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Optimal Linear-Quadratic Model Designs

John J. Borkowski

Department of Mathematical Sciences, Montana State University, Bozeman, MT 59717 USA

Author for correspondence; e-mail: jobo@math.montana.edu

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Abstract

Experimentation for achieving a robust process often involves signal variables which are controllable and internal to the process and noise variables which are generally external and routinely uncontrollable. To achieve a robust process, designs based on a combined array have been suggested by many authors. Many of these designs allow parameter estimation for the linear-quadratic (*LQ*) response surface model when the experimental design region is the hypercube. The *LQ* model contains the full quadratic model terms in the *Q* signal variables, the linear model terms in the *L* noise variables, and the signal by noise variable interaction terms. Because the quadratic regression model is just a special case of the *LQ* model when there are $L = 0$ noise variables, this article extends the optimal design theory regarding regression on the hypercube.

An approach similar to that of Farrell, Kiefer, and Walbran [13] will be taken in this article. A support of D- and G-optimal designs for the *LQ* model on the hypercube will be defined. Closed-form expressions for the generalized (D) and prediction (G) variance are derived. Using these closed-forms, D-optimal design weights are determined for barycentric subsets of points in the support. These weights and the corresponding optimal D-criterion values are tabled for $4 \le K \le 17$ design variables.

Keyword: combined array, crossed array, design efficiency, design optimality, generalized variance, prediction variance, robust design.

1. Introduction

Experimentation for achieving a robust process often considers two sets of process variables. "Signal" variables are internal to the manufacturing process with levels that can be controlled during routine operation of the process. "Noise" variables are, in general, external to the process and cannot be, or are difficult to, routinely control during the operation of the process. Despite the randomness of noise variables outside of the experimental situation, these variables can be controlled for experimental purposes.

The use of product or "crossed" orthogonal arrays (Taguchi [29], Myers and Montgomery [25]) is one experimental design approach for achieving a robust process. Alternatively, designs based on a single "combined" array have been discussed by many authors including Borkowski [2], Borkowski and Lucas [6], Lucas [21,22], Box and Jones [10], Myers et al. [24], Welch et al. [30,31], Shoemaker et al. [28], and Lorenzen and Villalobos [20]. In this paper, I consider the class of designs which allow estimation of the parameters in the following model when a design region is restricted to a $K = Q + L$ dimensional hypercube:

$$y = \beta_0 + \sum_{i=1}^{Q} \beta_i x_i + \sum_{i=1}^{Q} \beta_{ii} x_{ii}^2 + \sum_{i=1}^{Q-1} \sum_{j=i+1}^{Q} \beta_{ij} x_i x_j + \sum_{k=1}^{L} \delta_k z_k + \sum_{i=1}^{Q} \sum_{k=1}^{L} \delta_{ik} x_i z_k + \varepsilon \qquad (1)$$

This model will be called the **linear-by-quadratic model** or ***LQ* model** for signal variables $x_1,\ldots,x_Q$ and noise variables $z_1,\ldots,z_L$. The model is so named because it contains the

- Linear expression $\sum_{k=1}^{L} \delta_k z_k$ in the noise variables.
- Quadratic expression $\sum_{i=1}^{Q} \beta_i x_i + \sum_{i=1}^{Q} \beta_{ii} x_{ii}^2 + \sum_{i=1}^{Q-1} \sum_{j=i+1}^{Q} \beta_{ij} x_i x_j$ in the signal variables.
- Product expression $\sum_{i=1}^{Q} \sum_{k=1}^{L} \delta_{ik} x_i z_k$ in the Q signal and L noise variables.

Any design that can fit the *LQ* model will be referred to as an ***LQ* model design**. Like many response surface designs for fitting a full second order model, many *LQ* model designs are based on a combined array of factors. However, estimation of the squared z_i^2 terms and the interaction $z_i z_j$ terms among noise factors is not considered. Because *LQ* model designs require fewer design points than designs fitting the full second-order model, they are a compromise between the design size and being able to fit the additional z_i^2 and $z_i z_j$ terms of the full quadratic model. One benefit of combined array *LQ* model designs is that they always allow estimation of the potentially important signal-by-signal interaction terms while product orthogonal arrays do not always allow estimation of these interaction terms.

2. Design Optimality and Efficiency

Prior to the major contributions to the theory of optimal designs be Kiefer [16,17] and Kiefer and Wolfowitz [18,19], it was routinely assumed that each point in an experimental design was assigned an equal weight. However, Kiefer and his colleagues generalized this established concept to allow for alternate weighting schemes for the set of design points. Their research, often referred to as "approximate" design theory, developed concepts which treated a design as a probability measure ξ on the design space $\mathcal{X}$.

A design ξ is a **probability measure** on a compact design space $\mathcal{X}$ if it satisfies (i) $0 \le \xi(A) \le 1$ for all $\forall A \subset \mathcal{X}$, (ii) $\int_{\mathcal{X}} \xi(dx) = 1$, and (iii) if $\bigcap_{i=1}^{\infty} A_i \in \mathcal{X}$ for a disjoint sequence $A_1, A_2, \ldots$ of sets in $\mathcal{X}$, then $\xi(\bigcap_{i=1}^{\infty} A_i) = \sum_{i=1}^{\infty} \xi(A_i)$. An **approximate design** ξ on $\mathcal{X}$ is a probability measure that assigns weights $w_1, \ldots, w_N$ ($0 < w_i \le 1$) to the set of N experimental trials $x_1, \ldots, x_N$ and zero weight elsewhere. An **exact design** having N points is an approximate design for which the measure assigns weight r_i/N to each design point such that r_i is an integer ($i = 1, \ldots, N$) and $\sum r_i = N$.

Let f be a known $p \times 1$ vector of continuous functions $f_1, f_2, \ldots, f_p$ on the space $\mathcal{X}$, and let θ represent a $p \times 1$ vector of unknown real-valued parameters. For the *LQ* model:

$$f = [1, x_1, x_2, \ldots x_Q, x_1^2, x_2^2, \ldots, x_Q^2, x_1x_2, \ldots x_{Q-1}x_Q, z_1, z_2, \ldots z_L, x_1x_2, \ldots x_Q z_L]'$$

For design ξ, the **moment matrix** $\mathbf{M}(\xi) = [m_{ij}(\xi)]$ where $m_{ij}(\xi)$ is the $(i,j)^{\text{th}}$ entry of $\mathbf{M}(\xi)$ such that $m_{ij}(\xi) = \int_{\mathcal{X}} f_i(x) f_j(x)\, \xi(dx)$. (Note: For an exact *N*-point design with model matrix $\boldsymbol{X}$, the moment matrix $\mathbf{M}(\mathbf{X}) = (\mathbf{X'X})/N$. For nonsingular $\mathbf{M}(\xi)$, the **normalized prediction variance** function $V(x,\xi)$ is defined as

$$V(x,\xi) = f(x)'\, \mathbf{M}^{-1}(\xi)\, f(x). \quad (2)$$

Let $\lambda_1(\xi),\ldots,\lambda_k(\xi)$ be the eigenvalues of the moment matrix $\mathbf{M}(\xi)$. For nonsingular $\mathbf{M}(\xi)$, the optimality functionals are defined as

$$\Phi_t(\xi) = \left[\frac{1}{k} trace\ (\mathbf{M}^{-1}(\xi))\right]^{1/t} = \left[\frac{1}{k}\sum_{i=1}^{k}\lambda_i^{-t}(\xi)\right]^{1/t} \quad \text{for } 0 < t < \infty$$

$$\Phi_0(\xi) = \lim_{t\downarrow 0}\Phi_t(\xi) = \left|\ \mathbf{M}^{-1}(\xi)\ \right|$$

$$\Phi_\infty(\xi) = \lim_{t\to\infty}\Phi_t(\xi) = \max_i \lambda_i^{-1}(\xi).$$

$\Phi_0(\xi), \Phi_1(\xi),$ and $\Phi_\infty(\xi)$ correspond to the normalized D-, A- and E-optimality criteria (Pukelsheim [27]). A design $\xi^{(t)}$ is a $\Phi_t(\xi)$ - optimal design if it minimizes $\Phi_t(\xi)$. That is,

$$\xi^{(t)} \text{ is } \Phi_t(\xi)\text{-optimal if } \min_\xi \Phi_t(\xi) = \Phi_t(\xi^{(t)}) \quad \text{for } 0 \le t \le \infty$$

To evaluate the performance of design ξ with respect to some $\Phi_t(\xi)$ -optimality criterion, the $\Phi_t(\xi)$ - efficiency e_t is defined as

$$e_t(\xi) = \Phi_t(\xi)/\Phi_t(\xi^{(t)}) \quad \text{for } 0 \le t \le \infty.$$

$e_0(\xi)$, $e_1(\xi)$, and $e_\infty(\xi)$ are, respectively, referred to as the D, A, and E-efficiencies of a design ξ. Hence, any design ξ is considered acceptable for practical application if $e_t(\xi)$ is close to 1 for all values of t considered by the experimenter.

Additionally, there are the IV-optimality and G-optimality criteria $\overline{V}(\xi)$ and $V_G(\xi)$, which are, respectively, the average and maximum of $V(x,\xi)$ in $\mathcal{X}$. That is, for a design ξ, we define

$$\overline{V}(\xi) = \text{average}_{x\in\mathcal{X}} V(x,\xi) \quad \text{and} \quad V_G(\xi) = \max_{x\in\mathcal{X}} V(x,\xi)$$

A design ξ^* is IV-optimal or G-optimal if

$$\overline{V}(\xi^*) = \min_\xi \text{average}_{x\in\mathcal{X}} V(x,\xi) \quad \text{and} \quad V_G(\xi^*) = \min_\xi \max_{x\in\mathcal{X}} V(x,\xi) = p$$

The G-efficiency e_G of a design ξ is defined as $e_G(\xi) = p/V_G(\xi)$ where p is the number of model parameters. The fact that $V_G(\xi) = p$ for a G-optimal design ξ^* is a result of the Equivalence Theorem of Kiefer and Wolfowitz [19]:

Theorem 1 (Kiefer-Wolfowitz Equivalence Theorem): Conditions (I), (II), and (III) are equivalent.

I. ξ* is D-optimal if and only if $\mathbf{M}^{-1}(\xi)$ exists and $\max_{\xi} \left| \mathbf{M}(\xi) \right| = \left| \mathbf{M}(\xi^*) \right|$.

II. ξ* is G-optimal if and only if $\min_{\xi} \max_{x \in \mathcal{X}} V(x,\xi) = \max_{x \in \mathcal{X}} V(x,\xi^*)$.

III. A sufficient condition for ξ* to satisfy (II) is for $\max_{x \in \mathcal{X}} V(x,\xi^*) = p$.

Dette and O'Brien [12] introduced the I_L-optimality criterion which is analogous to the $\Phi_t(\xi)$ -criterion, but it is based on the prediction variance instead of eigenvalues. I_L-optimality is particularly useful for nonlinear regression models.

In practice, exact designs are implemented. Therefore, it is desirable that the D criterion $\Phi_0(\mathbf{X}) = \left(\left|\mathbf{X'X}/N\right|\right)^{1/p}$ and the G criterion $V_{\max}(\mathbf{X}) = N\ f(x)'(\mathbf{X'X})^{-1} f(x)$ that are evaluated for an exact design **X** to be close to the optimal D and G criteria values, i.e., we want an efficiency close to 1. Although a more appropriate comparison would be to compare the D and G values to the optimal exact *N*-trial design criteria values, it is unfortunate that optimal exact *N*-trial designs are not known for many response surface models, in particular, for quadratic and *LQ* models. An exception can be found in Borkowski [5] for which exact D, G, A, and IV-optimal exact designs for 1, 2, and 3 factors are given for the quadratic model assuming a hypercube design space. Efficiencies based on the approximate theory are, therefore, lower bounds for efficiencies based on the class of exact *N*-trial designs. The optimal D-criterion values will be presented in section 4. See Atkinson et al. [1] and Pukelsheim [27] for details on design optimality criteria, efficiencies, and the Kiefer-Wolfowitz Equivalence Theorem.

3. The Support of Optimal *LQ* Model Designs on the Hypercube

A **support** of a design measure ξ is defined to be any subset *S* in design space $\mathcal{X}$ for which $\xi(S)$ = 1. When considering a design as a probability measure, the complexities that usually occur with discrete set problems are reduced to those encountered with a continuous set problem. To aid in the discussion of the support of optimal designs, let

$$H_q = \left\{ (x_1, x_2, \ldots x_q) : \ |x_i| \le 1, \ \forall i \ \right\}$$

be the q-dimensional cube. A **barycenter of depth k** for $0 \le k \le q$ is a point with *k* coordinates equal to 0 and *q-k* coordinates equal to ±1. Thus, there are $\binom{q}{k} 2^{q-k}$ unique barycenters of depth k. The set of barycenters of depth k is denoted as $J(k)$ and the union of the sets of barycenters $J_q = \cup_{k=0}^{q} J(k)$. J_q is therefore the 3^q factorial array of q-tuples with coordinates 0 or ±1 or the **complete barycentric set** with q coordinates.

For $1 \le a \le q$ and for $1 \le b \le r$, a **barycenter set of depth (*a,b*)** is defined to be a point with $q + r$ coordinates such that

I. For the first q coordinates, a coordinates = 0 and q-a coordinates = ±1.

II. For the last r coordinates, b coordinates = 0 and r-b coordinates = ±1.

Thus, there are $\binom{q}{a}\binom{r}{b}2^{q+r-a-b}$ unique barycenters of depth (a,b). The set of barycenters of depth (a,b) will be denoted as $J(a,b)$. The barycentric points are crucial in the subsequent development of D-optimal *LQ* model designs.

For the *LQ* model, it will be shown that a D-optimal design can be supported by a subset of $J_Q \times J_L$, specifically, by the set of points in $J^* = J(0,0) \cup J(1,0) \cup J(Q,0)$.

The following two steps will be used to find D-optimal *LQ* designs:

1. Find closed-form expressions for $V(x,\xi)$ and $|\mathbf{M}(\xi)|$.
2. Find non-negative weights to assign to $J(0,0), J(1,0),$ and $J(Q,0)$ that maximize $|\mathbf{M}(\xi)|$.

Let ξ' be the design associated with the optimal weights. It will be shown that $\max_{x \in X} V(x,\xi') = p$. Thus, having satisfied Condition (III) of Theorem 1, the design ξ' is G-optimal and therefore D-optimal.

3.1 Closed-form Expressions for $V((x{:}z),\xi)$ and $|\mathbf{M}(\xi)|$

Recall that $J(a,b)$ is the set of barycenters of depth (a,b) for $1 \le a \le q$ and $1 \le b \le r$. We apply these sets in the *LQ* framework where $q = Q$ and $r = L$, and for brevity, let $J = J_{Q+L}$ be the complete barycentric set with $Q+L$ coordinates. It will be shown that $J^* = J(0,0) \cup J(1,0) \cup J(Q,0)$ will support an optimal *LQ* model design with $K=Q+L$ design variables. Let α_1, α_2, and α_3 correspond to the sets $J(0,0)$, $J(1,0)$, and $J(Q,0)$ so that

- a weight of $\frac{\alpha_1}{2^K}$ is assigned to each of the 2^K points in $J(0,0)$,
- a weight of $\frac{\alpha_2}{Q2^{K-1}}$ is assigned to each of the $Q2^{K-1}$ points in $J(1,0)$,
- a weight of $\frac{\alpha_3}{2^L}$ is assigned to each of the 2^L points in $J(Q,0)$.

Any $\{\alpha_1, \alpha_2, \alpha_3\}$ satisfying $\alpha_1+\alpha_2+\alpha_3= 1$ with $\alpha_i \geq 0$ for i =1,2,3 defines a discrete probability measure ξ on the design space $\mathcal{X}$. For notational simplicity, let $y = (x_1,\ldots,x_Q, z_1,\ldots,z_L)$. Because of the discrete design structure associated with ξ, the moments are defined to be:

$$u = \int x_i^2 \; \xi(dy) = \int x_i^4 \; \xi(dy) = \int x_i^2 z_k^2 \; \xi(dy) = \alpha_1 + \frac{Q-1}{Q}\alpha_2$$

$$v = \int x_i^2 x_j^2 \; \xi(dy) = \alpha_1 + \frac{Q-2}{Q}\alpha_2$$

and

$$\int z_k^2 \; \xi(dy) = \alpha_1 + \alpha_2 + \alpha_3 = 1$$

for all $1 \leq i < j \leq Q$ and $1 \leq k \leq L$. To see how u and v were calculated, consider $\int x_i^2 \; \xi(dy)$. By definition of the measure ξ, this integral equals $\sum_{j=1}^{M} x_{ij}^2 w_{ij}$ where $M = 2^K + Q2^{K-1} + 2^L$ = the number of points in J^*, and

$w_{ij} = \frac{\alpha_1}{2^K}$ for $j = 1,\ldots,2^K$ (i.e., the points in *J(0,0)*),

$w_{ij} = \frac{\alpha_2}{Q2^K}$ for $j = 2^K+1,\ldots, 2^K + Q2^{K-1}$ (i.e., the points in *J(1,0)*),

$w_{ij} = \frac{\alpha_3}{2^L}$ for $j = 2^K + Q2^{K-1}+1,\ldots,2^K + Q2^{K-1} + 2^L$ (i.e., the points in *J(Q,0)*).

Note that in *J(0,0)*, $x_{ij}^2 = 1$ for all 2^K values of j ; in *J(1,0)*, $x_{ij}^2 = 1$ for $(Q-1)2^{K-1}$ values of j and is 0 for the remaining 2^{K-1} values of j ; and in *J(Q,0)*, $x_{ij}^2 \equiv 0$ for all 2^L values of j. Thus,

$$\int x_i^2 \; \xi(dy) = \sum_{i=1}^{M} x_{ij}^2 w_{ij} = 2^K \frac{\alpha_1}{2^K} + (Q-1)2^{K-1}\frac{\alpha_2}{Q2^{K-1}} + (0)\frac{\alpha_3}{2^L} = \alpha_1 + \frac{Q-1}{Q}\alpha_2.$$

The other integrals associated with u and v are derived in similar fashion. In terms of u and v, the structure of the moment matrix $\mathbf{M}(\xi)$ and its inverse $\mathbf{M}^{-1}(\xi)$ are presented in Figures 1 and 2.

Figure 1: The Moment Matrix **M**(ξ)

Terms	1	x_i^2	$x_i x_j$	$x_i z_k$	x_i	z_k
1	1	$u\mathbf{J}'_Q$	0	0	0	0
x_i^2	$u\mathbf{J}_Q$	G	0	0	0	0
$x_i x_j$	0	0	$v\mathbf{I}_{Q(Q-1)/2}$	0	0	0
$x_i z_k$	0	0	0	$u\mathbf{I}_{Q\cdot L}$	0	0
x_i	0	0	0	0	$u\mathbf{I}_Q$	0
z_k	0	0	0	0	0	$\mathbf{I}_L$

where $G = (u - v)\mathbf{I}_Q + v\mathbf{J}_Q\mathbf{J}_Q'$

Figure 2: The Inverse Moment Matrix $\mathbf{M}^{-1}$(ξ)

Terms	1	x_i^2	$x_i x_j$	$x_i z_k$	x_i	z_k
1	A	$B\mathbf{J}'_Q$	0	0	0	0
x_i^2	$B\mathbf{J}_Q$	G^*	0	0	0	0
$x_i x_j$	0	0	$(1/v)\mathbf{I}_{Q(Q-1)/2}$	0	0	0
$x_i z_k$	0	0	0	$(1/u)\mathbf{I}_{Q\cdot L}$	0	0
x_i	0	0	0	0	$(1/u)\mathbf{I}_Q$	0
z_k	0	0	0	0	0	$\mathbf{I}_L$

where $A = \dfrac{(Q-1)v+u}{d^*}$ $B = -\dfrac{u}{d^*}$ $C = \dfrac{d^* + u^2 - v}{(u-v)d^*}$ $D = \dfrac{u^2 - v}{(u-v)d^*}$

$G^* = (C - D)\mathbf{I}_Q + D\mathbf{J}_Q\mathbf{J}_Q'$ $d^* = (Q-1)v + u - Qu^2$

Let (x:z) be the combined vector of control and noise variables. Using **M**(ξ) and $\mathbf{M}^{-1}$(ξ), closed-forms for the generalized variance |**M**(ξ)| and prediction variance V((x:z),ξ) can be derived as follows. Pre- and post-multiplying $\mathbf{M}^{-1}$(ξ) by $f'(x{:}z)$ and $f(x{:}z)$ in (2) yields the closed-form:

$$V((x:z),\xi) = \left(D + \frac{1}{2v}\right)\left(\sum_{i=1}^{Q} x_i^2\right)^2 + \left(2B + \frac{1}{u}\right)\sum_{i=1}^{Q} x_i^2 + \left(C - D - \frac{1}{2v}\right)\sum_{i=1}^{Q} x_i^4 + \sum_{k=1}^{L} z_k^2 + \frac{1}{u}\left(\sum_{i=1}^{Q} x_i^2\right)\left(\sum_{k=1}^{L} z_k^2\right) + A \tag{3}$$

Because u > 0 and v > 0, substitution of $z_k^2 \equiv 1$ (or $\sum z_k^2 = L$) in (3) yields the upper bound

$$max_{x\in\mathcal{X}} V((x:z),\xi) \le \left(D+\frac{1}{2v}\right)\left(\sum_{i=1}^{Q} x_i^2\right)^2 + \left(2B+\frac{L+1}{u}\right)\sum_{i=1}^{Q} x_i^2 + \left(C - D - \frac{1}{2v}\right)\sum_{i=1}^{Q} x_i^4 + A + L \quad (4)$$

Next, consider the further restriction of evaluating $V((x{:}z),\xi)$ at only those points in $J_{QL} = J_Q \times J_L(0)$. Then $z_k^2 \equiv 1$ and $x_i^2 = 0$ or ± 1. Thus, $x_i^2 \equiv x_i^4$. Substituting into (4) yields

$$V((x:z),\xi) = \left(D+\frac{1}{2v}\right)\left(\sum_{i=1}^{Q} x_i^2\right)^2 + \left(2B + C - D + \frac{L+1}{u} - \frac{1}{2v}\right)\sum_{i=1}^{Q} x_i^2 + A + L \quad (5)$$

for all $(x:z) \in J_{QL}$. The number of parameters in the LQ model is $p = 1+2Q+\binom{Q}{2}+L+QL$.

The goal is to show optimal weights $\{\alpha_1,\alpha_2,\alpha_3\}$ defining ξ^* on J^* exist such that ξ satisfies

$$p = max_{(x:z)\in J_{QL}} V((x:z),\xi)$$

$$= \max_{(x:z)\in J}\left[\left(D+\frac{1}{2v}\right)\left(\sum_{i=1}^{Q} x_i^2\right)^2 + \left(2B + C - D + \frac{L+1}{u} - \frac{1}{2v}\right)\sum_{i=1}^{Q} x_i^2 + A + L\right]$$

Once proven, Condition (III) of the Kiefer-Wolfowitz Equivalence Theorem will be satisfied stating that ξ^* will be both a D- and G-optimal design.

When searching for a D-optimal design, the goal is to maximize $|\mathbf{M}(\xi)|$. By exploiting the block structure of $\mathbf{M}(\xi)$ in Figure 1, we have the closed-form for $|\mathbf{M}(\xi)|$:

$$\left|\ \mathbf{M}(\xi)\ \right| = u^{Q(L+1)} \cdot v^{Q(Q-1)/2} \cdot (u-v)^{Q-1} \cdot \left[u + (Q-1)v - Qu^2\right]. \quad (6)$$

In Section 3.2, u, v and, hence, $\{\alpha_1, \alpha_2, \alpha_3\}$ values maximizing $|\mathbf{M}(\xi)|$ are determined.

3.2 Optimal Design Weights

The optimal weights $\{\alpha_1, \alpha_2, \alpha_3\}$ will be determined by studying the generalized variance $|\mathbf{M}(\xi)|$. The weights $\{\alpha_1, \alpha_2, \alpha_3\}$ are determined by maximizing $|\mathbf{M}(\xi)|$ with respect to u and v, or equivalently by maximizing $\mathcal{L}(u,v) = \log|\mathbf{M}(\xi)|$ with respect to u and v. From (6), we have

$$\mathcal{L}(u, v) = Q(L+1)\log(u) + \binom{Q}{2}\log(v) + (Q-1)\log(u-v) + \log[u + (Q-1)v - Qu^2]. \quad (7)$$

Taking partial derivatives of $\mathcal{L}(u,v)$ with respect to u and v yields

$$\frac{\partial \mathcal{L}}{\partial u} = \frac{Q(L+1)}{u} + \frac{Q-1}{u-v} + \frac{1-2Qu}{u+(Q-1)v-Qu^2}$$

$$\frac{\partial L}{\partial v} = \frac{\binom{Q}{2}}{v} - \frac{Q-1}{u-v} + \frac{Q-1}{u+(Q-1)v-Qu^2}$$

Equating the derivatives to b 0 yields

$$0 = \frac{Q(L+1)}{u} + \frac{Q-1}{u-v} + \frac{1-2Qu}{u+(Q-1)v-Qu^2} \quad (8)$$

$$0 = \frac{Q}{2v} - \frac{1}{u-v} + \frac{1}{u+(Q-1)v-Qu^2} \quad (9)$$

Applying MATLAB computational software [23], numerical solutions for the system of nonlinear equations defined by (8) and (9) were found. The resulting solutions $\{\alpha_1, \alpha_2, \alpha_3\}$ are presented in Table 1 for $4 \le K \le 17$ variables.

Next, it will be shown that each set of weights yields a D-optimal design. The first step is to restrict evaluation and maximization of $V((x{:}z),\xi)$ in (3) to $(x{:}z) \in J$. Note, however, that it is not necessary to evaluate $V((x{:}z),\xi)$ at all $(x{:}z) \in J$ due to sign and permutation invariance properties of $V(x{:}z)$. That is, (i) changing the sign of any x_i or z_k yields the same $V(x{:}z)$ and (ii) any permutation of the labels $i = 1,2,\ldots,Q$ for the control variables or any permutation of the labels $k = 1,2,\ldots,L$ for the noise variables yields the same $V(x{:}z)$. If we let

(i) $x^{(i)}$ be the Q-coordinate point such that the first i coordinates of $x^{(i)}$ are 0 and the last Q-i coordinates are 1,

(ii) $x^{(0)}$ be the L-coordinate point (1,1,…,1), and

(iii) J_{xz} be the set of (Q +1) points formed by the product $\{x^{(0)}, x^{(1)},\ldots x^{(Q)}\} \times z^{(0)}$,

then it is sufficient to evaluate $V((x{:}z),\xi)$ for only the (Q+1) points in J_{xz}. For each (Q,L) pair in Table 1, $V((x{:}z),\xi)$ was maximized over J_{xz} resulting in

$$\max_{(x:z)\in J_{xz}}\left[\left(D+\frac{1}{2v}\right)\left(\sum_{i=1}^{Q} x_i^2\right)^2 + \left(2B+C-D+\frac{L+1}{u}-\frac{1}{2v}\right)\sum_{i=1}^{Q} x_i^2 + A + L\right] = p$$

where p = the number of model parameters.

Therefore, for each $(\alpha_1, \alpha_2, \alpha_3)$ in Table 1, Condition (III) of the Kiefer-Wolfowitz Equivalence Theorem has been satisfied. Since Condition (III) is satisfied, then by equivalence of the three conditions, Conditions (I) and (II) are also satisfied, i.e., the design measure ξ determined by each $(\alpha_1, \alpha_2, \alpha_3)$ is D- and G-optimal. Thus, we know for $K \le 17$ design variables:

Table 1: Summary Table of D-Optimum Weights

Number of Design Variables and LQ Model Parameters				*Optimal Weights for Barycentric Subsets*			*Optimum D-criterion*	
Total	Signal	Noise		*J(0,0)*	*J(1,0)*	*J(Q,0)*		
K	*Q*	*L*	*p*	α_1	α_2	α_3	|M(x)|	
4	1	3	9	0.8333	0.1265	0.0402	0.6698	x 10-1
4	2	2	12	0.7055	0.2524	0.0421	0.4531	x 10-2
4	3	1	14	0.5779	0.3777	0.0444	0.3102	x 10-3
4	4	0	15	0.4505	0.5021	0.0474	0.2157	x 10-4
5	1	4	11	0.8571	0.1131	0.0297	0.5665	x 10-1
5	2	3	15	0.7432	0.2260	0.0308	0.3232	x 10-2
5	3	2	18	0.6293	0.3386	0.0321	0.1859	x 10-3
5	4	1	20	0.5156	0.4507	0.0337	0.1080	x 10-4
5	5	0	21	0.4021	0.5622	0.0358	0.6348	x 10-6
6	1	5	13	0.8750	0.1021	0.0229	0.4909	x 10-1
6	2	4	18	0.7723	0.2041	0.0236	0.2422	x 10-2
6	3	3	22	0.6697	0.3060	0.0244	0.1202	x 10-3
6	4	2	25	0.5671	0.4075	0.0253	0.6006	x 10-5
6	5	1	27	0.4647	0.5088	0.0265	0.3026	x 10-6
6	6	0	28	0.3624	0.6097	0.0279	0.1540	x 10-7
7	1	6	15	0.8889	0.0930	0.0181	0.4330	x 10-1
7	2	5	21	0.7955	0.1859	0.0186	0.1883	x 10-2
7	3	4	26	0.7022	0.2787	0.0191	0.8221	x 10-4
7	4	3	30	0.6089	0.3714	0.0198	0.3608	x 10-5
7	5	2	33	0.5157	0.4639	0.0205	0.1593	x 10-6
7	6	1	35	0.4225	0.5561	0.0213	0.7080	x 10-8
7	7	0	36	0.3295	0.6481	0.0224	0.3173	x 10-9
8	1	7	17	0.9000	0.0853	0.0147	0.3874	x 10-1
8	2	6	24	0.8144	0.1705	0.0150	0.1506	x 10-2
8	3	5	30	0.7289	0.2557	0.0154	0.5871	x 10-4
8	4	4	35	0.6434	0.3408	0.0158	0.2298	x 10-5
8	5	3	39	0.5579	0.4257	0.0163	0.9037	x 10-7
8	6	2	42	0.4725	0.5106	0.0169	0.3572	x 10-8
8	7	1	44	0.3871	0.5953	0.0176	0.1420	x 10-9
8	8	0	45	0.3019	0.6798	0.0183	0.5684	x 10-11
9	1	8	19	0.9091	0.0787	0.0122	0.3505	x 10-1
9	2	7	27	0.8302	0.1574	0.0124	0.1232	x 10-2
9	3	6	34	0.7512	0.2361	0.0127	0.4339	x 10-4
9	4	5	40	0.6724	0.3146	0.0130	0.1534	x 10-5
9	5	4	45	0.5935	0.3932	0.0133	0.5439	x 10-7
9	6	3	49	0.5146	0.4716	0.0137	0.1936	x 10-8
9	7	2	52	0.4358	0.5500	0.0142	0.6924	x 10-10
9	8	1	54	0.3571	0.6282	0.0147	0.2489	x 10-11
9	9	0	55	0.2784	0.7063	0.0153	0.8998	x 10-13

Table 1: (continued)

Number of Design Variables and LQ Model Parameters				*Optimal Weights for Barycentric Subsets*			*Optimum D-criterion*	
Total	Signal	Noise		*J(0,0)*	*J(1,0)*	*J(Q,0)*		
K	*Q*	*L*	*p*	α_1	α_2	α_3	|M(x)|	
10	1	9	21	0.9167	0.0731	0.0103	0.3200	x 10-1
10	2	8	30	0.8434	0.1461	0.0104	0.1026	x 10-2
10	3	7	38	0.7702	0.2192	0.0106	0.3298	x 10-4
10	4	6	45	0.6970	0.2921	0.0109	0.1062	x 10-5
10	5	5	51	0.6238	0.3651	0.0111	0.3433	x 10-7
10	6	4	56	0.5506	0.4380	0.0114	0.1112	x 10-8
10	7	3	60	0.4775	0.5108	0.0117	0.3617	x 10-10
10	8	2	63	0.4044	0.5836	0.0121	0.1181	x 10-11
10	9	1	65	0.3313	0.6563	0.0125	0.3872	x 10-13
10	10	0	66	0.2582	0.7288	0.0129	0.1276	x 10-14
11	1	10	23	0.9231	0.0682	0.0087	0.2944	x 10-1
11	2	9	33	0.8548	0.1363	0.0089	0.8681	x 10-3
11	3	8	42	0.7865	0.2045	0.0090	0.2565	x 10-4
11	4	7	50	0.7182	0.2726	0.0092	0.7593	x 10-6
11	5	6	57	0.6499	0.3406	0.0094	0.2253	x 10-7
11	6	5	63	0.5817	0.4087	0.0096	0.6702	x 10-9
11	7	4	68	0.5135	0.4767	0.0098	0.1999	x 10-10
11	8	3	72	0.4452	0.5447	0.0101	0.5982	x 10-12
11	9	2	75	0.3771	0.6126	0.0104	0.1796	x 10-13
11	10	1	77	0.3089	0.6804	0.0107	0.5414	x 10-15
11	11	0	78	0.2408	0.7482	0.0111	0.1639	x 10-16
12	1	11	25	0.9286	0.0639	0.0076	0.2726	x 10-1
12	2	10	36	0.8646	0.1277	0.0077	0.7440	x 10-3
12	3	9	46	0.8006	0.1916	0.0078	0.2034	x 10-4
12	4	8	55	0.7367	0.2554	0.0079	0.5571	x 10-6
12	5	7	63	0.6727	0.3192	0.0081	0.1529	x 10-7
12	6	6	70	0.6088	0.3830	0.0082	0.4203	x 10-9
12	7	5	76	0.5448	0.4468	0.0084	0.1158	x 10-10
12	8	4	81	0.4809	0.5105	0.0086	0.3200	x 10-12
12	9	3	85	0.4170	0.5742	0.0088	0.8866	x 10-14
12	10	2	88	0.3532	0.6378	0.0090	0.2464	x 10-15
12	11	1	90	0.2893	0.7014	0.0093	0.6870	x 10-17
12	12	0	91	0.2255	0.7649	0.0096	0.1923	x 10-18
13	1	12	27	0.9333	0.0601	0.0066	0.2538	x 10-1
13	2	11	39	0.8732	0.1202	0.0067	0.6448	x 10-3
13	3	10	50	0.8130	0.1802	0.0068	0.1640	x 10-4
13	4	9	60	0.7529	0.2403	0.0069	0.4180	x 10-6
13	5	8	69	0.6927	0.3003	0.0070	0.1067	x 10-7
13	6	7	77	0.6326	0.3603	0.0071	0.2727	x 10-9
13	7	6	84	0.5725	0.4203	0.0072	0.6986	x 10-11

Table 1: (continued)

Number of Design Variables and LQ Model Parameters				*Optimal Weights for Barycentric Subsets*			*Optimum D-criterion*	
Total *K*	Signal *Q*	Noise *L*	*p*	*J(0,0)* α_1	*J(1,0)* α_2	*J(Q,0)* α_3	|M(x)|	
13	8	5	90	0.5123	0.4803	0.0074	0.1793	x 10-12
13	9	4	95	0.4522	0.5402	0.0076	0.4613	x 10-14
13	10	3	99	0.3921	0.6001	0.0077	0.1190	x 10-15
13	11	2	102	0.3321	0.6600	0.0079	0.3076	x 10-17
13	12	1	104	0.2720	0.7198	0.0082	0.7980	x 10-19
13	13	0	105	0.2120	0.7796	0.0084	0.2077	x 10-20
14	1	13	29	0.9375	0.0567	0.0058	0.2374	x 10-1
14	2	12	42	0.8807	0.1134	0.0059	0.5641	x 10-3
14	3	11	54	0.8240	0.1701	0.0059	0.1342	x 10-4
14	4	10	65	0.7672	0.2268	0.0060	0.3198	x 10-6
14	5	9	75	0.7104	0.2834	0.0061	0.7628	x 10-8
14	6	8	84	0.6537	0.3401	0.0062	0.1822	x 10-9
14	7	7	92	0.5969	0.3967	0.0063	0.4361	x 10-11
14	8	6	99	0.5402	0.4534	0.0064	0.1045	x 10-12
14	9	5	105	0.4835	0.5100	0.0066	0.2511	x 10-14
14	10	4	110	0.4267	0.5666	0.0067	0.6042	x 10-16
14	11	3	114	0.3700	0.6231	0.0069	0.1457	x 10-17
14	12	2	117	0.3133	0.6796	0.0070	0.3524	x 10-19
14	13	1	119	0.2566	0.7361	0.0072	0.8544	x 10-21
14	14	0	120	0.2000	0.7926	0.0074	0.2078	x 10-22
15	1	14	31	0.9412	0.0537	0.0051	0.2230	x 10-1
15	2	13	45	0.8874	0.1074	0.0052	0.4977	x 10-3
15	3	12	58	0.8337	0.1610	0.0053	0.1112	x 10-4
15	4	11	70	0.7800	0.2147	0.0053	0.2488	x 10-6
15	5	10	81	0.7262	0.2684	0.0054	0.5571	x 10-8
15	6	9	91	0.6725	0.3220	0.0055	0.1249	x 10-9
15	7	8	100	0.6188	0.3757	0.0056	0.2805	x 10-11
15	8	7	108	0.5651	0.4293	0.0057	0.6309	x 10-13
15	9	6	115	0.5113	0.4829	0.0058	0.1421	x 10-14
15	10	5	121	0.4576	0.5365	0.0059	0.3206	x 10-16
15	11	4	126	0.4039	0.5901	0.0060	0.7248	x 10-18
15	12	3	130	0.3503	0.6436	0.0061	0.1642	x 10-19
15	13	2	133	0.2966	0.6972	0.0063	0.3727	x 10-21
15	14	1	135	0.2429	0.7507	0.0064	0.8484	x 10-23
15	15	0	136	0.1893	0.8042	0.0066	0.1936	x 10-24
16	1	15	33	0.9444	0.0510	0.0046	0.2102	x 10-1
16	2	14	48	0.8934	0.1019	0.0046	0.4424	x 10-3
16	3	13	62	0.8424	0.1529	0.0047	0.9318	x 10-5
16	4	12	75	0.7914	0.2039	0.0047	0.1965	x 10-6
16	5	11	87	0.7404	0.2548	0.0048	0.4146	x 10-8

Table 1: (continued)

Number of Design Variables and LQ Model Parameters				*Optimal Weights for Barycentric Subsets*			*Optimum D-criterion*	
Total	Signal	Noise		*J(0,0)*	*J(1,0)*	*J(Q,0)*		
K	*Q*	*L*	*p*	α_1	α_2	α_3	|M(x)|	
16	6	10	98	0.6894	0.3057	0.0049	0.8760	x 10-10
16	7	9	108	0.6384	0.3567	0.0049	0.1853	x 10-11
16	8	8	117	0.5874	0.4076	0.0050	0.3924	x 10-13
16	9	7	125	0.5364	0.4585	0.0051	0.8323	x 10-15
16	10	6	132	0.4854	0.5094	0.0052	0.1768	x 10-16
16	11	5	138	0.4344	0.5603	0.0053	0.3761	x 10-18
16	12	4	143	0.3834	0.6112	0.0054	0.8015	x 10-20
16	13	3	147	0.3325	0.6620	0.0055	0.1711	x 10-21
16	14	2	150	0.2815	0.7129	0.0056	0.3662	x 10-23
16	15	1	152	0.2306	0.7637	0.0057	0.7852	x 10-25
16	16	0	153	0.1796	0.8145	0.0059	0.1688	x 10-26
17	1	16	35	0.9474	0.0485	0.0041	0.1989	x 10-1
17	2	15	51	0.8988	0.0970	0.0042	0.3958	x 10-3
17	3	14	66	0.8503	0.1455	0.0042	0.7885	x 10-5
17	4	13	80	0.8017	0.1940	0.0043	0.1572	x 10-6
17	5	12	93	0.7532	0.2425	0.0043	0.3137	x 10-8
17	6	11	105	0.7046	0.2910	0.0044	0.6266	x 10-10
17	7	10	116	0.6561	0.3395	0.0044	0.1253	x 10-11
17	8	9	126	0.6075	0.3880	0.0045	0.2508	x 10-13
17	9	8	135	0.5590	0.4365	0.0045	0.5026	x 10-15
17	10	7	143	0.5105	0.4849	0.0046	0.1009	x 10-16
17	11	6	150	0.4619	0.5334	0.0047	0.2027	x 10-18
17	12	5	156	0.4134	0.5818	0.0048	0.4078	x 10-20
17	13	4	161	0.3649	0.6302	0.0049	0.8220	x 10-22
17	14	3	165	0.3164	0.6786	0.0050	0.1660	x 10-23
17	15	2	168	0.2679	0.7270	0.0051	0.3357	x 10-25
17	16	1	170	0.2194	0.7754	0.0052	0.6806	x 10-27
17	17	0	171	0.1709	0.8238	0.0053	0.1383	x 10-28

Theorem 2: The set of barycenter points $J(0,0) \cup J(1,0) \cup J(Q,0)$ supports D-optimal and G-optimal *LQ* model designs.

Because a closed-form solution for *u* and *v* has not been derived, solutions were determined using numerical optimization algorithms. These algorithms can no doubt be used to extend the results of Theorem 2 to *K* > 17 factors.

4. Applications

A weakness of many crossed-arrays (Kackar [14], Box [8], Nair [26] is the inability to estimate the full set of two-factor interactions among the controllable process variables. If any such interaction has a large effect on the response and is not estimable, adjustments cannot be made to account for it in the process variable settings. This is one motivation for considering *LQ* model designs. Consider a combined array of $K = Q + L$ two-level factors. Suppose a 2^{K-P} fractional factorial design allows estimation of the *LQ* model without the squared terms :

$$y = \beta_0 + \sum_{i=1}^{Q} \beta_i x_i + \sum_{i=1}^{Q-1} \sum_{j=i+1}^{Q} \beta_{ij} x_i x_j + \sum_{k=1}^{L} \delta_k z_k + \sum_{i=1}^{Q} \sum_{k=1}^{L} \delta_{ik} x_i z_k + \varepsilon$$

This design is called a 2^{K-P} **mixed resolution** or **MR** design (Borkowski [2], Lucas [22], Borkowski and Lucas [6], Borror and Montgomery [7] because the design is (i) at least Resolution V among the *Q* signal factors, (ii) at least Resolution III among the *L* noise factors, and (iii) each of the two factor interactions between a signal and a noise factor is not confounded with any main effect or any two factor interaction of signal, noise, or signal and noise factors.

Borkowski [2] and Borkowski and Lucas [6] developed a class of *LQ* model designs, called **composite mixed resolution** or **CMR** designs that are constructed analogously to the central composite designs (CCDs) of Box and Wilson [11]. These designs consist of

(i) 2^{K-P} points from a 2^{K-P} MR design with *Q* signal and *L* noise factors.

(ii) 2*Q* axial points with two axial points for each signal factor. An axial point sets a signal factor set at ±1 while all other factors are set at mid-level 0.

(iii) N_0 center points.

For more information on CCDs, see Borkowski [3,4], Montgomery and Myers [25], Khuri and Cornell [15], and Box and Draper [9].

As economical design size alternatives to Taguchi's crossed array designs, Box and Jones [10] also consider CMR designs when optimizing several loss functions, in particular, the integrated squared error loss function. Box and Jones use CMR designs of Resolution IV in the noise variables to protect against bias due to any $z_i z_j$ terms. Analogously, if the *LQ* model is true, a CMR design of Resolution III in the noise factors will produce unbiased estimates of the coefficients of terms involving the signal factors. Through their work, Box and Jones show that CMR designs can substantially reduce the design size for designing products robust to uncontrollable factors while preserving the response surface design approach to analysis.

By allowing the noise factors to be of Resolution III amongst themselves, smaller CMR designs for fitting the *LQ* model exist. It is noted that the cost of achieving these smaller designs is protection against model bias. However, for the majority of smallest CMR designs, the noise factors will be of Resolution IV or greater amongst themselves anyway. By allowing Resolution III for noise factors, the CMR designs have the net effect of reducing the overall fractional factorial design size by 1/2 of the number of points required by a Resolution IV design.

The results in this paper allow evaluation of D-efficiencies of CMR or any other designs based on the *LQ* model. Table 1 contains the D-criterion values necessary for calculating D-efficiencies for designs with $4 \le K = Q + L \le 17$ design variables. A catalog of CMR designs, a design size comparison to crossed arrays, and D-efficiencies for CMR designs can be found in Borkowski and Lucas [6].

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