average prediction variance as

$$\text{Average prediction variance} = 2^{-N} tr[(\mathbf{X'X})^{-1}\int_{\mathbf{x}\in\boldsymbol{\chi}}\mathbf{f}(\mathbf{x})\mathbf{f'}(\mathbf{x})d\mathbf{x}].$$

In general,

$$\text{Average prediction variance} \propto \mathrm{tr}\{(\mathbf{X'X})^{-1}\mathbf{B}\},$$

where

$$\boldsymbol{B} = \int_{\mathbf{x}\in[-\mathbf{1},+\mathbf{1}]^{\boldsymbol{N}}}\mathbf{f}(\mathbf{x})\mathbf{f'}(\mathbf{x})d\mathbf{x}.$$

$\boldsymbol{B}$ is called the moments matrix. When a model is a full quadratic model,

$$\boldsymbol{B} = \begin{bmatrix} \mathbf{1} & \mathbf{0}'_N & \mathbf{0}'_{N^*} & (1/3)\mathbf{1}'_N \\ \mathbf{0}_N & (1/3)\mathbf{I}_N & \mathbf{0}_{N\times N^*} & \mathbf{0}_{N\times N} \\ \mathbf{0}_{N^*} & \mathbf{0}_{N^*\times N} & (1/9)\mathbf{I}_{N^*} & \mathbf{0}_{N^*\times N} \\ (1/3)\mathbf{1}_N & \mathbf{0}_{N\times N} & \mathbf{0}_{N\times N^*} & (1/45)(4\mathbf{I}_N + 5\boldsymbol{J}_N) \end{bmatrix}$$

(Jones and Goos, 2012), where N is the number of factors, $N^* = N(N-1)/2$ is the number of two-factor interactions and $\boldsymbol{J}$ is an $N \times N$ matrix of ones.

I-efficiency of a design ξ is defined as

$$I_{eff} = \left(\frac{tr\{(\mathbf{X}(\xi^{\dagger\dagger})'\mathbf{X}(\xi^{\dagger\dagger})')^{-1}\mathbf{B}\}}{tr\{(\mathbf{X}(\xi)'\mathbf{X}(\xi))^{-1}\mathbf{B}\}} \right),$$

where $\xi^{\dagger\dagger}$ is the I-optimal design.

2.2.3 I_D-optimality criterion

Using two examples, Trinca and Gilmour (1999) pointed out that the pattern of the response is more interesting than the actual response, that is, how the response changes according to treatments is what of great importance. In particular, we are interested in the differences between the estimated response at standard condition and at other non-standard conditions. Based on this, the design should be chosen to minimize the average difference of prediction variances even if we are interested in the prediction of responses.

Let $\mathbf{x}_0$ represent standard operating conditions of the process and $\mathbf{x}$ be any other location. Then the differences between the estimated response at $\mathbf{x}_0$ and the estimated response at $\mathbf{x}$ is $y(\mathbf{x}) - y(\mathbf{x}_0)$. We are interested in minimizing the variances of differences in response, which is $var[\hat{y}(\mathbf{x}) - \hat{y}(\mathbf{x}_0)]$ (de Oliveira et al., 2019). The I_D-optimal design is defined as to minimize the average difference variance,

$$\text{Average difference variance} \propto \int_{\mathbf{x}\in\boldsymbol{\chi}} var[(\hat{y}(\mathbf{x}) - \hat{y}(\mathbf{x}_0))]d\mathbf{x}$$
$$= \int_{\mathbf{x}\in\boldsymbol{\chi}} [(\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{x}_0))]'(\mathbf{X}'\mathbf{X})^{-1}[(\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{x}_0))]d\mathbf{x}$$

(de Oliveira et al., 2019).

Since $[(\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{x}_0))]'(\mathbf{X}'\mathbf{X})^{-1}[(\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{x}_0))]$ is a scalar,

$$\begin{aligned}
& [(\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{x}_0))]'(\mathbf{X}'\mathbf{X})^{-1}[(\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{x}_0))] \\
= \; & tr\{[(\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{x}_0))]'(\mathbf{X}'\mathbf{X})^{-1}[(\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{x}_0))] \\
= \; & tr\{(\mathbf{X}'\mathbf{X})^{-1}[(\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{x}_0))]'[(\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{x}_0))]\}.
\end{aligned}$$

It follows that,

$$\begin{aligned}
& \int_{\mathbf{x}\in\boldsymbol{\chi}} [(\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{x}_0))]'(\mathbf{X}'\mathbf{X}+\mathbf{R})^{-1}[(\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{x}_0))]d\mathbf{x} \\
= \; & \int tr\{(\mathbf{X}'\mathbf{X})^{-1}[(\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{x}_0))]'[(\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{x}_0))]d\mathbf{x}\} \\
= \; & tr\{(\mathbf{X}'\mathbf{X})^{-1} \int [(\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{x}_0))]'[(\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{x}_0))]d\mathbf{x}\} \\
= \; & tr\{(\mathbf{X}'\mathbf{X})^{-1}\mathbf{B}_{I_D}\}
\end{aligned}$$

where $\mathbf{B}_{I_D} = \int[(\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{x}_0))]'[(\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{x}_0))]d\mathbf{x}$ and is the moment matrix $\mathbf{B}$ with the first row and the first column set to zero (de Oliveira et al., 2019). Thus I_D-optimal design minimizes

$$tr\{(\mathbf{X}'\mathbf{X})^{-1}\mathbf{B}_{I_D}\}.$$

I_D-efficiency of a design ξ is defined as

$$I_{D_{eff}} = \left(\frac{tr\{(\mathbf{X}(\xi^{\zeta\zeta})'\mathbf{X}(\xi^{\zeta\zeta})')^{-1}\mathbf{B}_{I_D}\}}{tr\{(\mathbf{X}(\xi)'\mathbf{X}(\xi))^{-1}\mathbf{B}_{I_D}\}}\right),$$

where $\xi^{\zeta\zeta}$ is the I_D-optimal design.

2.2.4 DP-optimality criterion

In early stages of experimentation unreplicated designs were popular due to their cost-effectiveness. But unreplicated designs cause a major problem since there is no reliable estimate for experimental error variance (Chai and Liao, 2009). Eventhough full replicated design is the best option to overcome this, full replicated designs lead to very costly experiments.

Wald (1943) introduced that maximizing determinant of the information matrix $\mathbf{X}'\mathbf{X}$ leads to minimize the volume of the joint confidence region for $\boldsymbol{\beta}$. Draper and Smith (1998) pointed out that the volume of a confidece interval region for $\boldsymbol{\beta}$ is proportional to $(F_{p,d;1-\alpha})^{p/2}|\mathbf{X}'\mathbf{X}|^{-1/2}$, where d is the pure error degrees of freedom and $F_{p,d;1-\alpha}$ is the $1-\alpha$ quantile of F distribution. Based on this idea, Gilmour and Trinca (2012) introduced a flexible strategy to obtain partially replicated designs. They modified D-criterion and defined DP-criterion which maximizes

$$\frac{|\mathbf{X}'\mathbf{X}|}{(F_{p,d;1-\alpha})^p}.$$

We have used α as 0.05 through out this thesis.

2.2.5 IP-Optimality criterion

Except for DP-criterion, Gilmour and Trinca (2012) also modified other optimality criteria for selecting replicated designs. In particular, they mentioned that I-criterion can be multiplied by $F_{1,d;1-\alpha}$ in order to choose replicated designs with high prediction efficiency. de Oliveira et al. (2019) formally defined IP-criterion which minimizes

$$tr\{(\mathbf{X}'\mathbf{X})^{-1}\mathbf{B}\}F_{1,d;1-\alpha}.$$

2.2.6 I_DP-optimality criterion

Similarly, de Oliveira et al. (2019) also defined I_DP-criterion which aims to minimize

$$tr\{(\mathbf{X}'\mathbf{X})^{-1}\mathbf{B}_{I_D}\}F_{1,d;1-\alpha}$$

.

2.2.7 Bayesian D-optimality criterion

Traditional optimal design approach assumes the model is known. This is a well-known drawback of the traditional approach. To overcome this, Bayesian optimality criteria, which have less dependence on an assumed model, have been introduced (DuMouchel and Jones, 1994).

Consider the traditional linear model split as

$$\boldsymbol{y} = \boldsymbol{X_1}\boldsymbol{\beta_1} + \boldsymbol{X_2}\boldsymbol{\beta_2} + \boldsymbol{\epsilon}, \tag{2.1}$$

where $\boldsymbol{X_1}$ is the $n \times p_1$ matrix of primary terms, $\boldsymbol{X_2}$ is the $n \times p_2$ matrix of potential terms, $\boldsymbol{\beta_1}$ is the $p_1 \times 1$ vector of parameters for primary terms and $\boldsymbol{\beta_2}$ is the $p_2 \times 1$ vector of parameters for potential terms.

Primary terms are considered as active terms by definition, therefore effects corresponding to the primary terms are given a arbitrary prior mean and a prior variance tending towards infinity. That is $\boldsymbol{\beta}_1 \sim N(\mathbf{0}_{p_1}, \gamma^2\mathbf{I}_{p_1)}$ where $\gamma^2 \to \infty$. Potential terms may or may not be active, hence the effects corresponding to potential terms are given a prior mean of zero and a finite prior variance. That is $\boldsymbol{\beta}_2 \sim N(\mathbf{0}_{p_2}, \tau^2\sigma^2)$ where τ^2 is a pre-defined value . Combining $\boldsymbol{\beta}_1$ and $\boldsymbol{\beta}_2$ the joint prior distribution of the unknown regression model parameters is $\boldsymbol{\beta}|\sigma^2$ $\sim N(\mathbf{0}\ , \sigma^2\mathbf{R}^{-1})$ (DuMouchel and Jones, 1994), where

$$\mathbf{R}^{-1} = \begin{bmatrix} \gamma^2\mathbf{I}_{p_1\times p_1} & \mathbf{0}_{p_1\times p_2} \\ \mathbf{0}_{p_2\times p_1} & \tau^2\mathbf{I}_{p_2\times p_2} \end{bmatrix}.$$

Since γ^2 approaches ∞, we have $\mathbf{R} = \mathbf{K}/\tau^2$, where

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

Different researchers have considered different values for τ^2. DuMouchel and Jones (1994) used $\tau^2 = 1$ while Leonard and Edwards (2017) used $\tau^2 = 3$. Since we consider two of the Bayesian criteria mentioned in Leonard and Edwards (2017) we also used $\tau^2 = 3$ for all Bayesian criteria in our thesis. In general, own sensitivity analysis for τ^2 is recommended.

Assuming conditional distribution $\boldsymbol{y}$ given $\boldsymbol{\beta}$ and σ^2 is $\boldsymbol{y}|(\boldsymbol{\beta}\ , \sigma^2) \sim N(\boldsymbol{X}\boldsymbol{\beta}\ , \sigma^2\boldsymbol{I})$, the posterior distribution for $\boldsymbol{\beta}|\boldsymbol{y}$ is given as

$$\boldsymbol{\beta}|\boldsymbol{y} \sim N[(\mathbf{X}'\mathbf{X} + \mathbf{R})^{-1}\mathbf{X}'\mathbf{y}\ , \sigma^2(\mathbf{X}'\mathbf{X} + \mathbf{R})^{-1})].$$

Thus Bayesian D-optimal design maximizes

$$|\mathbf{X}'\mathbf{X} + \mathbf{R}|.$$

2.2.8 Bayesian DP-optimality criterion

Leonard and Edwards (2017) introduced Bayesian approach to find replicated designs by adopting Gilmour and Trinca (2012)'s idea. They defined Bayesian DP-criterion, searched Bayesian DP-optimal designs, and compared them with D-, DP-, and Bayesian D-optimal designs.

Bayesian DP-optimal design seeks to maximize

$$\frac{|\mathbf{X}'\mathbf{X} + \mathbf{R}|}{(F_{p,d;1-\alpha})^p}.$$

2.2.9 Bayesian I-optimality criterion

From section 2.2.7, the variance of $\boldsymbol{\beta}|y$ is $(\mathbf{X}'\mathbf{X}+R)^{-1}$. Similar to the deviation in section 2.2.2, one can easily obtain that the average prediction variance is proportional to $tr\{(\mathbf{X}'\mathbf{X}+\mathbf{R})^{-1}\mathbf{B}\}$. Thus, Bayesian I-optimal design minimizes

$$tr\{(\mathbf{X}'\mathbf{X} + \mathbf{R})^{-1}\mathbf{B}\}.$$

2.3 Comparison measures

In this section, we will introduce some comparison measures which will be used to compare the differences among optimal designs.

2.3.1 $tr(\mathbf{AA}')$

Experimenters choose the model they are interested in sometimes. But it can be different to the true model. Assume that an experimenter fits the model $\boldsymbol{y} = \boldsymbol{X_1\beta_1} + \boldsymbol{\epsilon}^*$, which is different to the true model stated in (2.1). It is known that

$$E[\hat{\boldsymbol{\beta}}_{\mathbf{1}}] = \boldsymbol{\beta}_1 + \mathbf{A}\boldsymbol{\beta}_{\mathbf{2}},$$

where $\hat{\boldsymbol{\beta}}_{\mathbf{1}} = (\mathbf{X}_1'\mathbf{X}_1)^{-\mathbf{1}}\mathbf{X}_1'\mathbf{y}$ is the least square estimate of $\boldsymbol{\beta}_{\mathbf{1}}$ and $\mathbf{A} = (\mathbf{X}_1'\mathbf{X}_1)^{-\mathbf{1}}\mathbf{X}_1'\mathbf{X}_2$ is called the alias matrix which is considered to be responsible for transmitting bias to the estimate $\hat{\boldsymbol{\beta}}_{\mathbf{1}}$ (Jones and Nachtsheim, 2011). Bursztyn and Steinberg (2006) pointed out that $tr(\mathbf{AA}')$ value can be used to identify the potential impact of bias. Jones and Nachtsheim (2011) proposed to select an optimal design that has the minimal value of $tr(\mathbf{AA}')$ to minimize the aliasing among the effects.

2.3.2 Degrees of freedom

As the name suggests degrees of freedom is a measure of freedom to vary, that is, the number of observations in the data that are free to vary when estimating parameters. Pure error degrees of freedom denotes the total number of replicated design runs. Table 2.4 summarizes the calculation of degrees of freedom, where c is the number of distinct design runs.

Table 2.4: Calculation of degrees of freedom

Measure	Degrees of freedom
Lack of fit error	c-p
Pure error	n-c

2.4 Algorithm

Mainly there are two types of exchange algorithms such as coordinate exchange algorithm and point exchange algorithm (Jung and Yum, 1996; Cook and Nachtsheim, 1980). In coordinate exchange algorithm single entities of the design matrix is exchanged in each iteration, while in point exchange algorithm rows of the design matrix are exchanged. We have used the point exchange algorithm in our application and we utilized the full factorial design as the candidate set.

1. First randomly choose n runs from the candidate set with out replacement for starting design.

2. Use the starting design criterion value as the local optimal for comparison.

3. Perform the point exchange for each of the n runs. Point exchange is done by replacing the each row in the starting design with candidate set keeping all other rows of the starting design constant at the moment.

4. In each point exchange calculate the criterion value of the design and check with the existing local optimal criterion value whether the new value becomes optimal or not.

5. If the new design becomes optimal update the existing local optimal value with the new one and update the existing local optimal design with

the new design. If the new design is not becoming optimal go for next point exchange.

6. At the end of point exchange check the optimal value with existing optimal value and update accordingly.

7. Use the current local optimized design as the starting design and perform the point exchange until the design can not be optimized any further by replacing any of the rows with any row in the candidate set.

8. Update the current optimal value and the optimal design.

9. Omit the current optimal design from the candidate set and choose a new random design from the remaining runs in the candidate set. If candidate set's run size is less than 2n, then use the full candidate set to select the next random design without replacement.

10. Then perform the point exchange on new random start and update the optimal design.

11. Perform the same process for the pre-defined number of starting designs and obtain the global optimal design.

For obtaining optimal designs using this algorithm we utilized 3000-5000000 random starts depending on the optimal criterion, number of factors and the total number of runs. For each criterion we run the algorithm several times (5-10 times) until we get the same optimal value each time which we considered as the global optimum.

2.5 New Bayesian optimality criteria

In this section, we will introduce new Bayesian optimality criteria which can be used to select replicated designs with high prediction efficiency.

2.5.1 Bayesian I_D-optimality criterion

From section 2.2.7, we know that the variance of $\boldsymbol{\beta}|y$ is $(\mathbf{X}'\mathbf{X}+\mathbf{R})^{-1}$. Since the average difference variance of prediction is proportional to $\int_{\mathbf{x}\in\boldsymbol{\chi}} var[(\hat{y}(\mathbf{x})-\hat{y}(\mathbf{x}_0))]d\mathbf{x}$ (de Oliveira et al., 2019), we obtain $tr\{(\mathbf{X}'\mathbf{X}+\mathbf{R})^{-1}\mathbf{B}_{I_D}\}$.

$$\text{Average difference variance} \propto \int_{\mathbf{x}\in\boldsymbol{\chi}} var[(\hat{y}(\mathbf{x})-\hat{y}(\mathbf{x}_0))]d\mathbf{x}$$

$$= \int_{\mathbf{x}\in\boldsymbol{\chi}} [(\mathbf{f}(\mathbf{x})-\mathbf{f}(\mathbf{x}_0))]'(\mathbf{X}'\mathbf{X}+\mathbf{R})^{-1}[(\mathbf{f}(\mathbf{x})-\mathbf{f}(\mathbf{x}_0))]d\mathbf{x}.$$

since $[(\mathbf{f}(\mathbf{x})-\mathbf{f}(\mathbf{x}_0))]'(\mathbf{X}'\mathbf{X}+\mathbf{R})^{-1}[(\mathbf{f}(\mathbf{x})-\mathbf{f}(\mathbf{x}_0))]$ is a scalar,

$$\begin{aligned}
& [(\mathbf{f}(\mathbf{x})-\mathbf{f}(\mathbf{x}_0))]'(\mathbf{X}'\mathbf{X}+\mathbf{R})^{-1}[(\mathbf{f}(\mathbf{x})-\mathbf{f}(\mathbf{x}_0))] \\
= \;& tr\{[(\mathbf{f}(\mathbf{x})-\mathbf{f}(\mathbf{x}_0))]'(\mathbf{X}'\mathbf{X}+\mathbf{R})^{-1}[(\mathbf{f}(\mathbf{x})-\mathbf{f}(\mathbf{x}_0))] \\
= \;& tr\{(\mathbf{X}'\mathbf{X}+\mathbf{R})^{-1}[(\mathbf{f}(\mathbf{x})-\mathbf{f}(\mathbf{x}_0))]'[(\mathbf{f}(\mathbf{x})-\mathbf{f}(\mathbf{x}_0))]\}.
\end{aligned}$$

It follows that,

$$\begin{aligned}
&\int_{\mathbf{x}\in\boldsymbol{\chi}}[(\mathbf{f}(\mathbf{x})-\mathbf{f}(\mathbf{x}_0))]'(\mathbf{X}'\mathbf{X}+\mathbf{R})^{-1}[(\mathbf{f}(\mathbf{x})-\mathbf{f}(\mathbf{x}_0))]d\mathbf{x} \\
= & \int tr\{(\mathbf{X}'\mathbf{X}+\mathbf{R})^{-1}[(\mathbf{f}(\mathbf{x})-\mathbf{f}(\mathbf{x}_0))]'[(\mathbf{f}(\mathbf{x})-\mathbf{f}(\mathbf{x}_0))]d\mathbf{x}\} \\
= & \; tr\{(\mathbf{X}'\mathbf{X}+\mathbf{R})^{-1}\int[(\mathbf{f}(\mathbf{x})-\mathbf{f}(\mathbf{x}_0))]'[(\mathbf{f}(\mathbf{x})-\mathbf{f}(\mathbf{x}_0))]d\mathbf{x}\} \\
= & \; tr\{(\mathbf{X}'\mathbf{X}+\mathbf{R})^{-1}\mathbf{B}_{I_D}\},
\end{aligned}$$

where $\int[(\mathbf{f}(\mathbf{x})-\mathbf{f}(\mathbf{x}_0))]'[(\mathbf{f}(\mathbf{x})-\mathbf{f}(\mathbf{x}_0))]d\mathbf{x}=\mathbf{B}_{I_D}$ (de Oliveira et al., 2019). We define Bayesian I_D criterion which selects optimal designs with the minimum value of

$$tr\{(\mathbf{X}'\mathbf{X}+\mathbf{R})^{-1}\mathbf{B}_{I_D}\}.$$

2.5.2 Bayesian IP-optimality criterion and Bayesian I_DP-optimality criterion

To select designs that allow us to conduct inference, we adopt the idea in Gilmour and Trinca (2012) and define the Bayesian IP-criterion which seeks to minimize

$$tr\{(\mathbf{X}'\mathbf{X}+\mathbf{R})^{-1}\mathbf{B}\}F_{1,d;1-\alpha}.$$

Similarly, we define Bayesian I_DP-criterion which seeks to minimize

$$tr\{(\mathbf{X}'\mathbf{X}+\mathbf{R})^{-1}\mathbf{B}_{I_D}\}F_{1,d;1-\alpha}.$$

Chapter 3

First-Order Model With Two-Factor Interactions

In this chapter we consider two illustrative examples of two-level factor designs using I-, Bayesian I-, IP-, Bayesian IP-, I_D-, Bayesian I_D-, I_DP-, Bayesian I_DP-, D-, Bayesian D-, DP-, Bayesian DP-criteria (12 optimality criteria). First we consider 18 run designs with 6 factors and then we consider 24 run designs with 7 factors. For all non-Bayesian designs we used a priori main effects only model, while all Bayesian designs used the main effects with two-factor interactions model where main effects were specified as primary terms and the two-factor interactions were specified as potential terms. For each of these 12 optimality criteria we obtained optimal designs. We compare the differences of the optimal designs with various efficiency measures, degrees of freedom values and correlation measures.

3.1 18-run optimal designs with 6 two-level factors

We searched 18-run two-level optimal designs with 6 factors using 12 optimal criteria. Usually, for each optimality criterion, we can obtain one or more optimal designs. Table A.1 - Table A.6 in appendix A provide examples of the obtained optimal designs for each criterion. To see the difference of the optimal designs, we calculated the degrees of freedom of pure error, the degrees of freedom of lack of fit, I-efficiency, I_D-efficiency, $tr(\mathbf{AA}')$ and D-efficiency. The results are listed in Table 3.1.

From Table 3.1, we can see that except for the Bayesian IP-optimal design, all other optimal designs are above 85% I-efficient and above 90% D-efficient. It is found that IP- and Bayesian-I optimal designs are 100% I-efficient as well as 100% D-efficient. Bayesian IP-optimal design is 69.39% I-efficient and 75.68% D-efficient. Bayesian I_DP-optimal design is 86.75% I-efficient and 91.56% D-efficient. The advantage of the Bayesisn IP- and Bayesian I_DP-optimal designs is that there are replicated points in the designs so that we are able to do formal lack-of-fit tests.

Table 3.1: Comparison of 18-run two-level optimal designs with 6 factors

Criterion	df_{pe}	df_{LoF}	I-eff	I_D-eff	$tr(\mathbf{AA}')$	D-eff
I	0	11	1.0000	0.9986	4.0280	1.0000
I_D	0	11	0.9982	1.0000	3.9577	1.0000
IP	10	1	1.0000	0.9986	12.0744	1.0000
I_DP	10	1	0.9982	1.0000	12.0744	1.0000
BI	0	11	1.0000	0.9986	1.7388	1.0000
BI_D	0	11	0.9168	0.8767	0.6312	0.9512
BIP	5	6	0.6939	0.6320	3.5530	0.7568
BI_DP	6	5	0.8675	0.8470	2.6889	0.9156
D	2	9	0.9982	1.0000	5.5999	1.0000
DP	10	1	0.9982	1.0000	12.0744	1.0000
BD	0	11	0.9575	0.9320	1.7402	0.9711
BDP	6	5	0.8633	0.8412	2.6148	0.9156

Although Bayesian I- and Bayesian I_D-optimal designs have higher I-, I_D-, and D-efficiency values than Bayesian IP- and Bayesian I_DP-optimal designs, we did not observe any replicate points in Bayesian I- and Bayesian I_D-optimal designs. This results in absence of pure error degrees of freedom which will obstruct the experimenter to conduct formal tests for lack of fit. Thus inferences on these scenarios must be based on the residual mean square for the fitted model. Compared to Bayesian IP- and Bayesian I_DP-optimal designs, IP- and I_DP-optimal designs have higher I-, I_D-, and D-efficiency values too. However, their $tr(\mathbf{AA}')$ values are much higher than Bayesian optimal designs, which can be seen in Figure 3.1.

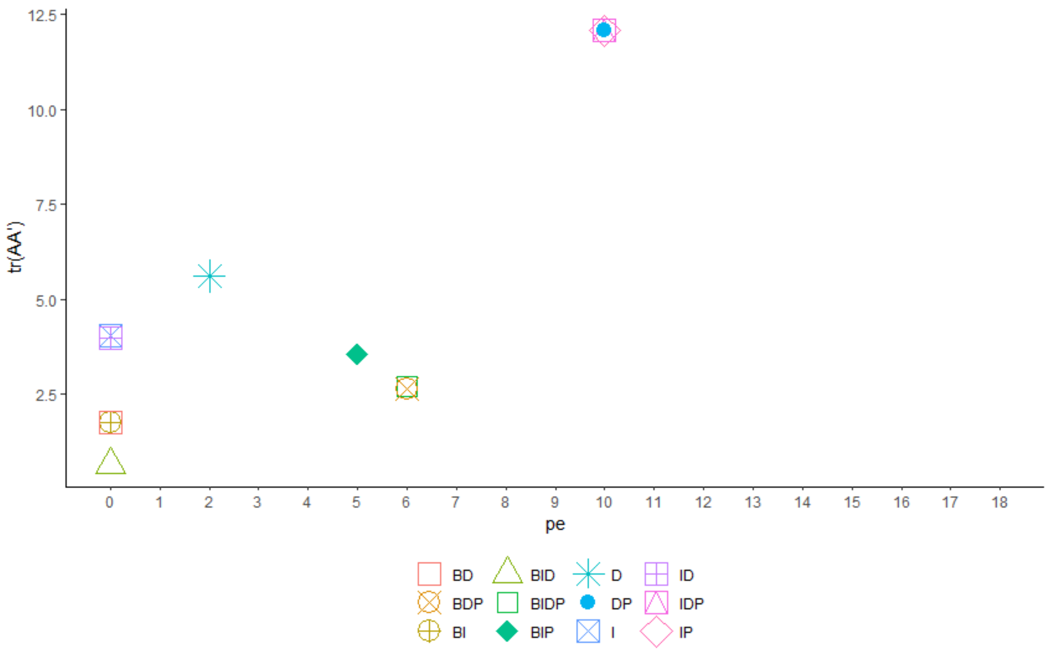
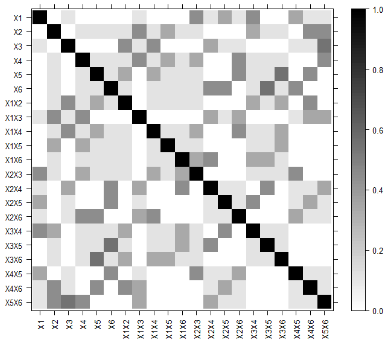
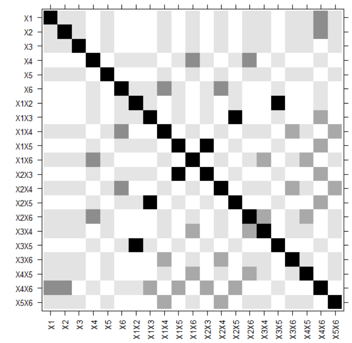


Figure 3.1: $tr(\mathbf{AA'})$ values of 18-run two-level optimal designs with 6 factors

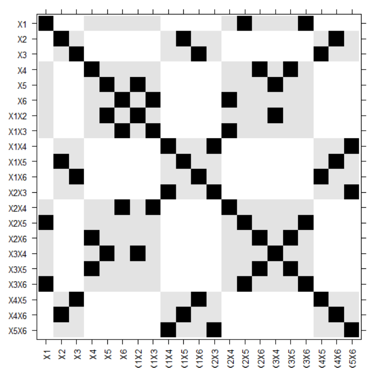
Furthermore, we obtained the absolute correlation graphs for each of the optimal designs in Table A.1 - Table A.6. The obtained graphs are in Figure 3.2. These correlation maps show the absolute correlation structure among main effects, among two-factor interactions and in between main effects and two-factor interactions. When we compare the correlation maps of Bayesian designs with the maps of corresponding non-Bayesian designs, it is clearly visible that pairwise correlations among main effects and two-factor interactions have been reduced in Bayesian designs. In particular, for IP- and I_DP-optimal designs, each main effect is fully confounded with two two-factor interactions, which is significantly reduced in Bayesian IP- and Bayesian I_DP-optimal designs, respectively.



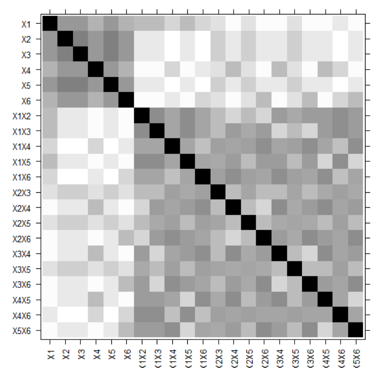
I



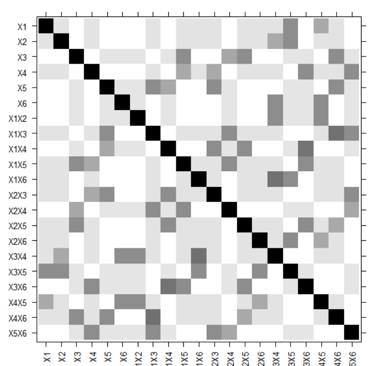
BI



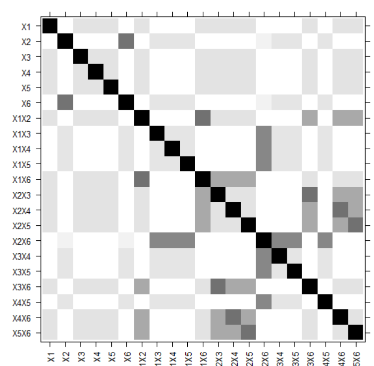
IP



BIP



I_D



BI_D

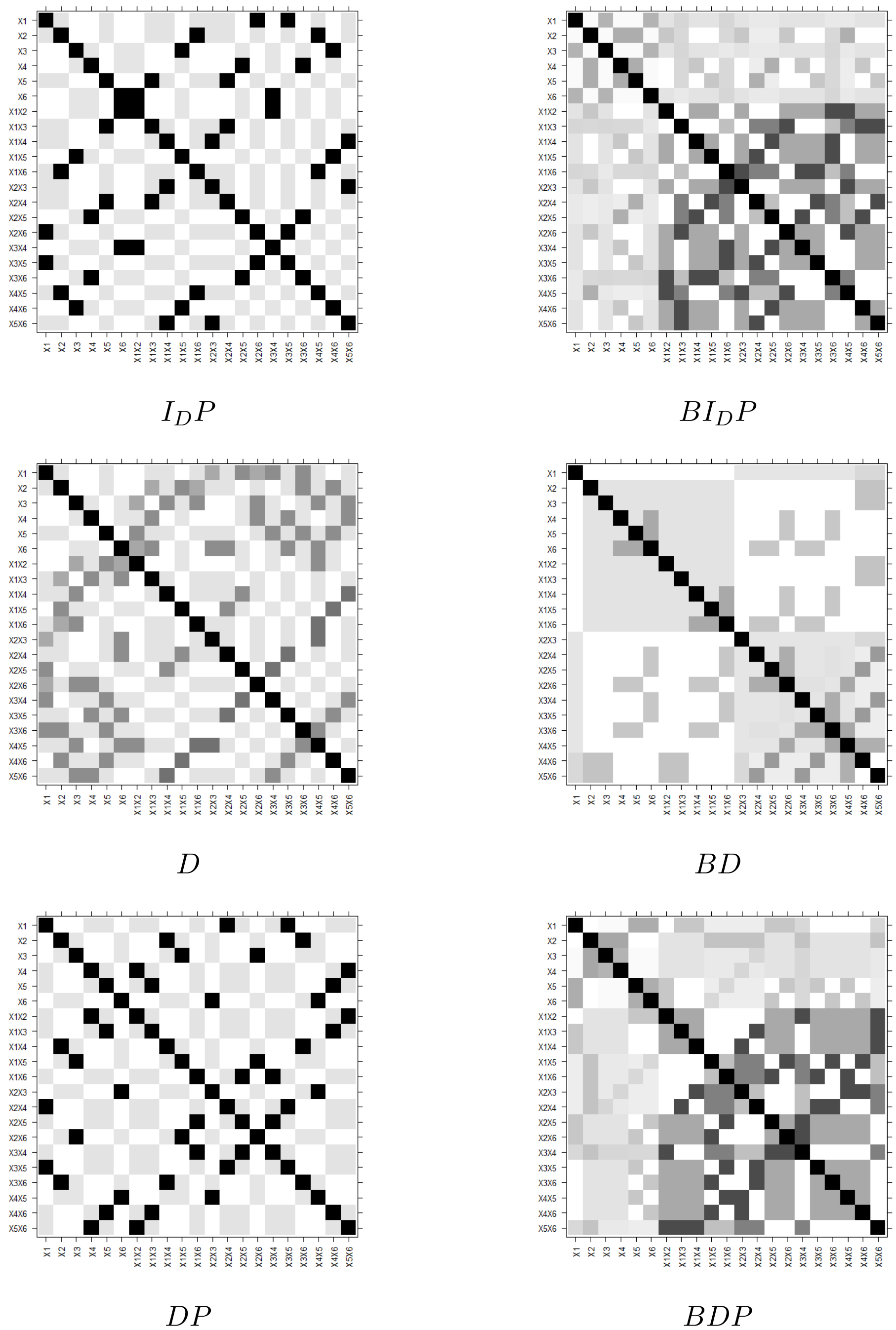


Figure 3.2: Absolute correlation maps of 18-run two-level optimal designs with 6 factors

The mean absolute correlations among primary terms, primary and potential terms and potential terms for the optimal designs are shown in Table 3.2.

Table 3.2: Mean absolute correlations of 18-run two-level optimal designs with 6 factors

Criterion	Primary & primary correlation	Primary & potential correlation	Potential & potential correlation
I	0.0511	0.1676	0.1088
I_D	0.0422	0.1284	0.1229
IP	0.0511	0.1741	0.1263
I_DP	0.0422	0.1726	0.1289
BI	0.0511	0.0849	0.1018
BI_D	0.0811	0.0542	0.1136
BIP	0.4015	0.1005	0.3400
BI_DP	0.1400	0.1097	0.2926
D	0.0422	0.1880	0.1034
DP	0.0422	0.1726	0.1289
BD	0.1037	0.0736	0.1119
BDP	0.1407	0.1148	0.2926

We have calculated the relative variance of coefficients for Bayesian optimal designs. The results are given in Table 3.3. One can see that the Bayesian I-optimal design estimates intercept, main effects, and nine out of 15 two-factor interactions more precisely than the Bayesian D-optimal design. Bayesian D-optimal design estimates the two-factor interactions X_1X_2, X_1X_3, X_1X_5, X_2X_3, and X_3X_5 more precisely than the Bayesian I-optimal design.

The Bayesian I_D-optimal design estimates main effects and ten out of 15 two-factor interactions more precisely than the Bayesian D-optimal designs.

Bayesian D-optimal design estimates the intercept and 5 out of 15 two-factor interactions more precisely than the Bayesian I_D-optimal design.

The Bayesian D-optimal design estimates the intercept and all two-factor interactions more precisely than the Bayesian DP-optimal design. The Bayesian DP-optimal design estimates all main effects more precisely than the Bayesian D-optimal design.

The Bayesian IP-optimal design estimates the intercept and the all two-factor interactions more precisely than the Bayesian DP-optimal designs. But the Bayesian DP-optimal design estimates all main effects more precisely than the Bayesian IP-optimal design.

The Bayesian I_DP-optimal design has equal estimation ability as the Bayesian DP-optimal design for the intercept, all the main effects and 7 out of the 15 two-factor interactions. Among the rest of the 15 two-factor interactions, the Bayesian I_DP-optimal design can estimate X_1X_5, X_2X_3, X_3X_4, and X_5X_6 more precisely than the Bayesian DP-optimal design and the Bayesian DP-optimal design can estimate X_1X_3, X_2X_5, X_3X_6, and X_4X_5 more precisely than the Bayesian I_DP-optimal design.

Table 3.3: Relative variance of factor effect estimates of 18-run two-level optimal designs with 6 factors

	BI	BI_D	BIP	BI_DP	BD	BDP
Intercept	0.0621	1.0842	0.2597	2.0625	0.2483	2.0625
X_1	0.1191	0.0623	0.0878	0.0749	0.1391	0.0749
X_2	0.1191	0.1221	0.1035	0.0749	0.2752	0.0750
X_3	0.0623	0.0623	0.1035	0.0749	0.2752	0.0750
X_4	0.1211	0.0623	0.0878	0.0749	0.5802	0.0750
X_5	0.0623	0.0623	0.1035	0.0749	0.5802	0.0749
X_6	0.1211	0.1221	0.0878	0.0749	1.2727	0.0749
X_1X_2	1.5154	1.1518	1.8143	1.9174	0.2653	1.9174
X_1X_3	1.5223	0.2183	1.8143	2.1423	0.2653	1.9174
X_1X_4	0.4538	0.2183	1.8124	1.9174	0.5580	1.9174
X_1X_5	1.5223	0.2183	1.8143	1.9174	0.5580	2.1423
X_1X_6	0.4538	1.1518	1.8124	2.1423	1.2225	2.1423
X_2X_3	1.5223	1.1518	1.8162	1.9174	0.1347	2.1423
X_2X_4	0.4538	1.1518	1.8143	2.1423	0.8423	2.1423
X_2X_5	1.5223	1.1518	1.8162	2.1423	0.8423	1.9174
X_2X_6	0.4538	2.0223	1.8143	1.9174	1.1992	1.9174
X_3X_4	0.4247	0.2183	1.8143	1.9174	0.8423	2.1423
X_3X_5	1.5154	0.2183	1.8162	1.9174	0.8423	1.9174
X_3X_6	0.4247	1.1518	1.8143	2.1423	1.1992	1.9174
X_4X_5	0.4247	0.2183	1.8143	2.1423	0.9996	1.9174
X_4X_6	0.2272	1.1518	1.8124	1.9174	1.3765	1.9174
X_5X_6	0.4247	1.1518	1.8143	1.9174	1.3765	2.1423

3.2 24-run optimal designs with 7 two-level factors

Following the same procedure as in section 3.1, we obtained 24-run two-level optimal designs with 7 factors using the 12-optimality criteria. Table A.7 - Table A.12 provide examples of the obtained optimal designs for each criterion.

To see the differences among each of these optimal designs we calculated the degrees of freedom of pure error, degrees of freedom of lack of fit, I-efficiency, I_D-efficiency, $tr(\mathbf{AA}')$ and D-efficiency for each optimal design. The results are listed in Table 3.4.

Table 3.4: Comparison of 24-run two-level optimal designs with 7 factors

Criterion	df_{pe}	df_{LoF}	I-eff	I_D-eff	$tr(\mathbf{AA}')$	D-eff
I	1	15	1.0000	1.0000	4.6667	1.0000
I_D	0	16	1.0000	1.0000	5.0000	1.0000
IP	16	0	1.0000	1.0000	21.0000	1.0000
I_DP	16	0	1.0000	1.0000	21.0000	1.0000
BI	0	16	0.9244	0.8953	1.1129	0.9501
BI_D	0	16	0.8794	0.8468	2.0505	0.9292
BIP	6	10	0.9281	0.9365	3.5917	0.9632
BI_DP	6	10	0.7796	0.7349	3.1255	0.8687
D	0	16	1.0000	1.0000	4.6667	1.0000
DP	16	0	1.0000	1.0000	21.0000	1.0000
BD	0	16	0.9244	0.8953	1.1129	0.9501
BDP	6	10	0.8511	0.8000	1.8730	0.9077

It can be seen that all the non-Bayesian optimal designs are 100% I-efficient, I_D-efficient and D-efficient. When considering Bayesian designs, except for the Bayesian I_DP-optimal design, all other Bayesian optimal designs are above 85% I-efficient and above 90% D-efficient. I_D-, Bayesian I-, Bayesian I_D-, D- and Bayesian D-optimal designs do not show any replicate points which prevent the experimenter to conduct formal lack of fit tests. On the other hand, I-, IP-, I_DP-, Bayesian IP-, Bayesian I_DP-, DP- and Bayesian DP-optimal designs provide replicated points which allows the experimenter to conduct formal lack of fit tests. IP-, I_DP- and DP-optimal designs show higher $tr(\mathbf{AA}')$ value compared to Bayesian optimal designs. This is clearly visible in Figure 3.3.

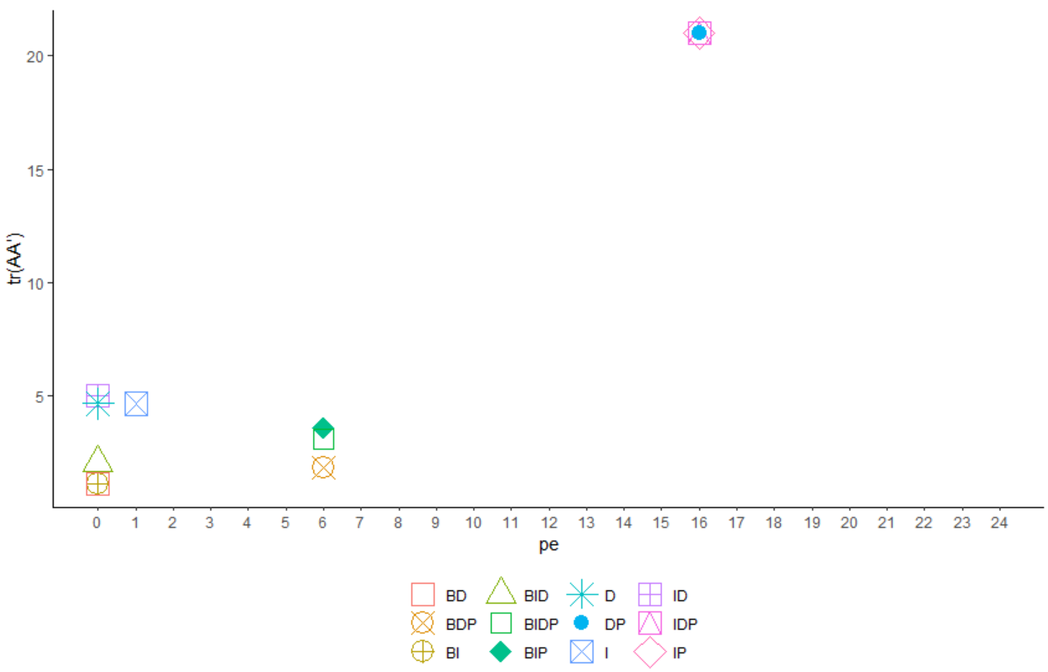
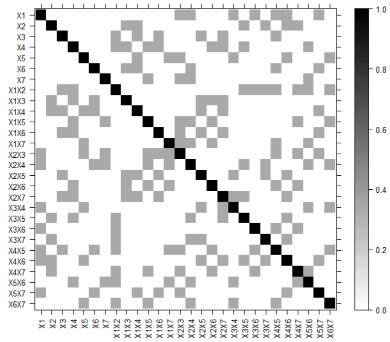
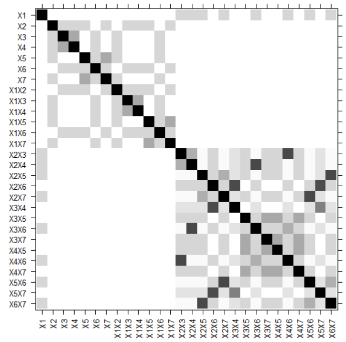


Figure 3.3: $tr(\mathbf{AA}')$ values of 24-run two-level optimal designs with 7 factors

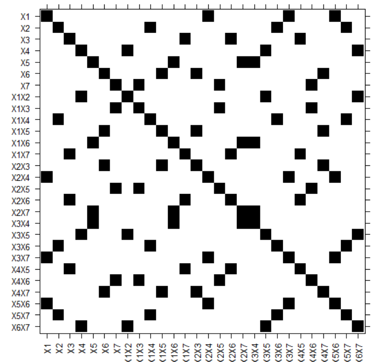
Furthermore, we calculated the absolute correlation graphs for each of the optimal designs, which are shown in Figure 3.4.



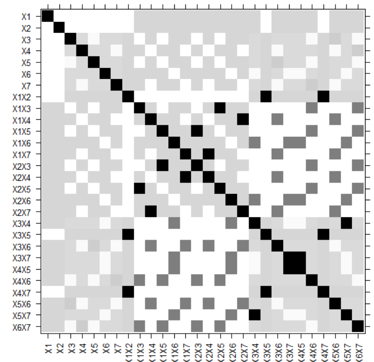
I



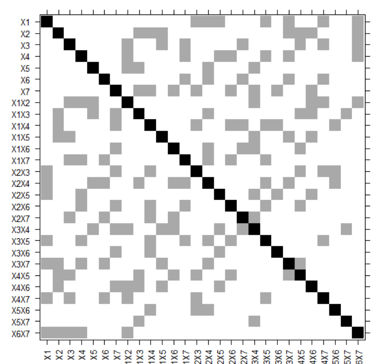
BI



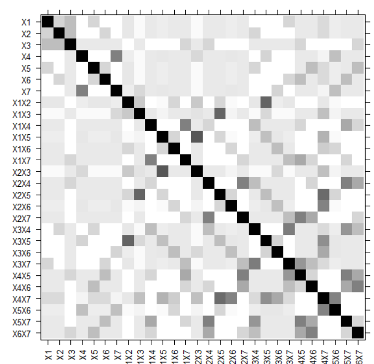
IP



BIP



I_D



BI_D

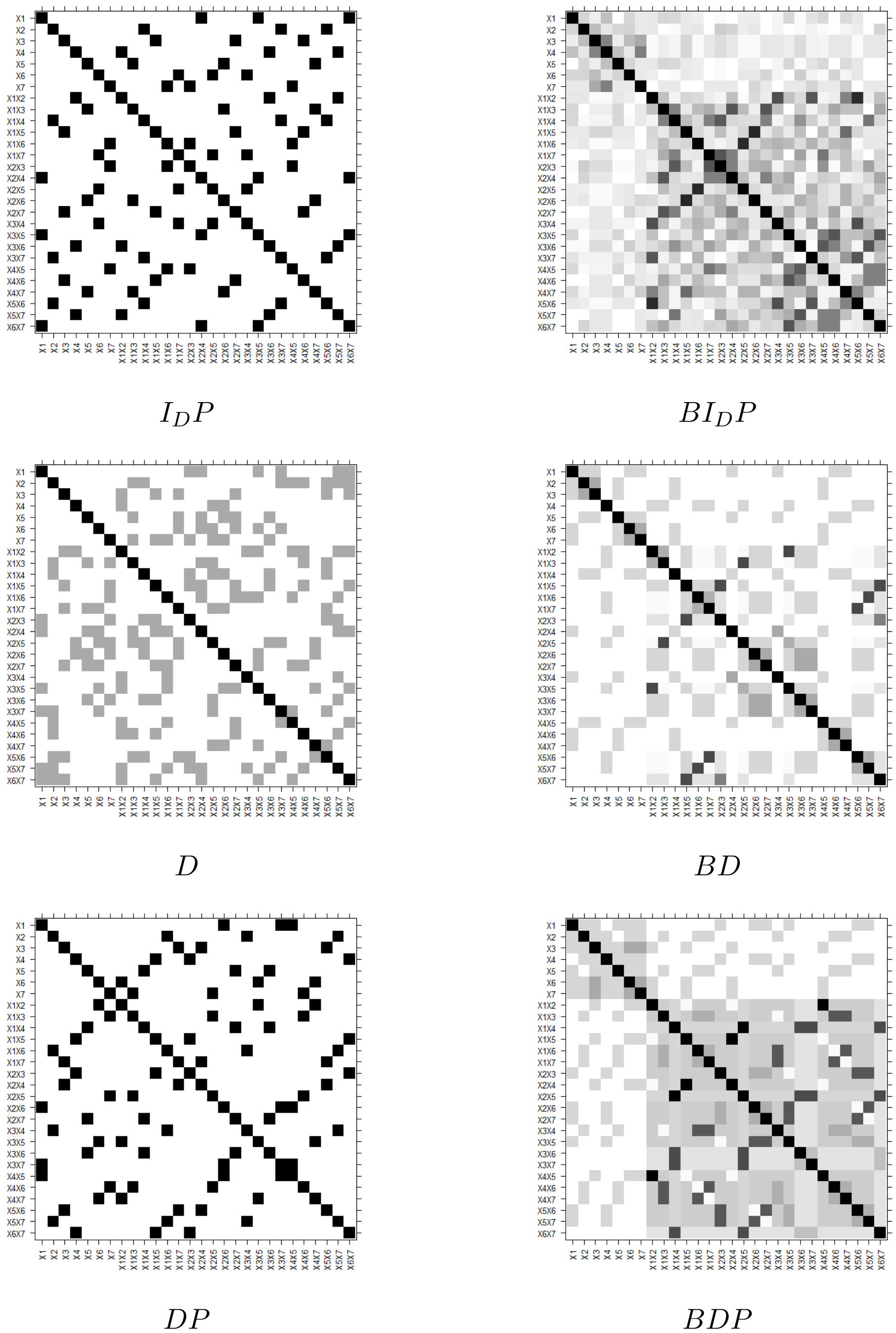


Figure 3.4: Absolute correlation maps of 24-run two-level optimal designs with 7 factors

According to the results it can be seen that all non-Bayesian designs are orthogonal, which indicates that main effects are not correlated in those designs. These orthogonal designs are 100% I-efficient, I_D-efficient and D-efficient. The orthogonality is lost in Bayesian designs. However, the pairwise correlations among main effects and two-factor interactions have been reduced in Bayesian designs when compared to corresponding non-Bayesian designs. In particular, for IP-, IDP- and DP-optimal designs, each main effect is fully confounded with three two-factor interactions which are significantly reduced in corresponding Bayesian designs.

We have also calculated the mean absolute correlation among primary terms, primary and potential terms and potential terms for the optimal designs which are shown in Table 3.5.

Table 3.5: Mean absolute correlations of 24-run two-level optimal designs with 7 factors

Criterion	Primary & primary correlation	Primary & potential correlation	Potential & potential correlation
I	0.0000	0.0952	0.0810
I_D	0.0000	0.1020	0.0619
IP	0.0000	0.1429	0.1000
I_DP	0.0000	0.1429	0.1000
BI	0.0952	0.0273	0.0918
BI_D	0.0981	0.0778	0.1153
BIP	0.0571	0.1262	0.1599
BI_DP	0.1845	0.0717	0.2314
D	0.0000	0.1088	0.0714
DP	0.0000	0.1429	0.1000
BD	0.0952	0.0273	0.0918
BDP	0.1746	0.0414	0.2280

The relative variance of coefficients for the optimal designs are given in Table 3.6. It is observed that Bayesian I- and Bayesian D-optimal designs gave similar estimates. For example, X_1 of Bayesian I-optimal design and X_4 of Bayesian D-optimal designs have the same estimate 0.0468. Similarly X_1X_2 to X_1X_7 of Bayesian I-optimal design and X_1X_4, X_2X_4, X_3X_4, X_4X_5, X_4X_6 and X_4X_7 have the same estimate 0.0491. Bayesian I-and Bayesian D-optimal designs show a higher precision of estimating the intercept and main effects than the other designs. Bayesian D-optimal design estimates the intercept, all main effects and 9 out of 21 two-factor interactions more precisely than the Bayesian I_D-optimal design while Bayesian I_D-optimal design estimates 12 out of 21 two-factor interactions more precisely than the Bayesian D-optimal design. Bayesian I_D-optimal design estimates 9 out of 21 two-factor interactions more precisely than the Bayesian I-optimal design and most of the two-factor interactions more precisely than the Bayesian IP-, Bayesian I_DP- and Bayesian DP-optimal designs.

Table 3.6: Relative variance of factor effect estimates of 24-run two-level optimal designs with 7 factors

	BI	BI_D	BIP	BI_DP	BD	BDP
Intercept	0.0622	0.8114	0.0526	1.1883	0.0622	1.3744
X_1	0.0468	0.0537	0.0693	0.0602	0.0499	0.5521
X_2	0.0499	0.0536	0.0693	0.0755	0.0500	0.5521
X_3	0.0500	0.0538	0.0677	0.0931	0.0500	0.0555
X_4	0.0500	0.0909	0.0677	0.0857	0.0468	0.5521
X_5	0.0500	0.0626	0.0677	0.0602	0.0499	0.5521
X_6	0.0499	0.0515	0.0923	0.0755	0.0500	0.0555
X_7	0.0500	0.0893	0.0677	0.0852	0.0500	0.0555
X_1X_2	0.0491	0.8885	2.0075	1.6461	1.0532	1.7929
X_1X_3	0.0491	0.8917	1.7617	1.6526	1.0532	1.6383
X_1X_4	0.0491	0.4811	1.7617	1.7254	0.0491	2.2055
X_1X_5	0.0491	0.5093	1.7617	1.5171	1.5116	1.7929
X_1X_6	0.0491	0.0943	1.0478	1.4103	1.0532	1.6383
X_1X_7	0.0491	0.4850	1.7617	1.4996	1.0532	1.6383
X_2X_3	1.0532	0.6822	1.7617	1.6949	1.1472	1.6383
X_2X_4	1.0532	1.0591	1.7617	1.4992	0.0491	1.7929
X_2X_5	1.0532	1.0299	1.7617	1.4103	1.0532	2.2055
X_2X_6	1.5116	0.1041	1.0478	1.4686	0.7770	1.6383
X_2X_7	1.0532	1.0595	1.7617	1.4921	0.7770	1.6383
X_3X_4	1.1472	0.7612	1.7617	1.8421	0.0491	1.6383
X_3X_5	0.7770	1.0287	2.0075	1.6526	1.0532	1.6383
X_3X_6	1.0532	0.0985	1.0460	1.6949	0.7770	0.6877
X_3X_7	0.7770	0.7560	1.7617	1.6044	0.7770	0.6877
X_4X_5	0.7770	1.0670	1.7617	1.7254	0.0491	1.7929
X_4X_6	1.0532	1.0585	1.0460	1.4992	0.0491	1.6383
X_4X_7	0.7770	1.4667	2.0075	1.7177	0.0491	1.6383
X_5X_6	1.0532	0.2458	1.0460	1.6461	1.0532	1.6383
X_5X_7	1.1472	1.0692	1.7617	1.4996	1.0532	1.6383
X_6X_7	1.0532	1.0612	1.0460	1.4921	1.1472	0.6877

Chapter 4

The Second-Order Model With Two-Factor Interactions

When quadratic effects are introduced to a model, experimenters prefer to use three-level factors. In this chapter we consider two illustrative examples of three-level factor designs using the 12 optimality criteria. First we consider 24-run designs with 3 factors and then we consider 30-run designs with 4 factors. For non-Bayesian designs we used main effects and the second-order terms only model. For Bayesian designs we used the model with main effects, second-order terms and two-factor interactions while main effects and second-order terms are specified as primary terms and two-factor interactions are specified as potential terms. For each of these 12 optimality criteria we obtained optimal designs and differences among them are compared with various efficiency measures, degrees of freedom values and correlation measures.

4.1 24-run optimal designs with 3 three-level factors

Similar to the two-level scenario we searched 24-run three-level optimal designs with 3 factors using the 12 optimality criteria. Examples of the obtained optimal designs for each criterion are listed in Table A.13 - Table A.15. The degrees of freedom of pure error, the degrees of freedom of lack of fit and the values of I-efficiency, I_D-efficiency, $tr(\mathbf{AA}')$ and D-efficiency of the optimal designs are listed in Table 4.1.

Table 4.1: Comparison of 24-run three-level optimal designs with 3 factors

Criterion	df_{pe}	df_{LoF}	I-eff	I_D-eff	$tr(\mathbf{AA}')$	D-eff
I	6	11	1.0000	0.9507	0.4118	0.9549
I_D	4	13	0.9162	1.0000	0.8333	0.9877
IP	15	2	0.9946	0.9545	2.3517	0.9277
I_DP	14	3	0.9162	1.0000	1.6875	0.9877
BI	3	14	0.9568	0.9958	0.1645	0.9703
BI_D	3	14	0.9162	1.0000	0.0000	0.9877
BIP	10	7	0.9916	0.9418	0.0000	0.9691
BI_DP	10	7	0.7594	0.9179	0.0503	0.9375
D	6	11	0.8696	0.9120	1.4821	1.0000
DP	15	2	0.8696	0.9120	3.7551	1.0000
BD	7	10	0.6545	0.8536	0.3155	0.9292
BDP	13	4	0.6002	0.7599	0.0000	0.8586

From Table 4.1, we can see that I_D-, IP-, I_DP-, Bayesian I_D- and Bayesian IP-optimal designs are all above 90% I-efficient and D-efficient.

$tr(\mathbf{AA'})$ values show the same pattern like in the examples in chapter 3. Highest values are showed by DP-, IP- and I_DP-optimal designs. IP- and I_DP-optimal designs show much higher value compared to other Bayesian designs. This is clearly visible in Figure 4.1.

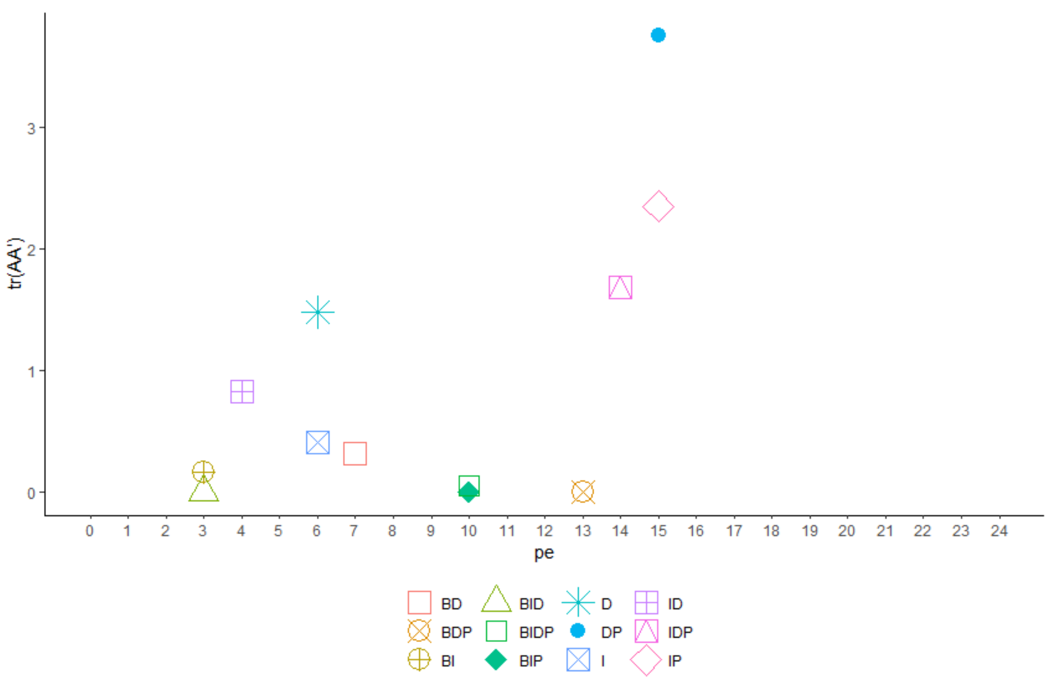
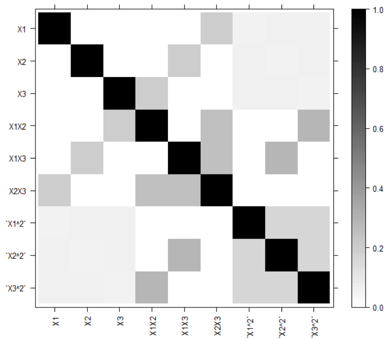
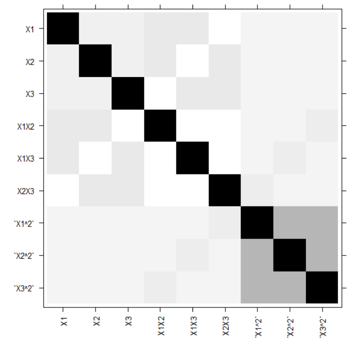


Figure 4.1: $tr(\mathbf{AA'})$ values of 24-run three-level optimal designs with 3 factors

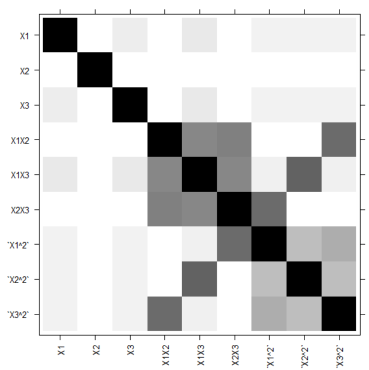
The absolute correlation graphs for each of the optimal designs are shown in Figure 4.2.



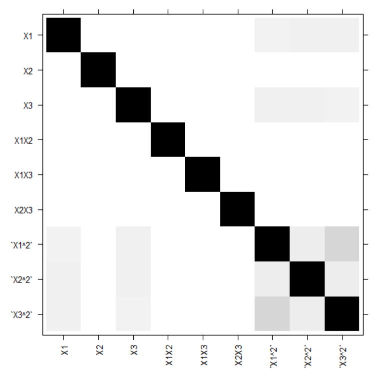
I



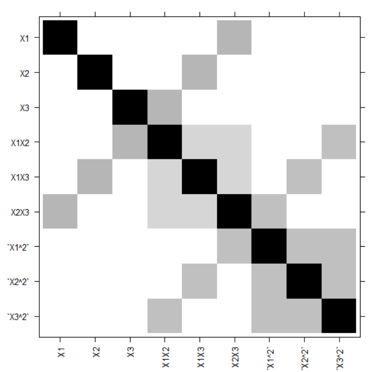
$B\mathrm{I}$



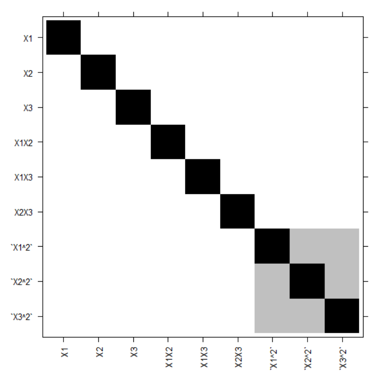
IP



BIP



I_D



BI_D

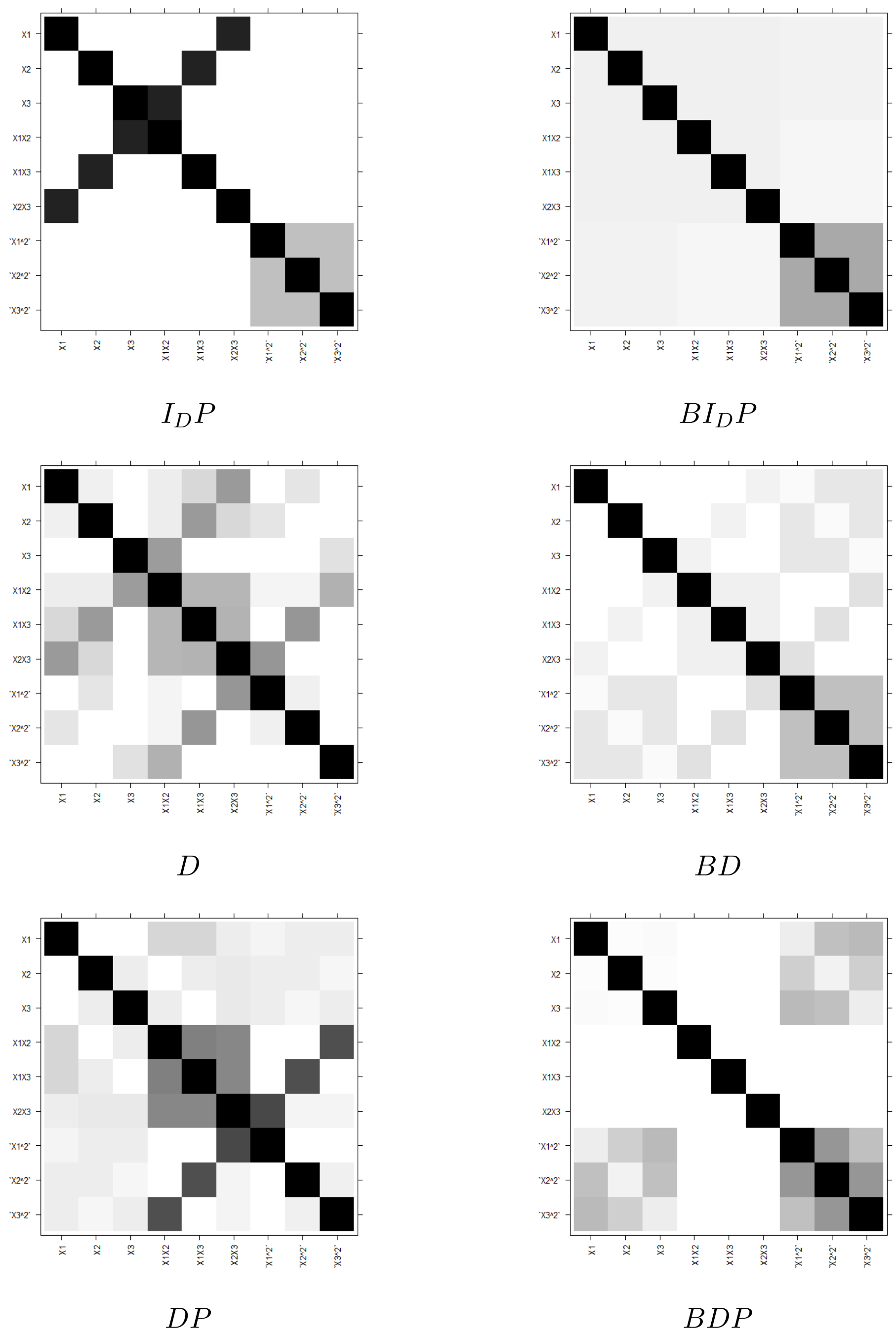


Figure 4.2: Absolute correlation maps of 24-run three-level optimal designs with 3 factors

From Figure 4.2 and the mean absolute correlation results in Table 4.2, it is clearly visible that correlations among primary and potential terms are reduced in Bayesian designs compared to corresponding non-Bayesian designs. I-, Bayesian IP-, I_D-, Bayesian I_D-, I_DP, and Bayesian D- optimal designs are orthogonal designs which had no correlation among main effects. Bayesian I_D-, Bayesian IP- and Bayesian DP-optimal designs show correlations only among primary terms.

Table 4.2: Mean absolute correlations of 24-run three-level optimal designs with 3 factors

Criterion	Primary & primary correlation	Primary & potential correlation	Potential & potential correlation
I	0.0679	0.0649	0.1667
I_D	0.0500	0.0898	0.1667
IP	0.0818	0.1153	0.4817
I_DP	0.0500	0.1443	0.0000
BI	0.0962	0.0569	0.0038
BI_D	0.0500	0.0000	0.0000
BIP	0.0445	0.0000	0.0000
BI_DP	0.1132	0.0484	0.0696
D	0.0310	0.1586	0.2911
DP	0.0476	0.1610	0.4851
BD	0.0902	0.0305	0.0625
BDP	0.1828	0.0000	0.0000

We have calculated the relative variance of coefficients for Bayesian designs. The results are in Table 4.3.

Table 4.3: Relative variance of factor effect estimates of 24-run three-level optimal designs with 3 factors

	BI	BI_D	BIP	BI_DP	BD	BDP
Intercept	0.1694	0.2017	0.1685	0.2604	0.3565	0.3373
X_1	0.069	0.0625	0.0781	0.0584	0.0538	0.0616
X_2	0.069	0.0625	0.0714	0.0584	0.0538	0.0617
X_3	0.069	0.0625	0.0781	0.0584	0.0538	0.0616
X_1X_2	0.094	0.0833	0.1250	0.0691	0.0642	0.0625
X_1X_3	0.094	0.0833	0.1250	0.0691	0.0642	0.0625
X_2X_3	0.094	0.0833	0.1250	0.0691	0.0642	0.0625
X_1^2	0.1938	0.1938	0.1646	0.2460	0.2619	0.3125
X_2^2	0.1938	0.1938	0.1648	0.2460	0.2619	0.3092
X_3^2	0.1938	0.1938	0.1646	0.2460	0.2619	0.3125

According to the results in Table 4.3, it is observed that Bayesian I_D-optimal design estimates all two-factor interactions and the second-order effects more precisely than Bayesian I-optimal design while Bayesian I-optimal design estimates the intercept more precisely than Bayesian I_D-optimal design.

Bayesian D-optimal design estimates the main effects more precisely than any other designs while Bayesian DP-optimal design estimates the two-factor interactions more precisely than other designs. Bayesian IP-optimal design estimates 2 out of the 3 second order effects and the intercept more precisely than other designs.

4.2 30-run optimal designs with 4 three-level factors

Using the 12 optimality criteria, we obtained 30-run three-level optimal designs with 4 factors. Table A.16 - Table A.21 show the examples of obtained optimal designs for each criterion.

To see the differences among each of these optimal designs we calculated the degrees of freedom of pure error, the degrees of freedom of lack of fit, the values of I-efficiency, I_D-efficiency, $tr(\mathbf{AA}')$ and D-efficiency of the optimal designs, which are listed in Table 4.4.

Table 4.4: Comparison of 30-run three-level optimal designs with 4 factors

Criterion	df_{pe}	df_{LoF}	I-eff	I_D-eff	$tr(\mathbf{AA}')$	D-eff
I	3	18	1.0000	0.9402	1.1921	0.9313
I_D	2	19	0.9251	1.0000	2.1284	0.9596
IP	20	1	0.9992	0.9767	6.6543	0.9568
I_DP	21	0	0.9901	1.0000	12.0000	0.9804
BI	5	16	0.9720	0.9850	0.1004	0.9347
BI_D	4	17	0.8726	0.9802	0.4437	0.9355
BIP	11	10	0.9662	0.9546	0.6510	0.9286
BI_DP	11	10	0.8380	0.9355	0.9810	0.9179
D	0	21	0.8020	0.8971	1.2377	1.0000
DP	21	0	0.8103	0.8802	10.5000	0.9991
BD	1	20	0.4766	0.7144	0.6055	0.9012
BDP	15	6	0.4081	0.5780	7.2044	0.8019

According to the results in Table 4.4, it is interesting to see that, except for D-optimal design, all other designs show replicate points. However, the number of replicate points are reduced relatively for I-, I_D-, Bayesian I-, D- and Bayesian D-optimal designs comparing to the 24-run three-level designs with 3 factors. This is due to the run size of 24 is relatively large compared to three-level 3 factors full factorial design run size 27. 30 runs is relatively small compared to three-level 4 factors full factorial run size which is 81.

When comparing I-efficiency and D-efficiency, except for the Bayesian D- and Bayesian DP-optimal designs, all other designs are above 80% I-efficient and above 90% D-efficient.

I_DP-, DP- and IP-optimal designs show the highest $tr(\mathbf{AA'})$ values. Bayesian designs show lower $tr(\mathbf{AA'})$ values compared to non-Bayesian designs in general. This can be clearly seen in Figure 4.3.

Absolute correlation graphs of the optimal designs are shown in Figure 4.4. From Figure 4.4 and the mean absolute correlation results in Table 4.5, one can see that it follows the same pattern as the previous cases where pairwise correlations between primary and potential terms are reduced in Bayesian designs compared to corresponding non-Bayesian designs. The I_DP-optimal design shows orthogonality and shows no correlation among main effects and two-factor interactions. The Bayesian I-optimal design shows no correlation among its potential terms.

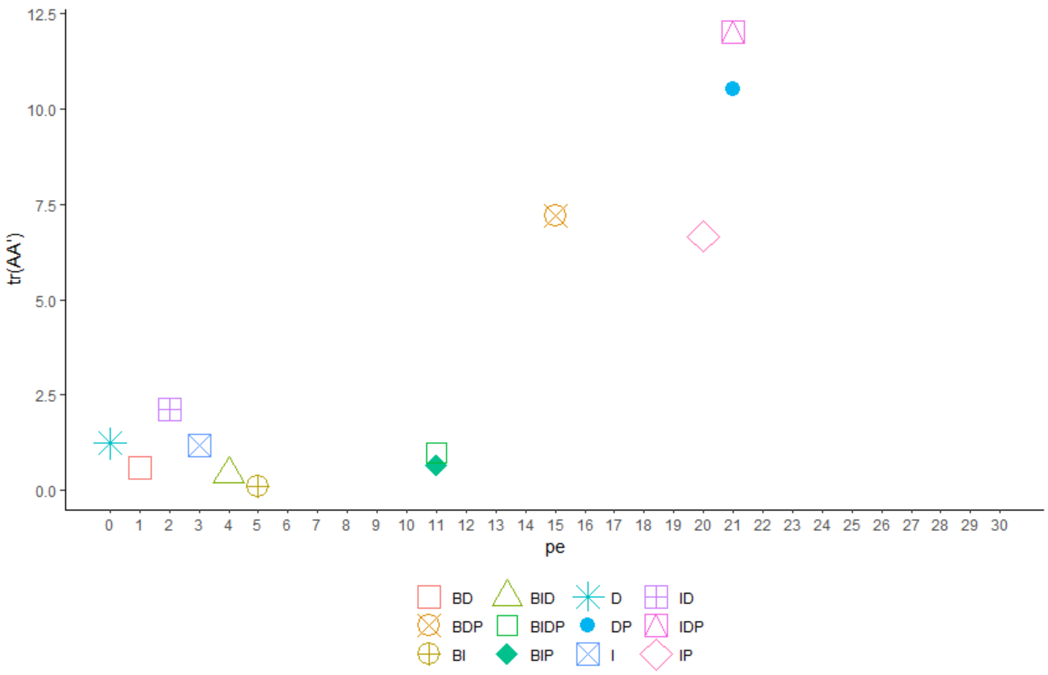
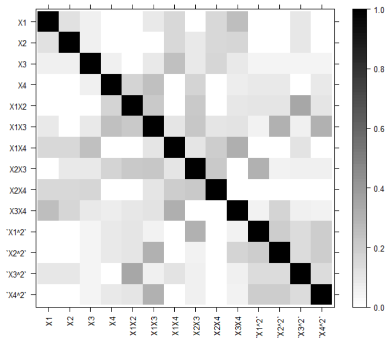
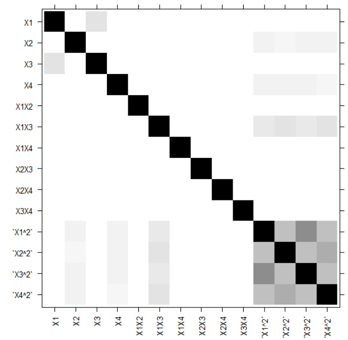


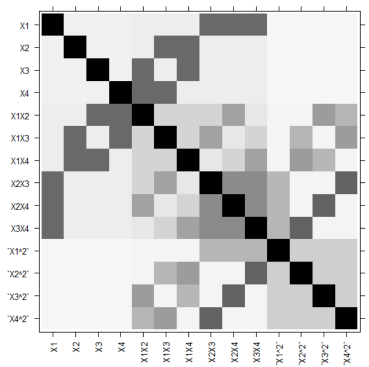
Figure 4.3: $tr(\mathbf{AA'})$ values of 30-run three-level optimal designs with 4 factors



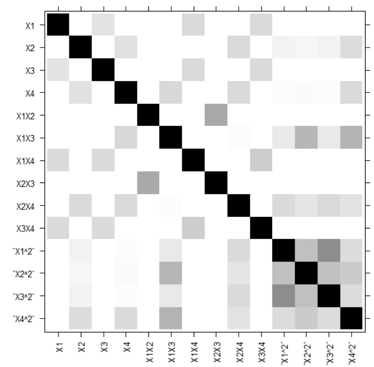
I



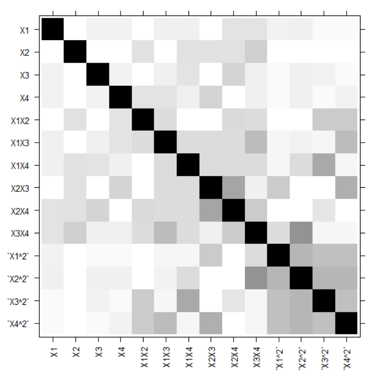
BI



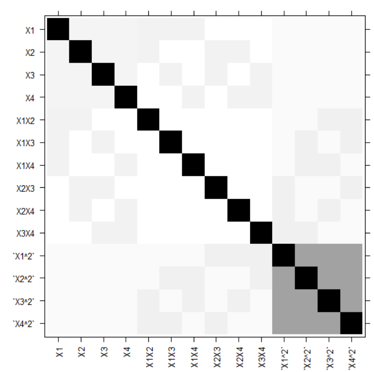
IP



BIP



I_D



BI_D

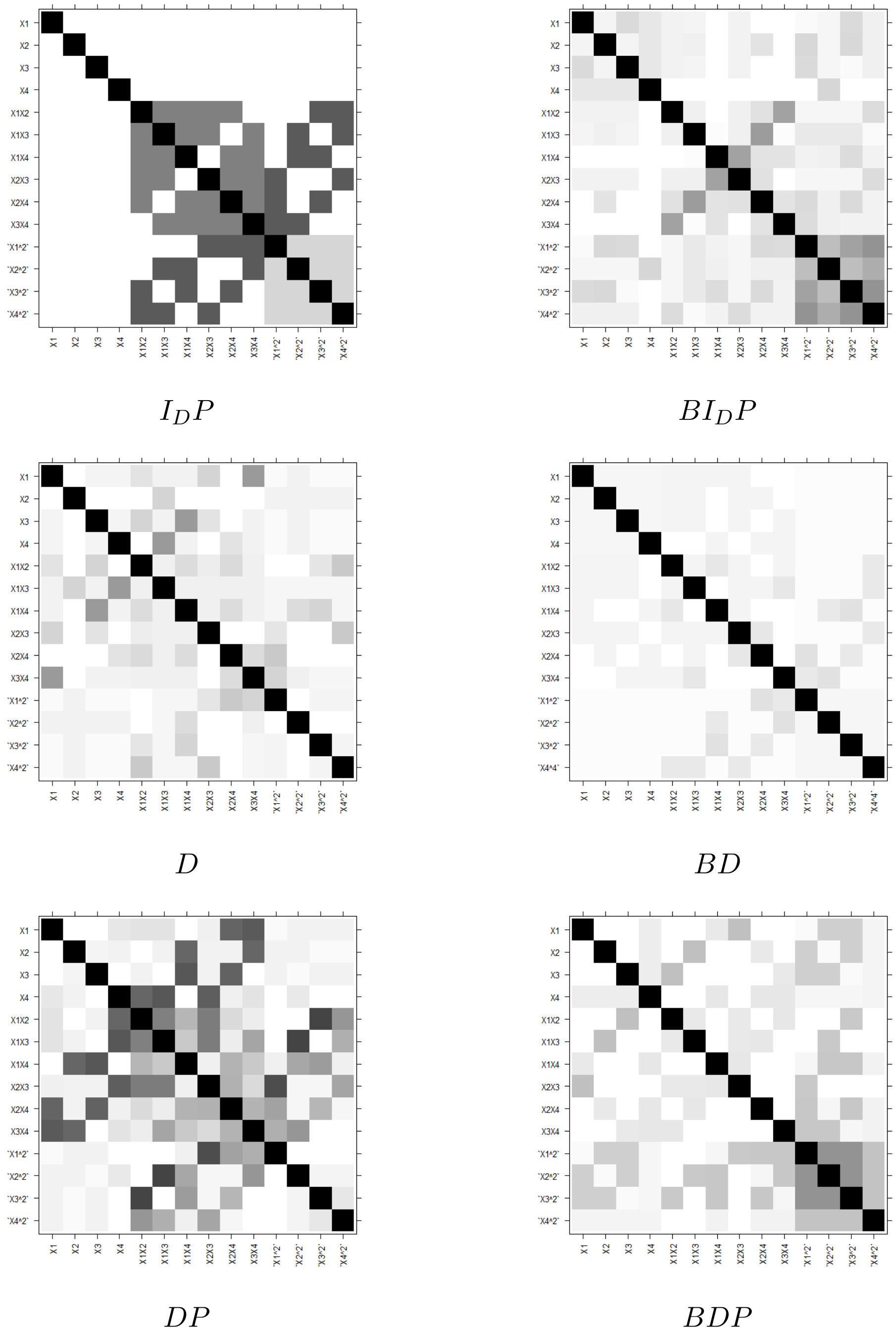


Figure 4.4: Absolute correlation maps of 30-run three-level optimal designs with 4 factors

Table 4.5: Mean absolute correlations of 30-run three-level optimal designs with 4 factors

Criterion	Primary & primary correlation	Primary & potential correlation	Potential & potential correlation
I	0.0687	0.1024	0.1286
I_D	0.0834	0.0953	0.1428
IP	0.0750	0.2435	0.2547
I_DP	0.0357	0.1614	0.4000
BI	0.0808	0.0082	0.0000
BI_D	0.1030	0.0374	0.0020
BIP	0.0763	0.0478	0.0363
BI_DP	0.1321	0.0500	0.1292
D	0.0330	0.0848	0.0782
DP	0.0374	0.2498	0.2681
BD	0.0262	0.0380	0.0378
BDP	0.1315	0.0738	0.0375

We have calculated the relative variance of coefficients for Bayesian designs. The results are in Table 4.6. From the results in Table 4.6, it can be seen that Bayesian I_D-optimal design estimates the main effects and two-factor interactions more precisely than the Bayesian I-optimal design while Bayesian I-optimal design estimates the intercept and the second order effects more precisely than all other designs. Bayesian D-optimal design estimates main effects and the two-factor interactions more precisely than all other designs.

Bayesian I_D-optimal design estimates intercept and second-order effects more precisely than Bayesian D-optimal design, while Bayesian D-optimal design estimates main effects and two-factor interactions more precisely than Bayesian I_D-optimal design. Bayesian IP-optimal design estimates intercept and second-order effects more precisely than Bayesian DP-optimal design while Bayesian DP-optimal design estimates main effects and two-factor interactions more precisely than the Bayesian IP-optimal design. Bayesian DP-optimal design estimates main effects, second-order terms and two-factor interactions more precisely than Bayesian I_DP-optimal design while Bayesian I_DP-optimal design estimates intercept more precisely than Bayesian DP-optimal design.

Table 4.6: Relative variance of factor effect estimates of 30-run three-level optimal designs with 4 factors

	BI	BI_D	BIP	BI_DP	BD	BDP
Intercept	0.1321	0.1791	0.1346	0.1899	0.5921	0.6936
X_1	0.0563	0.0486	0.0590	0.0514	0.0405	0.0455
X_2	0.0595	0.0486	0.0620	0.0565	0.0405	0.0455
X_3	0.0563	0.0486	0.0590	0.0514	0.0405	0.0455
X_4	0.0595	0.0504	0.0726	0.0479	0.0405	0.0487
X_1X_2	0.0833	0.0608	0.0938	0.0813	0.0490	0.0493
X_1X_3	0.0752	0.0608	0.0921	0.0716	0.0490	0.0493
X_1X_4	0.0833	0.061	0.1079	0.0693	0.0495	0.0631
X_2X_3	0.0833	0.0603	0.0938	0.0815	0.0490	0.0493
X_2X_4	0.0811	0.0596	0.1078	0.0776	0.0487	0.0618
X_3X_4	0.0811	0.0596	0.1042	0.0677	0.0487	0.0618
X_1^2	0.1700	0.2004	0.1694	0.2128	0.2287	0.4370
X_2^2	0.1531	0.1968	0.1650	0.1672	0.2288	0.4371
X_3^2	0.1700	0.1968	0.1694	0.2129	0.2288	0.4371
X_4^2	0.1531	0.1943	0.1599	0.2335	0.2288	0.1768

Chapter 5

Conclusion and Future Work

Constructing partially replicated designs is important in order to estimate the experimental error by conducting formal lack of fit tests. Prediction efficiency has gained greater importance in industry. In this thesis we have introduced three new optimality criteria to construct partially replicated designs with high prediction efficiency. Four illustrative examples are discussed to compare the performances of newly introduced criteria with existing criteria. Moreover, Bayesian I-optimal designs are compared with Bayesian D-optimal designs.

When comparing Bayesian I_D-optimal designs Bayesian D-optimal designs have higher D-efficiency and I-efficiency values in the first order model, but those efficiency values are very close. However, in the second order model, Bayesian I_D-optimal designs have higher I-efficiency and D-efficiency values than Bayesian D-optimal designs. In both models, minimal $tr(\mathbf{AA}')$ values are observed in Bayesian I_D-optimal designs.

In comparison with Bayesian D-optimal designs, we see that Bayesian IP-

and Bayesian I_DP-optimal designs have higher I-efficiency and D-efficiency values and minimal $tr(\mathbf{AA}')$ values in the second order model. But we did not see any pattern in the first order model.

In comparison with Bayesian I-optimal designs with Bayesian D-optimal designs, it is visible that Bayesian I-optimal designs always have equal or higher I-efficiency and D-efficiency values. In addition, the $tr(\mathbf{AA}')$ values of Bayesian I-optimal designs are smaller or equal to that of Bayesian D-optimal designs.

In general, based on our results, it can be seen that the newly introduced Bayesian IP and Bayesian I_DP optimality criteria select optimal designs that have replicated points, which allows the experimenter to conduct formal lack of fit tests. Bayesian I type of optimal designs (Bayesian I-, Bayesian IP-, Bayesian I_D- and Bayesian I_DP-optimal designs) are better than Bayesian D type of optimal designs (Bayesian D- and Bayesian DP-optimal designs) since Bayesian I type of optimal designs have higher D-efficiency, but Bayesian D type of optimal designs have very low I-efficiency. In terms of factor effect estimates, Bayesian I type of designs performed better in estimating the second order effects for the second order model.

We also found that $tr(\mathbf{AA}')$ values are higher in DP-, I_DP- and IP-optimal designs compared to the optimal designs obtained using other 9 optimality criteria we discussed. From the correlation maps it is clearly visible that correlations among primary and potential terms are reduced in Bayesian designs compared to the corresponding non-Bayesian designs.

In our research, we select optimal designs using one optimality criterion. One possible future work is to select optimal designs using compound criteria which combine two or more criteria based on different interests of experimenters. For example, we can use both I-efficiency and $tr(\mathbf{AA}')$ to obtain efficient designs with both high I-efficiency and low bias values.

Graphical methods like variance dispersion graphs (VDG) (Jensen and Myers, 1989) and difference variance dispersion graphs (DVDGs) (Trinca and Gilmour, 1999) can also be used to select designs with high prediction efficiency. VDG plots the minimum, mean and maximum variances of prediction while DVDG plots the variances of response difference. In addition, fractional design space (FDS) plots (Zahran et al., 2003) and difference fraction of design space (DFDS) plots (de Oliveira et al., 2019) can also be used to illustrate the response prediction properties of designs. FDS plots show the prediction variance against the relative volume of region while DFDS plots show the prediction variances of estimated response differences against fraction of design space. DFDS plots are capable of showing the properties of a design for each part of the design region. Another possible future work is to extend the graphical methods to Bayesian designs.

Our proposed new criteria helps to select partially replicated optimal designs. It is particularly useful for screening designs. This can been seen from the examples in chapter 3. However, for the second order model in chapter 4, due to the high computation time and the problem of calculating $(X'X)^{-1}$ and $(X'X+R)^{-1}$ using R software, we cannot provide examples that have large number of factors, but with relatively smaller run sizes. This is one of the major limitation we come across with our research. Different computer software like Python may help to calculate the $(X'X)^{-1}$ and $(X'X+R)^{-1}$ values for large number of factors. This might be one possible future work.

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Appendix A

Appendix

Table A.1: 18-run two-level I- and Bayesian I-optimal designs with 6 factors.

Run	I						BI					
	X_1	X_2	X_3	X_4	X_5	X_6	X_1	X_2	X_3	X_4	X_5	X_6
1	-1	-1	-1	1	1	1	-1	-1	-1	1	-1	1
2	-1	1	-1	-1	-1	1	1	-1	-1	1	1	1
3	1	1	1	-1	1	-1	1	1	-1	-1	-1	1
4	-1	1	-1	-1	-1	-1	-1	1	1	-1	-1	-1
5	1	-1	-1	-1	1	1	1	-1	1	1	-1	-1
6	-1	-1	1	1	1	1	-1	1	1	1	-1	1
7	1	-1	1	-1	-1	1	1	-1	-1	-1	1	-1
8	-1	-1	1	1	-1	-1	-1	1	-1	1	1	-1
9	-1	1	-1	-1	1	-1	-1	-1	-1	-1	-1	-1
10	1	1	1	-1	1	-1	-1	-1	1	1	1	1
11	-1	-1	1	-1	-1	1	-1	-1	1	-1	1	-1
12	1	-1	-1	1	-1	-1	1	-1	1	-1	-1	1
13	1	-1	-1	1	-1	-1	-1	1	-1	-1	1	1
14	1	1	-1	1	1	1	1	1	-1	1	-1	-1
15	-1	1	1	1	1	-1	1	1	1	-1	1	1
16	-1	-1	1	-1	1	-1	-1	1	-1	1	1	1
17	1	1	1	1	-1	1	1	-1	1	1	-1	1
18	-1	1	1	1	-1	1	1	1	1	1	1	-1

Table A.2: 18-run two-level IP- and Bayesian IP-optimal designs with 6 factors.

Run	IP						BIP					
	X_1	X_2	X_3	X_4	X_5	X_6	X_1	X_2	X_3	X_4	X_5	X_6
1	-1	1	1	-1	1	-1	1	-1	1	1	-1	-1
2	-1	-1	1	1	-1	-1	-1	-1	1	1	-1	1
3	-1	1	1	-1	1	-1	1	-1	1	1	-1	1
4	1	-1	-1	1	1	-1	1	1	1	1	-1	1
5	-1	-1	-1	-1	-1	1	-1	1	-1	-1	-1	-1
6	-1	-1	-1	-1	-1	1	1	-1	-1	1	-1	1
7	1	-1	1	-1	1	1	-1	-1	-1	-1	1	-1
8	1	1	-1	-1	-1	-1	1	-1	1	-1	-1	1
9	-1	1	1	-1	1	-1	-1	1	-1	-1	1	1
10	-1	1	-1	1	1	1	-1	-1	1	1	-1	1
11	1	-1	-1	1	1	-1	-1	1	-1	1	1	-1
12	1	1	1	1	-1	1	-1	1	1	-1	1	-1
13	-1	-1	1	1	-1	-1	1	-1	1	1	-1	1
14	1	1	1	1	-1	1	1	-1	1	1	-1	1
15	1	1	1	1	-1	1	1	1	-1	-1	1	-1
16	-1	1	-1	1	1	1	1	-1	1	1	-1	-1
17	1	1	-1	-1	-1	-1	1	-1	1	-1	-1	1
18	1	-1	1	-1	1	1	1	-1	1	1	1	1

Table A.3: 18-run two-level I_D- and Bayesian I_D-optimal designs with 6 factors.

Run	I_D						BI_D					
	X_1	X_2	X_3	X_4	X_5	X_6	X_1	X_2	X_3	X_4	X_5	X_6
1	-1	1	1	-1	-1	-1	1	-1	-1	-1	-1	-1
2	-1	1	1	-1	-1	1	-1	-1	-1	1	-1	1
3	-1	-1	-1	-1	1	-1	-1	1	-1	-1	-1	1
4	-1	-1	1	1	1	1	1	1	1	-1	-1	1
5	1	-1	-1	1	-1	-1	1	1	-1	1	-1	1
6	1	-1	1	1	1	1	1	-1	1	1	-1	-1
7	-1	-1	1	1	-1	-1	1	1	-1	-1	1	1
8	-1	-1	-1	-1	-1	1	1	1	1	1	1	1
9	-1	1	-1	1	1	-1	-1	1	1	-1	1	1
10	-1	1	-1	1	1	1	-1	-1	-1	-1	1	-1
11	1	1	-1	-1	1	1	-1	1	1	1	-1	1
12	1	-1	1	-1	1	-1	-1	1	-1	1	-1	-1
13	-1	1	1	1	-1	-1	1	-1	-1	1	1	-1
14	1	1	-1	1	-1	-1	-1	-1	1	1	1	-1
15	1	1	1	1	-1	1	1	1	1	-1	1	-1
16	1	-1	1	-1	-1	-1	1	-1	1	-1	1	1
17	1	1	1	-1	1	-1	-1	-1	1	-1	-1	-1
18	1	-1	-1	-1	-1	1	-1	1	-1	1	1	1

Table A.4: 18-run two-level I_DP- and Bayesian I_DP-optimal designs with 6 factors.

Run	I_DP						BI_DP					
	X_1	X_2	X_3	X_4	X_5	X_6	X_1	X_2	X_3	X_4	X_5	X_6
1	-1	1	1	-1	1	-1	-1	-1	-1	1	1	-1
2	-1	-1	1	1	1	1	-1	1	-1	1	-1	1
3	-1	1	1	-1	1	-1	1	1	1	-1	-1	1
4	1	-1	1	-1	-1	-1	-1	1	1	1	-1	-1
5	-1	1	1	-1	1	-1	1	1	1	1	1	1
6	1	1	1	1	-1	1	1	-1	-1	-1	1	1
7	-1	-1	1	1	1	1	-1	1	-1	-1	1	-1
8	1	1	1	1	-1	1	-1	1	1	1	-1	-1
9	1	1	-1	-1	1	1	-1	-1	-1	-1	-1	-1
10	1	-1	-1	1	1	-1	1	1	-1	1	-1	-1
11	-1	-1	-1	-1	-1	1	1	-1	1	1	-1	1
12	-1	-1	-1	-1	-1	1	1	-1	1	-1	1	-1
13	1	-1	1	-1	-1	-1	1	1	-1	1	-1	-1
14	-1	1	-1	1	-1	-1	-1	-1	-1	1	1	-1
15	1	-1	-1	1	1	-1	-1	1	-1	1	-1	1
16	1	-1	1	-1	-1	-1	-1	-1	-1	-1	-1	-1
17	-1	1	-1	1	-1	-1	-1	-1	1	-1	1	1
18	1	1	-1	-1	1	1	-1	1	-1	-1	1	-1

Table A.5: 18-run two-level D- and Bayesian D-optimal designs with 6 factors.

Run	D						BD					
	X_1	X_2	X_3	X_4	X_5	X_6	X_1	X_2	X_3	X_4	X_5	X_6
1	-1	1	1	1	1	-1	-1	1	-1	-1	-1	-1
2	1	-1	-1	1	1	1	1	-1	1	-1	-1	1
3	1	1	1	1	-1	-1	-1	-1	1	1	1	1
4	-1	1	-1	1	1	-1	-1	-1	1	-1	1	-1
5	1	-1	-1	1	1	-1	-1	-1	-1	-1	-1	1
6	1	-1	1	-1	1	-1	1	-1	-1	1	-1	1
7	1	1	-1	-1	1	1	1	1	1	1	-1	-1
8	-1	-1	1	-1	1	1	-1	1	-1	-1	1	1
9	1	1	-1	1	-1	1	1	1	-1	-1	-1	1
10	1	1	1	-1	-1	1	-1	1	-1	1	-1	1
11	-1	-1	1	1	-1	1	1	1	-1	1	1	-1
12	-1	1	-1	-1	1	1	-1	-1	1	1	-1	-1
13	-1	-1	-1	-1	-1	-1	-1	1	1	1	1	-1
14	1	1	1	-1	1	-1	1	-1	-1	-1	1	-1
15	-1	1	-1	-1	-1	-1	1	1	1	-1	1	1
16	-1	-1	-1	-1	-1	-1	-1	-1	-1	1	1	-1
17	1	-1	-1	-1	-1	-1	1	-1	1	1	1	-1
18	-1	-1	1	1	-1	1	-1	1	1	-1	-1	1

Table A.6: 18-run two-level DP- and Bayesian DP-optimal designs with 6 factors.

Run	DP						BDP					
	X_1	X_2	X_3	X_4	X_5	X_6	X_1	X_2	X_3	X_4	X_5	X_6
1	1	-1	-1	-1	1	1	1	1	-1	1	-1	1
2	-1	-1	1	1	1	-1	-1	-1	-1	1	-1	-1
3	-1	1	-1	-1	-1	-1	1	1	1	-1	1	1
4	-1	-1	-1	1	-1	1	1	-1	1	-1	-1	-1
5	-1	-1	-1	1	-1	1	-1	1	-1	-1	-1	-1
6	-1	1	1	-1	1	1	1	-1	1	1	1	1
7	1	1	-1	1	1	-1	-1	-1	1	-1	1	-1
8	1	1	-1	1	1	-1	-1	-1	1	-1	-1	1
9	-1	1	-1	-1	-1	-1	1	-1	1	1	1	1
10	1	-1	-1	-1	1	1	1	-1	-1	-1	1	1
11	1	1	1	1	-1	1	1	1	-1	1	-1	1
12	1	-1	1	-1	-1	-1	-1	1	-1	1	1	1
13	1	-1	1	-1	-1	-1	-1	-1	-1	1	-1	-1
14	-1	-1	1	1	1	-1	1	1	-1	1	1	-1
15	1	1	1	1	-1	1	1	-1	-1	-1	1	1
16	-1	1	1	-1	1	1	-1	1	1	1	-1	-1
17	1	1	-1	1	1	-1	-1	1	-1	1	1	1
18	-1	1	-1	-1	-1	-1	1	1	-1	1	1	-1

Table A.7: 24-Run two-level I and Bayesian I-Optimal designs with 7 factors.

Run	I							Bayesian I						
	X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_1	X_2	X_3	X_4	X_5	X_6	X_7
1	-1	1	-1	1	-1	1	-1	-1	-1	1	1	1	1	-1
2	-1	-1	-1	-1	-1	1	-1	-1	1	1	1	-1	-1	1
3	1	1	-1	1	-1	-1	1	-1	-1	-1	-1	1	1	-1
4	-1	1	-1	1	1	-1	-1	1	-1	1	-1	1	1	-1
5	-1	1	1	1	1	-1	1	1	1	-1	-1	1	-1	-1
6	-1	-1	-1	1	1	1	1	1	1	1	1	1	-1	-1
7	1	1	-1	-1	-1	-1	-1	-1	1	1	-1	-1	1	-1
8	1	1	-1	-1	-1	1	1	-1	-1	1	-1	1	-1	-1
9	1	-1	1	1	-1	1	-1	1	-1	1	1	-1	1	1
10	-1	1	1	-1	-1	-1	1	-1	1	-1	-1	-1	-1	1
11	-1	-1	-1	1	1	1	1	-1	-1	1	-1	-1	1	1
12	1	1	-1	-1	1	1	-1	1	-1	1	-1	-1	-1	-1
13	-1	1	1	-1	1	1	1	1	-1	1	-1	1	-1	1
14	-1	-1	1	-1	1	-1	-1	-1	-1	-1	1	1	-1	1
15	1	1	1	-1	1	1	1	1	-1	-1	-1	-1	1	1
16	1	-1	1	-1	1	1	-1	1	1	-1	1	-1	1	-1
17	1	-1	1	1	-1	-1	1	1	1	-1	1	-1	-1	1
18	-1	1	1	1	-1	1	-1	-1	1	-1	1	1	-1	-1
19	1	-1	1	1	-1	1	1	1	-1	-1	1	1	-1	-1
20	1	1	1	1	1	-1	-1	1	1	1	-1	-1	1	1
21	-1	-1	-1	-1	-1	-1	1	-1	1	-1	1	-1	1	1
22	-1	-1	1	-1	-1	-1	-1	1	1	-1	1	1	1	1
23	1	-1	-1	-1	1	-1	1	-1	1	1	-1	1	1	1
24	1	-1	-1	1	1	-1	-1	-1	-1	-1	1	-1	-1	-1

Table A.8: 24-run two-level IP- and Bayesian IP-ptimal designs with 7-factors.

Run	IP							Bayesian IP						
	X1	X2	X3	X4	X5	X6	X7	X1	X2	X3	X4	X5	X6	X7
1	-1	1	1	-1	1	1	-1	-1	1	1	1	1	-1	-1
2	1	-1	1	-1	1	-1	1	1	1	-1	-1	1	-1	-1
3	1	-1	1	-1	1	-1	1	1	1	1	1	-1	-1	1
4	-1	-1	-1	1	1	1	1	1	1	-1	1	1	1	1
5	1	-1	-1	-1	-1	1	-1	1	-1	-1	1	-1	-1	-1
6	1	1	-1	1	1	-1	-1	-1	-1	-1	1	1	-1	1
7	-1	-1	-1	1	1	1	1	-1	1	1	-1	1	1	1
8	-1	1	1	-1	1	1	-1	1	1	-1	-1	1	-1	-1
9	1	-1	-1	-1	-1	1	-1	1	-1	1	1	1	1	-1
10	-1	1	-1	-1	-1	-1	1	-1	-1	-1	1	1	-1	1
11	1	1	1	1	-1	1	1	-1	-1	1	1	-1	1	1
12	1	1	1	1	-1	1	1	-1	-1	-1	-1	1	1	-1
13	-1	-1	1	1	-1	-1	-1	-1	1	-1	1	-1	-1	-1
14	1	-1	1	-1	1	-1	1	1	1	1	1	-1	-1	1
15	-1	-1	-1	1	1	1	1	-1	1	-1	1	-1	-1	-1
16	1	-1	-1	-1	-1	1	-1	1	-1	-1	1	-1	1	-1
17	-1	1	1	-1	1	1	-1	1	-1	1	-1	1	1	1
18	1	1	1	1	-1	1	1	1	-1	-1	1	-1	-1	-1
19	1	1	-1	1	1	-1	-1	1	-1	-1	-1	-1	-1	1
20	-1	-1	1	1	-1	-1	-1	-1	-1	1	-1	-1	-1	-1
21	-1	-1	1	1	-1	-1	-1	1	1	1	-1	-1	1	-1
22	1	1	-1	1	1	-1	-1	-1	1	-1	-1	-1	1	1
23	-1	1	-1	-1	-1	-1	1	-1	1	-1	1	-1	1	-1
24	-1	1	-1	-1	-1	-1	1	-1	-1	1	-1	-1	-1	-1

Table A.9: 24-run two-level I_D- and Bayesian I_D-optimal designs with 7-factors.

Run	I_D							Bayesian I_D						
	X1	X2	X3	X4	X5	X6	X7	X1	X2	X3	X4	X5	X6	X7
1	1	-1	-1	1	1	1	1	1	1	1	-1	1	-1	1
2	1	-1	-1	1	-1	-1	-1	1	1	1	-1	-1	1	-1
3	1	-1	-1	-1	-1	1	1	1	-1	1	-1	1	-1	-1
4	-1	-1	1	-1	-1	-1	1	-1	1	1	-1	1	1	-1
5	-1	1	-1	-1	1	1	1	-1	1	1	1	1	-1	-1
6	-1	-1	1	1	1	1	1	1	1	-1	1	1	-1	-1
7	1	1	-1	1	-1	1	-1	1	1	-1	-1	1	-1	-1
8	-1	1	-1	1	1	-1	-1	1	1	1	1	-1	-1	1
9	-1	1	-1	-1	1	1	-1	-1	1	-1	-1	-1	1	-1
10	1	-1	-1	-1	1	-1	1	1	-1	-1	-1	-1	-1	-1
11	-1	-1	1	-1	-1	-1	-1	-1	1	1	-1	-1	-1	-1
12	-1	-1	-1	1	-1	1	1	1	-1	-1	-1	1	1	-1
13	1	1	1	-1	1	-1	1	-1	-1	-1	-1	1	-1	-1
14	1	1	1	-1	1	1	-1	1	1	-1	1	1	1	1
15	1	1	-1	-1	-1	-1	1	1	-1	-1	1	-1	1	-1
16	-1	1	1	1	-1	1	1	-1	1	1	-1	1	-1	1
17	1	-1	1	1	1	1	-1	1	-1	1	1	1	1	1
18	1	1	1	1	-1	-1	1	1	-1	-1	-1	-1	1	1
19	-1	1	1	1	1	-1	1	-1	1	-1	1	-1	-1	1
20	-1	-1	1	-1	-1	1	-1	-1	-1	1	1	-1	-1	1
21	-1	-1	-1	-1	1	-1	-1	1	-1	-1	1	1	-1	1
22	1	-1	1	1	1	-1	-1	-1	-1	1	-1	-1	1	-1
23	-1	1	-1	1	-1	-1	-1	-1	-1	-1	1	1	1	1
24	1	1	1	-1	-1	1	-1	-1	1	1	1	-1	1	1

Table A.10: 24-run two-level $I_D P$- and Bayesian $I_D P$-ptimal designs with 7-factors.

Run	$I_D P$							Bayesian $I_D P$						
	X1	X2	X3	X4	X5	X6	X7	X1	X2	X3	X4	X5	X6	X7
1	-1	-1	-1	-1	-1	1	-1	1	-1	-1	1	1	1	1
2	1	-1	-1	1	1	-1	-1	1	1	1	-1	-1	1	1
3	1	1	-1	-1	1	1	1	-1	1	1	-1	1	1	-1
4	1	1	1	-1	-1	-1	-1	-1	-1	1	-1	1	-1	-1
5	-1	-1	1	-1	1	-1	1	-1	-1	1	1	-1	1	1
6	1	-1	-1	1	1	-1	-1	1	1	1	1	-1	1	-1
7	1	-1	1	1	-1	1	1	-1	1	-1	1	-1	-1	1
8	1	-1	1	1	-1	1	1	1	-1	-1	1	-1	-1	1
9	-1	-1	-1	-1	-1	1	-1	-1	1	1	-1	-1	-1	-1
10	-1	-1	-1	-1	-1	1	-1	-1	-1	-1	-1	1	-1	1
11	-1	1	-1	1	-1	-1	1	-1	1	1	-1	-1	-1	-1
12	1	1	-1	-1	1	1	1	1	-1	1	-1	1	1	-1
13	-1	-1	1	-1	1	-1	1	1	1	1	1	1	-1	1
14	1	-1	1	1	-1	1	1	1	1	-1	-1	1	-1	-1
15	1	1	-1	-1	1	1	1	-1	-1	-1	1	1	-1	-1
16	-1	1	-1	1	-1	-1	1	1	-1	-1	1	-1	-1	1
17	-1	1	-1	1	-1	-1	1	-1	1	-1	1	-1	-1	1
18	1	1	1	-1	-1	-1	-1	1	-1	1	-1	-1	-1	-1
19	-1	1	1	1	1	1	-1	1	-1	-1	1	1	1	1
20	1	1	1	-1	-1	-1	-1	-1	1	1	-1	1	-1	1
21	-1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	1	-1
22	-1	-1	1	-1	1	-1	1	1	-1	1	-1	1	1	-1
23	-1	1	1	1	1	1	-1	-1	-1	1	-1	1	1	1
24	1	-1	-1	1	1	-1	-1	-1	1	1	-1	1	1	-1

Table A.11: 24-run two-level D and Bayesian D-optimal designs with 7-factors.

Run	D							Bayesian D						
	X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_1	X_2	X_3	X_4	X_5	X_6	X_7
1	-1	1	-1	1	-1	1	1	1	-1	1	-1	-1	1	1
2	-1	-1	1	1	-1	-1	-1	-1	1	1	1	-1	1	-1
3	1	-1	-1	1	-1	1	-1	-1	1	-1	-1	1	1	1
4	-1	1	-1	-1	-1	-1	1	1	-1	-1	-1	1	1	-1
5	1	-1	1	1	1	1	1	-1	-1	1	1	1	1	1
6	1	1	1	1	-1	1	1	-1	1	1	-1	-1	-1	1
7	-1	1	-1	1	-1	-1	1	1	1	-1	1	-1	1	1
8	1	-1	-1	-1	-1	1	-1	1	-1	1	1	-1	-1	1
9	-1	1	1	-1	1	-1	-1	-1	-1	-1	1	-1	1	-1
10	-1	-1	1	-1	-1	1	1	-1	1	-1	1	-1	-1	1
11	1	1	1	-1	-1	-1	-1	1	1	-1	1	-1	-1	-1
12	1	1	1	-1	1	1	1	-1	1	-1	-1	-1	1	-1
13	1	1	-1	-1	1	-1	-1	-1	1	-1	-1	1	-1	-1
14	1	-1	-1	1	1	-1	-1	1	-1	1	-1	-1	-1	-1
15	-1	1	1	1	1	1	-1	-1	-1	1	-1	1	1	-1
16	1	1	1	1	-1	-1	-1	-1	-1	-1	-1	-1	-1	1
17	-1	-1	-1	-1	1	-1	1	1	-1	1	1	1	1	-1
18	-1	-1	-1	-1	-1	1	-1	-1	-1	1	1	1	-1	-1
19	1	1	-1	-1	1	1	1	1	-1	1	-1	1	-1	1
20	-1	-1	1	1	1	-1	1	1	1	-1	-1	-1	-1	1
21	-1	-1	1	-1	1	1	-1	1	-1	-1	1	1	-1	1
22	1	-1	-1	1	1	-1	1	1	1	1	1	1	-1	1
23	1	-1	1	-1	-1	-1	1	-1	1	-1	1	1	1	-1
24	-1	1	-1	1	1	1	-1	1	1	1	-1	1	1	-1

Table A.12: 24-run two-level DP- and Bayesian DP-optimal designs with 7-factors.

Run	DP							Bayesian DP						
	X1	X2	X3	X4	X5	X6	X7	X1	X2	X3	X4	X5	X6	X7
1	1	-1	1	1	-1	1	1	1	1	-1	1	-1	-1	-1
2	-1	-1	1	1	1	-1	-1	1	-1	1	-1	-1	-1	-1
3	1	1	-1	1	-1	-1	-1	1	-1	-1	-1	-1	1	-1
4	-1	1	-1	1	1	1	1	1	-1	1	1	1	1	1
5	1	1	-1	1	-1	-1	-1	-1	-1	1	-1	1	1	1
6	-1	-1	-1	-1	-1	-1	1	-1	-1	1	-1	1	1	1
7	1	-1	-1	-1	1	1	-1	-1	-1	1	1	-1	-1	1
8	1	1	-1	1	-1	-1	-1	1	1	1	1	-1	1	1
9	1	-1	1	1	-1	1	1	1	1	1	-1	1	-1	1
10	-1	-1	-1	-1	-1	-1	1	-1	1	-1	-1	-1	-1	-1
11	1	-1	1	1	-1	1	1	-1	-1	-1	1	-1	1	1
12	-1	1	-1	1	1	1	1	-1	1	-1	-1	-1	-1	-1
13	1	1	1	-1	1	-1	1	1	1	-1	1	-1	-1	-1
14	-1	1	1	-1	-1	1	-1	-1	-1	-1	-1	1	-1	-1
15	-1	1	1	-1	-1	1	-1	-1	-1	1	1	-1	1	-1
16	1	-1	-1	-1	1	1	-1	1	1	-1	-1	1	1	1
17	1	-1	-1	-1	1	1	-1	1	1	1	-1	1	1	-1
18	1	1	1	-1	1	-1	1	1	1	1	1	-1	1	1
19	-1	-1	1	1	1	-1	-1	-1	1	-1	1	1	1	-1
20	1	1	1	-1	1	-1	1	-1	-1	-1	-1	1	-1	-1
21	-1	-1	1	1	1	-1	-1	1	-1	-1	-1	-1	-1	1
22	-1	1	1	-1	-1	1	-1	-1	1	-1	1	1	-1	1
23	-1	-1	-1	-1	-1	-1	1	1	-1	1	1	1	1	1
24	-1	1	-1	1	1	1	1	-1	1	1	1	1	-1	-1

Table A.13: 24-run three-level I-, Bayesian I-, IP-, and Bayesian IP-optimal designs with 3-factors.

Run	I			Bayesian I			IP			Bayesian IP		
	X1	X2	X3	X1	X2	X3	X1	X2	X3	X1	X2	X3
1	0	1	1	1	-1	1	0	0	0	0	-1	0
2	-1	-1	0	1	-1	-1	0	0	0	1	0	0
3	1	0	0	0	0	-1	1	1	1	0	-1	0
4	1	-1	1	0	0	0	0	0	0	1	0	0
5	1	1	-1	0	0	0	1	0	-1	0	0	1
6	0	-1	1	1	1	1	1	0	-1	1	-1	-1
7	-1	0	-1	0	0	0	1	1	1	0	-1	0
8	-1	0	-1	0	1	-1	0	0	0	0	0	-1
9	-1	1	0	-1	0	1	0	0	0	-1	-1	-1
10	0	0	0	1	1	0	0	-1	1	0	0	1
11	0	0	0	-1	0	-1	-1	1	0	-1	0	0
12	1	0	1	0	-1	0	0	0	0	0	0	-1
13	-1	1	1	1	0	1	-1	-1	-1	-1	-1	1
14	0	0	0	0	-1	1	1	-1	0	-1	0	0
15	0	1	-1	-1	1	1	0	1	-1	0	1	0
16	1	1	0	0	0	0	-1	0	1	1	-1	1
17	0	-1	0	-1	-1	1	0	-1	1	0	1	0
18	-1	-1	0	-1	1	-1	-1	-1	-1	0	0	-1
19	0	0	0	-1	1	0	-1	1	0	-1	0	0
20	1	-1	-1	1	0	0	0	0	0	-1	1	1
21	0	-1	-1	-1	-1	0	1	0	-1	-1	1	-1
22	0	0	-1	0	1	1	-1	0	1	1	1	-1
23	-1	0	1	1	1	-1	0	1	-1	0	1	0
24	0	0	0	-1	-1	-1	1	-1	0	1	1	1

Table A.14: 24-run three-level I_D-, Bayesian I_D-, I_DP-, and Bayesian I_DP-optimal designs with 3-factors.

Run	I_D			Bayesian I_D			I_DP			Bayesian I_DP		
	X1	X2	X3	X1	X2	X3	X1	X2	X3	X1	X2	X3
1	0	0	0	1	1	1	0	0	1	1	-1	1
2	-1	1	1	-1	-1	1	1	-1	1	1	1	1
3	0	0	0	0	0	0	1	-1	1	1	-1	-1
4	1	0	-1	0	0	0	1	1	-1	-1	1	-1
5	-1	1	1	1	1	-1	1	-1	1	1	-1	-1
6	-1	-1	-1	0	0	0	-1	-1	-1	-1	-1	-1
7	0	1	-1	1	-1	-1	-1	-1	-1	-1	-1	-1
8	0	-1	0	0	1	1	-1	1	1	-1	1	1
9	0	0	-1	0	0	0	0	-1	0	-1	1	1
10	1	-1	1	1	-1	1	-1	0	0	0	0	-1
11	-1	0	1	-1	0	1	-1	1	1	1	0	0
12	-1	1	-1	-1	0	-1	-1	0	0	0	1	0
13	1	1	-1	1	1	0	0	0	1	-1	-1	1
14	1	1	0	1	-1	0	0	-1	0	1	0	0
15	1	-1	-1	-1	1	-1	0	0	-1	1	-1	1
16	0	1	0	-1	-1	-1	-1	1	1	1	1	1
17	1	0	0	0	-1	1	-1	-1	-1	1	1	-1
18	-1	-1	0	-1	1	0	1	1	-1	0	0	-1
19	1	-1	1	1	0	1	1	1	-1	0	1	0
20	0	-1	1	-1	-1	0	0	0	-1	-1	0	0
21	-1	0	0	1	0	-1	0	1	0	-1	1	-1
22	0	0	1	0	1	-1	0	1	0	0	0	1
23	-1	-1	-1	-1	1	1	1	0	0	1	1	-1
24	1	1	1	0	-1	-1	1	0	0	0	-1	0

Table A.15: 24-Run three-level D, Bayesian D-, DP-, and Bayesian DP-optimal designs with 3-factors.

Run	D			Bayesian D			DP			Bayesian DP		
	X_1	X_2	X_3	X_1	X_2	X_3	X_1	X_2	X_3	X_1	X_2	X_3
1	-1	0	0	-1	1	1	-1	1	-1	1	-1	1
2	0	0	1	1	-1	1	-1	-1	0	-1	1	-1
3	1	-1	1	-1	1	1	0	1	1	-1	1	1
4	-1	1	-1	-1	0	0	0	1	1	0	1	0
5	0	-1	-1	-1	-1	1	0	-1	-1	-1	1	1
6	0	0	0	-1	-1	1	0	-1	-1	0	1	0
7	-1	1	-1	-1	-1	-1	1	-1	1	0	0	1
8	1	-1	0	1	-1	1	1	1	0	1	-1	-1
9	0	1	0	1	0	0	-1	0	1	1	-1	1
10	-1	-1	1	1	-1	-1	-1	0	1	0	0	1
11	1	1	0	1	1	-1	0	1	1	-1	0	0
12	1	-1	-1	-1	1	-1	-1	-1	0	-1	-1	-1
13	-1	-1	0	-1	1	-1	1	1	0	1	1	1
14	1	0	-1	1	1	1	1	0	-1	1	1	-1
15	1	0	0	1	1	0	1	0	-1	1	-1	-1
16	-1	1	-1	0	0	-1	1	1	0	0	0	1
17	0	1	1	0	0	1	1	-1	1	-1	-1	-1
18	0	0	-1	1	0	-1	-1	1	-1	-1	0	0
19	1	1	1	1	1	1	0	-1	-1	1	1	1
20	0	-1	-1	0	-1	0	0	0	0	1	1	-1
21	1	0	-1	0	1	-1	0	0	0	-1	-1	1
22	0	1	0	-1	-1	-1	0	0	0	-1	0	0
23	-1	-1	0	1	-1	-1	-1	1	-1	-1	-1	1
24	-1	0	1	0	1	0	1	0	-1	-1	1	-1

Table A.16: 30-run three-level I- and Bayesian I-optimal designs with 4-factors.

Run	I				Bayesian I			
	X_1	X_2	X_3	X_4	X_1	X_2	X_3	X_4
1	0	0	1	-1	0	0	0	1
2	0	0	0	0	1	1	-1	-1
3	0	0	-1	0	0	0	0	0
4	-1	-1	0	-1	1	-1	0	-1
5	0	-1	0	0	0	0	0	0
6	0	0	0	0	0	-1	1	1
7	0	1	-1	1	1	1	1	0
8	1	1	0	-1	1	0	-1	0
9	0	0	0	0	1	1	0	1
10	-1	1	1	-1	1	0	1	1
11	-1	0	1	0	0	-1	-1	-1
12	-1	0	0	1	0	1	-1	1
13	-1	-1	0	1	-1	1	1	1
14	1	0	-1	1	-1	1	-1	0
15	0	-1	1	1	-1	0	-1	1
16	-1	-1	-1	0	0	0	0	0
17	-1	1	-1	0	1	-1	-1	1
18	1	-1	-1	-1	0	0	0	0
19	0	1	0	0	-1	-1	1	-1
20	1	1	1	1	-1	1	0	-1
21	0	-1	0	-1	0	0	0	0
22	1	0	-1	-1	0	1	0	0
23	0	1	-1	-1	1	0	1	-1
24	1	1	0	0	-1	0	1	0
25	0	0	0	0	-1	0	-1	-1
26	1	0	0	0	-1	-1	-1	0
27	1	-1	1	0	0	0	0	0
28	0	0	0	1	0	1	1	-1
29	0	0	1	0	1	-1	1	0
30	-1	0	0	-1	-1	-1	0	1

Table A.17: 30-run three-level IP- and Bayesian IP-optimal designs with 4-factors.

Run	IP				Bayesian IP			
	X1	X2	X3	X4	X1	X2	X3	X4
1	0	-1	1	0	0	1	0	0
2	0	-1	1	0	-1	0	1	1
3	0	0	-1	1	1	0	0	0
4	1	0	0	0	-1	0	0	0
5	1	0	0	0	-1	1	1	-1
6	1	1	1	1	0	0	0	-1
7	0	1	0	-1	0	0	0	-1
8	1	-1	-1	-1	-1	-1	-1	0
9	1	-1	-1	-1	0	0	0	-1
10	-1	0	1	-1	-1	1	-1	-1
11	0	0	0	0	-1	-1	-1	0
12	0	0	0	0	0	-1	0	1
13	-1	-1	0	1	1	1	-1	-1
14	-1	1	-1	0	0	1	0	0
15	1	1	1	1	1	0	-1	1
16	0	0	0	0	0	0	-1	0
17	-1	-1	0	1	1	1	1	-1
18	-1	0	1	-1	0	-1	0	1
19	1	-1	-1	-1	0	0	1	0
20	-1	1	-1	0	0	0	1	0
21	0	0	-1	1	1	-1	-1	-1
22	0	1	0	-1	0	0	-1	0
23	0	0	-1	1	-1	-1	1	-1
24	0	-1	1	0	-1	0	0	0
25	0	0	0	0	1	-1	1	0
26	-1	0	1	-1	1	1	1	1
27	1	0	0	0	0	1	0	0
28	0	1	0	-1	1	0	0	0
29	-1	-1	0	1	1	-1	1	0
30	-1	1	-1	0	-1	1	-1	1

Table A.18: 30-run three-level I_D- and Bayesian I_D-optimal designs with 4-factors.

Run	I_D				Bayesian I_D			
	X_1	X_2	X_3	X_4	X_1	X_2	X_3	X_4
1	0	0	0	0	-1	1	1	1
2	1	-1	-1	0	-1	1	-1	-1
3	0	0	1	0	0	-1	0	0
4	0	0	0	0	-1	1	-1	1
5	-1	1	0	1	-1	1	1	-1
6	1	1	1	1	-1	-1	-1	-1
7	0	-1	-1	-1	1	-1	1	1
8	0	0	-1	1	1	1	1	1
9	0	0	1	-1	-1	-1	-1	1
10	1	-1	1	1	1	1	-1	-1
11	-1	1	-1	-1	1	1	-1	1
12	-1	0	0	0	1	-1	1	-1
13	-1	1	1	0	1	-1	-1	1
14	0	1	1	0	-1	-1	1	1
15	-1	0	1	-1	-1	0	0	-1
16	1	0	0	-1	0	0	1	0
17	0	-1	0	0	1	1	1	-1
18	-1	-1	1	1	1	0	0	0
19	-1	-1	-1	-1	0	0	0	1
20	-1	-1	1	-1	-1	-1	1	-1
21	1	-1	1	1	0	-1	0	0
22	-1	0	-1	1	1	-1	-1	-1
23	1	0	-1	0	-1	0	-1	0
24	0	1	0	-1	0	1	-1	0
25	1	1	-1	1	-1	1	0	0
26	1	1	-1	-1	0	0	0	1
27	0	0	0	1	0	0	1	0
28	1	-1	0	-1	1	0	0	0
29	1	1	1	-1	0	0	-1	-1
30	1	0	0	0	0	1	0	-1

Table A.19: 30-run three-level I_DP- and Bayesian I_DP-Optimal designs with 4-factors.

Run	I_DP				Bayesian I_DP			
	X1	X2	X3	X4	X1	X2	X3	X4
1	0	0	0	0	0	0	0	0
2	1	0	1	-1	0	0	0	0
3	0	1	-1	-1	1	-1	1	0
4	0	1	-1	-1	1	1	1	-1
5	0	0	0	0	-1	-1	0	-1
6	-1	0	-1	1	1	0	-1	-1
7	1	1	0	1	-1	1	-1	-1
8	-1	-1	0	-1	0	0	0	0
9	1	1	0	1	0	-1	-1	1
10	0	0	0	0	-1	1	1	0
11	0	0	0	0	0	0	0	0
12	-1	0	-1	1	1	1	-1	1
13	0	-1	1	1	-1	1	-1	-1
14	1	0	1	-1	-1	-1	1	1
15	0	0	0	0	-1	-1	-1	0
16	0	1	-1	-1	1	0	1	1
17	0	-1	1	1	1	0	1	1
18	-1	0	-1	1	0	1	1	1
19	-1	-1	0	-1	0	0	0	0
20	1	-1	-1	0	-1	-1	0	-1
21	-1	1	1	0	1	-1	0	1
22	1	-1	-1	0	-1	0	-1	1
23	-1	1	1	0	-1	0	-1	1
24	0	0	0	0	1	1	-1	1
25	0	-1	1	1	-1	1	0	1
26	-1	1	1	0	1	1	1	-1
27	-1	-1	0	-1	1	-1	-1	-1
28	1	0	1	-1	0	-1	1	-1
29	1	1	0	1	0	-1	1	-1
30	1	-1	-1	0	-1	0	1	-1

Table A.20: 30-run three-level D- and Bayesian D-optimal designs with 4-factors.

Run	D				Bayesian D			
	X_1	X_2	X_3	X_4	X_1	X_2	X_3	X_4
1	-1	-1	0	1	1	1	-1	1
2	0	1	-1	0	-1	-1	-1	1
3	1	-1	-1	0	-1	1	1	1
4	1	1	0	-1	1	-1	1	1
5	-1	-1	-1	0	1	1	-1	-1
6	0	0	0	-1	1	-1	-1	1
7	0	1	-1	1	1	-1	-1	-1
8	0	-1	1	1	1	1	1	1
9	0	0	0	0	-1	1	-1	1
10	0	1	1	0	1	-1	1	0
11	-1	1	0	1	-1	-1	1	1
12	0	0	1	1	1	1	1	-1
13	1	-1	0	0	0	1	-1	-1
14	-1	1	1	-1	-1	-1	1	-1
15	1	-1	1	1	-1	1	1	-1
16	1	0	0	1	-1	0	-1	-1
17	-1	-1	-1	1	0	0	0	1
18	1	-1	1	-1	1	-1	0	-1
19	1	0	1	0	0	-1	-1	0
20	0	-1	0	-1	0	-1	1	-1
21	-1	0	1	0	-1	-1	-1	-1
22	1	1	-1	-1	-1	1	-1	0
23	-1	-1	1	-1	1	0	-1	1
24	1	0	-1	-1	-1	1	0	-1
25	-1	0	-1	1	-1	-1	0	1
26	-1	0	-1	-1	-1	0	1	0
27	-1	0	1	-1	1	-1	1	1
28	1	1	1	1	1	0	1	-1
29	0	-1	-1	-1	0	1	1	1
30	-1	1	0	0	1	1	0	0

Table A.21: 30-run three-level DP- and Bayesian BDP-optimal designs with 4-factors.

Run	DP				Bayesian DP			
	X_1	X_2	X_3	X_4	X_1	X_2	X_3	X_4
1	1	1	0	0	1	-1	-1	-1
2	1	1	0	0	-1	1	-1	-1
3	-1	1	-1	1	1	-1	-1	1
4	1	1	0	0	1	-1	-1	-1
5	-1	-1	0	-1	-1	1	-1	1
6	1	0	-1	-1	-1	-1	1	1
7	1	0	-1	-1	-1	-1	1	-1
8	-1	0	1	0	-1	-1	1	-1
9	0	1	1	-1	-1	1	1	0
10	0	-1	-1	0	1	1	1	-1
11	0	-1	-1	0	1	1	1	-1
12	-1	1	-1	1	1	-1	-1	1
13	-1	0	1	0	1	1	0	1
14	0	0	0	1	-1	-1	-1	0
15	-1	-1	0	-1	1	1	0	1
16	1	0	-1	-1	1	0	1	1
17	0	1	1	-1	-1	1	-1	-1
18	0	-1	-1	0	1	0	1	1
19	1	-1	1	1	-1	-1	1	1
20	0	0	0	1	1	-1	1	0
21	-1	-1	0	-1	1	1	-1	0
22	1	-1	1	1	1	1	-1	0
23	-1	0	1	0	1	-1	1	0
24	0	0	0	1	-1	1	1	0
25	1	0	-1	-1	0	1	1	1
26	1	-1	1	1	-1	-1	-1	0
27	-1	1	-1	1	0	0	0	-1
28	1	1	0	0	0	1	1	1
29	-1	1	-1	1	0	0	0	-1
30	0	1	1	-1	-1	1	-1	1