

Useful Numerical Statistics of Some Response Surface Methodology Designs

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Abstract

Useful numerical evaluations associated with three categories of Response Surface Methodology designs are presented with respect to five commonly encountered alphabetic optimality criteria. The first-order Plackett-Burman designs and the 2^k Factorial designs are examined for the main effects models and the complete first-order models respectively. The second-order Central Composite Designs are examined for second-order models. The A-, D-, E-, G- and T-optimality criteria are employed as commonly encountered optimality criteria summarizing how good the experimental designs are. Relationships among the optimality criteria are pointed out with regards to the designs and the models. Generally the designs do not show uniform preferences in terms of the considered optimality criteria. However, one interesting finding is that central composite designs defined on cubes and hypercubes with unit axial distances are uniformly preferred in terms of E-optimality and G-optimality criteria.

Keywords: Plackett-Burman design, 2^k Factorial design, Central Composite Design, A-optimality criterion, D-optimality criterion, E-optimality criterion, G-optimality criterion and T-optimality criterion.

1. Introduction

First- and second-order models are the most frequently utilized approximating models in response surface methodology. In most cases, they adequately represent the true unknown functional relationship between the response variable and the control or independent variables. Designs for fitting the first-order models and the second-order models are called the first-order designs and the second-order designs, respectively. The use of first-order designs is vital in preliminary stage of experimentation involving several factors. Commonly encountered first-order designs are the 2^k Factorial designs, 2^{k-p} Fractional factorial designs and the Plackett-Burman designs, where k is the number of control variables and p is the number of defining relations. The 2^k Factorial design involves k factors measured at 2 levels each. As the number of control variables increases, the use of full factorial designs becomes very demanding and burdensome. This then requires running only the 2^{k-p} Fractional factorial designs which are subsets of the full factorial designs, where each subset could be made up of one-half, one-quarter and so on, of the full factorial design.

Plackett-Burman designs, due to Plackett and Burman (1946), are also two level factorial designs but used for studying up to $k = N-1$ response variables in N runs, where N is a multiple of 4. Each of Plackett-Burman design, 2^k Factorial design and 2^{k-p} Fractional factorial design plays a vital role in experiments involving several factors and where the interest is to examine the joint effects of the factors on a response variable. They are very suitable in screening experiments for the purpose of identifying factors that contribute significantly to the process under study thereby screening out less influential factors. The 2^k factorial designs require large experimental runs when compared to 2^{k-p} fractional factorial designs and the Plackett-Burman designs in k variables. In fact, the Plackett-Burman designs are very economical as each requires a much smaller number of experimental runs, especially for large control variables k , where $N=k+1$. In this wise, the Plackett-Burman designs are considered saturated. Although Plackett-Burman designs exist for multiples of 4, they are equivalent to 2^{k-p} Fractional factorial designs for N that is powers of 2.

Whereas first-order Response Surface Methodology designs exhibit lack of fits in the presence of curvature and hence inadequate at such stage of experimentation, second-order designs are considered suitable for addressing the quadratic effects. One commonly encountered second-order response surface methodology design is the Central Composite Design due to Box and Wilson (1951). The Central Composite Designs have been extensively studied and there exist vast literature on the subject. For reference purpose, see Dette and Grigoriev (2014), Chigbu and Nduka (2006), Iwundu (2015), Lucas (1976), Myer *et al.* (1992), Giovannitti-Jensen and Myers (1989), Zahran *et al.* (2003), Chigbu *et al.* (2009) and Ukaegbu and Chigbu (2015). We investigate in this paper the optimality properties of three categories of

Response Surface Methodology designs namely, the Plackett-Burman designs, 2^k Factorial design and the Central Composite Designs. Rady *et al.* (2009) presented a survey on optimality criteria that are often encountered in the theory of designing experiments as well as the relationships among several optimality criteria. Although concise enough, no illustrative examples were presented. The aim of this paper is thus to present useful numerical values associated with the three categories of Response Surface Methodology designs, with respect to some commonly encountered alphabetic optimality criteria.

2. Methodology

Most early stages of experimentation assume the absence of curvature in the system and thus utilize the main effects models or complete first-order models to serve as some “good” representation of the response surface in a small region of experimentation. Plackett-Burman designs and the full Factorial designs shall be examined for the main effects models and the complete first-order models respectively, in k factors. The Plackett-Burman designs shall be examined for $k = 3, 7, 11, 15$. The 2^k Factorial designs shall be examined for $k = 2, 3, 4$. However when k exceeds 4 the Fractional factorial designs should be encouraged. In a similar fashion, the central composite designs shall be examined for second-order models in k factors ($k = 2, 3, 4$) and at varying α values. Five alphabetic optimality criteria, namely A-, D-, E-, G- and T-optimality criteria shall be employed in the numerical evaluations as optimality criteria summarize how good experimental designs are. As reported in Khuri and Mukhopadhyay (2010), optimal designs are constructed on the basis of optimality criteria. Rady *et al.* (2009) remarked that optimal designs are model dependent as designs are generally optimal only with respect to specific statistical models. As can be seen in most standard literatures on optimal designs such as Raymond *et al.* (2009) and Rady *et al.* (2009), D-optimality criterion focuses on good model parameter estimation. A D-optimal design is one in which the determinant of the moment matrix

$$M = \frac{X^T X}{N}$$

is maximized over all designs, where X represents the design matrix associated with the design and X^T represents its transpose. The criterion of D-optimality equivalently minimizes the determinant of M^{-1} . A-optimality criterion also focuses on good model parameter estimation. However unlike the D-optimality criterion, it does not take into account the covariances among model coefficients. A-optimality criterion is one in which the sum of the variances of the model coefficients is minimized. It is defined as

$$\text{Min tr}(M^{-1})$$

where Min implies that minimization is over all designs and tr represents trace.

E-optimality criterion aims at finding a design which maximizes the minimum eigen value of M or equivalently finds a design which minimizes the maximum eigen value of M^{-1} . By E-optimality, the maximum variance of all possible normalized linear combinations of parameter estimates is minimized. E-optimality criterion is defined by

$$\text{Max } \lambda_{\min}(M) \equiv \text{Min } \lambda_{\max}(M^{-1})$$

where λ_{\min} and λ_{\max} represent minimum eigen value and maximum eigen value, respectively. On the other hand, G-optimality criterion considers designs whose maximum scaled prediction variance, $v(\underline{x})$, in the region of the design is not too large. Hence, a G-optimal design minimizes the maximum scaled prediction variance and is defined by

$$\text{Min}\{\max_{\underline{x} \in R} v(\underline{x})\}$$

The concept of scaled prediction variance has been well explained in Myers *et al.* (2009). Finally, the T-optimality criterion aims at finding a design that maximizes the trace of M .

The first-order main effects model to be employed in this study is

$$y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \varepsilon \quad ; -1 \leq x_i \leq 1 \quad (1)$$

where the model parameters retain their usual definitions as contained in standard textbooks on response surface methodology. The first-order complete model (main effects and interactions model) to be employed in this study is

$$y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \{ \sum_{i=1}^{k-1} \sum_{j=i+1}^k \beta_{ij} (x_i x_j) \} + \{ \sum_i \sum_j \sum_k \beta_{ijk} (x_i x_j x_k) \} + \dots + \varepsilon \quad ; -1 \leq x_i \leq 1 \quad (2)$$

The second-order complete model (main effects, interaction effects and quadratic effects model) to be employed in this study is

$$y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \{ \sum_{i=1}^{k-1} \sum_{j=i+1}^k \beta_{ij} (x_i x_j) \} + \sum_{i=1}^k \beta_{ii} x_i^2 + \varepsilon \quad ; -\alpha \leq x_i, x_j \leq \alpha \quad (3)$$

The real value α represents the axial distance associated with central composite design. According to Myers *et al.* (2009; pg.298) the value of the axial distance generally lies between 1.0 and \sqrt{k} . An α value of 1.0 places the axial points on the cube or hypercube and an α value of \sqrt{k} places all points on a common sphere. To achieve rotatability of designs,

the axial distance is set at $\alpha = F^{\frac{1}{4}}$, where F is the number of factorial points contained in the design.

3. Results

We present in this section some useful numerical evaluations for the considered response surface methodology designs.

3.1 Main Effects Model and the Plackett-burman Design

Case 1: K=3, N=4

The 4-point Plackett-Burman design in three controllable variables is

$$\xi = \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \\ -1 & -1 & -1 \end{pmatrix}$$

Using the design and the model in (1) yields the normalized information matrix

$$M = \begin{pmatrix} 1.0000 & 0 & 0 & 0 \\ 0 & 1.0000 & 0 & 0 \\ 0 & 0 & 1.0000 & 0 \\ 0 & 0 & 0 & 1.0000 \end{pmatrix}$$

For the purpose of evaluating the optimality measures the following computations are made.

The Eigen values of M are

1.0000

1.0000

1.0000

1.0000

The determinant value and the trace of M are respectively 1.0000 and 4.0000.

The variance of prediction at each corresponding design point in ξ is respectively

4.0000

4.0000

4.0000

4.0000

$$M^{-1} = \begin{pmatrix} 1.0000 & 0 & 0 & 0 \\ 0 & 1.0000 & 0 & 0 \\ 0 & 0 & 1.0000 & 0 \\ 0 & 0 & 0 & 1.0000 \end{pmatrix}$$

The Eigen values of M^{-1} are

1.0000

1.0000

1.0000

1.0000

The determinant value and the trace of M^{-1} are respectively 1.0000 and 4.0000.

Case 2: K=7, N=8

$$\xi = \begin{pmatrix} 1 & 1 & 1 & -1 & 1 & -1 & -1 \\ -1 & 1 & 1 & 1 & -1 & 1 & -1 \\ -1 & -1 & 1 & 1 & 1 & -1 & 1 \\ 1 & -1 & -1 & 1 & 1 & 1 & -1 \\ -1 & 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 & -1 & -1 & 1 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 \end{pmatrix}$$

Using the design and the model in (1) yields the normalized information matrix

$$M = \begin{pmatrix} 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 \end{pmatrix}$$

The Eigen values of M are

1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000

The determinant value and the trace of M are respectively 1.0000 and 8.0000

The variance of prediction at each corresponding design point in ξ is respectively

8.0000
8.0000
8.0000
8.0000
8.0000
8.0000
8.0000
8.0000

$$M^{-1} = \begin{pmatrix} 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 \end{pmatrix}$$

The Eigen values of M^{-1} are

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

The determinant value and the trace of M^{-1} are respectively 1.0000 and 8.0000.

Case 3: K=11, N=12

The 12-point Plackett-Burman design in eleven controllable variables is

$$\xi = \begin{pmatrix} 1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 \\ 1 & -1 & 1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & 1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & 1 & 1 & -1 \\ -1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & 1 & 1 \\ 1 & -1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 & -1 & 1 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \end{pmatrix}$$

Using the design and the model in (1) yields the normalized information matrix

$$M = \begin{pmatrix} 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 \end{pmatrix}$$

The Eigen values of M are 1.0000

1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000

The determinant value and the trace of M are respectively 1.0000 and 12.0000.

The variance of prediction at each corresponding design point in ξ is respectively

12
12
12
12
12
12
12
12
12
12
12
12
12

$M^{-1} = \begin{pmatrix} 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 \end{pmatrix}$

The Eigen values of M^{-1} are

1.0000
1.0000
1.0000
1.0000
1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

The determinant value and the trace of M^{-1} are respectively 1.0000 and 12.0000.

Case 4: K=15, N=16

The 16-point Plackett-Burman design in fifteen controllable variables is

$$\xi = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 \\ 1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 \\ 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 \\ 1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 \\ 1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \end{pmatrix}$$

Using the design and the model in (1) yields the normalized information matrix

$$M = \begin{pmatrix} 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 \end{pmatrix}$$

The Eigen values of M are

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

The determinant value and the trace of M are respectively 1.0000 and 16.0000

The variance of prediction at each corresponding design point in ξ is respectively

16

16

16

16

16

16

16

16

16

16

16

16

16

16

16

16

$$M^{-1} = \begin{pmatrix} 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 \end{pmatrix}$$

The Eigen values of M^{-1} are

1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000

The determinant value and the trace of M^{-1} are respectively 1.0000 and 16.0000

3.2 Complete Model and the 2^k Factorial Design

Case 1: $k=2$, $N=4$

The 4-point full factorial design is

$$\xi = \begin{pmatrix} -1 & -1 \\ 1 & -1 \\ -1 & 1 \\ 1 & 1 \end{pmatrix}$$

Using the design and the model in (2) yields the normalized information matrix

$$M = \begin{pmatrix} 1.0000 & 0 & 0 & 0 \\ 0 & 1.0000 & 0 & 0 \\ 0 & 0 & 1.0000 & 0 \\ 0 & 0 & 0 & 1.0000 \end{pmatrix}$$

The Eigen values of M are

1.0000
1.0000
1.0000
1.0000

The determinant value and the trace of M are respectively 1.0000 and 4.0000.

The variance of prediction at each corresponding design point in ξ is respectively

4.0000
4.0000
4.0000
4.0000

$$\mathbf{M}^{-1} = \begin{pmatrix} 1.0000 & 0 & 0 & 0 \\ 0 & 1.0000 & 0 & 0 \\ 0 & 0 & 1.0000 & 0 \\ 0 & 0 & 0 & 1.0000 \end{pmatrix}$$

The Eigen values of \mathbf{M}^{-1} are

1.0000

1.0000

1.0000

1.0000

The determinant value and the trace of \mathbf{M}^{-1} are respectively 1.0000 and 4.0000.

Case 2: $k=3$, $N=8$

The 8-point full factorial design is

$$\xi = \begin{pmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$

Using the design and the model in (2) yields the normalized information matrix

$$\mathbf{M} = \begin{pmatrix} 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 \end{pmatrix}$$

The Eigen values of \mathbf{M} are

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

The determinant value and the trace of \mathbf{M} are respectively 1.0000 and 8.0000.

The variance of prediction at each corresponding design point in ξ is respectively

8.0000
8.0000
8.0000
8.0000
8.0000
8.0000
8.0000
8.0000

$$\mathbf{M}^{-1} = \begin{pmatrix} 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 \end{pmatrix}$$

The Eigen values of \mathbf{M}^{-1} are

1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000
1.0000

The determinant value and the trace of \mathbf{M}^{-1} are respectively 1.0000 and 8.0000.

Case 3: $k=4$, $N=16$

The 16-point full factorial design is

$$\xi = \begin{pmatrix} -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & 1 & 1 & -1 \\ -1 & -1 & -1 & 1 \\ 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}$$

Using the design and the model in (2) yields the normalized information matrix

$M =$

1.0000	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	1.0000	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	1.0000	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	1.0000	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	1.0000	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	1.0000	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	1.0000	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	1.0000	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	1.0000	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	1.0000	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	1.0000	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	1.0000	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	1.0000	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	1.0000	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.0000	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.0000

The Eigen values of M are

- 1.0000
- 1.0000
- 1.0000
- 1.0000
- 1.0000
- 1.0000
- 1.0000
- 1.0000
- 1.0000
- 1.0000
- 1.0000
- 1.0000
- 1.0000
- 1.0000
- 1.0000
- 1.0000

The determinant value and the trace of M are respectively 1.0000 and 16.0000.

The variance of prediction at each corresponding design point in ξ is respectively

- 16
- 16
- 16
- 16
- 16
- 16
- 16
- 16
- 16
- 16
- 16
- 16
- 16
- 16
- 16
- 16

16

16

16

16

16

$$M^{-1} = \begin{pmatrix} 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0000 \end{pmatrix}$$

The Eigen values of M^{-1} are

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

1.0000

The determinant value and the trace of M^{-1} are respectively 1.0000 and 16.0000.

3.3 Second Order Model and the Central Composite Design

Case 1: $K=2$, $N=9$; $\alpha=1$

The 9-point central composite design is

$$\xi = \begin{pmatrix} -1 & -1 \\ 1 & -1 \\ -1 & 1 \\ 1 & 1 \\ 1 & 0 \\ -1 & 0 \\ 0 & 0 \\ 0 & -1 \\ 0 & 0 \end{pmatrix}$$

Using the design and the model in (3) yields the normalized information matrix

$$\mathbf{M} = \begin{pmatrix} 1.0000 & 0 & 0 & 0 & 0.6667 & 0.6667 \\ 0 & 0.6667 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.6667 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.4444 & 0 & 0 \\ 0.6667 & 0 & 0 & 0 & 0.6667 & 0.4444 \\ 0.6667 & 0 & 0 & 0 & 0.4444 & 0.6667 \end{pmatrix}$$

The Eigen values of \mathbf{M} are

0.1111

0.2222

0.4444

0.6667

0.6667

2.0000

The determinant value and the trace of \mathbf{M} are respectively 0.0098 and 4.1111.

The variance of prediction at each corresponding design point in ξ is respectively

7.2500

7.2500

7.2500

7.2500

5.0000

5.0000

5.0000

5.0000

$$\mathbf{M}^{-1} = \begin{pmatrix} 5.0000 & 0 & 0 & 0 & -3.0000 & -3.0000 \\ 0 & 1.5000 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.5000 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2.2500 & 0 & 0 \\ -3.0000 & 0 & 0 & 0 & 4.5000 & 0 \\ -3.0000 & 0 & 0 & 0 & 0 & 4.5000 \end{pmatrix}$$

The Eigen values of \mathbf{M}^{-1} are

0.5000

1.5000

1.5000

2.2500

4.5000

9.0000

The determinant value and the trace of \mathbf{M}^{-1} are respectively 102.5156 and 19.2500.

Case 2: $K=2$, $N=9$; $\alpha=1.414$

The 9-point central composite design is

$$\xi = \begin{pmatrix} -1 & -1 \\ 1 & -1 \\ -1 & 1 \\ 1 & 1 \\ 1.414 & 0 \\ -1.414 & 0 \\ 0 & 1.414 \\ 0 & -1.414 \\ 0 & 0 \end{pmatrix}$$

Using the design and the model in (3) yields the normalized information matrix

$$\mathbf{M} = \begin{pmatrix} 1.0000 & 0 & 0 & 0 & 0.8888 & 0.8888 \\ 0 & 0.8888 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.8888 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.4444 & 0 & 0 \\ 0.8888 & 0 & 0 & 0 & 1.3328 & 0.4444 \\ 0.8888 & 0 & 0 & 0 & 0.4444 & 1.3328 \end{pmatrix}$$

The Eigen values of M are

0.0730

0.4444

0.8884

0.8888

0.8888

2.7042

The determinant value and the trace of M are respectively 0.0616 and 5.8875.

The variance of prediction at each corresponding design point in ξ is respectively

5.6257

5.6257

5.6257

5.6257

5.6243

5.6243

5.6243

5.6243

9.0000

$$\mathbf{M}^{-1} = \begin{pmatrix} 9.0000 & 0 & 0 & 0 & -4.5007 & -4.5007 \\ 0 & 1.1252 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.1252 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2.2500 & 0 & 0 \\ -4.5007 & 0 & 0 & 0 & 3.0949 & 1.9692 \\ -4.5007 & 0 & 0 & 0 & 1.9692 & 3.0949 \end{pmatrix}$$

The Eigen values of M^{-1} are

13.6942

0.3698

1.1257

1.1252

1.1252

2.2500

The determinant value and the trace of M^{-1} are respectively 16.2379 and 19.6902.

Case 3: $K=3$, $N=15$; $\alpha=1$

The 15-point central composite design is

$$\xi = \begin{pmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix}$$

Using the design and the model in (3) yields the normalized information matrix

$$M = \begin{pmatrix} 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0.6667 & 0.6667 & 0.6667 \\ 0 & 0.6667 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.6667 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.6667 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.5333 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.5333 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.5333 & 0 & 0 & 0 \\ 0.6667 & 0 & 0 & 0 & 0 & 0 & 0 & 0.6667 & 0.5333 & 0.5333 \\ 0.6667 & 0 & 0 & 0 & 0 & 0 & 0 & 0.5333 & 0.6667 & 0.5333 \\ 0.6667 & 0 & 0 & 0 & 0 & 0 & 0 & 0.5333 & 0.5333 & 0.6667 \end{pmatrix}$$

The Eigen values of M are

0.1333

0.1333

0.1551

0.5333

0.5333

0.5333

0.6667

0.6667

0.6667

2.5782

The determinant value and the trace of M are respectively 3.1964e-004 and 6.6000.

The variance of prediction at each corresponding design point in ξ is respectively

11.9583

11.9583

11.9583

11.9583

11.9583

11.9583

11.9583

11.9583

8.3333

8.3333

8.3333

8.3333

8.3333

8.3333

4.3333

$$M^{-1} = \begin{pmatrix} 4.3333 & 0 & 0 & 0 & 0 & 0 & 0 & -1.6667 & -1.6667 & -1.6667 \\ 0 & 1.5000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.5000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.5000 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.8750 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.8750 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.8750 & 0 & 0 & 0 \\ -1.6667 & 0 & 0 & 0 & 0 & 0 & 0 & 5.8333 & -1.6667 & -1.6667 \\ -1.6667 & 0 & 0 & 0 & 0 & 0 & 0 & -1.6667 & 5.8333 & -1.6667 \\ -1.6667 & 0 & 0 & 0 & 0 & 0 & 0 & -1.6667 & -1.6667 & 5.8333 \end{pmatrix}$$

The Eigen values of M^{-1} are

6.4455

0.3879

7.5000

7.5000

1.5000

1.5000

1.5000

1.8750

1.8750

1.8750

The determinant value and the trace of M^{-1} are respectively 3.1285e+003 and 31.9583.

Case 4: N=15 P=10, 1.682= α , K=3

The 15-point central composite design is

$$\xi = \begin{pmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ 1.682 & 0 & 0 \\ -1.682 & 0 & 0 \\ 0 & 1.682 & 0 \\ 0 & -1.682 & 0 \\ 0 & 0 & 1.682 \\ 0 & 0 & -1.682 \\ 0 & 0 & 0 \end{pmatrix}$$

Using the design and the model in (3) yields the normalized information matrix

$$\mathbf{M} = \begin{pmatrix} 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0.9105 & 0.9105 & 0.9105 \\ 0 & 0.9105 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.9105 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.9105 & 0 & 0 & 0 & 0 & 0 & 0.0000 \\ 0 & 0 & 0 & 0 & 0.5333 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.5333 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.5333 & 0 & 0 & 0 \\ 0.9105 & 0 & 0 & 0 & 0 & 0 & 0 & 1.6005 & 0.5333 & 0.5333 \\ 0.9105 & 0 & 0 & 0 & 0 & 0 & 0 & 0.5333 & 1.6005 & 0.5333 \\ 0.9105 & 0 & 0 & 0 & 0 & 0 & 0 & 0.5333 & 0.5333 & 1.6005 \end{pmatrix}$$

The Eigen values of M are

0.0497

0.5333

0.5333

0.5333

0.9105

0.9105

0.9105

1.0672

1.0672

3.6175

The determinant value and the trace of M are respectively 0.0235 and 10.1332.

The variance of prediction at each corresponding design point in ξ is respectively

10.0532

10.0532

10.0532

10.0532

10.0532

10.0532

10.0532

10.0532

9.1247

9.1247

9.1247

9.1247

9.1247

9.1247

14.8269

$$M^{-1} = \begin{pmatrix} 14.8268 & 0 & 0 & 0 & 0 & 0 & 0 & -5.0617 & -5.0617 & -5.0617 \\ 0 & 1.0982 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.0982 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.0982 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.8750 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.8750 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.8750 & 0 & 0 & 0 \\ -5.0617 & 0 & 0 & 0 & 0 & 0 & 0 & 2.4777 & 1.5406 & 1.5406 \\ -5.0617 & 0 & 0 & 0 & 0 & 0 & 0 & 1.5406 & 1.5406 & 1.5406 \\ -5.0617 & 0 & 0 & 0 & 0 & 0 & 0 & 1.5406 & 1.5406 & 2.4777 \end{pmatrix}$$

The Eigen values of M^{-1} are

20.1094

0.2764

1.0982

0.9370

0.9370

1.0982

1.0982

1.8750

1.8750

1.8750

The determinant value and the trace of M^{-1} are respectively 42.6197 and 31.1796.

Case 5 :N=15, P=10, 1.7321= α , K=3

The 15-point central composite design is

$$\xi = \begin{pmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ 1.7321 & 0 & 0 \\ -1.7321 & 0 & 0 \\ 0 & 1.7321 & 0 \\ 0 & -1.7321 & 0 \\ 0 & 0 & 1.7321 \\ 0 & 0 & -1.7321 \\ 0 & 0 & 0 \end{pmatrix}$$

Using the design and the model in (3) yields the normalized information matrix

$$M = \begin{pmatrix} 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0.9334 & 0.9334 & 0.9334 \\ 0 & 0.9334 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.9334 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.9334 & 0 & 0 & 0 & 0 & 0 & -0.0000 \\ 0 & 0 & 0 & 0 & 0.5333 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.5333 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.5333 & 0 & 0 & 0 \\ 0.9334 & 0 & 0 & 0 & 0 & 0 & 0 & 1.7335 & 0.5333 & 0.5333 \\ 0.9334 & 0 & 0 & 0 & 0 & 0 & 0 & 0.5333 & 1.7335 & 0.5333 \\ 0.9334 & 0 & 0 & 0 & 0 & 0 & 0 & 0.5333 & 0.5333 & 1.7335 \end{pmatrix}$$

The Eigen values of M are

0.0498

0.5333

0.5333

0.5333

0.9334

0.9334

0.9334

1.2001

1.2001

3.7504

The determinant value and the trace of M are respectively 0.0332 and 10.6005.

The variance of prediction at each corresponding design point in ξ is respectively

9.9106

9.9106

9.9106

9.9106

9.9106

9.9106

9.9106

9.9106

9.2859

9.2859

9.2859

9.2859

9.2859

9.2859

15.000

 $M^{-1} =$

$$\begin{pmatrix}
 15.0000 & 0 & 0 & 0 & 0 & 0 & 0 & -4.9999 & -4.9999 & -4.9999 \\
 0 & 1.0714 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 1.0714 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 1.0714 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 1.8750 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 1.8750 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 1.8750 & 0 & 0 & 0 \\
 -4.9999 & 0 & 0 & 0 & 0 & 0 & 0 & 2.3411 & 1.5079 & 1.5079 \\
 -4.9999 & 0 & 0 & 0 & 0 & 0 & 0 & 1.5079 & 2.3411 & 1.5079 \\
 -4.9999 & 0 & 0 & 0 & 0 & 0 & 0 & 1.5079 & 1.5079 & 2.3411
 \end{pmatrix}$$

The Eigen values of M^{-1} are

20.0902

0.2666

1.0714

0.8332

0.8332

1.0714

1.8750

1.8750

1.8750

The determinant value and the trace of M^{-1} are respectively 30.1510 and 30.8625.

Case 6:K=4 , I.0 P=15, N=25

The 15-point central composite design is

$$\xi = \begin{pmatrix}
 -1 & -1 & -1 & -1 \\
 1 & -1 & -1 & -1 \\
 -1 & 1 & -1 & -1 \\
 1 & 1 & -1 & -1 \\
 -1 & -1 & 1 & -1 \\
 1 & -1 & 1 & -1 \\
 -1 & 1 & 1 & -1 \\
 1 & 1 & 1 & -1 \\
 -1 & -1 & -1 & 1 \\
 1 & -1 & -1 & 1 \\
 -1 & 1 & -1 & 1 \\
 1 & 1 & -1 & 1 \\
 -1 & -1 & 1 & 1 \\
 1 & -1 & 1 & 1 \\
 -1 & 1 & 1 & 1 \\
 1 & 1 & 1 & 1 \\
 1 & 0 & 0 & 0 \\
 -1 & 0 & 0 & 0 \\
 0 & 1 & 0 & 0 \\
 0 & -1 & 0 & 0 \\
 0 & 0 & 1 & 0 \\
 0 & 0 & -1 & 0 \\
 0 & 0 & 0 & 1 \\
 0 & 0 & 0 & -1 \\
 0 & 0 & 0 & 0
 \end{pmatrix}$$

Using the design and the model in (3) yields the normalized information matrix

$$M = \begin{pmatrix} 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.7200 & 0.7200 & 0.7200 & 0.7200 \\ 0 & 0.7200 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.7200 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.7200 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.7200 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.6400 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.6400 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.6400 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.6400 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.6400 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.6400 & 0 & 0 & 0 & 0 \\ 0.7200 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.7200 & 0.6400 & 0.6400 & 0.6400 \\ 0.7200 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.6400 & 0.7200 & 0.6400 & 0.6400 \\ 0.7200 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.6400 & 0.6400 & 0.7200 & 0.6400 \\ 0.7200 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.6400 & 0.6400 & 0.6400 & 0.7200 \end{pmatrix}$$

The Eigen values of M are

0.0800

0.0800

0.0800

0.1629

0.6400

0.6400

0.6400

0.6400

0.6400

0.6400

0.7200

0.7200

0.7200

0.7200

3.4771

The determinant value and the trace of M are respectively 5.3555×10^{-6} and 10.6000.

The variance of prediction at each corresponding design point in ξ is respectively

16.4842

16.4842

16.4842

16.4842

16.4842

16.4842

16.4842

16.4842

16.4842

16.4842

16.4842

16.4842

16.4842

16.4842

16.4842

16.4842

17.4905

17.4905

17.4905

17.4905

17.4905

17.4905

17.4905

17.4905

4.6610

$$M^{-1} = \begin{pmatrix} 4.6610 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1.2712 & -1.2712 & -1.2712 & -1.2712 \\ 0 & 1.3889 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.3889 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.3889 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.3889 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.5625 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.5625 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.5625 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.5625 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.5625 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.5625 & 0 & 0 & 0 & 0 & 0 \\ -1.2712 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9.8164 & -2.6836 & -2.6836 & -2.6836 & -2.6836 \\ -1.2712 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2.6836 & 9.8164 & -2.6836 & -2.6836 & -2.6836 \\ -1.2712 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2.6836 & -2.6836 & 9.8164 & -2.6836 & -2.6836 \\ -1.2712 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2.6836 & -2.6836 & -2.6836 & 9.8164 & -2.6836 \end{pmatrix}$$

The Eigen values of M^{-1} are

0.2876

6.1390

12.500

12.500

12.500

1.3889

1.3889

1.3889

1.3889

1.5625

1.5625

1.5625

1.5625

1.5625

1.5625

The determinant value and the trace of M^{-1} are respectively 1.8672e+005 and 58.8571

Case 7: K=4, 2, P=15, N=25

The 9-point central composite design is

$$\xi = \begin{pmatrix} -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & 1 & 1 & -1 \\ -1 & -1 & -1 & 1 \\ 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 2 & 0 & 0 & 0 \\ -2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & -2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & -2 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Using the design and the model in (3) yields the normalized information matrix

$$M = \begin{pmatrix} 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.9600 & 0.9600 & 0.9600 & 0.9600 \\ 0 & 0.9600 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.9600 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.9600 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.9600 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.6400 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.6400 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.6400 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.6400 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.6400 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.6400 & 0 & 0 & 0 & 0 \\ 0.9600 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.9200 & 0.6400 & 0.6400 & 0.6400 \\ 0.9600 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.6400 & 1.9200 & 0.6400 & 0.6400 \\ 0.9600 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.6400 & 0.6400 & 1.9200 & 0.6400 \\ 0.9600 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.6400 & 0.6400 & 0.6400 & 1.9200 \end{pmatrix}$$

The Eigen values of M are

0.0319

0.6400

0.6400

0.6400

0.6400

0.6400

0.6400

0.9600

0.9600

0.9600

0.9600

1.2800

1.2800

1.2800

4.8081

The determinant value and the trace of M are respectively 0.0188 and 16.3600.

The variance of prediction at each corresponding design point in ξ is respectively

14.5833

14.5833

14.5833

14.5833

14.5833

14.5833

14.5833

14.5833

14.5833

14.5833

14.5833

14.5833

14.5833

14.5833

14.5833

14.5833

18.8802

18.8802

18.8802

18.8802

18.8802

18.8802

18.8802

18.8802

25.0000

$$M^{-1} = \begin{pmatrix} 25.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -6.2500 & -6.2500 & -6.2500 & -6.2500 \\ 0 & 1.0417 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.0417 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.0417 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.0417 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.5625 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.5625 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.5625 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.5625 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.5625 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.5625 & 0 & 0 & 0 & 0 & 0 \\ -6.2500 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2.2135 & 1.4323 & 1.4323 & 1.4323 & 1.4323 \\ -6.2500 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.4323 & 2.2135 & 1.4323 & 1.4323 & 1.4323 \\ -6.2500 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.4323 & 1.4323 & 2.2135 & 1.4323 & 1.4323 \\ -6.2500 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.4323 & 1.4323 & 1.4323 & 2.2135 & 1.4323 \end{pmatrix}$$

The Eigen values of M^{-1} are

31.3024

0.2080

0.7813

0.7813 + 0.0000i

0.7813 - 0.0000i

1.0417

1.0417

1.0417

1.0417

1.5625

1.5625

1.5625

1.5625

1.5625

1.5625

The determinant value and the trace of M^{-1} are respectively 53.1881 and 47.3958.

We summarize in Table 1 some optimality constants for the three categories of designs considered.

Table 1. Optimality Constants for Response Surface Methodology Designs

Model Type	Experimental Design	Control Variables k, Axial distance α	Design Size N	A-Optimality constant	D-Optimality constant		E-Optimality constant	G-Optimality constant	T-Optimality constant
				(Trace of M^{-1})	(Determinant of M)	(Determinant of M^{-1})	(minimum Eigen value of M)	(maximum scaled predictive variance)	(Trace of M)
Main effects model	Plackett-Burman design	k=3	4	4.0	1.0	1.0	1.0	4.0	4.0
		k=7	8	8.0	1.0	1.0	1.0	8.0	8.0
		k=11	12	12.0	1.0	1.0	1.0	12.0	12.0
		k=15	16	16.0	1.0	1.0	1.0	16.0	16.0
First-order Complete model	2^k Factorial design	k=2	4	4.0	1.0	1.0	1.0	4.0	4.0
		k=3	8	8.0	1.0	1.0	1.0	8.0	8.0
		k=4	16	16.0	1.0	1.0	1.0	16.0	16.0
Second-order complete model	Central Composite Design	k=2 ($\alpha=1.0$)	9	19.2500	0.0098	102.5156	0.1111	7.2500	4.1111
		k=2 ($\alpha=1.414$)	9	19.6900	0.0616	16.2379	0.0730	9.0000	5.8875
		k=3 ($\alpha=1.0$)	15	31.1796	3.1954×10^{-4}	3.1285×10^3	0.1333	11.9583	6.6000
		k=3 ($\alpha=1.682$)	15	31.1796	0.0235	42.6197	0.0497	14.8269	10.1332
		k=3 ($\alpha=1.7321$)	15	30.8625	0.0332	30.1510	0.0498	15.0000	10.6005
		k=4 ($\alpha=1.0$)	25	58.8571	5.3555×10^{-6}	1.8672×10^5	0.0800	17.4906	10.6000
		k=4 ($\alpha=2.0$)	15	53.1881	0.0188	53.1881	0.0319	25.0000	16.3600

4. Discussion

Many areas of Mathematical Science deal with approximation properties and asymptotic behaviours as could be seen in Mishra (2007), Mishra and Mishra (2012), Mishra *et al.* (2013) and Deepmala (2014)). With regards to estimation problems and asymptotic behaviours of optimality criteria, several literatures on optimal design of experiments have theoretically shown that relationships exist among the optimality criteria. However, in reviewing the literatures, there arose the need for concise numerical illustrations appreciably relating many of the criteria. In this paper, illustrative examples have been considered and presented with helpful evaluations thus offering first-hand information regarding response surface methodology designs and their optimality properties. As mentioned in the introduction, Plackett-Burman designs and the 2^k factorial designs are suitable for modeling first order effects. These categories of designs share similar optimality properties as seen in this paper. For all N-point k variable Plackett-Burman designs, the information matrices were diagonal and hence orthogonal with uniform diagonal elements. The Plackett-Burman designs exhibit uniform precision as the variance of prediction at each design point remained constant. Moreover, the maximum variance of prediction in each case was exactly equal to the number of model parameters. These two properties of the Plackett-Burman designs indicate D-optimality and G-optimality of the designs respectively. In fact, the design matrices being orthogonal satisfy rotatability requirements for first order designs. For each normalized information matrix, the determinant value and the minimum Eigen value were unity. These were also true for the determinant values of the variance-covariance matrices. The maximum scaled predictive variance, the trace of information matrix and the trace of the variance-covariance matrix shared the property of being equal to the number of design size. Each of these properties was also exhibited by the 2^k factorial designs.

Unlike the first-order designs, the second-order central composite designs do not show orthogonality of associated information matrices. This is true from existing literatures. However, the central composite designs have nice variance property of having the same variance of prediction at any two design points that are equidistant from the center point. For $k=2$, the 9-point design with $\alpha=1.0$ which was A-optimal when compared with the 9-point design with $\alpha=1.414$ was also E- and G-optimal. Hence the design with $\alpha=1.0$ which minimized the trace of the variance-covariance matrix, M^{-1} , also maximized the minimum Eigen value of the information matrix as well as minimizing the maximum scaled predictive variance. On the other hand, the 9-point design with $\alpha=1.414$ showed preference over the 9-point design with $\alpha=1.0$ under the criteria of D- and T-optimality as the design with $\alpha=1.414$ which maximized the determinant of information matrix also maximized the trace of information matrix.

For $k=3$. The design with $\alpha=1.7321$, which minimized the trace of the variance-covariance matrix also maximized the determinant of the information matrix and correspondingly maximized the trace of the information matrix. By these, the design with $\alpha=1.7321$ showed preference in terms of A-, D- and T-optimality criteria when compared with the designs with $\alpha=1.0$ and $\alpha=1.682$. However, design with $\alpha=1.0$ was preferred in terms of E- and G-optimality criteria. For $k=4$, design with $\alpha=1.0$ was again preferred in terms of E- and G-optimality criteria when compared with the design with $\alpha=2.0$. The design with $\alpha=2.0$ was preferred in terms of A-, D- and T-optimality criteria when compared with design with $\alpha=1.0$. It was observed as mentioned in existing literatures that designs that maximized the determinant of information matrices equivalently minimized the determinant of the variance-covariance matrices. One interesting finding is that central composite designs defined on cubes and hypercubes (i.e. with unit axial distance) were uniformly preferred in terms of E-optimality and G-optimality criteria.

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