# ON THE CONSTRUCTION OF $G_{r m}$-OPTIMAL DESIGNS 

Dale Song and Weng Kee Wong<br>Department of Biostatistics, UCLA


#### Abstract

We consider the problem of finding an efficient design for estimating the model parameters and the mean response surface simultaneously when the true degree of the polynomial model is unknown. A precision constraint is imposed on one of these estimates and the optimal design is found using the theory of canonical moments. Robustness properties of the optimal designs to model assumptions and their performances relative to similar designs are studied.


Key words and phrases: Canonical moment, continuous design, D-optimality, Goptimality, robust design criteria.

## 1. Introduction

Suppose an experiment is run and $N$ independent observations of the response $y$ are measured according to the model

$$
\begin{equation*}
y_{i}=f^{T}\left(x_{i}\right) \beta+e_{i}, \quad x_{i} \in[0,1] \text { and } i=1,2, \ldots, N . \tag{1.1}
\end{equation*}
$$

Here $f^{T}(x)=\left(1, x, x^{2}, \ldots, x^{m}\right), \beta$ is the vector of unknown parameters and the $e_{i}$ 's are unobservable random errors with mean zero and constant variance. The problem of interest here is how to find an efficient design for estimating the model parameters and the mean response surface simultaneously when the true degree of the model (i.e. $m$ ) is unknown.

Some pioneering work addressing design issues when there is model uncertainty are Atwood (1971), Stigler (1971) and Läuter (1974). Both Atwood and Stigler's work are seminal; they formalized the concepts of robust design and found optimal designs for some simple models. Läuter (1974) proposed algorithms for generating $D$-optimal designs when it is possible to postulate the true model is in a class of models. Subsequent works include Studden (1982), Lee (1988), and Rosenberger and Pukelsheim (1993), where efficient designs are found when the mean regression function is not known precisely.

Stigler (1971) proposed two robust design criteria when there is model uncertainty. They were generalized by Studden (1982) as $D_{r m}$ and $G_{r m}$-optimality. These designs are optimal for estimating the model parameters and the mean response surface respectively when the assumed model is a polynomial of degree $r$ but, at the same time, also ensure a certain level of precision for estimating
if additional terms $x^{r+1}, \ldots, x^{m}$ are needed. Studden (1982) used the theory of canonical moments and found closed form descriptions for $D_{r m}$-optimal designs when $m>r$ and $r=1,2$. Stigler (1971) and Studden (1982) noted that the $D_{r m}$-optimal designs are 'somewhat simpler to calculate than the $G_{r m}$-optimal designs'. Except in the simplest case, when $m=2$ and $r=1$, no other $G_{r m}{ }^{-}$ optimal designs were found. One of the difficulties is that the $G$-optimality criterion is not differentiable and standard algorithms cannot be used to find the optimal design.

In this paper, we construct $G_{r m}$-optimal designs and derive explicit analytic formulae in terms of canonical moments, for any $m>r$ and $r=1,2$. In addition, we show that $D_{1 m}$ and $G_{1 m}$-optimal designs are equivalent for any $m>1$. Robustness properties of $G_{r m}$-optimal designs to model assumptions are studied, and their performances relative to $D_{r m}$-optimal designs and the constrained designs in Pukelsheim and Rosenberger (1993) are compared.

## 2. The $D_{r m}$ and $G_{r m}$-optimality Criteria

Let $\xi$ denote a design with $n_{j}$ observations at the point $x_{j} \varepsilon[0,1], j=1, \ldots, J$, subject to $\sum n_{j}=N$. We will treat $\xi$ as a probability measure which puts mass $\xi_{j}$ at $x_{j}$ without insisting that each $N \xi_{j}$ is an integer, subject to the constraint that they sum to 1 . Such designs are called continuous designs and, they are easier to study and generate than the traditional discrete designs (Kiefer (1959)). The information matrix of $\xi$ is

$$
M_{m}(\xi)=\int_{0}^{1} f(x) f(x)^{T} \xi(d x)
$$

and the covariance matrix of the LSE (least squares estimate) of $\beta$ is proportional to $M_{m}(\xi)^{-1}$, if $M_{m}(\xi)$ is non-singular. Designs are non-singular if their information matrices are non-singular.

Various optimality criteria have been proposed, and many are formulated as convex functions of $M_{m}(\xi)$. For instance, a design is $D$-optimal if it maximizes $\left|M_{m}(\xi)\right|$ over the set $\Xi$ containing all designs on $[0,1]$. Another criterion is $G$ optimality, which seeks to minimize over $\Xi$, the maximum of the standardized variance function $d_{m}(x, \xi)=f^{T}(x) M_{m}(\xi)^{-1} f(x)$. Thus, $D$-optimal designs are useful for parameter estimation and $G$-optimal designs are useful for estimating the response surface. Kiefer and Wolfowitz (1960) showed that $D$ and $G$-optimal designs are equivalent when the model is homoscedastic.

Let $f^{T}(x)=\left(f_{1}^{T}(x), f_{2}^{T}(x)\right)$ where $f_{1}^{T}(x)=\left(1, x, \ldots, r^{r}\right), f_{2}^{T}(x)=\left(x^{r+1}, \ldots\right.$, $\left.x^{m}\right)$ and $\beta^{T}=\left(\beta_{1}^{T}, \beta_{2}^{T}\right)$. The model of interest becomes $E y=f_{1}^{T}(x) \beta_{1}+f_{2}^{T}(x) \beta_{2}$. For any arbitrary design $\xi$, its information matrix can be partitioned as

$$
M_{m}(\xi)=\left(\begin{array}{ll}
M_{11}(\xi) & M_{12}(\xi) \\
M_{21}(\xi) & M_{22}(\xi)
\end{array}\right)
$$

where $M_{11}(\xi)$ has size $r+1$ and $M_{22}(\xi)$ has size $m-r$. The covariance matrix of the LSE of $\beta_{1}$ is proportional to $M_{11}(\xi)^{-1}$ if the polynomial model of degree $r$ is fitted. In this case, the standardized variance function of the design $\xi$ at the point $x$ is given by $d_{r}(x, \xi)=f_{1}^{T}(x) M_{11}(\xi)^{-1} f_{1}(x)$. On the other hand, if the polynomial model of degree $m$ is fitted, the covariance matrix of the LSE of $\beta_{2}$ is proportional to $M_{22.1}(\xi)^{-1}$, where

$$
M_{22.1}(\xi)=M_{22}(\xi)-M_{21}(\xi) M_{11}(\xi)^{-1} M_{12}(\xi)
$$

Let $\bar{d}_{r}(\xi)=\max _{0 \leq x \leq 1} d_{r}(x, \xi)$ whenever $M_{11}(\xi)^{-1}$ exists.
Definition 2.1. (The $D_{r m}$-problem) A design is called $D_{r m}$-optimal if it

$$
\text { maximizes }\left|M_{11}(\xi)\right| \text { subject to }\left|M_{22.1}(\xi)\right| \geq \rho^{m-r} \max _{\eta \in \Xi}\left|M_{22.1}(\eta)\right|
$$

Definition 2.2. (The $G_{r m}$-problem) A design is called $G_{r m}$-optimal if it

$$
\text { minimizes } \bar{d}_{r}(\xi) \text { subject to }\left|M_{22.1}(\xi)\right| \geq \rho^{m-r} \max _{\eta \in \Xi}\left|M_{22.1}(\eta)\right|
$$

These definitions are motivated by design efficiencies: Recall that if the $D$-optimal design for model (1.1) is $\xi^{*}$, then the $D$ and $G$-efficiency of a nonsingular design $\xi$ is $\left\{\left|M_{m}(\xi)\right| /\left|M_{m}\left(\xi^{*}\right)\right|\right\}^{1 /(m+1)}$ and $(m+1) / \bar{d}_{m}(\xi)$ respectively. The reciprocal of these numbers represent how many times the design $\xi$ has to be replicated for it to do as well as the optimal design. Clearly, designs with high efficiencies are sought. It follows that the inequalities in the above definitions ensure that the $D_{r m}$ and $G_{r m}$-optimal design has a guaranteed $D$-efficiency of at least $\rho$ for estimating $\beta_{2}$, while still being as close to optimal as possible under the other criterion. If $\rho=0(1)$, this corresponds to the case when estimating $\beta_{1}\left(\beta_{2}\right)$ is the only goal: intermediate values of $\rho$ represent a compromised goal of balancing model uncertainty and precision of the various estimates. We will call the set of all information matrices that satisfy the inequality constraint in the above definitions as the constrained set.

## 3. Canonical Moments

We now define and review properties of canonical moments useful for finding $G_{r m}$-optimal designs. For an arbitrary design $\xi$ on $[0,1]$, let $c_{k}$ denote the $k$ th ordinary moment of $\xi, k=0,1, \ldots$ Given a set of moments $c_{0}, c_{1}, \ldots, c_{i-1}$, let $c_{i}^{+}$be the maximum value of the $i$ th moment over the set of designs having the given moments $c_{0}, c_{1}, \ldots, c_{i-1}$. Similarly, let $c_{i}^{-}$be the corresponding minimum. The canonical moments are defined by

$$
p_{i}=\left(c_{i}-c_{i}^{-}\right) /\left(c_{i}^{+}-c_{i}^{-}\right) \quad i=1,2, \ldots
$$

Note that $0 \leq p_{i} \leq 1$ and if $c_{i}^{-}=c_{i}^{+}, p_{i}$ is left undefined and the sequence is terminated. There are many interesting properties of canonical moments; for example, if $p_{2 m}=1$, the design is supported at $(m+1)$ points (Dette and Roeder (1996)). Other pertinent facts about canonical moments include the following.

Property 3.1. (Skibinsky (1986)) Every probability measure on $[0,1]$ is uniquely determined by its canonical moment sequence.

Property 3.2. (Skibinsky (1969), Lau (1983)) The canonical moments are invariant under linear transformations, and all odd canonical moments of a design on $[0,1]$ are equal to $1 / 2$ if and only if the design is symmetric about $x=1 / 2$.

Property 3.3. (Lau (1983)) For the polynomial regression model of degree $m$, $\left|M_{m}(\xi)\right|=\prod_{i=1}^{m}\left(\zeta_{2 i-1} \zeta_{2 i}\right)^{m+1-i}$ where $\zeta_{i}=p_{i} q_{i-1}, q_{i}=1-p_{i}, i=1,2, \ldots$ and $q_{0}=1$.

Property 3.3 is useful because it facilitates the calculation of the optimal design; each $p_{i}$ varies independently over the space $[0,1]$ so the determinant can be maximized by maximizing each $p_{i}$ one at a time. Once the canonical moments are found, the optimal design is recovered using standard technique (see, for example, the appendix in Dette and Roeder (1996)).

## 4. $G_{r m}$-optimal Designs

In general it is quite laborious to find $G_{r m}$-optimal designs. The following lemmas help reduce the complexity of the problem.

Lemma 1. There exists a symmetric $G_{r m}$-optimal design about the midpoint of the design space $[0,1]$.

Proof. We observe that the constrained set is convex because $\log \left|M_{22.1}(\xi)\right|$ is concave on the set $\left\{M_{m}(\xi) \mid \xi \in \Xi\right.$ and $\left.\left|M_{11}(\xi)\right|>0\right\}$ (Pázman (1986), p. 104) and the logarithm function is an increasing function. This implies that the set of all $G_{r m}$-optimal designs is convex and consequently, there exists a symmetric $G_{r m}$ optimal design since $\bar{d}_{r}(\xi)$ is strictly convex on $\left\{M_{11}(\xi) \mid \xi \in \Xi\right.$ and $\left.\left|M_{11}(\xi)\right|>0\right\}$ (Pázman (1986), p. 86).
Lemma 2. If $\xi$ is a symmetric non-singular design on $[0,1]$, then the standardized variance function $d_{m}(x, \xi)$ is symmetric about $x=1 / 2$.
Proof. This is immediate if the design is transformed linearly onto $[-1,1]$, observing that the resulting variance function is symmetric with respect to 0 .
Lemma 3. The information matrix of a $G_{r m}$-optimal design is on the boundary of the constrained set. In other words, if $\xi^{*}$ is a $G_{r m}$-optimal design, then

$$
\left|M_{22.1}\left(\xi^{*}\right)\right|=\rho^{m-r} \max _{\eta \in \Xi}\left|M_{22.1}(\eta)\right|
$$

Proof. Since $\bar{d}_{r}(\xi)$ is strictly convex on $\left\{M_{11}(\xi) \mid \xi \in \Xi\right.$ and $\left.\left|M_{11}(\xi)\right|>0\right\}$ (Pázman (1986), p. 86), it is also strictly convex on $\left\{M_{m}(\xi) \mid \xi \in \Xi\right.$ and $\left|M_{11}(\xi)\right|>$ $0\}$. If $M_{m}\left(\xi^{*}\right)$ is an interior point of the constrained set, then clearly $\bar{d}_{r}\left(\xi^{*}\right)$ is the global minimum and hence $\xi^{*}$ is a unconstrained $G$-optimal design for the problem when $\rho=0$. Since $f_{1}(x)$ is a polynomial of degree $r$, $\xi^{*}$ is supported at $r+1$ points. This implies $\left|M_{22.1}\left(\xi^{*}\right)\right|=\left|M_{m}\left(\xi^{*}\right)\right| /\left|M_{11}\left(\xi^{*}\right)\right|=0$ because $m>r$ by assumption. This is impossible and so $M_{m}\left(\xi^{*}\right)$ is on the boundary of the constrained set.

We now consider the problem of finding $G_{1 m}$ and $G_{2 m}$-optimal designs (though the procedure can be generalized to find $G_{r m}$-designs when $m>r>2$ ). Theorem 4.1 assumes a simple linear model but some protection is needed for the terms $\beta_{2}, \beta_{3}, \ldots, \beta_{m}$. The result extends the equivalence result found by Stigler (1971) where he showed $G_{12}$ and $D_{12}$-optimal designs coincide.

Theorem 4.1. For any $\rho$ and $m$, the $G_{1 m}$ and $D_{1 m}$-optimal designs are equivalent.

Proof. By Lemma 1 and Property 3.2, we only need to consider designs $\xi$, which are symmetric and non-singular. Since $c_{1}=p_{1}, c_{2}=p_{1}\left(p_{1}+q_{1} p_{2}\right)$, we have

$$
M_{11}(\xi)^{-1}=\frac{1}{p_{2}}\left(\begin{array}{cc}
1+p_{2} & -2 \\
-2 & 4
\end{array}\right)
$$

and the standardized variance function is $d_{1}(x, \xi)=\left(4 x^{2}-4 x+1+p_{2}\right) / p_{2}$.
By definition, the constrained set for the $G_{1 m}$ problem is the same constrained set as the $D_{1 m}$-problem. Since $\bar{d}_{1}(\xi)=d_{1}(0, \xi)=1+1 / p_{2}$, the $G_{1 m}$ optimal design minimizes $1+1 / p_{2}$, or maximizes $p_{2}$, among all designs whose information matrices are in the constrained set. But Studden (1982) showed the $D_{1 m}$-optimal design maximizes $p_{2}$ among designs from the same set; consequently their sequences of canonical moments coincide and by Property 3.1, the $G_{1 m}$ and $D_{1 m}$-optimal designs are equivalent. Formulas for $D_{1 m}$-optimal designs are given in Studden (1982).

We now state and prove the results for $G_{2 m}$-optimal design.
Theorem 4.2. Let $\rho$, $m$ be given, let $R(p)=\{1+\sqrt{1-\rho /[4 p(1-p])}\} / 2$ and let $p_{2}$ be the root bounded between $(1 \pm \sqrt{1-\rho}) / 2$ of the following equation:

$$
\begin{equation*}
\frac{d}{d p}\left\{\frac{1}{p}+\frac{1-p}{p R(p)}\right\}=0 \quad \text { if } \quad \rho>0.96 \tag{4.0}
\end{equation*}
$$

or

$$
\begin{equation*}
2 p-1-(1-p) R(p)=0 \quad \text { if } \quad \rho \leq 0.96 \tag{4.1}
\end{equation*}
$$

The $G_{2 m}$-optimal design has canonical moments given by $p_{2 i-1}=1 / 2, i=$ $1,2, \ldots, m, p_{2}$ (above), $p_{4}=R\left(p_{2}\right), p_{2 i}=(m-i+1) /(2 m-2 i+1), i=3, \ldots, m-1$ and $p_{2 m}=1$.

Proof. We prove the result for $m=3$ first. The first diagonal block of the information matrix of any design for the $G_{23}$-problem is $3 \times 3$ and can be expressed in terms of canonical moments. Replacing all odd canonical moments by $1 / 2$, a direct calculation shows the standardized variance function is

$$
\begin{aligned}
d_{2}(x, \xi)=\{ & \left(p_{2}-2 p_{2}^{2}+p_{2}^{3}+p_{2} q_{2} p_{4}+p_{2}^{2} q_{2} p_{4}\right)+4\left(2 p_{2}^{2}-2 p_{2}-p_{2} q_{2} p_{4}\right) x \\
& \left.+4\left(6 p_{2}-2 p_{2}^{2}+p_{2} q_{2} p_{4}\right) x^{2}-32 p_{2} x^{3}+16 p_{2} x^{4}\right\} / p_{2}^{2} q_{2} p_{4} .
\end{aligned}
$$

This function depends only on the second and fourth canonical moments of $\xi$ and it is instructive to write $d_{2}(x, \xi)$ as $d_{2}\left(x, p_{2}, p_{4}\right)$ in what is to follow. By property 3.3, we have $\left|M_{22.1}(\xi)\right|=\left(p_{1} q_{1}\right)\left(p_{2} q_{2}\right)\left(p_{3} q_{3}\right)\left(p_{4} q_{4}\right)\left(p_{5} q_{5}\right) p_{6}$. Thus, when we replace the odd moments by $1 / 2$ and set $p_{6}=1$, the problem is reduced to

$$
\begin{equation*}
\operatorname{minimize} \bar{d}_{2}(\xi) \quad \text { subject to } p_{2} q_{2} p_{4} q_{4}=\rho / 16 \tag{4.2}
\end{equation*}
$$

by Lemma 3 . The nature of the constraint implies that for each $p_{2}$ satisfying

$$
\begin{equation*}
L=\{1-\sqrt{1-\rho}\} / 2 \leq p_{2} \leq\{1+\sqrt{1-\rho}\} / 2=U \tag{4.3}
\end{equation*}
$$

we must have $p_{4}=R\left(p_{2}\right)$ or $r\left(p_{2}\right)$ where

$$
R\left(p_{2}\right)=\frac{1}{2}+\frac{1}{2} \sqrt{1-\frac{\rho}{4 p_{2} q_{2}}} \text { and } r\left(p_{2}\right)=\frac{1}{2}-\frac{1}{2} \sqrt{1-\frac{\rho}{4 p_{2} q_{2}}} .
$$

It follows that for each $p_{2}$ satisfying (4.3), it suffices to compare $\bar{d}_{2}\left(p_{2}, R\left(p_{2}\right)\right)$ and $\bar{d}_{2}\left(p_{2}, r\left(p_{2}\right)\right)$. Because $d_{2}\left(x, p_{2}, p_{4}\right)$ is a 4 th order polynomial with positive coefficient of $x^{4}$ and symmetric about $x=0.5$ (Lemma 2), this function attains its maximum at 0 and 1 , and/or at $x=0.5$; thus $d_{2}\left(x, p_{2}, R\left(p_{2}\right)\right)$ and $d_{2}\left(x, p_{2}, r\left(p_{2}\right)\right)$ are maximized at $x=0$ and 1 and/or 0.5 . A direct calculation shows $d_{2}\left(0, p_{2}, p_{4}\right)=1+1 / p_{2}+q_{2} /\left(p_{2} p_{4}\right)$ and $d_{2}\left(0.5, p_{2}, p_{4}\right)=1+p_{2} /\left(q_{2} p_{4}\right)$. Since $R\left(p_{2}\right)>r\left(p_{2}\right)$, we have $d_{2}\left(0, p_{2}, R\left(p_{2}\right)\right)<d_{2}\left(0, p_{2}, r\left(p_{2}\right)\right)$ and $d_{2}\left(0.5, p_{2}, R\left(p_{2}\right)\right)<$ $d_{2}\left(0.5, p_{2}, r\left(p_{2}\right)\right)$. Hence, $\bar{d}_{2}\left(p_{2}, R\left(p_{2}\right)\right)<\bar{d}_{2}\left(p_{2}, r\left(p_{2}\right)\right)$ for all $p_{2}$ satisfying (4.3).

To find the $G_{2,3}$-optimal design, we search for $p_{2}$ in (4.3) to minimize $\bar{d}_{2}\left(p_{2}\right.$, $\left.R\left(p_{2}\right)\right)$ or equivalently to minimize $\max \left\{d_{2}\left(0, p_{2}, R\left(p_{2}\right)\right), d_{2}\left(0.5, p_{2}, R\left(p_{2}\right)\right)\right\}$.
Claim. If $\rho \geq 0.96, \max \left\{d_{2}\left(0, p_{2}, R\left(p_{2}\right)\right), d_{2}\left(0.5, p_{2}, R\left(p_{2}\right)\right)\right\}=d_{2}\left(0, p_{2}, R\left(p_{2}\right)\right)$ for all $p_{2}$ satisfying (4.3).

Proof. Let $g\left(p_{2}\right)=d_{2}\left(0.5, p_{2}, R\left(p_{2}\right)\right)-d_{2}\left(0, p_{2}, R\left(p_{2}\right)\right)=2 p_{2}-1-\left(1-p_{2}\right) R\left(p_{2}\right)$, ignoring an unimportant positive constant. For $L \leq p_{2} \leq 1 / 2$, observe that
$g\left(p_{2}\right) \leq 0-\left(1-p_{2}\right) R\left(p_{2}\right) \leq 0$ and so $\bar{d}_{2}\left(p_{2}, R\left(p_{2}\right)\right)=d_{2}\left(0, p_{2}, R\left(p_{2}\right)\right)$. If $1 / 2 \leq$ $p_{2} \leq U, R\left(p_{2}\right)$ is a decreasing function and so $g\left(p_{2}\right)$ is an increasing function. This implies $g(U)=2 U-1-(1-U) R(U)=2 U-1-(1 / 2)(1-U)=(5 U-3) / 2 \leq 0$ if $U \leq 0.6$, or equivalently if $\rho \geq 0.96$. Thus, $\bar{d}_{2}\left(p_{2}, R\left(p_{2}\right)\right)=d_{2}\left(0, p_{2}, R\left(p_{2}\right)\right)$ for all $p_{2}$ satisfying (4.3) as claimed.

The optimal $p_{2}$ is the one which minimizes $d_{2}\left(0, p_{2}, R\left(p_{2}\right)\right)$ in the interval $[L, U]$. It can be verified that this value is the root of the equation in (4.0); its existence is guaranteed since
$\lim _{p \rightarrow L} \frac{d}{d p}\{1 / p+(1-p) /(p R(p))\}=-\infty$ and $\lim _{p \rightarrow U} \frac{d}{d p}\{1 / p+(1-p) /(p R(p))\}=\infty$.
On the other hand, if $\rho<0.96$, we have $L \leq 0.4, U \geq 0.6, g(L) \leq 0$ and $g(U) \geq 0$. This implies the optimal value of $p_{2}$ is found by solving $g(p)=0$ given in (4.1). Again, the existence of a root between $U$ and $L$ is assured since $g(U) g(L)=(5 U-3)(5 L-3) / 4<0$. This completes the proof when $m=3$.

To obtain $G_{2, m \text {-optimal designs when } m>3 \text {, a direct calculation yields }}$ $\left|M_{22.1}(\xi)\right|=\left(p_{1} q_{1} p_{2} q_{2} p_{3} q_{3} p_{4} q_{4} p_{5} q_{5}\right)^{m-2} p_{6}^{m-2} q_{6}^{m-3}\left(p_{7} q_{7}\right)^{m-3} p_{8}^{m-3} q_{8}^{m-4} \cdots p_{2 m}$. If we replace all odd moments by $1 / 2$ and set $p_{2 k}=(m-k+1) /(2 m-2 k+1)$, $k=3, \ldots, m-1, p_{2 m}=1$, the problem is reduced exactly to (4.2). Thus, the $G_{2, m}$-optimal design has the same $p_{2}$ and $p_{4}$ as $G_{23}$ has, with $p_{2 k}=(m-k+$ $1) /(2 m-2 k+1), k=3, \ldots, m$. This completes the proof of the theorem.

As an example, suppose $\rho=0.8$. The $G_{23 \text {-optimal design has canonical }}$ moments $p_{1}=p_{3}=p_{5}=1 / 2, p_{2}=0.6282, p_{4}=0.6896$ and $p_{6}=1$. Table 1 shows some $G_{23}$-optimal designs. All designs are supported at $0,1-t, t$ and 1 with mass $w, 1 / 2-w, 1 / 2-w$ and $w$ respectively. The corresponding numbers for the $D_{23 \text {-optimal design are given in Studden (1982) and are displayed in }}$ parentheses.

Table 1. $G_{23}\left(D_{23}\right)$-optimal designs for various values of $\rho$.

| $\rho$ | $p_{2}$ | $p_{4}$ | $t$ | $w$ |
| :--- | :---: | :---: | :---: | :---: |
| 0.1 | $0.6634(0.6633)$ | $0.9712(0.9712)$ | $0.5691(0.5691)$ | $0.3284(0.3284)$ |
| 0.2 | $0.6600(0.6595)$ | $0.9408(0.9408)$ | $0.5988(0.5988)$ | $0.3231(0.3229)$ |
| 0.3 | $0.6562(0.6551)$ | $0.9085(0.9087)$ | $0.6225(0.6223)$ | $0.3171(0.3166)$ |
| 0.4 | $0.6520(0.6499)$ | $0.8739(0.8743)$ | $0.6434(0.6429)$ | $0.3104(0.3094)$ |
| 0.5 | $0.6474(0.6436)$ | $0.8363(0.8373)$ | $0.6628(0.6618)$ | $0.3028(0.3010)$ |
| 0.6 | $0.6422(0.6357)$ | $0.7946(0.7968)$ | $0.6816(0.6797)$ | $0.2939(0.2908)$ |
| 0.7 | $0.6360(0.6254)$ | $0.7470(0.7515)$ | $0.7006(0.6971)$ | $0.2831(0.2782)$ |
| 0.8 | $0.6282(0.6109)$ | $0.6896(0.6992)$ | $0.7208(0.7143)$ | $0.2691(0.2616)$ |
| 0.9 | $0.6168(0.5872)$ | $0.6096(0.6339)$ | $0.7454(0.7318)$ | $0.2476(0.2371)$ |
| 0.98 | $0.5675(0.5450)$ | $0.5212(0.5548)$ | $0.7606(0.7463)$ | $0.2031(0.1996)$ |

Table 1 shows that the second canonical moments of the $D_{23^{-}}$and $G_{23^{-}}$ optimal design are different; thus by Property $3.1, G_{2 m}$ and $D_{2 m \text {-optimal designs }}$ are no longer equivalent.

## 5. Discussion

To see if $G_{r m}$-optimal designs are robust to model misspecification, we consider the case where $r=2$ and the true model is of degree 1,2 and 3 . Let $\xi_{G, 2 m}$ denote the $G_{2 m}$-optimal design. From Property 3.3 , the $D$-efficiencies of $\xi_{G, r m}$ for the $k$ th degree polynomial can be expressed in terms of canonical moments. When $k=1,2$ and 3 , these expression are respectively given by, for all $m>2$,

$$
\begin{aligned}
& e_{1}^{D}\left(\xi_{G, 2 m}\right)=p_{2}^{1 / 2}, \quad e_{2}^{D}\left(\xi_{G, 2 m}\right)=3\left(0.25 p_{2}^{2} q_{2} p_{4}\right)^{1 / 3}, \\
& e_{3}^{D}\left(\xi_{G, 2 m}\right)=\{(m-2) /(2 m-5)\}^{1 / 4} e_{3}^{D}\left(\xi_{G, 23}\right)
\end{aligned}
$$

and

$$
e_{3}^{D}\left(\xi_{G, 23}\right)=0.5\left(5^{5} p_{2}^{3} q_{2}^{2} p_{4}^{2} q_{4}\right)^{1 / 4}
$$

A similar argument shows that the $G$-efficiencies of $\xi_{G, r m}$ for the simple and quadratic models are independent of $m$ if $m>2$, and are $e_{1}^{G}\left(\xi_{G, 2 m}\right)=2 p_{2} /\left(1+p_{2}\right)$ and $e_{2}^{G}\left(\xi_{G, 2 m}\right)=3 p_{2}^{2} q_{2} p_{4} /\left(p_{2}-2 p_{2}^{2}+p_{2}^{3}+p_{2} q_{2} p_{4}+p_{2}^{2} q_{2} p_{4}\right)$, respectively. Table 2 shows the $D$ - and $G$-efficiencies of the $G_{23}$-optimal designs for various $\rho$ under different model assumptions. Note that the fourth column is specific to the $G_{23}{ }^{-}$ optimal designs only; the entries in the other columns apply to $G_{2 m}$-optimal designs for any $m>2$. Unlike the other columns, the entries in the fourth column increase as $\rho$ increases until $\rho$ is roughly 0.8 and it decreases after that. The rationale for this observation is that for very high values of $\rho$, one essentially estimates only the cubic coefficient in the cubic model and therefore the efficiency for estimating all the parameters declines. This pattern is also reflected in Table 3 of Studden (1982) for $D_{r m}$-optimal designs.

Table 2. Selected $D$ and $G$-efficiencies of $G_{r m}$-optimal designs.

| $\rho$ | $e_{1}^{D}\left(\xi_{G, 2 m}\right)$ | $e_{2}^{D}\left(\xi_{G, 2 m}\right)$ | $e_{3}^{D}\left(\xi_{G, 23}\right)$ | $e_{1}^{G}\left(\xi_{G, 2 m}\right)$ | $e_{2}^{G}\left(\xi_{G, 2 m}\right)$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 0.1 | 0.8145 | 0.9903 | 0.6474 | 0.7977 | 0.9902 |
| 0.2 | 0.8124 | 0.9798 | 0.7637 | 0.7951 | 0.9795 |
| 0.3 | 0.8101 | 0.9683 | 0.8377 | 0.7924 | 0.9675 |
| 0.4 | 0.8075 | 0.9556 | 0.8914 | 0.7894 | 0.9541 |
| 0.5 | 0.8046 | 0.9414 | 0.9320 | 0.7860 | 0.9387 |
| 0.6 | 0.8014 | 0.9250 | 0.9627 | 0.7821 | 0.9207 |
| 0.7 | 0.7975 | 0.9055 | 0.9846 | 0.7775 | 0.8986 |
| 0.8 | 0.7926 | 0.8806 | 0.9970 | 0.7716 | 0.8695 |
| 0.9 | 0.7854 | 0.8434 | 0.9940 | 0.7630 | 0.8241 |

Note that for the quadratic model, all $G_{2 m}$-optimal designs have very high $D$ and $G$-efficiencies for small $\rho$, and the efficiencies decrease rather slowly as $\rho$ increases. For the cubic model, these efficiencies grow rather fast as $\rho$ increases. In any case, all the efficiencies remain quite stable if the linear model is assumed.

We also evaluate the $D$ and $G$-efficiency of $\xi_{G, 2 m}$ relative to the $D_{2 m}$-optimal design $\xi_{D, r m}$ when the assumed polynomial model is of degree $k$. For any two designs $\xi_{1}$ and $\xi_{2}$, these relative $D$-efficiencies are defined by $\left\{\left|M_{k}\left(\xi_{1}\right)\right| /\right.$ $\left.\left|M_{k}\left(\xi_{2}\right)\right|\right\}^{1 /(k+1)}$ and $\bar{d}\left(\xi_{2}\right) / \bar{d}\left(\xi_{1}\right)$. Since the canonical moments of $\xi_{G, 2 m}$ and $\xi_{D, 2 m}$ differ only in $p_{2}$ and $p_{4}$, the above for these designs are independent of $m$ for $k=1$ and 2. Our calculation showed these efficiencies range from 0.99 to 1.05 when $0.1 \leq \rho \leq 0.9$, suggesting that the $G_{2 m}$ and $D_{2 m}$-optimal designs have almost identical performances if we have simple, quadratic or cubic models. This means the $D_{2 m}$ and the $G_{2 m}$-optimal designs are roughly optimal for both parameter estimation and response surface estimation, and at the same time offer some protection against model miss-specification for low order polynomial models.

Finally, we compare our designs with the constrained optimal designs obtained by Pukelsheim and Rosenberger (1993). We follow their notation and let $\Theta_{3}$ denote the 'cubic' coefficient, let $\Theta_{(A)}$ denote the vector of parameters in the quadratic model and let $\Theta_{(B)}^{T}=\left(\Theta_{(A)}^{T}, \Theta_{3}\right)$. They reported the efficiencies of two $D$-optimal designs for $\Theta_{(A)}$, (a) and (b) below, which guarantee a $50 \%$ efficiency for estimating $\Theta_{3}$. In our case, the $G_{23}$-optimal design with $\rho=0.5$ is symmetrically supported on $\pm 1$ and $\pm 0.3256$ with mass 0.3208 at 1 and 0.1972 at 0.3256 respectively. Table 3 , row (c), shows this design performs similarly to theirs and has the same numerical efficiencies with the $D_{23}$-optimal design.

Table 3. Comparing some properties of $G_{r m}$-optimal designs with those obtained by Pukelsheim and Rosenberger (1993).

|  | design description | Efficiencies |  |  |
| :--- | :--- | :---: | :---: | :---: |
|  |  |  | $\Theta_{3}$ | $\Theta_{(B)}$ |
| $\Theta_{(A)}$ |  |  |  |  |
| $(\mathrm{a})$ | $D$-optimal for $\Theta_{(A)}, 50 \%$ efficient for $\Theta_{3}$ on $[-1,1]$ | 0.50 | 0.93 | 0.94 |
| $(\mathrm{~b})$ | $D$-optimal for $\Theta_{(A)}, 50 \%$ for $\Theta_{3}$ on $\pm 1, \pm 1 / 2,0$ | 0.50 | 0.92 | 0.93 |
| $(\mathrm{c})$ | $G$-optimal for $\Theta_{(A)}, 50 \%$ for $\Theta_{3}$ on $[-1,1]$ | 0.50 | 0.93 | 0.94 |

## Acknowledgements

The authors would like to thank the referees for their constructive comments leading to an improved version of this paper. The research of Wong is partially supported by a NIH FIRST award.

## References

Atwood, C. L. (1971). Robust procedures and estimating polynomial regression. J. Amer. Statist. Assoc. 66, 855-860.
Dette, H. and Roder, I. (1996). Optimal product designs for multivariate regression with missing terms. Scandinavian J. Statist. 23, 195-208.
Kiefer, J. (1959). Optimum experimental designs. J. Roy. Statist. Soc. Ser. B 21, 272-319.
Kiefer, J. and Wolfowitz, J. (1960). The equivalence of two extremum problems. Canadian J. Math. 12, 363-366.
Lau, T. S. (1983). Theory of Canonical Moments and Its Applications in Polynomial Regression. Purdue University Technical Report No. 83-23, No. 83-24.
Läuter, E. (1974). Experimental planning in a class of models. Math. Operationsfosh. und Statist. 36, 1627-1655.
Lee, C. M. S. (1988). Constrained optimal designs. J. Statist. Plann. Inference 18, 377-389.
Pázman, A. (1986). Foundations of Optimum Experimental Design. Reidel, Boston.
Pukelsheim, F. and Rosenberger, J. L. (1993). Experimental designs for model discrimination. J. Amer. Statist. Assoc. 88, 9642-9649.

Skibinsky, M. (1969). Some striking properties of binomial and beta moments. Ann. Math. Statist. 40, 1753-1764.
Skibinsky, M. (1986). Principal representations and canonical moment sequences on an interval. J. Math. Anal. Approx. 120, 95-120.

Stigler, S. M. (1971). Optimal experimental design for polynomial regression. J. Amer. Statist. Assoc. 66, 311-318.
Studden, W. J. (1982). Some robust-type $D$-optimal designs in polynomial regression. J. Amer. Statist. Assoc. 77, 916-921.

Department of Biostatistics, School of Public Health, University of California, 10833 Le Conte Avenue, Los Angeles, CA 90095-1772, U.S.A.
E-mail: wkwong@sunlab.ph.ucla.edu
E-mail: song@ucla.edu
(Received August 1996; accepted February 1998)

