



Comparison of Designs for Response Surface Models with Random Block Effects

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Abstract: The purpose of this article is to compare designs for response surface models with a random block effect. To assess the quality of prediction associated with a given design, the scaled prediction variance is considered as a design criterion. The proposed approach is based on using quantiles of this design criterion on concentric surfaces within the experimental region. The dependence of these quantiles on the unknown value of the ratio of two variance components, namely, the ones for the block effect and the experimental error, is depicted by plotting the so-called quantile dispersion graphs (QDGs). These plots provide a clear assessment of the quality of prediction associated with a given design. A numerical example is presented to illustrate the proposed methodology.

Keywords: Design dependence problem, quantile dispersion graphs, response surface design, scaled prediction variance, second-order designs, variance components.

1. Introduction

Khuri [10] discussed the analysis of a response surface model in the presence of a random block effect. Giovannitti-Jensen and Myers [7] introduced the so-called variance dispersion graphs (VDGs) to assess the overall prediction capability of a response surface design inside a region of interest, R . The VDGs are two-dimensional plots of the maximum and minimum values of the prediction variance on several concentric spheres inside R . In an effort to provide more information concerning the prediction variance on such spheres, Khuri *et al.* [13] proposed the use of the quantile plots of the prediction variance on the spheres. Such plots describe the entire distribution of the prediction variance and thereby give more complete assessment of the effect of the design on the prediction variance.

For response surface models with random block effects, quantiles of the prediction variance depend, unfortunately, on an unknown parameter, namely, the ratio of two unknown variance components, as will be seen later. Consequently, the assessment of the design effect on the prediction variance depends on the value of the unknown parameter.

This dependence problem is a common feature of designs for variance component estimation, and for designs for nonlinear models, including generalized linear models. There are several approaches to deal with this dependence problem in general. These approaches include the use of

- (i). locally optimal designs by specifying initial values of the unknown parameters.
- (ii). the sequential method, which allows the experimenter to obtain updated estimates of

the unknown parameters in successive stages following the use of the initial values in the first stage.

- (iii). the Bayesian methodology, which requires the specification of some prior distribution on the unknown parameters.
- (iv). quantile dispersion graphs (QDGs), which describe the dispersion in the quantile values of a particular design criterion function over a certain parameter space associated with the unknown parameter. The use of this approach was first introduced in Khuri [11] for the comparison of designs for a random two-way model. See also Lee and Khuri [15, 16].

The design dependence problem in the case of GLMs was recently addressed in a review article by Khuri *et al.* [14]. Cheng [4], Atkins and Cheng [1], and Goos and Vandebroek [8] considered designs for response surface models with random block effects.

In this article, we adapt the use of the QDG approach to the comparison of designs for response surface models with a random block effect. Section 2 describes these models and the corresponding notation. Section 3 gives details of the QDG approach. A discussion concerning the construction of the parameter space, mentioned earlier in (iv), is given in Section 4. A numerical example to describe the implementation of the QDG approach is presented in Section 5. Finally, concluding remarks are given in Section 6.

2. Model and Notation

Khuri [10] considered the following model of order $d (\geq 1)$ in k input variables x_1, x_2, \dots, x_k . The experimental runs in the associated design are arranged in b blocks of sizes n_1, n_2, \dots, n_b :

$$\mathbf{y} = \beta_0 \mathbf{1}_n + \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\varepsilon}, \quad (1)$$

where \mathbf{y} is a vector of $n = (\sum_{l=1}^b n_l)$ observations on the response, β_0 and $\boldsymbol{\beta} = (\beta_1, \beta_2, \dots, \beta_p)'$ are unknown parameters associated with the polynomial portion of the model, $\boldsymbol{\gamma} = (\gamma_1, \gamma_2, \dots, \gamma_b)'$, where γ_l denotes the effect of the l^{th} block ($l=1, 2, \dots, b$), and $\boldsymbol{\varepsilon}$ is a random error vector. Here, \mathbf{X} and \mathbf{Z} are known matrices of orders $n \times p$ and $n \times b$ and ranks p and b , respectively. The rows of \mathbf{X} consist of the values of $f'(\mathbf{x}_u)$, a vector whose elements are powers and crossproducts of powers of x_1, x_2, \dots, x_k of degree d evaluated at \mathbf{x}_u , the vector of design settings at the u^{th} experimental run ($u=1, 2, \dots, n$). The matrix \mathbf{Z} is of the form:

$$\mathbf{Z} = \text{diag}(\mathbf{1}_{n_1}, \mathbf{1}_{n_2}, \dots, \mathbf{1}_{n_b}). \quad (2)$$

Note that the columns of \mathbf{Z} sum to $\mathbf{1}_n$. The random vector $\boldsymbol{\gamma}$ is assumed to be distributed as $N(\mathbf{0}, \sigma_\gamma^2 \mathbf{I}_b)$ independently of $\boldsymbol{\varepsilon}$, which is assumed to follow the normal distribution $N(\mathbf{0}, \sigma_\varepsilon^2 \mathbf{I}_n)$.

Let us rewrite the model (1) as

$$E(\mathbf{y}) = \mathbf{W}\boldsymbol{\tau} + \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\varepsilon}, \quad (3)$$

where $\boldsymbol{\tau} = (\beta_0, \boldsymbol{\beta})'$ and $\mathbf{W} = [\mathbf{1}_n : \mathbf{X}]$. Hence,

$$E(\mathbf{y}) = \boldsymbol{\mu} = \beta_0 \mathbf{1}_n + \mathbf{X}\boldsymbol{\beta} = \mathbf{W}\boldsymbol{\tau} \quad (4)$$

$$V(\mathbf{y}) = \Sigma = \sigma_\varepsilon^2 \mathbf{I}_n + \sigma_\gamma^2 \mathbf{Z}\mathbf{Z}' = \sigma_\varepsilon^2 \mathbf{A}, \quad (5)$$

where

$$\mathbf{A} = \text{diag}(\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_b), \quad (6)$$

$$\mathbf{A}_l = \mathbf{I}_{n_l} + \eta \mathbf{J}_{n_l} \quad (l=1, 2, \dots, b), \text{ and } \eta = \sigma_\gamma^2 / \sigma_\varepsilon^2.$$

If $\eta = \sigma_\gamma^2 / \sigma_\varepsilon^2$ is known, then the *best linear unbiased estimator* (BLUE) of τ is the generalized least squares estimator $\hat{\tau}$ given by

$$\hat{\tau} = (\mathbf{W}'\mathbf{A}^{-1}\mathbf{W})^{-1} \mathbf{W}'\mathbf{A}^{-1} \mathbf{y}. \quad (7)$$

Its variance-covariance matrix is

$$\text{Var}(\hat{\tau}) = (\mathbf{W}'\mathbf{A}^{-1}\mathbf{W})^{-1} \sigma_\varepsilon^2. \quad (8)$$

Let $\hat{y}(\mathbf{x}) = \mathbf{g}'(\mathbf{x})\hat{\tau}$ denote the predicted response at a point \mathbf{x} in the experimental region R , where $\mathbf{g}'(\mathbf{x}) = [1, f'(\mathbf{x})]$. The prediction variance, $\text{Var}[\hat{y}(\mathbf{x})]$, is of the form

$$\text{Var}[\hat{y}(\mathbf{x})] = \mathbf{g}'(\mathbf{x})(\mathbf{W}'\mathbf{A}^{-1}\mathbf{W})^{-1} \mathbf{g}(\mathbf{x})\sigma_\varepsilon^2. \quad (9)$$

We define the scaled prediction variance as

$$\frac{n}{\sigma_\varepsilon^2} \text{Var}[\hat{y}(\mathbf{x})] = n[\mathbf{g}'(\mathbf{x})(\mathbf{W}'\mathbf{A}^{-1}\mathbf{W})^{-1} \mathbf{g}(\mathbf{x})]. \quad (10)$$

It is to be noted that the division of the prediction variance by σ_ε^2 makes this quantity scale free. The multiplication by n aids in theoretical comparisons of designs with continuous optimal designs (see, for example, Khuri and Cornell [12, p.434] and Myers and Montgomery [18, Section 8.2.1]). However, if no comparison is to be made with continuous designs, then scaling the prediction variance by just σ_ε^2 can be considered.

3. Quantile Dispersion Graphs

We shall use the scaled prediction variance given in (10) as a design criterion for comparing designs for model (1). Note that $\text{Var}[\hat{y}(\mathbf{x})]$ depends on \mathbf{x} (through $\mathbf{g}(\mathbf{x})$), D (the design under consideration) through the matrix \mathbf{W} , and η . Let us therefore denote $n\text{Var}[\hat{y}(\mathbf{x})]/\sigma_\varepsilon^2$ by $\Delta_D(\mathbf{x}, \eta)$, where n is the total number of experimental runs. If design D is used to fit the model, the prediction capability of D can be assessed by considering the quantiles of the distribution of $\Delta_D(\mathbf{x}, \eta)$ over concentric surfaces within the experimental region R . To address the problem of unknown η , we consider several values of η that belong to a parameter space C . We choose C to be a $(1-\alpha)100\%$ confidence interval on η . Such a confidence interval can be constructed using response data obtained under an initial design. A method by Harville and Fenech [9] is used to construct such a confidence interval, as will be shown in Section 4.

In order to study the performance of a design D throughout R , we consider several concentric surfaces denoted by R_λ located within R . These surfaces are obtained by reducing the boundary of R using a shrinkage factor λ . The prediction capability of D can then be evaluated by considering the distribution of $\Delta_D(\mathbf{x}, \eta)$, as determined by its quantiles on R_λ , for a given η in C . Small values of $\Delta_D(\mathbf{x}, \eta)$ are obviously desirable.

For a given design D and a given value of η in C , let $Q_D(p, \eta, \lambda)$ denote the p^{th} quantile of the distribution of the values of $\Delta_D(\mathbf{x}, \eta)$ on R_λ for a specified λ . The dependence of these quantiles on η is investigated by computing $Q_D(p, \eta, \lambda)$ for several values of η selected from C . We then calculate

$$\begin{aligned} Q_D^{\min}(p, \lambda) &= \min_{\eta \in C} Q_D(p, \eta, \lambda), \\ Q_D^{\max}(p, \lambda) &= \max_{\eta \in C} Q_D(p, \eta, \lambda). \end{aligned} \quad (11)$$

By plotting $Q_D^{\max}(p, \lambda)$ and $Q_D^{\min}(p, \lambda)$ against p for each D and λ we obtain the so-called *quantile dispersion graphs* (QDGs). Such plots can be constructed for two given designs, D_1 and D_2 , and for each of several values of λ . The plots provide a comprehensive assessment of the prediction capabilities of D_1 and D_2 throughout the region R . Clearly, D_1 is preferred over D_2 if the QDGs for D_1 show smaller values of $Q_{D_1}^{\max}(p, \lambda)$ and $Q_{D_1}^{\min}(p, \lambda)$ than those for D_2 . Furthermore, the closeness of $Q_{D_1}^{\max}(p, \lambda)$ to $Q_{D_1}^{\min}(p, \lambda)$ for a given design indicates robustness, or lack of sensitivity, that is induced by the design of the scaled prediction variance to changes in the parameter values over the parameter space C .

4. Confidence Interval for η

Harville and Fenech [9] derived a confidence interval for a variance ratio for an unbalanced mixed linear model. We now briefly outline their procedure for constructing such an interval for η . Let us consider the general model in Eq. (3). Define $r = \text{rank}(\mathbf{W}, \mathbf{Z}) - \text{rank}(\mathbf{W})$, $p^* = \text{rank}(\mathbf{W})$, and $f = n - \text{rank}(\mathbf{W}, \mathbf{Z})$. From Eq. (5) it follows that

$$\text{Var}(\mathbf{y}) = \sigma_e^2 (\mathbf{I} + \eta \mathbf{Z}\mathbf{Z}'). \quad (12)$$

In order to derive the confidence interval for η , let

$$S_\tau = \mathbf{y}' \mathbf{P}_W \mathbf{y}$$

$$S_\gamma = \tilde{\gamma}' \mathbf{q}$$

$$SS_E = \mathbf{y}' \mathbf{y} - S_\tau - S_\gamma$$

$$m = \frac{1}{r} \text{tr}(\mathbf{M})$$

$$\mathbf{P}_W = \mathbf{W}(\mathbf{W}'\mathbf{W})^{-1} \mathbf{W}'$$

$$\mathbf{M} = \mathbf{Z}'(\mathbf{I} - \mathbf{P}_W)\mathbf{Z}$$

$$\mathbf{q} = \mathbf{Z}'(\mathbf{I} - \mathbf{P}_W)\mathbf{y},$$

where $\tilde{\gamma}$ is any solution to the equation $\mathbf{M}\tilde{\gamma} = \mathbf{q}$, which is obtained from the normal equations that can be derived by treating γ , like τ , as a vector of unknown parameters and applying the method of ordinary least squares (Harville and Fenech [9, Eq. 2.3]). An interesting property of the matrix \mathbf{M} is that $\text{rank}(\mathbf{M}) = r$ (Marsaglia and Styan [17]). Also note that $S_\gamma = R(\gamma|\tau) = R(\gamma, \tau) - R(\tau)$ and $S_\tau = R(\tau)$, where $R(\gamma|\tau)$ denotes the reduction in the sum of squares due to fitting γ after τ , $R(\gamma, \tau)$ is the total regression

sum of squares obtained from both the fixed and random effects in the model, $R(\boldsymbol{\tau})$ is the regression sum of squares due to fitting a model with just the fixed effects, and SS_E is the corresponding residual sum of squares. Applying Formula (79) of Searle [19, p. 445], we have:

$$E[S_{\boldsymbol{\gamma}} / r] = \sigma_{\varepsilon}^2 + \frac{1}{r} \text{tr}(\mathbf{M})\sigma_{\boldsymbol{\gamma}}^2 = \sigma_{\varepsilon}^2 + m\sigma_{\boldsymbol{\gamma}}^2,$$

$$E[SS_E / f] = \sigma_{\varepsilon}^2.$$

It is well known from the theory of distribution of quadratic forms that $SS_E / \sigma_{\varepsilon}^2 \sim \chi_f^2$. Suppose that we are interested in testing the null hypothesis that $\eta = 0$. If this hypothesis is true, then $S_{\boldsymbol{\gamma}} / (\sigma_{\varepsilon}^2 + m\sigma_{\boldsymbol{\gamma}}^2) \sim \chi_r^2$. However, if the null hypothesis is false, then the distribution of $S_{\boldsymbol{\gamma}} / (\sigma_{\varepsilon}^2 + m\sigma_{\boldsymbol{\gamma}}^2)$ is not χ_r^2 , but is a linear combination of two or more independently distributed chi-squared random variables. In what follows, we obtain a pivotal quantity which can be used for constructing a confidence interval for η .

Recall that $r = \text{rank}(\mathbf{M})$. Let $\Delta_1, \dots, \Delta_r$ denote the nonzero eigenvalues of \mathbf{M} and let $\mathbf{D} = \text{diag}(\Delta_1, \dots, \Delta_r)$ with $0 < \Delta_1 \leq \dots \leq \Delta_r$. Define \mathbf{N} as a $b \times r$ matrix such that $\mathbf{N}'\mathbf{N} = \mathbf{I}_r$ and $\mathbf{M}\mathbf{N} = \mathbf{N}\mathbf{D}$, that is, the columns of \mathbf{N} are orthonormal eigenvectors of \mathbf{M} corresponding to the eigenvalues $\Delta_1, \dots, \Delta_r$. Treating $\boldsymbol{\gamma}$ like $\boldsymbol{\tau}$ as a vector of unknown parameters, Harville and Fenech [9, p. 140] concluded the following: (i) a necessary and sufficient condition for a linear function $\mathbf{g}'\boldsymbol{\gamma}$ to be estimable is the existence of a vector \mathbf{h} such that $\mathbf{g}' = \mathbf{h}'\mathbf{M}$, and (ii) there exists an $r \times 1$ (where $r = \text{rank}(\mathbf{M})$) vector of linearly independent estimable functions of $\boldsymbol{\gamma}$. One such $r \times 1$ vector is $\mathbf{t} = (t_1, \dots, t_r)'$ where

$$\mathbf{t} = \mathbf{D}^{1/2}\mathbf{N}'\boldsymbol{\gamma} = \mathbf{D}^{-1/2}\mathbf{N}\mathbf{M}\boldsymbol{\gamma}. \tag{13}$$

Since $\tilde{\boldsymbol{\gamma}}$ is a solution to the linear equation $\mathbf{M}\tilde{\boldsymbol{\gamma}} = \mathbf{q}$, $\mathbf{t} = (t_1, \dots, t_r)'$ can be estimated by $\tilde{\mathbf{t}} = (\tilde{t}_1, \dots, \tilde{t}_r)'$, where

$$\tilde{\mathbf{t}} = \mathbf{D}^{1/2}\mathbf{N}'\tilde{\boldsymbol{\gamma}} = \mathbf{D}^{-1/2}\mathbf{N}\mathbf{M}\tilde{\boldsymbol{\gamma}} = \mathbf{D}^{-1/2}\mathbf{N}\mathbf{q}, \tag{14}$$

which will be used to obtain a pivotal quantity for constructing a confidence interval for η . Noting that $\mathbf{P}_W\mathbf{W} = \mathbf{W}$, $\mathbf{P}_W = \mathbf{P}'_W = \mathbf{P}^2_W$, it can be shown that the distribution of \mathbf{q} is a multivariate normal with

$$E(\mathbf{q}) = \mathbf{0}$$

$$\text{Var}(\mathbf{q}) = \sigma_{\varepsilon}^2\mathbf{Z}'(\mathbf{I} - \mathbf{P}_W)(\mathbf{I} + \eta\mathbf{Z}\mathbf{Z}')(\mathbf{I} - \mathbf{P}_W)\mathbf{Z}$$

$$= \sigma_{\varepsilon}^2(\mathbf{M} + \eta\mathbf{M}^2),$$

where, if we recall, $\sigma_{\varepsilon}^2(\mathbf{I} + \eta\mathbf{Z}\mathbf{Z}')$ is equal to $\text{Var}(\mathbf{y})$. As a result, the distribution of $\tilde{\mathbf{t}}$ is a multivariate normal with

$$E(\tilde{\mathbf{t}}) = \mathbf{0},$$

$$\text{Var}(\tilde{\mathbf{t}}) = \sigma_{\varepsilon}^2\mathbf{D}^{-1/2}\mathbf{N}'(\mathbf{M} + \eta\mathbf{M}^2)\mathbf{N}\mathbf{D}^{-1/2}$$

$$= \sigma_{\varepsilon}^2(\mathbf{I} + \eta\mathbf{D}).$$

Let us now define $G(\eta; \mathbf{y})$ as

$$\begin{aligned} G(\eta; \mathbf{y}) &= \frac{(1/r)\tilde{\mathbf{t}}'(\mathbf{I} + \eta\mathbf{D})^{-1}\tilde{\mathbf{t}}}{(1/f)SS_E} \\ &= \left(\frac{f}{r}\right)^{\sum_{i=1}^r \tilde{t}_i^2 / (1 + \eta\Delta_i)} \frac{1}{SS_E}. \end{aligned} \quad (15)$$

It can be shown that $\tilde{\mathbf{t}}'(\mathbf{I} + \eta\mathbf{D})^{-1}\tilde{\mathbf{t}} / \sigma_\varepsilon^2 = \tilde{\mathbf{t}}'[Var(\tilde{\mathbf{t}})]^{-1}\tilde{\mathbf{t}} \sim \chi_r^2$ and hence $G(\eta; \mathbf{y}) \sim F(r; f)$. Note that although the matrix \mathbf{N} is not unique, $Var(\tilde{\mathbf{t}}) = \sigma_\varepsilon^2(\mathbf{I} + \eta\mathbf{D})$ is invariant to the choice of \mathbf{N} . As the distribution of $G(\eta; \mathbf{y})$ does not depend on any unknown parameters except η , it can be used as a pivotal quantity for constructing a confidence interval for η .

Burdick *et al.* [3] used the so-called bisection method to compute the aforementioned exact interval. The exact two-sided $(1-\alpha)100\%$ confidence interval on η is given by $[l^*, u^*]$, where l^*, u^* are, respectively, the roots of the following equations:

$$\begin{aligned} G(\eta; \mathbf{y}) &= F_{1-\alpha/2; r, f}, \\ G(\eta; \mathbf{y}) &= F_{\alpha/2; r, f}. \end{aligned} \quad (16)$$

Note that $G(\eta; \mathbf{y})$ can be rewritten as

$$G(\eta; \mathbf{y}) = \left(\frac{f}{r}\right)^{\sum_{i=1}^r \tilde{t}_i^2 (\Delta_i^{-1} + \eta)^{-1} / \Delta_i} \frac{1}{SS_E}. \quad (17)$$

The function $G(\eta; \mathbf{y})$ is convex and monotonically nonincreasing with respect to η for $0 \leq \eta < \infty$ and $G(0; \mathbf{y}) = f \sum_{i=1}^r \tilde{t}_i^2 / (rSS_E)$. If we replace $(\Delta_i^{-1} + \eta)^{-1}$ with $(\Delta_1^{-1} + \eta)^{-1}$ and $(\Delta_r^{-1} + \eta)^{-1}$ we get the functions $G_1(\eta; \mathbf{y})$ and $G_r(\eta; \mathbf{y})$, respectively, such that $G_1(\eta; \mathbf{y}) \leq G(\eta; \mathbf{y}) \leq G_r(\eta; \mathbf{y})$. This is true because $0 < \Delta_1 \leq \dots \leq \Delta_r$.

The bisection method makes use of the bounds l_1, l_r, u_1, u_r (see Eqs. (19)), which are obtained by equating $G_1(\eta; \mathbf{y})$ and $G_r(\eta; \mathbf{y})$ with $F_{1-\alpha/2; r, f}$ and $F_{\alpha/2; r, f}$, respectively. Thus by replacing η with l_1, l_r, u_1, u_r we get the following equations:

$$\begin{aligned} G_1(l_1; \mathbf{y}) &= F_{1-\alpha/2; r, f} \\ G_r(l_r; \mathbf{y}) &= F_{1-\alpha/2; r, f} \\ G_1(u_1; \mathbf{y}) &= F_{\alpha/2; r, f} \\ G_r(u_r; \mathbf{y}) &= F_{\alpha/2; r, f}. \end{aligned} \quad (18)$$

The above equations yield the following bounds

$$l_1 = \frac{f \sum_{i=1}^r \tilde{t}_i^2 / \Delta_i}{rSS_E F_{1-\alpha/2; r, f}} - 1 / \Delta_1$$

$$\begin{aligned}
 l_r &= \frac{f \sum_{i=1}^r \tilde{t}_i^2 / \Delta_i}{rSS_E F_{1-\alpha/2;r,f}} - 1 / \Delta_r \\
 u_1 &= \frac{f \sum_{i=1}^r \tilde{t}_i^2 / \Delta_i}{rSS_E F_{\alpha/2;r,f}} - 1 / \Delta_1 \\
 u_r &= \frac{f \sum_{i=1}^r \tilde{t}_i^2 / \Delta_i}{rSS_E F_{\alpha/2;r,f}} - 1 / \Delta_r.
 \end{aligned} \tag{19}$$

For example, $G_1(l_1; \mathbf{y}) = F_{1-\alpha/2;r,f}$ implies that (see Eq. (17))

$$\begin{aligned}
 \left(\frac{f}{r}\right) \frac{\sum_{i=1}^r \tilde{t}_i^2 (\Delta_1^{-1} + l_1)^{-1} / \Delta_i}{SS_E} &= F_{1-\alpha/2;r,f} \\
 \left(\frac{f}{r}\right) \frac{\sum_{i=1}^r \tilde{t}_i^2 / \Delta_i}{SS_E} &= (l_1 + \Delta_1^{-1}) F_{1-\alpha/2;r,f} \\
 \frac{f \sum_{i=1}^r \tilde{t}_i^2 / \Delta_i}{rSS_E F_{1-\alpha/2;r,f}} - 1 / \Delta_1 &= l_1.
 \end{aligned}$$

Since $G_1(\eta; \mathbf{y}) \leq G(\eta; \mathbf{y}) \leq G_r(\eta; \mathbf{y})$, $l_1 \leq l^* \leq l_r$ and $u_1 \leq u^* \leq u_r$, where l^*, u^* are the roots of Eq. (16). Instead of solving the two non-linear equations, the bisection method uses these lower and upper bounds to compute l^* and u^* . A demonstration of these calculations is given in Burdick and Graybill ([2], Appendix B).

5. Example

A numerical example describing the analysis of a response surface model with a random block effect was given in Khuri [10]. The example investigated the effects of two factors, temperature (x_1) and curing time (x_2), on the shear strength of the bonding of galvanized steel bars with a certain adhesive. The galvanized steel bars were selected over a period of 12 days. Each batch of steel bars was selected at random on a given date. Hence, the 12 dates were treated as random blocks. Three levels were chosen for each of the two factors according to a 3^2 factorial design. The same design was used on each of these 12 dates, except that on certain days, replications were taken at the design center in order to test for lack of fit of the fitted model. We refer to this 3^2 factorial design as D_1 . A complete second-degree model was fitted to the data. The actual data set, consisting of $n=118$ observations in 12 blocks, is given in Khuri ([10], Table 1) and is reproduced here in Table 1. Note that x_1 and x_2 denote the coded values of temperature and time, respectively, namely,

$$x_1 = \frac{\text{temperature} - 400}{25}, \quad x_2 = \frac{\text{time} - 35}{5}.$$

The settings of x_1 and x_2 from the 3^2 design are $-1, 0, 2$ for x_1 , and $-1, 0, 1$ for x_2 .

Table 1. Design settings and response values (shear strength in psi).

Block(Batch)							
Temp x_1	Time x_2	1 (July 11)	2 (July 16)	3 (July 20)	4 (Aug. 7)	5 (Aug. 8)	6 (Aug. 14)
-1	-1	1226	1075	1172	1213	1282	1142
0	-1	1898	1790	1804	1961	1940	1699
2	-1	2142	1843	2061	2184	2095	1935
-1	0	1472	1121	1506	1606	1572	1608
0	0	2010, 1882 1915, 2106	2175	2279	2450, 2355 2420, 2240	2291	2374
2	0	2352	2274	2168	2298	2147	2413
-1	1	1491	1691	1707	1882	1741	1846
0	1	2078	2513	2392	2531	2366	2392
2	1	2531	2588	2617	2609	2431	2408
Block(Batch)							
Temp x_1	Time x_2	7 (Aug. 20)	8 (Aug. 22)	9 (Sep. 11)	10 (Sep. 24)	11 (Oct. 3)	12 (Oct.10)
-1	-1	1281	1305	1091	1281	1305	1207
0	-1	1833	1774	1588	1992	2011	1742
2	-1	2116	2133	1913	2213	2192	1995
-1	0	1502	1580	1343	1691	1584	1486
0	0	2471	2393	2205,2268 2103	2142	2052, 2032 2190	2339
2	0	2430	2440	2093	2208	2201	2216
-1	1	1645	1688	1582	1692	1744	1751
0	1	2392	2413	2392	2488	2392	2390
2	1	2517	2604	2477	2601	2588	2572

Note: The original design settings of x_1 corresponding to -1, 0, 2 are 375° F, 400° F, and 450° F, respectively; those for x_2 corresponding to -1, 0, 1 are 30, 35, and 40 sec., respectively. (Source: Khuri [10, Table 1])

Table 2. Design settings for D_1 , D_2 , D_3 , D_4 and D_5 .

D_1^a		D_2^b		D_3^c		D_4^d		D_5^e	
x_1	x_2	x_1	x_2	x_1	x_2	x_1	x_2	x_1	x_2
-1	-1	-1	-1	-1	0	-1	-1	0.54	0.14
0	-1	0.5	-1	1	-1	0.5	1	0.33	0.99
2	-1	2	-1	1	1	2	-1	0.09	-0.77
-1	0	-1	0	-0.5	1	0.5	-1	-0.91	0.53
0	0	0.5	0	-0.5	-1	-1	1	0.96	-0.22
2	0	2	0	2	0	2	1	-0.38	-0.30
-1	1	-1	1	0	0	0.5	0	-0.80	-0.38
0	1	0.5	1	0	0	0.5	0	-0.10	0.52
2	1	2	1	0	0	0.5	0	0.59	0.09

- a: D_1 is the original design shown in Table 1.
b: D_2 is the same as D_1 , but the settings of x_1 are -1, 0.5, 2.
c: D_3 is the semi-uniform shell 1 design.
d: D_4 is the semi-uniform shell 2 design.
e: D_5 is the randomly generated design.

In this section, we compare D_1 with four other second-order designs. The designs were chosen so that a second-degree model can be fitted. They include the designs D_2 , D_3 , D_4 , and D_5 . The first one is similar to D_1 with the only difference being that the coded settings of x_1 are equally spaced having the values $-1, 0.5, 2$. Designs D_3 and D_4 are modified versions of the so-called uniform shell designs which were developed by Doehlert [5] and Klee (Doehlert and Klee [6]). The original uniform shell designs consist of points that are distributed on concentric spherical shells. In two-dimensional spaces, these designs are obtained from the points of a double simplex with a center point. The proposed modified design points for D_3 and D_4 resemble the points of a two-dimensional uniform shell design, but they are not located on the same sphere. Therefore, we refer to D_3 and D_4 as semi-uniform shell 1 and semi-uniform shell 2 designs, respectively. The fourth design is D_5 , which is obtained by randomly generating points in the design space of D_1 . The design settings for $D_1 - D_5$ are presented in Table 2 and the corresponding design points are shown in Figure 1.

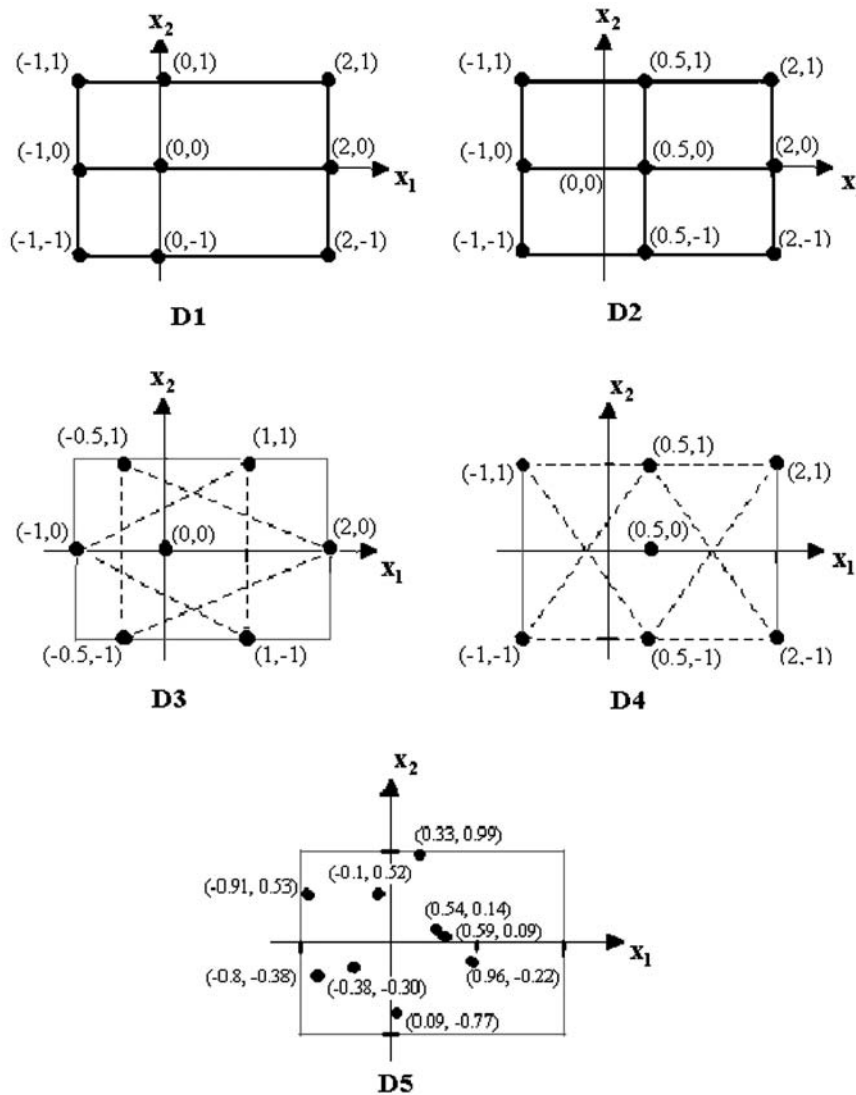


Figure 1. Plots of the design points for D_1 , D_2 , D_3 , D_4 and D_5 .

The experimental region, R , is rectangular with $-1 \leq x_1 \leq 2$, $-1 \leq x_2 \leq 1$. For each design, we consider the distribution of $\Delta_D(x, \eta)$ on each of several concentric rectangles, R_λ , which are obtained by a reduction of the boundary of R using a shrinkage factor λ , $0.5 < \lambda \leq 1$. Thus R_λ is determined by the inequalities

$$a_i + (1 - \lambda)(b_i - a_i) \leq x_i \leq b_i - (1 - \lambda)(b_i - a_i), \quad i = 1, 2,$$

where a_i and b_i are the bounds on x_i in R ($i = 1, 2$). In order to investigate the dependence of $\Delta_D(x, \eta)$ on η , a parameter space for η is established. For this purpose, we use the method described in Section 4 to construct a confidence interval for η . Using the data set in Table 1, we obtain the 95% confidence interval, C , namely $(l^*, u^*) = (0.0763243, 0.9667678)$. For each design and a selected value of η in C , quantiles of the distribution of $\Delta_D(x, \eta)$ are obtained for $x \in R_\lambda$, where λ is one of several values of λ chosen from the interval $(0.5, 1]$. The number of points chosen on each R_λ was 2000 consisting of 500 on each side. The quantiles are calculated for $p = 0(0.05)1$. The procedure is repeated for other values of η in C . Then $Q_D^{max}(p, \lambda)$ and $Q_D^{min}(p, \lambda)$ are calculated using the formulas in Eq. (11). The R software was used in conducting the numerical investigation and obtaining the actual plots.

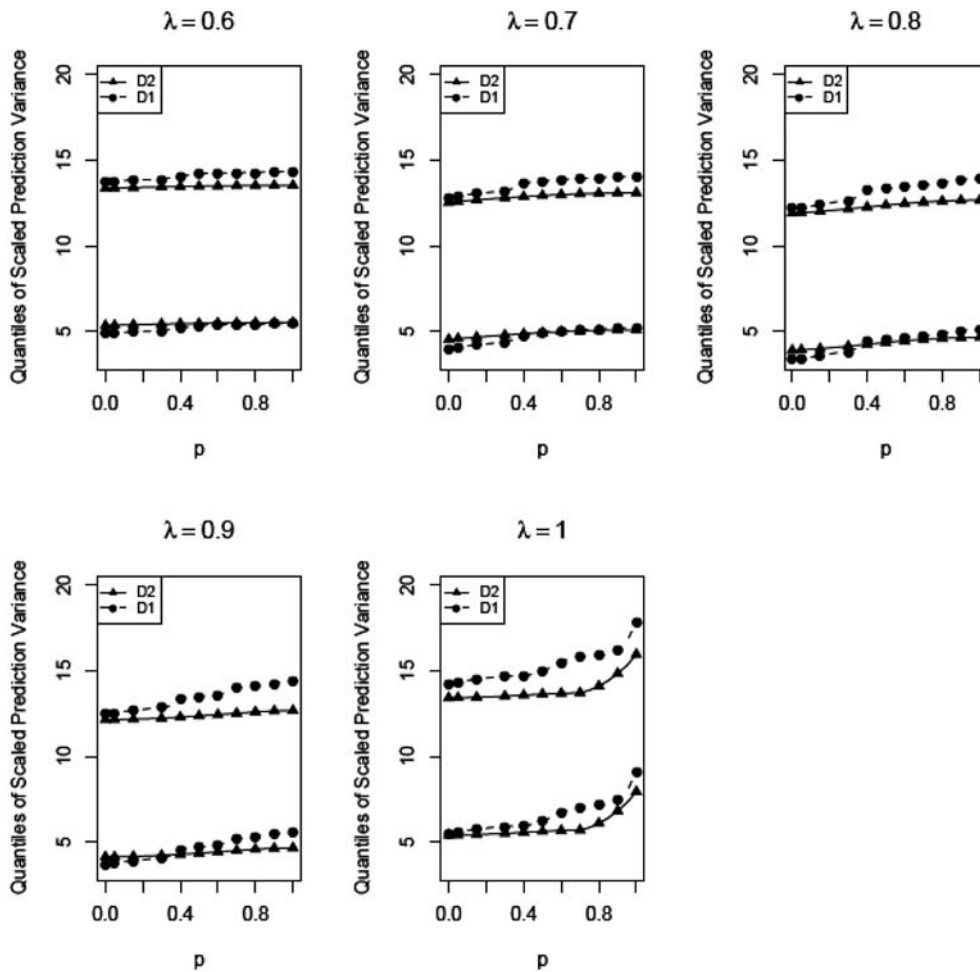


Figure 2. Quantile dispersion graphs for D_1 and D_2 .

The QDGs for the comparison of design D_1 with D_2 , D_3 , D_4 , and D_5 are given in Figures 2, 3, 4 and 5, respectively. The QDGs for the comparison of D_3 with D_4 , and D_4 with D_5 are presented in Figures 6 and 7, respectively. From Figure 2, it is evident that for small values of λ (less than 0.9), D_2 performs slightly better than D_1 . For $\lambda = 0.9$ and 1, the difference in prediction capability is distinctly evident in favor of D_2 . Figures 3 and 4 suggest that the semi-uniform shell designs, D_3 and D_4 , perform better than D_1 for $\lambda = 0.6, 0.7$ and 0.8 . However, for $\lambda = 0.9$ and 1 and high values of p , D_1 has better prediction capability than D_3 and D_4 . The QDGs for the comparison of design D_1 with D_5 (see Figure 5) clearly depict better prediction capability with design D_1 . Figures 6 and 7 indicate that design D_4 is better than D_3 and D_5 . It should be noted that changing the confidence coefficient for the confidence interval C from 0.95 to 0.90 or 0.99 did not change much the pattern of the QDGs. This indicates that the QDGs are not sensitive to changes in the bounds of the confidence interval on η .

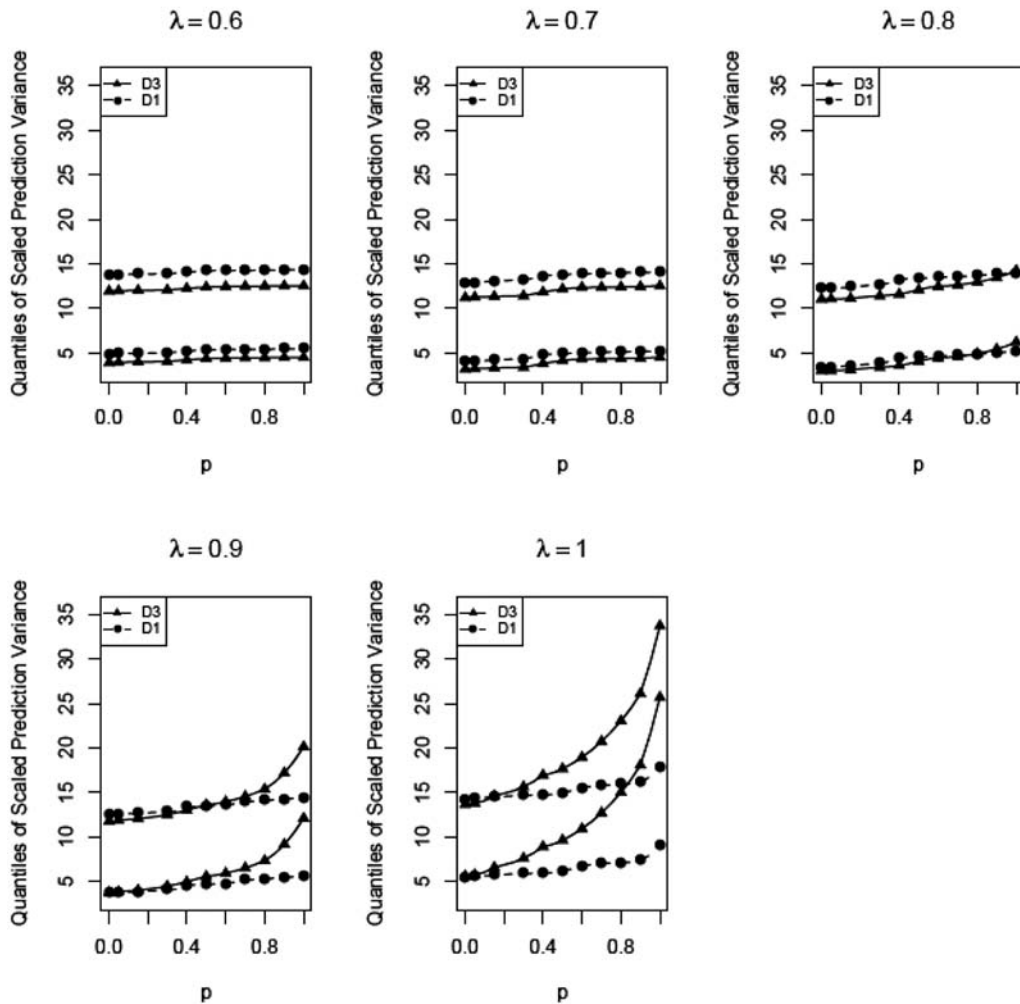


Figure 3. Quantile dispersion graphs for D_1 and D_3 (semi-uniform shell 1).

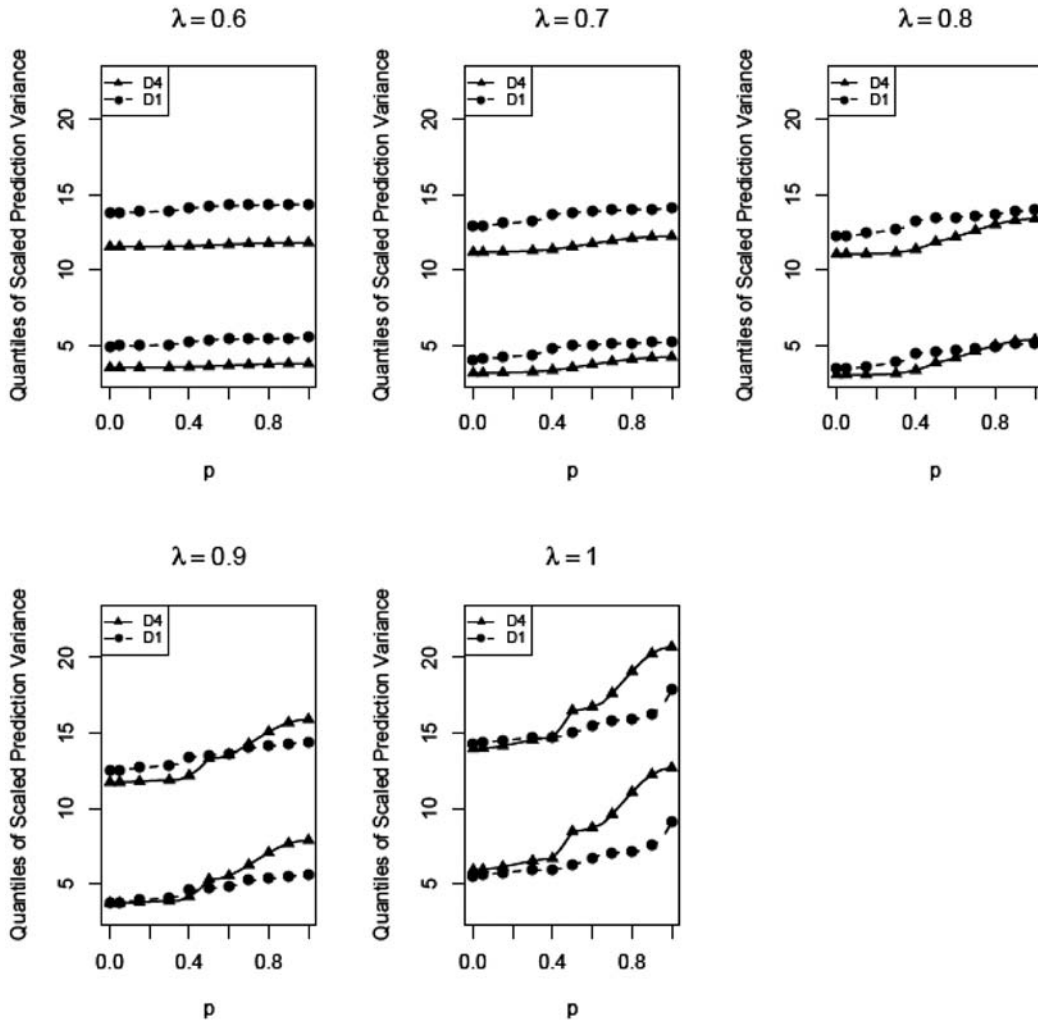


Figure 4. Quantile dispersion graphs for D_1 and D_4 (semi-uniform shell 2).

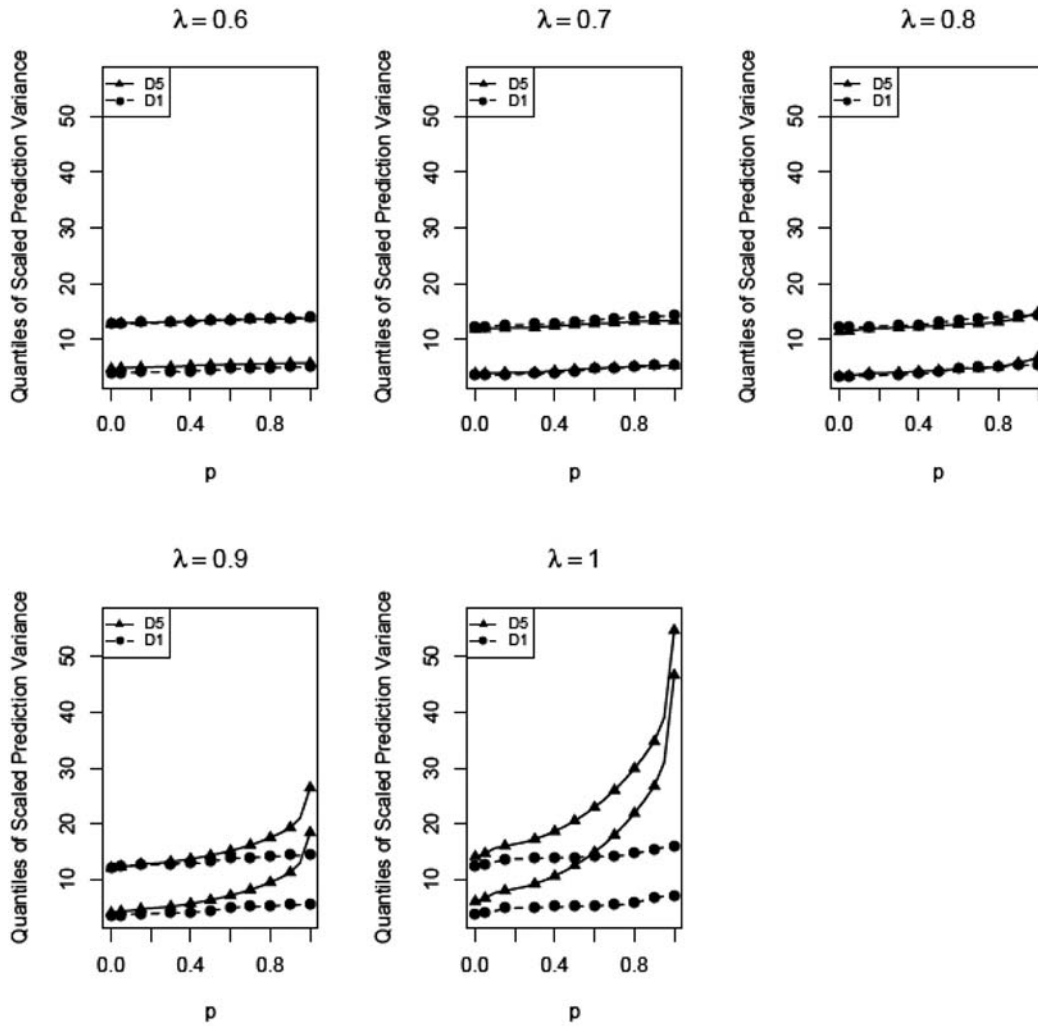


Figure 5. Quantile dispersion graphs for D_1 and D_5 (randomly generated).

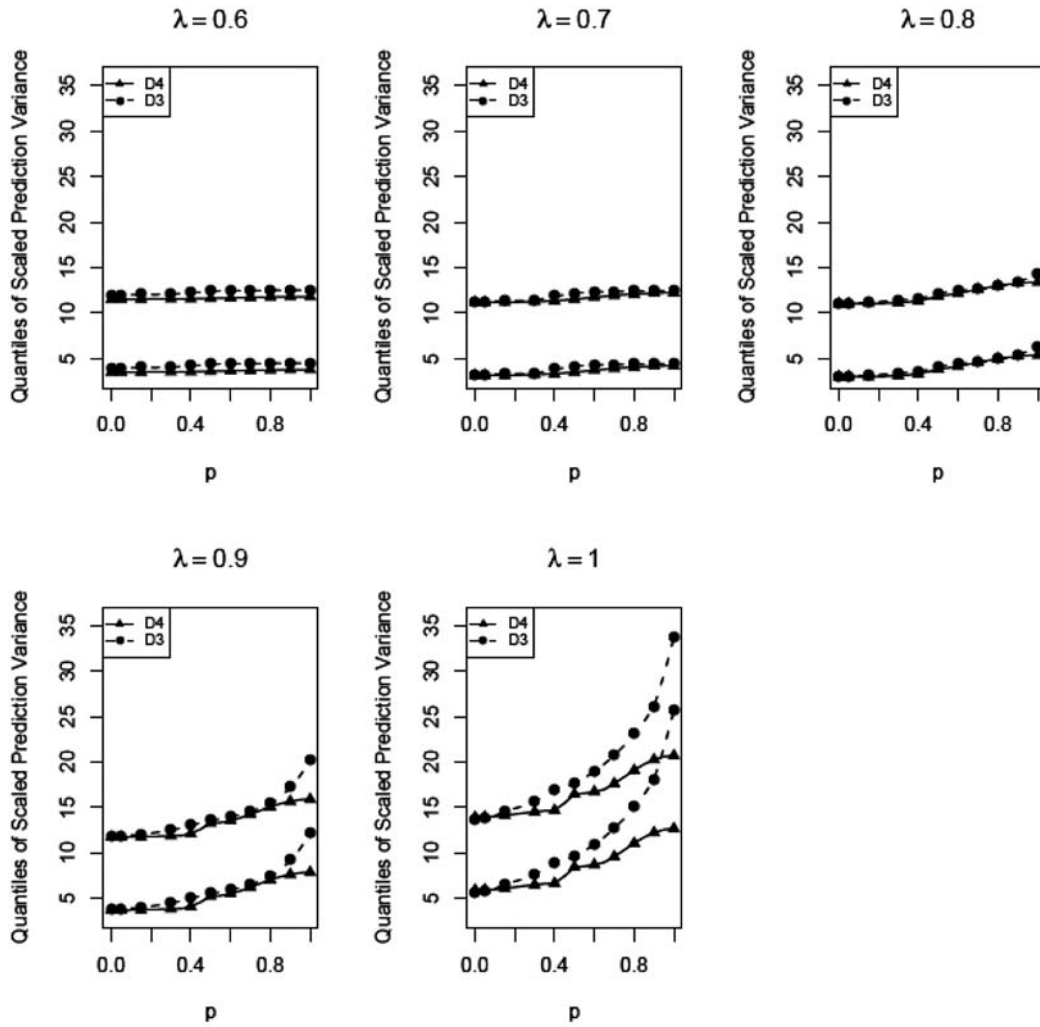


Figure 6. Quantile dispersion graphs for D_3 (semi-uniform shell 1) and D_4 (semi-uniform shell 2).

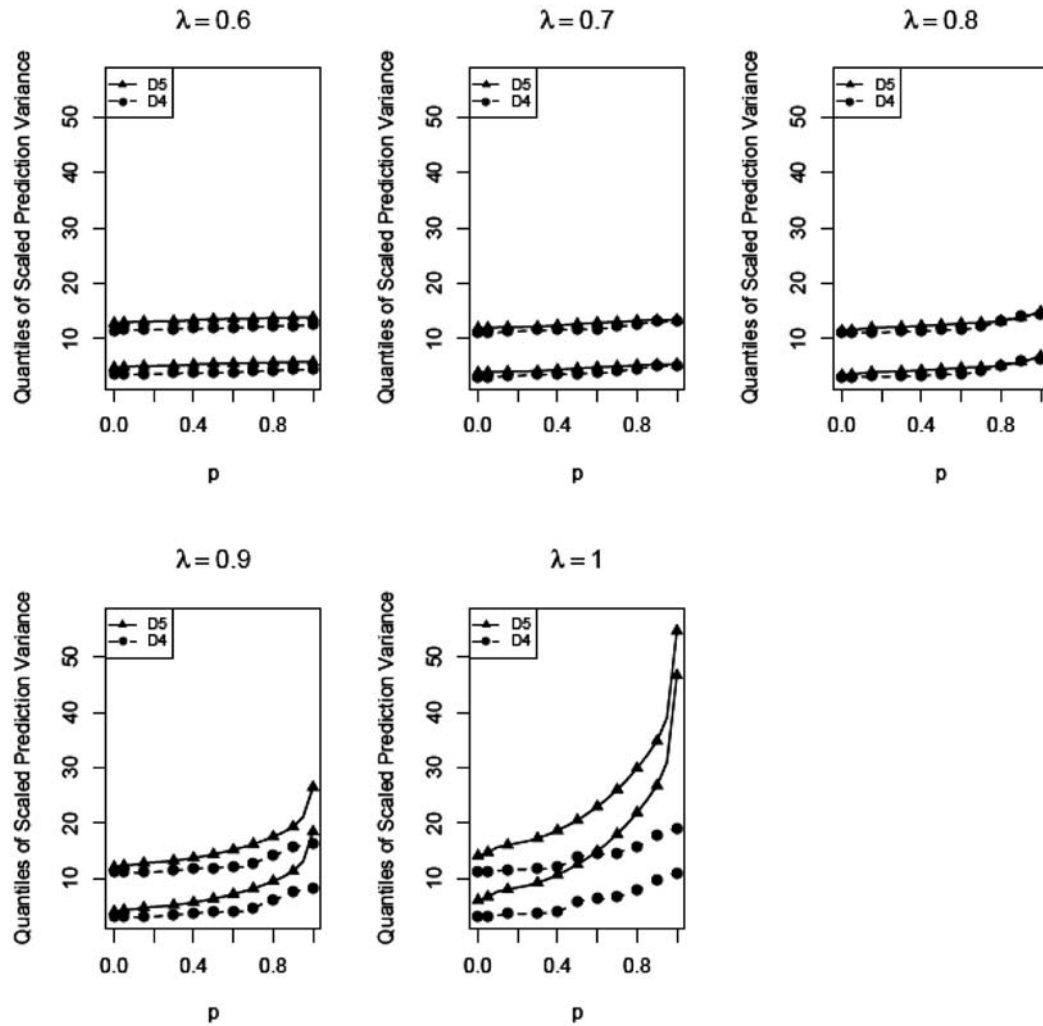


Figure 7. Quantile dispersion graphs for D_4 (semi-uniform shell 2) and D_5 (randomly generated).

6. Concluding Remarks

The QDGs provide a powerful graphical tool for comparing designs for response surface models with random block effects. The design dependence problem was circumvented by the consideration of the dispersion of the quantiles of the scaled prediction variance over a certain parameter space associated with the unknown parameter, η .

The experimental error variance in a response surface model with a block effect has traditionally been assumed to be constant. However, in many experimental situations, this variance may not be the same for the different blocks that make up the associated design. We would like to extend the proposed methodology to study the choice of designs for such models with heterogeneous error variances.

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