First and Second Order Rotatability of Experimental Designs, Moment Matrices, and Information Surfaces

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1 Introduction

Balancedness and symmetry properties are among the most useful and pleasing features that an experimental design can possess. In the present paper we discuss the classical linear model of uncorrelated homoscedastic observations for fitting a polynomial response of some selected order,

$$\eta(t,\theta) = \theta_0 + t_1\theta_1 + \ldots + t_m\theta_m + t_1^2\theta_{11} + t_1t_2\theta_{12} + \ldots \quad . \tag{1.1}$$

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This is a polynomial in the values $t_1, \ldots, t_m$ that m factors can attain, with coefficients $\theta_0, \theta_1, \ldots, \theta_m, \theta_{11}, \theta_{12}, \ldots$ to be estimated.

The levels $t_1, \ldots, t_m$ jointly form the m-dimensional vector of experimental conditions $t \in \mathbb{R}^m$. An experimental design for sample size N then enumerates N vectors of experimental conditions at which to draw an observation. More generally, we shall consider approximate designs which assign, to a finite number of experimental conditions, positive weights which sum to one. The weights determine the proportions of all observations to be taken under the corresponding vector of experimental conditions.

For a polynomial fit the notion of symmetry which has received the greatest attention in the literature requires that the statistical performance of an experimental design remain the same when the experimental conditions $t \in \mathbb{R}^m$ undergo an arbitrary rotation, that is, an arbitrary orthogonal transformation. In the present paper, we provide a detailed study of this concept as it pertains to polynomial fits of first and second order.

The orthogonal matrices Q, where $Q'Q = I$, form an infinite, though compact, group of nonsingular matrices. Our main result is that, for second order fits, invariance with respect to the finite subset of sign changes, permutations, and the orthodiagonal reflection implies rotatability. For two factors, $m = 2$, the orthodiagonal reflection is replaced by a rotation of 45°.

For our mathematical analysis it is convenient to shift emphasis from the experimental conditions $t \in \mathbb{R}^m$ to the regression vectors $x = f(t) \in \mathbb{R}^k$, where the vector $f(t)$ is composed of the mixed powers in the variables $t_1, \ldots, t_m$ which appear in the response surface representation (1.1). Let $\mathscr{X} \subseteq \mathbb{R}^k$ be the regression range of vectors $f(t)$ which result when the experimental conditions t vary over an experimental domain $\mathscr{T} \subseteq \mathbb{R}^m$. A design ξ on $\mathscr{X}$, or τ on $\mathscr{T}$, is taken to be a probability measure which has a finite support. The support of a design is the set of points which are assigned a positive weight, and is denoted by $\operatorname{supp} \xi \subseteq \mathscr{X}$ or $\operatorname{supp} \tau \subseteq \mathscr{T}$, respectively.

We call f the regression function associated with (1.1), and take its dimensionality to be equal to k. In the present paper we discuss first and second order models,

$$f(t) = \begin{pmatrix} 1 \\ t \end{pmatrix} \in \mathbb{R}^k \ , \qquad k = 1 + m \ , \tag{1.2}$$

$$f(t) = \begin{pmatrix} 1 \\ t \\ t \otimes t \end{pmatrix} \in \mathbb{R}^k \ , \quad k = 1 + m + m^2 \ , \tag{1.3}$$

respectively. The second order regression function (1.3) utilizes the Kronecker product $t \otimes t$. This representation repeats the mixed second order terms twice, as $t_i t_j$ and as $t_j t_i$ if $i \neq j$. We prefer this representation for discussing rotatability because of the simple calculus that evolves. We show in Section 9 that the results are the same had we cancelled all repetitions, or had we used the Schläflian power notation.

Our considerations of rotability allow us to derive measures of rotatability, that is, measures which indicate how well the moments of any given design compare to those of a rotatable design. The criteria are presented in Section 6. An alternative presentation together with practical examples is given by Draper and Pukelsheim (1990).

We first provide a brief discussion of those aspects which are common to all invariant design problems.

2 Invariant Design Problems

Let ξ be a design on a regression range $\mathscr{X} \subseteq \mathbb{R}^k$, and let Q be a nonsingular $k \times k$ matrix. All invariance considerations amount to comparing the two designs ξ and ξ^Q, where the latter is the rotation of ξ under Q given by

$$\xi^Q(y) = \xi(Q^{-1}y) \ .$$

In a classical linear model the performance of a design ξ is evaluated through its moment matrix

$$M(\xi) = \sum_{x \in \operatorname{supp} \xi} \xi(x) x x' \ .$$

Our first lemma relates the support sets and the moment matrices of a design and its rotation in a quite simpler manner.

Lemma 2.1. Let ξ be a design on $\mathscr{X} \subseteq \mathbb{R}^k$, and let Q be a nonsingular $k \times k$ matrix. Then the support of the rotated design ξ^Q is equal to the image under Q of the support of ξ,

$$\operatorname{supp} \xi^Q = Q(\operatorname{supp} \xi) \ ,$$

and the moment matrix of ξ^Q is obtained from the moment matrix of ξ by a congruence transformation,

$$M(\xi^Q) = QM(\xi)Q' \ . \qquad \square$$

Now let $\mathcal{Q}$ be a set of nonsingular $k \times k$ matrices. (At his point we do not require $\mathcal{Q}$ to be a group yet.) Then a design ξ is called invariant under $\mathcal{Q}$ when

$$\xi^Q = \xi \quad \text{for all} \quad Q \in \mathcal{Q} \ ;$$

and a symmetric $k \times k$ matrix M is called invariant under $\mathcal{Q}$ when

$$QMQ' = M \quad \text{for all} \quad Q \in \mathcal{Q} \ .$$

The set of all invariant symmetric $k \times k$ matrices is denoted by $\mathrm{Sym}\,(k, \mathcal{Q})$.

It follows from Lemma 2.1 that an invariant design possesses an invariant moment matrix. However, the converse is not true. Moreover, the fact that an invariant moment matrix may be generated by a non-invariant design is often the source of great economy. The rotatable central composite design of Box and Hunter (1957) provide well-known examples: Although these designs are not themselves invariant under all rotations, their moment matrices are. Thus the notion of invariant matrices carries further than that of invariant designs.

Next we show that the invariant matrices form a subspace of symmetric matrices.

Lemma 2.2. Let $\mathcal{Q}$ be a set of nonsingular $k \times k$ matrices. Then the set $\mathrm{Sym}\,(k, \mathcal{Q})$ of invariant matrices forms a subspace of symmetric matrices. If all matrices in $\mathcal{Q}$ are orthogonal, then the subspace $\mathrm{Sym}\,(k, \mathcal{Q})$ is a quadratic subspace of symmetric matrices, that is,

$$M^2 \in \mathrm{Sym}\,(k, \mathcal{Q}) \quad \text{for all} \quad M \in \mathrm{Sym}\,(k, \mathcal{Q}) \ . \qquad \square$$

The notion of quadratic subspaces of symmetric matrices is due to Seely (1971). Quadratic subspaces of symmetric matrices have a number of pleasant properties. For instance, with every member M they also contain the Moore-Penrose inverse M^+. For our invariant subspaces $\mathrm{Sym}\,(k, \mathcal{Q})$ this is also easily seen directly, since if Q is orthogonal then $QM^+Q' = (QMQ')^+ = M^+$. Lemma 1.6 of Seely (1971) provides another important property. If a member M of a quadratic subspace has an eigenvalue decomposition

$$M = \sum_{i=1}^{l} \mu_i P_i \ ,$$

with l distinct eigenvalues μ_i, then each projection matrix P_i also is a member of the quadratic subspace. This entails that, if $\mathrm{Sym}(k, \mathscr{Q})$ has dimension l, then every invariant symmetric matrix M can have at most l distinct eigenvalues, and the associated projection matrices P_i are themselves invariant.

A major result of the present paper is that we can always make do with *finitely many* transformations Q. For rotatability in first and second order models these are given in Theorems 4.1 and 6.1, respectively. The following theorem ascertains that the reduction from arbitrarily many to finitely many transformations is always mathematically feasible, even though it does not provide a practical way for carrying out this reduction.

Theorem 2.3. Let $\mathscr{Q}$ be a set of nonsingular $k \times k$ matrices. Then $\mathscr{Q}$ contains a finite subset $\{Q_1, \ldots, Q_l\}$, say, such that $\mathscr{Q}$ and $\{Q_1, \ldots, Q_l\}$ share the same subspace of invariant symmetric matrices, that is,

$$\mathrm{Sym}(k, \mathscr{Q}) = \mathrm{Sym}(k, \{Q_1, \ldots, Q_l\}) \ .$$

Proof: For $Q \in \mathscr{Q}$ we define the mapping T_Q from $\mathrm{Sym}(k)$ into $\mathrm{Sym}(k)$ by $T_Q(A) = QAQ' - A$. Then M is invariant under $\mathscr{Q}$ if and only if

$$T_Q(M) = 0 \quad \text{for all} \quad Q \in \mathscr{Q} \ . \tag{2.1}$$

Evidently T_Q is a member of the space $\mathscr{L}$ of all linear mappings from $\mathrm{Sym}(k)$ into $\mathrm{Sym}(k)$. Hence (2.1) extends to the subspace $\mathscr{L}(\mathscr{Q})$ generated by $T_Q, Q \in \mathscr{Q}$. Thus (2.1) becomes the same as

$$T(M) = 0 \quad \text{for all} \quad T \in \mathscr{L}(\mathscr{Q}) \ . \tag{2.2}$$

But $\mathscr{L}(\mathscr{Q})$, being a subspace of the finite dimensional space $\mathscr{L}$, has finite dimension l, say. Therefore the generator $\{T_Q : Q \in \mathscr{Q}\}$ contains a basis $\{T_{Q_1}, \ldots, T_{Q_l}\}$, whence (2.2) reduces to

$$T_{Q_i}(M) = 0 \quad \text{for all} \quad i = 1, \ldots, l \ . \tag{2.3}$$

The equivalence of (2.1) and (2.3) proves the assertion. □

In our investigations the sets $\mathscr{Q}$ will often be subgroups of orthogonal matrices. Before turning to our statistical problems, we first list those subgroups that will be of relevance to us.

3 Finite Subgroups of Orthogonal Matrices

The transformations of the regression vectors $x \in \mathbb{R}^k$ are induced by transformations of the experimental conditions $t \in \mathbb{R}^m$. We shall be interested in the following groups acting on the experimental domain $\mathscr{T} \subseteq \mathbb{R}^m$:

$$\begin{aligned}
\mathrm{GL}(m) &= \{Q \in \mathbb{R}^{m \times m} : \det Q \neq 0\} , && \\
\mathrm{Orth}(m) &= \{Q \in \mathbb{R}^{m \times m} : Q'Q = I_m\} && \subseteq \mathrm{GL}(m) , \\
\mathrm{Sign}(m) &= \{\Delta_\varepsilon \in \mathbb{R}^{m \times m} : \varepsilon \in \{\pm 1\}^m\} && \subseteq \mathrm{Orth}(m) , \\
\mathrm{Perm}(m) &= \left\{ \sum_{j \leq m} e_{\pi(j)} e_j' : \pi \in \mathscr{S}_m \right\} && \subseteq \mathrm{Orth}(m) , \\
\mathrm{Refl}(1_m) &= \left\{ I_m, I_m - \frac{2}{m} 1_m 1_m' \right\} && \subseteq \mathrm{Orth}(m) , \\
\mathrm{Rot}(45°) &= \left\{ \begin{pmatrix} \cos(j45°) & -\sin(j45°) \\ \sin(j45°) & \cos(j45°) \end{pmatrix} : j = 0, \ldots, 7 \right\} && \subseteq \mathrm{Orth}(2) .
\end{aligned} \tag{3.1}$$

GL (m) is the general linear group of nonsingular $m \times m$ matrices. Orth (m) is the orthogonal group consisting of all orthogonal matrices. Sign (m) is the sign change group, composed as follows. Let $\varepsilon = (\varepsilon_1, \ldots, \varepsilon_m)'$ be a vector with components ± 1, and let Δ_ε be the diagonal matrix with the vector ε on the diagonal. Then Δ_ε acts as a sign change transformation on a vector $t \in \mathbb{R}^m$, that is, $\Delta_\varepsilon t = (\varepsilon_1 t_1, \ldots, \varepsilon_m t_m)'$.

Perm (m) is the permutation group where, in its definition, we have referred to permutations π of the subscripts $1, \ldots, m$ and the Euclidean unit vectors $e_j \in \mathbb{R}^m$. The reflection group Refl (1_m) describes the reflection at the hyperplane orthogonal to the unity vector 1_m; the transformation $I_m - \frac{2}{m} 1_m 1_m'$ is called the orthodiagonal reflection. Finally, in the plane $m = 2$, we need the rotation group Rot (45°) which rotates the axes by half a right angle and which is generated by the special case $j = 1$.

The groups differ considerably in size. GL (m) is infinite and noncompact, Orth (m) is infinite but compact. The remaining four subgroups are finite: Sign (m) has order 2^m, Perm (m) has order $m!$, Refl (1_m) has order 2, and Rot (45°) has order 8.

Straightforward verification shows that the subspaces of symmetric matrices which are invariant under these groups are the following:

$$\mathrm{Sym}\,(m,\mathcal{Q}) = \begin{cases} \{0\} & \text{for } \mathcal{Q} = \mathrm{GL}\,(m)\ , \\ \{\alpha I_m : \alpha \in \mathbb{R}\} & \text{for } \mathcal{Q} = \mathrm{Orth}\,(m)\ , \\ \{\Delta_t : t \in \mathbb{R}^m\} & \text{for } \mathcal{Q} = \mathrm{Sign}\,(m)\ , \\ \{\alpha I_m + \beta 1_m 1_m' : \alpha, \beta \in \mathbb{R}\} & \text{for } \mathcal{Q} = \mathrm{Perm}\,(m)\ , \\ \{A \in \mathrm{Sym}\,(m) : A 1_m = \alpha 1_m, \alpha \in \mathbb{R}\} & \text{for } \mathcal{Q} = \mathrm{Refl}\,(1_m)\ , \\ \{\alpha I_2 : \alpha \in \mathbb{R}\} & \text{for } \mathcal{Q} = \mathrm{Rot}\,(45°)\ . \end{cases} \tag{3.2}$$

In particular, Sign (m) is associated with the subspace of all diagonal matrices, Perm (m) with all completely symmetric matrices, that is, those of the form $\alpha I_m + \beta 1_m 1_m'$. A matrix A is invariant relative to Refl (1_m) if and only if the unity vector 1_m is an eigenvector of A, that is, A has constant row and column sums.

The experimental domains $\mathcal{T} \subseteq \mathbb{R}^m$ which are invariant under these groups have familiar geometric shapes. Orth (m) is associated with the closed balls $\mathcal{T} = \left\{ t \in \mathbb{R}^m : \sum_{j \le m} t_j^2 \le r \right\}$; Perm (m) with cubes $\mathcal{T} = [0, r]^m$. Together, the two groups Sign (m) and Perm (m) come with symmetrized cubes $\mathcal{T} = [-r, r]^m$. Most often the radius $r > 0$ is scaled to be equal to unity.

4 First Order Rotatability

The simplest case is that of a first order polynomial fit, sometimes called multiple linear regression. Here the quantities mentioned before specialize as follows:

experimental conditions	$t \in \mathbb{R}^m$
experimental domain	$\mathcal{T} \subseteq \mathbb{R}^m$
regression vectors	$x = f(t) = \begin{pmatrix} 1 \\ t \end{pmatrix} \in \mathbb{R}^k\ , \quad k = 1 + m$
regression range	$\mathcal{X} = \{f(t) : t \in \mathcal{T}\} \subseteq \mathbb{R}^k$
transformation group	$\mathcal{Q} = \left\{ \begin{pmatrix} 1 & 0 \\ 0 & R \end{pmatrix} : R \in \mathrm{Orth}\,(m) \right\}\ .$

For a first order fit the regression range lies in $\mathbb{R}^k$, with $k = 1 + m$. The $k \times k$ matrix Q that is induced by an $m \times m$ rotation R is abbreviated by

$$Q_R = \begin{pmatrix} 1 & 0 \\ 0 & R \end{pmatrix} .$$

We call a symmetric $k \times k$ matrix M (first order) rotatable when M is invariant under $\mathcal{Q}$. A design τ is called first order rotatable when its moment matrix $M(\tau) = \int_{\mathcal{T}} f(t) f(t') d\tau$ is first order rotatable.

Hence a design τ inherits its rotatability properties through its moment matrix $M(\tau)$. Our definition does not mean or imply that a rotatable design τ is invariant under the group $\mathcal{Q}$.

We first study which symmetric matrices are invariant, and then specialize the result to moment matrices.

Theorem 4.1. Let M be a symmetric $k \times k$ matrix. Then the following three statements are equivalent:

(i) M is first order rotatable.
(ii) M is invariant under the finitely many matrices Q_R, where R is any sign change matrix or the orthodiagonal reflection.
(iii) There exists scalars $\alpha, \beta \in \mathbb{R}$ such that M has the form

$$M = \begin{pmatrix} \alpha & 0 \\ 0 & \beta I_m \end{pmatrix} . \tag{4.1}$$

Proof: It is clear that (i) implies (ii), since (ii) involves fewer transformations than (i).

Next we show that (ii) implies (iii). To this end write M in the form

$$M = \begin{pmatrix} \alpha & a' \\ a & B \end{pmatrix} . \tag{4.2}$$

A congruence transformation using Q_R then yields

$$Q_R M Q_R' = \begin{pmatrix} \alpha & a'R' \\ Ra & RBR' \end{pmatrix} .$$

Invariance entails that $Ra = a$ for $R = -I_m$, whence a vanishes. Letting R vary over all sign change matrices, the matrix B is seen to be diagonal. But B is also invariant under the orthodiagonal reflection and hence must be a multiple of the identity matrix, $B = \beta I_m$.

That (iii) implies (i) is plainly verified. □

The two scalars α and β (with multiplicity m) are the $k = m+1$ eigenvalues of the matrix M in (4.1). Also the nonvanishing blocks in (4.1) correspond to the design moments of order 0 and 2, whence it is convenient to represent invariant matrices using the two symmetric $k \times k$ matrices

$$V_0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad V_2 = \frac{1}{\sqrt{m}} \begin{pmatrix} 0 & 0 \\ 0 & I_m \end{pmatrix}. \tag{4.3}$$

It is easily verified that the pair V_0 and V_2 form an orthonormal system in the space Sym (k) of all symmetric $k \times k$ matrices, that is, $\langle V_0, V_2 \rangle = \text{trace } V_0 V_2 = 0$ and $\langle V_i, V_i \rangle = \text{trace } V_i^2 = 1$ for $i = 0, 2$.

Corollary 4.2. Let M be a symmetric $k \times k$ matrix. Then the following three statements are equivalent:

(i) M is first order rotatable.
(ii) There exist scalars $\alpha, \beta \in \mathbb{R}$ such that $M = \alpha V_0 + \beta V_2$.
(iii) $M = (\text{trace } M V_0) V_0 + (\text{trace } M V_2) V_2$. □

Next we apply these results to moment matrices.

Let τ be a design on the experimental domain $\mathscr{T}$. If its moment matrix $M(\tau)$ has the form (4.1) then $\alpha = 1$, and β is the second moment λ_2 common to the components t_j of the experimental conditions t, that is, for all $j \le m$ we have

$$\sum_{t \in \text{supp } \tau} \tau(t) t_j^2 = \beta = \lambda_2 . \tag{4.4}$$

In particular, when the design τ is realizable for sample size N with experimental conditions $t_u \in \mathbb{R}^m$ for $u = 1, \ldots, N$, then (4.4) may be written as

$$\sum_{u \le N} t_{uj}^2 = N \lambda_2 . \tag{4.5}$$

In summary, it is easy to recognize rotatable moment matrices as follows.

Corollary 4.3. Let M be a symmetric $k \times k$ matrix. Then the following three statements are equivalent:

(i) M is a first order rotatable moment matrix on some experimental domain $\mathscr{T} \subseteq \mathbb{R}^m$.

(ii) There exists a scalar $\lambda_2 \geq 0$ such that $M = V_0 + \lambda_2 \sqrt{m}\, V_2$.
(iii) M is a nonnegative definite matrix such that $M = V_0 + (\operatorname{trace} M V_2)\, V_2$. □

It follows that the first order rotatable moment matrices form a shifted convex cone with tip in V_0, parametrized by $\lambda_2 \geq 0$. The interior of the cone, $\lambda_2 > 0$, corresponds to those moment matrices which have a maximum rank, k.

Many authors scale the design so that the second moment λ_2 is equal to unity. With this scaling, any first order rotatable moment matrix becomes the identity matrix, $M = V_0 + \sqrt{m}\, V_2 = I_k$. In our exposition we stick to an experimental domain $\mathscr{T}$ which is fixed and given in advance. The best second moment λ_2 then is the maximum $\lambda_2(\mathscr{T})$ that can be achieved among all designs τ which have zero first moments and which satisfy the symmetry condition (4.4). Corollary 4.3(ii) does not show this upper bound, in the sense that an arbitrarily large second moment λ_2 can be achieved provided the experimental domain $\mathscr{T}$ becomes arbitrarily large.

A design on the experimental domain $\mathscr{T}$ that has moment matrix $V_0 + \lambda_2(\mathscr{T}) \sqrt{m}\, V_2$ is universally optimal in the sense of Pukelsheim (1987b). This means that any other design τ with moment matrix M may first be improved in the direction of a more balanced matrix (say) $\bar{M} = V_0 + (\operatorname{trace} M V_2)\, V_2$, followed by an improvement in the Löwner ordering towards $V_0 + \lambda_2(\mathscr{T})\, V_2$.

For various shapes of the experimental domain $\mathscr{T}$ we may determine the maximal second moment $\lambda_2(\mathscr{T})$, and the first order rotatable designs τ that achieve this maximal second moment. For example, if $\mathscr{T}$ is the ball of radius r then $\lambda_2(\mathscr{T}) = r^2/m$. An identical value holds for a hypercube whose vertices are on the ball.

So far we have concentrated on moment matrices. A function which is of considerable statistical interest is the information surface which is induced by a moment matrix M. It is defined by

$$i_M(t) = \left\{ (1, t') M^{-1} \begin{pmatrix} 1 \\ t \end{pmatrix} \right\}^{-1} \quad \text{for all} \quad t \in \mathbb{R}^m , \tag{4.6}$$

provided M is positive definite. Such a (first order) information surface i_M is called rotatable when $i_M(Rt) = i_M(t)$ for all $R \in \operatorname{Orth}(m)$ and $t \in \mathbb{R}^m$.

The study of information surfaces is aided by first discussing the quadratic form q_M induced by M, given by

$$q_M(t) = (1, t') M \begin{pmatrix} 1 \\ t \end{pmatrix} \quad \text{for all} \quad t \in \mathbb{R}^m . \tag{4.7}$$

This quadratic form makes sense for every symmetric $k \times k$ matrix M, and does not require nonsingularity. A quadratic form q_M is called rotatable when $q_M(Rt) = q_M(t)$ for all $R \in \operatorname{Orth}(m)$ and $t \in \mathbb{R}^m$.

Rotatability of a matrix M coincides with rotatability of its quadratic form q_M or its information surface i_M. For first order models this result holds for all symmetric matrices, for higher order models it is restricted to moment matrices, only. Therefore the following argument does not carry over to second order models, compare Section 7.

Theorem 4.4. A symmetric $k \times k$ matrix M is first order rotatable if and only if its induced quadratic form q_M from (4.7) is rotatable. A nonsingular symmetric $k \times k$ matrix M is first order rotatable if and only if the information surface i_M from (4.6) is rotatable.

Proof: A rotatable moment matrix as in (4.1) has quadratic form $q_M(t) = \alpha + \beta t't$ which clearly is rotatable.

Conversely, write M in the partitioned form (4.2). Its quadratic form is $q_M(t) = \alpha + 2t'a + t'Bt$. Fix $R \in \mathrm{Orth}(m)$ and $t \in \mathbb{R}^m$. Then $q_M(\mu Rt)$ and $q_M(\mu t)$ form two polynomials in $\mu \in \mathbb{R}$ which, by the invariance assumption, are identical. Equating coefficients we obtain

$$t'R'a = t'a \quad \text{and} \quad t'R'BRt = t'Bt \quad \text{for all} \quad R \in \mathrm{Orth}(m) \quad \text{and} \quad t \in \mathbb{R}^m \ .$$

As in the proof of Theorem 4.1 it follows that I. $a = 0$ and II. $B = \beta I_m$ for some scalar β. Hence M has the form (4.1).

Now we assume M to be nonsingular and rotatable. Then

$$M^{-1} = \begin{pmatrix} \frac{1}{\alpha} & 0 \\ 0 & \frac{1}{\beta} I_m \end{pmatrix}$$

is rotatable. Hence $1/i_M = q_{M^{-1}}$, and the information surface i_M is rotatable. Conversely, if i_M is rotatable then so is $q_{M^{-1}}$. Therefore the matrix M^{-1} is rotatable, and then M must be rotatable as well. □

In summary, the notion of first order rotatability of designs τ is the same whether it pertains their moment matrices $M(\tau)$, the quadratic forms $q_{M(\tau)}$, or the information surfaces $i_{M(\tau)}$.

We now turn to the corresponding results for second order rotatability. First we review some convenient tools from matrix algebra.

5 Kronecker Products and Vectorization of Matrices

We arrange the second order terms as a Kronecker square,

$$t \otimes t = (t_1^2, t_1 t_2, t_1 t_3, \ldots, t_1 t_m; t_2 t_1, t_2^2, t_2 t_3, \ldots, t_2 t_m; \ldots, t_m^2)' \ . \tag{5.1}$$

Thus the mixed second order terms $t_i t_j$, for $i \neq j$, are represented twice, as $t_i t_j$ and $t_j t_i$. This representation is redundant. But the powerful properties of the Kronecker product make it vastly superior to any other representation, for our manipulations.

The Kronecker* product of two matrices $A \in \mathbb{R}^{k \times p}$ and $B \in \mathbb{R}^{m \times q}$ is

$$A \otimes B = \begin{pmatrix} a_{11} B & \ldots & a_{1p} B \\ \vdots & & \\ a_{k1} B & \ldots & a_{kp} B \end{pmatrix} \in \mathbb{R}^{km \times pq} \ . \tag{5.2}$$

For vectors $s \in \mathbb{R}^k$ and $t \in \mathbb{R}^m$ this simplifies to

$$s \otimes t = \begin{pmatrix} s_1 t \\ \vdots \\ s_k t \end{pmatrix} \in \mathbb{R}^{km} \ . \tag{5.3}$$

The most important property of the Kronecker product is that it conforms with matrix multiplication by way of

$$(A \otimes B)(s \otimes t) = (As) \otimes (Bt) \ , \tag{5.4}$$

provided the dimensions match appropriately. It is a consequence of (5.4) that the transpose (inverse, generalized inverse, Moore-Penrose inverse) of a Kronecker product is equal to the Kronecker products of the transposes (inverses, generalized inverses, Moore-Penrose inverses).

The same cross products $s_i t_j$ which appear in $s \otimes t$ also appear, in a different arrangement, in the rank-one matrix st'. For an easy transition between the two arrangements we define the vectorization operator

$$\operatorname{vec}(st') = s \otimes t \ . \tag{5.5}$$

* This product is actually due to Zehfuß; see Henderson, Pukelsheim and Searle (1983).

In other words, the matrix st' is converted into a column vector by writing one row after the other, followed by a transposition. This procedure extends to the vectorization of any matrix, according to

$$\operatorname{vec} A = (\text{first row of } A; \text{ second row of } A; \ldots; \text{last row of } A)' . \tag{5.6}$$

This is a vector representing the entries of the matrix A in lexicographic order; see Pukelsheim (1977), or the alternative treatment in Searle (1982, p. 332) who defines $\operatorname{vec} A$ to be the column vector obtained from stacking the columns of A one under the other. The vectorization operator also preserves the inner products between vectors and between matrices,

$$(\operatorname{vec} A)'(\operatorname{vec} B) = \operatorname{trace} A'B \quad \text{for all} \quad A, B \in \mathbb{R}^{k \times m} . \tag{5.7}$$

Vectorization, matrix products and Kronecker products go together in the formula

$$\operatorname{vec}(ABC) = (A \otimes C')(\operatorname{vec} B) , \tag{5.8}$$

provided dimensions match appropriately.

All these properties are proved best by first establishing them for Euclidean unit vectors e_i with i^{th} entry unity and zeros elsewhere, and Euclidean unit matrices

$$E_{ij} = e_i e_j'$$

with $(i,j)^{\text{th}}$ entry unity and zeros elsewhere. As a prototype proof we derive (5.8):

$$\begin{aligned} \operatorname{vec}(AE_{ij}C) &= (Ae_i) \otimes (C'e_j) && \text{by (5.5)} \\ &= (A \otimes C')(e_i \otimes e_j) && \text{by (5.4)} \\ &= (A \otimes C')(\operatorname{vec} E_{ij}) && \text{by (5.5)} . \end{aligned}$$

For an arbitrary matrix $B = \sum \sum b_{ij} E_{ij}$ this immediately extends to formula (5.8), by linearity; compare BenIsrael and Greville (1974, p. 42).

In second order moment matrices, the submatrix corresponding to fourth moments is conveniently displayed using the three matrices

$$I_m \otimes I_m = \sum \sum E_{ii} \otimes E_{jj} , \tag{5.9}$$

$$I_{m,m} = \sum \sum E_{ij} \otimes E_{ji} , \tag{5.10}$$

$$(\mathrm{vec}\, I_m)(\mathrm{vec}\, I_m)' = \sum \sum E_{ij} \otimes E_{ij} . \tag{5.11}$$

The matrix $I_{m,m}$ in (5.10) is called the vec permutation matrix, for the reason that

$$\begin{aligned} I_{m,m}(\mathrm{vec}\, E_{kl}) &= \sum_i \sum_j \{(e_i \otimes e_j)(e_j \otimes e_i)'\}(e_k \otimes e_l) && \text{by (5.10) and (5.5)} \\ &= e_l \otimes e_k && \text{by (5.4)} \\ &= \mathrm{vec}\, E_{lk} && \text{by (5.5)} . \end{aligned}$$

Linearity extends this to $I_{m,m}(\mathrm{vec}\, A) = \mathrm{vec}\, A'$ for all square matrices $A \in \mathbb{R}^{m \times m}$; see Henderson and Searle (1981, p. 279).

It is convenient to define the $m^2 \times m^2$ matrix

$$F_m = (I_m \otimes I_m) + I_{m,m} + (\mathrm{vec}\, I_m)(\mathrm{vec}\, I_m)' . \tag{5.12}$$

The matrix F_m will reflect the fourth moment structure in case of rotatability. It is nonnegative definite, as follows from

$$\begin{aligned} (\mathrm{vec}\, A)' F_m (\mathrm{vec}\, A) &= \mathrm{trace}(A'A) + \mathrm{trace}\,(A^2) + (\mathrm{trace}\, A)^2 \\ &= \tfrac{1}{2}\mathrm{trace}\,(A'+A)'(A'+A) + (\mathrm{trace}\, A)^2 \qquad (5.13) \\ &\geq 0 \end{aligned}$$

for all square matrices $A \in \mathbb{R}^{m \times m}$. In (5.13) equality holds if and only if $A' = -A$, whence F_m has rank $m(m+1)/2$.

With these tools we now turn to models for fitting a second order response surface.

6 Second Order Rotatability of Moment Matrices

We first list the pertinent quantities for an m-way second order polynomial fit model:

experimental conditions	$t \in \mathbb{R}^m$
experimental domain	$\mathscr{T} \subseteq \mathbb{R}^m$
regression vectors	$x = f(t) = \begin{pmatrix} 1 \\ t \\ t \otimes t \end{pmatrix} \in \mathbb{R}^k, \quad k = 1+m+m^2$
regression range	$\mathscr{X} = \{f(t) : t \in \mathscr{T}\} \subseteq \mathbb{R}^k$
transformation group	$\mathscr{Q} = \left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & R & 0 \\ 0 & 0 & R \otimes R \end{pmatrix} : R \in \mathrm{Orth}\,(m) \right\}.$

Here the regression range lies in $\mathbb{R}^k$, with $k = 1+m+m^2$. For brevity we write

$$Q_R = \begin{pmatrix} 1 & 0 & 0 \\ 0 & R & 0 \\ 0 & 0 & R \otimes R \end{pmatrix}$$

for the transformation of the regression range which is induced by the rotation R of the experimental domain.

A symmetric $k \times k$ matrix M is called (second order) rotatable when M is invariant under $\mathscr{Q}$. A design τ on $\mathscr{T}$ is called second order rotatable when its moment matrix $M(\tau) = \int_{\mathscr{T}} f(t) f(t)' \, d\tau$ is second order rotatable.

Again we first tackle the purely matrix oriented problem of characterizing second order rotatable matrices.

Theorem 6.1. Let M be a symmetric $k \times k$ matrix. Then the following three statements are equivalent:

(i) M is second order rotatable.
(ii) M is invariant under the finitely many matrices Q_R where R is any sign change matrix, any permutation matrix, or the orthodiagonal reflection (which, for $m = 2$, is replaced by the 45° rotation).
(iii) There exist scalars α, β, γ, δ_1, δ_2, $\delta_3 \in \mathbb{R}$ such that M has the form

$$M = \begin{pmatrix} \alpha & 0 & \gamma \operatorname{vec}' I_m \\ 0 & \beta I_m & 0 \\ \gamma \operatorname{vec} I_m & 0 & F(\delta_1, \delta_2, \delta_3) \end{pmatrix}, \tag{6.1}$$

where $F(\delta_1, \delta_2, \delta_3) = \delta_1 (I_m \otimes I_m) + \delta_2 I_{m,m} + \delta_3 (\operatorname{vec} I_m)(\operatorname{vec} I_m)'$.

Proof: Part (i) implies (ii), since (ii) comprises fewer transformations than (i). Part (iii) implies part (i), since by (5.8) and (5.4) we have

$$(R\otimes R)(\operatorname{vec} I_m) = \operatorname{vec}(RR') = \operatorname{vec} I_m \ ,$$
$$(R\otimes R)(I_m\otimes I_m)(R'\otimes R') = (RR')\otimes(RR') = I_m\otimes I_m \ ,$$
$$(R\otimes R)I_{m,m}(R'\otimes R') = I_{m,m} \ .$$

The latter property, invariance of the vec permutation matrix $I_{m,m}$, is seen best by postmultiplying by $\operatorname{vec} A$ with an arbitrary square matrix $A\in\mathbb{R}^{m\times m}$, to obtain

$$\begin{aligned}(R\otimes R)I_{m,m}(R'\otimes R')(\operatorname{vec} A) &= (R\otimes R)I_{m,m}(\operatorname{vec} R'AR)\\ &= (R\otimes R)\operatorname{vec}(R'A'R)\\ &= \operatorname{vec}(RR'A'RR')\\ &= \operatorname{vec} A'\\ &= I_{m,m}(\operatorname{vec} A)\ .\end{aligned}$$

Hence $F(\delta_1,\delta_2,\delta_3)$ is invariant under $R\otimes R$, and M is invariant under Q_R.

It remains to show that part (ii) implies part (iii). To this end write M in the partioned form

$$M = \begin{pmatrix} \alpha & a' & b' \\ a & B & C' \\ b & C & D \end{pmatrix} \ . \tag{6.2}$$

A transformation by Q_R transforms M into

$$Q_R M Q_R' = \begin{pmatrix} \alpha & a'R' & b'(R'\otimes R') \\ Ra & RBR' & RC'(R'\otimes R') \\ (R\otimes R)b & (R\otimes R)CR' & (R\otimes R)D(R'\otimes R') \end{pmatrix} \ . \tag{6.3}$$

I. If, in the invariance relation $Ra = a$, we insert the reflection $R = -I_m$, then $a = 0$.
II. The invariance property $RBR' = B$, for all sign changes and the orthodiagonal reflection, entails $B = \beta I_m$ for some scalar β, by (4.2).
III. The vector b has m^2 entries and hence may be written as $b = \operatorname{vec} A$ for some square matrix $A\in\mathbb{R}^{m\times m}$. The invariance property $(R\otimes R)b = b$ thus turns into $\operatorname{vec}(RAR') = \operatorname{vec} A$. Varying R over all sign changes and the orthodiagonal reflection, we see that $A = \gamma I_m$ for some scalar γ, again by (4.2). Hence $b = \gamma \operatorname{vec} I_m$.

IV. If in the invariance relation $(R\otimes R)CR'=C$ we insert the reflection $R=-I_m$, then we obtain $-C=C$, that is, $C=0$.
V. It remains to exploit the invariance property

$$D=(R\otimes R)D(R'\otimes R') \ ,$$

for the transformations R mentioned in part (ii). In terms of its entries

$$d_{ij,kl}=(e_i\otimes e_j)'D(e_k\otimes e_l) \ , \tag{6.4}$$

the matrix D takes the form

$$\begin{aligned} D&=\sum_{i,j,k,l}(e_i\otimes e_j)(e_i\otimes e_j)'D(e_k\otimes e_l)(e_k\otimes e_l)' \\ &=\sum_{i,j,k,l} d_{ij,kl}E_{ik}\otimes E_{jl} \ . \end{aligned} \tag{6.5}$$

Va. First we consider the sign changes $R=\Delta_\varepsilon$ with $\varepsilon=(\varepsilon_1,\ldots,\varepsilon_m)'$. This yields

$$\begin{aligned} d_{ij,kl}&=(e_i\otimes e_j)'D(e_k\otimes e_l) \\ &=(e_i\otimes e_j)'(R\otimes R)D(R'\otimes R')(e_k\otimes e_l)=\varepsilon_i\varepsilon_j\varepsilon_k\varepsilon_l d_{ij,kl} \ . \end{aligned} \tag{6.6}$$

Inserting $\varepsilon_i=\pm 1$ etc. we see that $d_{ij,kl}$ vanishes provided we have four distinct subscripts, or three distinct subscripts, or two distinct subscripts of which one has multiplicity 1 and the other one has multiplicity 3. Because of $\varepsilon_i^2\varepsilon_j^2=\varepsilon_i^4=1$ no reduction occurs for two distinct pairs of subscripts nor for a single subscript of multiplicity 4. This reduces the subscript ranges in (6.5) to $i=k\neq j=l$, $i=l\neq j=k$, $i=j\neq k=l$, and $i=j=k=l$,

$$D=\sum_{i\neq j}\{d_{ij,ij}E_{ii}\otimes E_{jj}+d_{ij,ji}E_{ij}\otimes E_{ji}+d_{ii,jj}E_{ij}\otimes E_{ij}\}+\sum_i d_{ii,ii}E_{ii}\otimes E_{ii} \ , \tag{6.7}$$

and leaves $3m(m-1)+m=3m^2-2m$ coefficients to be determined.
Vb. Now we let R run through the permutation group $\mathrm{Perm}(m)$. With $R=\sum e_je'_{\pi(j)}$ for some permutation π we have $R'e_i=e_{\pi(i)}$, and thus obtain

$$d_{ij,kl}=(e_i\otimes e_j)'(R\otimes R)D(R'\otimes R')(e_k\otimes e_l)=d_{\pi(i)\pi(j),\pi(k)\pi(l)} \ . \tag{6.8}$$

For the subscript ranges of the four terms in (6.7) this entails

$$\begin{aligned} d_{ij,ij} &= \text{const} = \delta_1\ , \quad \text{say}\ , \quad \text{for all} \quad i \neq j\ , \\ d_{ij,ji} &= \text{const} = \delta_2\ , \quad \text{say}\ , \quad \text{for all} \quad i \neq j\ , \\ d_{ii,jj} &= \text{const} = \delta_3\ , \quad \text{say}\ , \quad \text{for all} \quad i \neq j\ , \\ d_{ii,ii} &= \text{const} = \delta_4\ , \quad \text{say}\ , \quad \text{for all} \quad i\ . \end{aligned} \tag{6.9}$$

This reduces representation (6.7) of the matrix D to

$$D = \sum_{i \neq j} \{\delta_1 E_{ii} \otimes E_{jj} + \delta_2 E_{ij} \otimes E_{ji} + \delta_3 E_{ij} \otimes E_{ij}\} + \delta_4 \sum_i E_{ii} \otimes E_{ii} \tag{6.10}$$

which leaves us with 4 coefficients.

Vc. For our final argument we concentrate on the top left element $d_{11,11}$. From

$$(e_1 \otimes e_1)'(R \otimes R)(E_{ik} \otimes E_{jl})(R' \otimes R')(e_1 \otimes e_1) = r_{1i}r_{1j}r_{1k}r_{1l} \tag{6.11}$$

and (6.10) we get

$$d_{11,11} = (\delta_1 + \delta_2 + \delta_3) \sum_{i \neq j} r_{1i}^2 r_{1j}^2 + \delta_4 \sum_i r_{1i}^4\ . \tag{6.12}$$

The choice $R = I_m$ yields $d_{11,11} = \delta_4$. For $m > 2$ another choice is the orthodiagonal reflection $R = I_m - \frac{2}{m} 1_m 1_m'$. Comparing the resulting value for $d_{11,11}$ with δ_4 we obtain

$$0 = 8(m-1)(m-2)(\delta_1 + \delta_2 + \delta_3 - \delta_4)/m^3\ . \tag{6.13}$$

Because $m > 2$ it follows that $\delta_4 = \delta_1 + \delta_2 + \delta_3$. Now (6.10) turns into $D = F(\delta_1, \delta_2, \delta_3)$, and M takes the form claimed in (6.1). This completes the proof when the experimental conditions have $m > 2$ components.

Vd. If $m = 2$ we use the 45° rotation $R = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$. The top left hand entry $d_{11,11}$ equals δ_4 before the transformation, and $(\delta_1 + \delta_2 + \delta_3 + \delta_4)/2$ after the transformation. This again yields $\delta_4 = \delta_1 + \delta_2 + \delta_3$. □

The representation from Theorem 6.1(iii) takes a special form in case of moment matrices.

Theorem 6.2. Let M be a symmetric $k\times k$ matrix. Then M is a second order rotatable moment matrix on some experimental domain $\mathscr{T}\subseteq \mathbb{R}^m$ if and only if there exist scalars $\lambda_2\geq 0$ and $\lambda_4\geq \frac{m}{m+2}\lambda_2^2$ such that, with F_m from (5.12), M takes the form

$$M=\begin{pmatrix} 1 & 0 & \lambda_2 \operatorname{vec}' I_m \\ 0 & \lambda_2 I_m & 0 \\ \lambda_2 \operatorname{vec} I_m & 0 & \lambda_4 F_m \end{pmatrix} . \tag{6.14}$$

Proof: For the direct part assume M to be a rotatable matrix as well as the moment matrix of a design τ, say. Then, in (6.1), we must have $\gamma=\beta=\lambda_2$, as given by (4.4). Similarly, the coefficients for the right bottom block satisfy, for $i\neq j$,

$$\delta_1 = d_{ij,ij} = (e_i\otimes e_j)\mathrm{E}_\tau[(t\otimes t)(t\otimes t)'](e_i\otimes e_j) = \int_{\mathscr{T}} t_i^2 t_j^2 d\tau = \lambda_4 , \tag{6.15}$$

and $\delta_2=\delta_3=\lambda_4$ as well.

Nonnegative definiteness of the variance-covariance matrix of $t\otimes t$ under the design τ yields

$$\begin{aligned} V_\tau[t\otimes t] &= \mathrm{E}_\tau[(t\otimes t)(t\otimes t)'] - \mathrm{E}_\tau[t\otimes t]\mathrm{E}_\tau[t\otimes t]' \\ &= \lambda_4 F_m - \lambda_2^2 (\operatorname{vec} I_m)(\operatorname{vec} I_m)' . \end{aligned} \tag{6.16}$$

Hence the variance of $t't=(\operatorname{vec} I_m)'(t\otimes t)$ becomes

$$\begin{aligned} \mathrm{Var}_\tau[t't] &= \lambda_4(\operatorname{vec} I_m)'F_m(\operatorname{vec} I_m) - \lambda_2^2(\operatorname{vec} I_m)'(\operatorname{vec} I_m)(\operatorname{vec} I_m)'(\operatorname{vec} I_m) \\ &= \lambda_4(m+m+m^2) - \lambda_2^2 m^2 \\ &= m\{(m+2)\lambda_4 - m\lambda_2^2\} . \end{aligned} \tag{6.17}$$

It follows that $\lambda_4\geq \frac{m}{m+2}\lambda_2^2$, and the lower bound is attainable, for example, for the point arrangements mentioned in Box and Draper (1987, p. 489).

Conversely, let $\lambda_2 \geq 0$ and $\lambda_4 \geq \frac{m}{m+2}\lambda_2^2$ be given. Clearly the matrix M in (6.14) is rotatable. We need to find a design τ which has M for its moment matrix. To this end we define

$$\alpha = \frac{m}{m+2}\frac{\lambda_2^2}{\lambda_4} \in [0,1] \ , \tag{6.18}$$

and choose τ to be the probability measure assigning mass $1-\alpha$ to the origin and distributing the remaining mass α uniformly over the sphere of radius

$$r = \sqrt{(m+2)\frac{\lambda_4}{\lambda_2}} \ . \tag{6.19}$$

Clearly the probability measure τ is invariant under all rotations, whence its moment matrix $M(\tau)$ is rotatable. Furthermore, the moments $\lambda_2(\tau)$ and $\lambda_4(\tau)$ of τ satisfy

$$\begin{aligned} m\lambda_2(\tau) &= \sum_{i=1}^{m} \int t_i^2 d\tau = \int t' t \, d\tau = \alpha r^2 = m\lambda_2 \ ; \\ (m-1)\lambda_4(\tau) &= \sum_{i>1} \int t_i^2 t_1^2 d\tau = \int t' t t_1^2 d\tau - \int t_1^4 d\tau = r^2 \lambda_2(\tau) - 3\lambda_4(\tau) \\ &= (m+2)\lambda_4 - 3\lambda_4(\tau) \ . \end{aligned}$$

It follows that $\lambda_2(\tau) = \lambda_2$ and $\lambda_4(\tau) = \lambda_4$. Hence $M(\tau) = M$, and the proof is complete. □

Another convenient representation uses the following matrices corresponding to the design moments of orders 0, 2, 4, respectively:

$$V_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \ , \tag{6.20}$$

$$V_2 = \frac{1}{\sqrt{3m}} \begin{pmatrix} 0 & 0 & \operatorname{vec}' I_m \\ 0 & I_m & 0 \\ \operatorname{vec} I_m & 0 & 0 \end{pmatrix} \ , \tag{6.21}$$

$$V_4 = \frac{1}{\sqrt{3m(m+2)}} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & F_m \end{pmatrix} . \tag{6.22}$$

It is easy to check that the matrices V_0, V_2, V_4 form an orthonormal system in the space Sym (k) with inner product $\langle V_i, V_j \rangle = \text{trace } V_i V_j$.

Corollary 6.3. For a moment matrix $M = \sum_{t \in \text{supp } \tau} \tau(t) f(t) f(t)'$ with $r^2 = \max\{t't : t \in \text{supp } \tau\}$, the following three statements are equivalent:

(i) M is second order rotatable.

(ii) There exist scalars $\lambda_2 \geq 0$, $\lambda_4 \in \left[\frac{m}{m+2} \lambda_2^2, \frac{r^2}{m+2} \lambda_2 \right]$ such that $M = V_0 + \lambda_2 \sqrt{3m}\, V_2 + \lambda_4 \sqrt{3m(m+2)}\, V_4$.

(iii) $M = V_0 + (\text{trace } M V_2) V_2 + (\text{trace } M V_4) V_4$.

Proof: It only remains to establish the upper bound on λ_4. But, assuming that (i) holds, we obtain

$$(m-1)\lambda_4 = \sum_{i>1} \int t_i^2 t_1^2 d\tau = \int t' t t_1^2 d\tau - \int t_1^4 d\tau \leq r^2 \lambda_2 - 3\lambda_4 . \qquad \square$$

The second order rotatable moment matrix M in (6.14) has eigenvalues λ_2 with multiplicity m, and $2\lambda_4$ with multiplicity $\frac{1}{2}m(m+1)-1$. The associated projection matrices are, respectively,

$$P_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & I_m & 0 \\ 0 & 0 & 0 \end{pmatrix} , \quad P_4 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & G_m \end{pmatrix} , \tag{6.23}$$

where $G_m = \frac{1}{2}(I_m \otimes I_m + I_{m,m}) - \frac{1}{m}(\text{vec } I_m)(\text{vec } I_m)'$. This accounts for all but two of the $\frac{1}{2}(m+1)(m+2)$ degrees of freedom. In order to investigate the remaining two eigenvalues we observe that

$$M = STS' + \lambda_2 P_2 + 2\lambda_4 P_4 , \tag{6.24}$$

where

$$S = \begin{pmatrix} I & 0 \\ 0 & 0 \\ 0 & \operatorname{vec} I_m \end{pmatrix} , \quad T = \begin{pmatrix} 1 & \lambda_2 \\ \lambda_2 & \frac{m+2}{m}\lambda_4 \end{pmatrix} . \tag{6.25}$$

The nonvanishing eigenvalues of STS' are the same as those of the 2×2 matrix $S'ST$, and the latter has determinant

$$\det(S'ST) = (m+2)\lambda_4 - m\lambda_2^2 = d , \quad \text{say} . \tag{6.26}$$

Hence the rank of M can attain only three values,

$$\operatorname{rank} M = \begin{cases} 1 & \text{for} \quad \lambda_4 = \lambda_2 = 0 ; \\ \frac{1}{2}(m+1)(m+2) - 1 & \text{for} \quad \lambda_4 = \frac{m}{m+2}\lambda_2^2 > 0 ; \\ \frac{1}{2}(m+1)(m+2) & \text{for} \quad \lambda_4 > \frac{m}{m+2}\lambda_2^2 > 0 . \end{cases} \tag{6.27}$$

When $\lambda_4 > \frac{m}{m+2}\lambda_2^2 > 0$ the rank of M is maximal. From (6.24), the Moore-Penrose inverse of M then is

$$M^+ = S(S'S)^{-1}T^{-1}(S'S)^{-1}S' + \frac{1}{\lambda_2}P_2 + \frac{1}{2\lambda_4}P_4 . \tag{6.28}$$

With d given by (6.26), M^+ thus has form (6.1) with

$$\begin{aligned} \alpha &= \frac{(m+2)\lambda_4}{d} ; \\ \beta &= \frac{1}{\lambda_2} ; \\ \gamma &= -\frac{\lambda_2}{d} ; \\ \delta_1 &= \frac{1}{4\lambda_4} = \delta_2 ; \\ \delta_3 &= \frac{1}{md} - \frac{1}{2m\lambda_4} . \end{aligned} \tag{6.29}$$

The results of the present section also provide the foundation for the measures of rotatability discussed in Draper and Pukelsheim (1990). Given an arbitrary moment matrix M its rotatable part, $\bar{M}$ say, is the projection of M onto the subspace of rotatable matrices, namely

$$\bar{M} = V_0 + (\text{trace}\, M V_2)\, V_2 + (\text{trace}\, M V_4)\, V_4 \ . \tag{6.30}$$

Hence the rotatable part $\bar{M}$ can be interpreted as the fitted value obtained by regressing M on V_0, V_2, and V_4. Measures of rotatability that suggest themselves in this context are the squared distance

$$\delta^2 = \|M - \bar{M}\|^2 = \text{trace}\,(M - \bar{M})^2 \ , \tag{6.31}$$

or the R^2-type statistic

$$Q^* = \frac{\|\bar{M} - V_0\|^2}{\|M - V_0\|^2} \ . \tag{6.32}$$

Hence, for rotatability the following statements are equivalent:

(i) M is second order rotatable,
(ii) $M = \bar{M}$,
(iii) $\delta^2 = 0$,
(iv) $Q^* = 1$.

For the practical uses to which Q^* may be applied, see Draper and Pukelsheim (1990).

Alternatively the rotatable part $\bar{M}$ is obtained by averaging $Q_R M Q_R'$ over all rotations R,

$$\bar{M} = \int_{\text{Orth}\,(m)} Q_R M Q_R' dR \ , \tag{6.33}$$

where dR is Haar probability measure on the orthogonal group Orth (m). This fits into the majorization orderings of experimental designs discussed by Giovagnoli and Wynn (1981; 1985 a, b), Bondar (1983), Giovagnoli, Pukelsheim and Wynn (1987), and Pukelsheim (1987 a, b, c). From this point of view, if A is a matrix in the set

$$\text{conv}\,\{Q_R M Q_R' : R \in \text{Orth}\,(m)\} \ , \tag{6.34}$$

– the convex hull of the orbit of M under rotations – then A is called more rotatable than M. The rotatable part $\bar{M}$ is the barycenter of the set (6.34).

So far we have concentrated on second order moment matrices. Next we turn to their associated information surfaces.

7 Second Order Rotatability of Information Surfaces

Due to our choice of second order representation which involves $t \otimes t$, all our second order moment matrices are singular. Hence before we define information surfaces, we prove a result which allows us to replace regular inverses by generalized inverses.

Lemma 7.1. Let M be a moment matrix of rank $\frac{1}{2}(m+1)(m+2)$. Then the information surface

$$i_M(t) = \left\{ (1, t', t' \otimes t') M^- \begin{pmatrix} 1 \\ t \\ t \otimes t \end{pmatrix} \right\}^{-1}, \quad t \in \mathbb{R}^m , \tag{7.1}$$

is well defined, that is, the expression in braces is invariant to the choice of generalized inverse M^- of M, and is positive.

Proof: The idempotent and symmetric matrix

$$P_m = \begin{bmatrix} 1 & 0 & 0 \\ 0 & I_m & 0 \\ 0 & 0 & \frac{1}{2}(I_m \otimes I_m + I_{m,m}) \end{bmatrix}, \tag{7.2}$$

say, is the orthogonal projector onto its range (column space) $\mathscr{L} \subseteq \mathbb{R}^k$, say. The dimension of $\mathscr{L}$ is rank P_m = trace $P_m = \frac{1}{2}(m+1)(m+2)$. For every vector $t \in \mathbb{R}^m$ we have $P_m f(t) = f(t)$, as is seen by straightforward verification.

As a consequence, every moment matrix M has a range that is a subspace of $\mathscr{L}$. Our assumption that rank $M = \frac{1}{2}(m+1)(m+2)$ makes the range of M is equal to $\mathscr{L}$, entailing

$$MM^+ = P_m . \tag{7.3}$$

Hence given $t \in \mathbb{R}^m$, we define $a = M^+ f(t)$. Then we have $Ma = MM^+ f(t) = P_m f(t) = f(t)$, and therefore $f(t)'M^- f(t) = a'MM^- Ma = a'Ma$, independently of the specific choice of M^-.

Furthermore the quantity $f(t)'M^- f(t)$ is positive, since otherwise $a'Ma = 0$ leads to the contradiction

$$0 = Ma = f(t) \neq 0 \ . \qquad \square$$

We call (7.1) the information surface of M and say that it is rotatable when $i_M(Rt) = i_M(t)$ for all $R \in \mathrm{Orth}(m)$ and $t \in \mathbb{R}^m$. Rotatability of the information surface is implied by rotatability of moment matrices, as follows.

Theorem 7.2. Let M be a second order rotatable moment matrix (6.14), with $\lambda_2 > 0$ and $\lambda_4 > \frac{m}{m+2} \lambda_2^2$. Then the information surface i_M is rotatable. More precisely, with d from (6.26) the information surface is, for $t \in \mathbb{R}^m$,

$$i_M(t) = d / \left\{ (m+2)\lambda_4 + (m+2) \left(\frac{\lambda_4}{\lambda_2} - \lambda_2 \right) t't + \frac{1}{2} \left[m+1-(m-1)\frac{\lambda_2^2}{\lambda_4} \right] (t't)^2 \right\}. \tag{7.4}$$

Proof: A rotatable moment matrix M has a Moore-Penrose inverse M^+ of the form (6.1), with coefficients as given by (6.29). Inserting this representation into $i_M(t) = \{f(t)'M^+ f(t)\}^{-1}$ establishes (7.4) which clearly is rotatable. $\square$

When the second moments are scaled to unity, $\lambda_2 = 1$, formula (7.4) reduces to a result due to Box and Hunter (1957, p. 213, Eq. (48)).

Box and Hunter (1957, pp. 207–208) demand as a starting point that the variance surface

$$v_M(t) = \frac{1}{i_M(t)} = (1, t', t' \otimes t') M^- \begin{pmatrix} 1 \\ t \\ t \otimes t \end{pmatrix} \tag{7.5}$$

is rotatable, and then deduce that the moment matrix M is rotatable, too. Their brief argument suggests a trivial conclusion. However, there is more to prove than there seems at first glance.

At this point it becomes crucial whether we admit moment matrices M, only, or whether we endeavor to cover arbitrary nonnegative definit $k \times k$ matrices A. A second glance at the proof of Lemma 7.1 reveals that it makes sense to speak of the information surface i_A whenever the nonnegative definite $k \times k$ matrix A has the same range as the projector P_m in (7.2). However, the hypothesis is false that, for any such matrix A, rotatability if i_A implies rotatability of A.

The issue becomes more transparent in terms of the form

$$q_A(t) = (1, t', t' \otimes t')A \begin{pmatrix} 1 \\ t \\ t \otimes t \end{pmatrix} . \tag{7.6}$$

Since the rotatable symmetric matrices form a quadratic subspace by Lemma 2.2, rotatability of A forces rotatability of A^+. Hence our hypothesis would entail that rotatability of q_{A^+}, via rotatability of A, implies rotatability of A^+. Therefore a simpler version of our hypothesis is that rotatability of the form q_A implies rotatability of the matrix A.

The following counterexample is adapted from Koll (1980).

Counterexample 7.3. For $m = 2$ we have $k = 7$. Define the 7×7 matrix

$$A(\varepsilon) = \begin{pmatrix} 2 & 0 & 0 & -\frac{1}{2} & -\frac{\varepsilon}{2} & -\frac{\varepsilon}{2} & -\frac{1}{2} \\ 0 & 1 & \varepsilon & 0 & 0 & 0 & 0 \\ 0 & \varepsilon & 1 & 0 & 0 & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ -\frac{\varepsilon}{2} & 0 & 0 & 0 & \frac{1}{4} & \frac{1}{4} & 0 \\ -\frac{\varepsilon}{2} & 0 & 0 & 0 & \frac{1}{4} & \frac{1}{4} & 0 \\ -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{pmatrix} . \tag{7.7}$$

According to (6.29) the matrix $A(0)$ is the Moore-Penrose inverse of the moment matrix (6.14) with $\lambda_2 = \lambda_4 = 1$. Augmenting some of its entries by ε or $-\varepsilon/2$ produces $A(\varepsilon)$ as shown in (7.7). Straightforward evaluation yields, for $x = (x_1, \ldots, x_7)' \in \mathbb{R}^7$,

$$x'A(\varepsilon)x = \frac{1}{2}(2-\varepsilon)x_1^2 + \frac{1}{2}(x_1 - x_4)^2 + \frac{1}{2}(x_1 - x_7)^2 + \frac{\varepsilon}{2}(x_1 - x_5 - x_6)^2$$
$$+ (1-\varepsilon)(x_2^2 + x_3^2) + \varepsilon(x_2 + x_3)^2 + \frac{1}{2}\left(\frac{1}{2} - \varepsilon\right)(x_5 + x_6)^2 . \tag{7.8}$$

Hence if $\varepsilon \in [0, \frac{1}{2}]$ then $A(\varepsilon)$ is nonnegative definite, and since its nullspace is spanned by the vector $x \in \mathbb{R}^7$ with components

$$x_1 = x_2 = x_3 = x_4 = x_7 = 0 \ , \quad x_5 = -x_6 \ , \tag{7.9}$$

we see that $A(\varepsilon)$ has the same range as P_2 in (7.2).

All of the forms $q_{A(\varepsilon)}$ are rotatable, as follows from

$$q_{A(\varepsilon)}(t) = q_{A(0)}(t) + 2\varepsilon t_1 t_2 - 2\varepsilon t_1 t_2 = q_{A(0)}(t) \tag{7.10}$$

and the rotatability of the matrix $A(0)$. The latter is verified by inspection from (6.1). In the same way we see that the matrices $A(\varepsilon)$ with $\varepsilon \in (0, \frac{1}{2}]$ are not rotatable. □

The problem is resolved by restricting attention to moment matrices M, only. Since the moment matrix property of M does not tell us enough of the structure of M^+, we cannot present a unified treatment as in the first order discussion of Theorem 4.4. Instead we offer two separate derivations depending on whether we assume rotatability of i_M, or of q_M. The proof of the converse of Theorem 7.2 is based on a matrix lemma.

Lemma 7.4. Let A be a nonnegative definite $k \times k$ matrix. Then A is idempotent if and only if

$$\operatorname{trace} A = \operatorname{trace} A^+ = \operatorname{rank} A \ . \tag{7.11}$$

Proof: The direct part is folklore. For the converse part let $y_1, \ldots, y_r$ be the positive eigenvalues of A, repeated according to their multiplicities. Then (7.11) entails

$$\sum_{j=1}^{r} \left(y_j + \frac{1}{y_j} \right) = \operatorname{trace} A + \operatorname{trace} A^+ = 2 \operatorname{rank} A = 2r \ . \tag{7.12}$$

Since for $y > 0$ the minimum of $y + 1/y$ equals 2 and is attained only at $y = 1$, it follows from (7.12) that $y_1 = \ldots = y_r = 1$. Hence A is idempotent. □

Theorem 7.5. A moment matrix M of rank $(m+1)(m+2)/2$ is second order rotatable if and only if the information surface i_M or the variance surface v_M is rotatable.

Proof: The direct part is Theorem 7.2. For the converse part fix a rotation $R \in \mathrm{Orth}(m)$ and define

$$A = M^{1/2} Q_R' M^+ Q_R M^{1/2} \ . \tag{7.13}$$

There is a design τ which has moment matrix M. Rotatability of $v_M(t) = f(t)'M^+ f(t)$ entails

$$\begin{aligned} \operatorname{trace} A &= \operatorname{trace} M Q_R' M^+ Q_R \\ &= \sum_{i=1}^{l} \tau(t_i) f(t_i)' Q_R' M^+ Q_R f(t_i) = \sum_{i=1}^{l} \tau(t_i) f(t_i)' M^+ f(t_i) \\ &= \operatorname{trace} M M^+ = \operatorname{rank} P_m \ , \end{aligned} \tag{7.14}$$

by (7.3). Next we observe that the matrices Q_R and P_m commute, $Q_R P_m = P_m Q_R$. This is easily seen to be equivalent to $(R \otimes R) I_{m,m} = I_{m,m}(R \otimes R)$, and the latter follows by postmultiplying with $\operatorname{vec} A$ where A is an arbitrary square $m \times m$ matrix:

$$\begin{aligned} (R \otimes R) I_{m,m} \operatorname{vec} A &= (R \otimes R) \operatorname{vec}(A') = \operatorname{vec}(RA'R') \\ &= I_{m,m} \operatorname{vec}(RAR') = I_{m,m}(R \otimes R) \operatorname{vec} A \ . \end{aligned}$$

Therefore we obtain

$$Q_R M^{1/2} M^{+1/2} Q_R' = Q_R P_m Q_R' = P_m \ . \tag{7.15}$$

Hence the Moore-Penrose inverse of A is easily verified to be

$$A^+ = M^{+1/2} Q_R' M Q_R M^{+1/2} \ . \tag{7.16}$$

With $Q_R' = Q_{R'}$ the invariance of v_M yields, as in (7.14),

$$\operatorname{trace} A^+ = \operatorname{trace} M Q_R M^+ Q_R' = \operatorname{trace} M M^+ = \operatorname{rank} P_m \ . \tag{7.17}$$

From $Q_{R'} P_m = P_m Q_{R'}$ and nonsingularity of $Q_{R'}$ we get

$$\operatorname{rank} A = \operatorname{rank} M^{1/2} Q'_R M^{+1/2} = \operatorname{rank} M^{+1/2} M^{1/2} Q'_R M^{+1/2} M^{1/2}$$
$$= \operatorname{rank} P_m Q'_R P_m = \operatorname{rank} P_m \ . \tag{7.18}$$

Thus (7.14), (7.17), and (7.18) verify (7.11) whence A is idempotent.

Inserting (7.13) into $A^2 = A$ we get

$$M^{1/2} Q'_R M^+ Q_R M Q'_R M^+ Q_R M^{1/2} = M^{1/2} Q'_R M^+ Q_R M^{1/2} \ . \tag{7.19}$$

In view of (7.15) this simplifies by pre- and postmultiplication with $Q_R M^{+1/2}$ and $M^{+1/2} Q'_R$, respectively,

$$M^+ Q_R M Q'_R M^+ = M^+ \ . \tag{7.20}$$

Finally we pre- and postmultiply by M. Becaue of $MM^+ Q_R = P_m Q_R = Q_R P_m$ we obtain $Q_R M Q'_R = M$. Since $R \in \operatorname{Orth}(m)$ is arbitrary, M is rotatable. □

Our final result shows that rotatability of the form q_M implies rotatability of M provided M is a moment matrix.

Theorem 7.6. A moment matrix M is second order rotatable if and only if the form q_M of (7.6) is rotatable.

Proof: If M is rotatable then from (6.14) we get $q_M(t) = 1 + 3\lambda_2 t't + 3\lambda_4 (t't)^2$ which is clearly rotatable.

Conversely let q_M be rotatable, and fix a transformation Q_R. Then we have

$$\operatorname{trace} Q'_R M Q_R f(t) f(t)' = \operatorname{trace} M f(t) f(t)' \ , \quad \text{for all} \quad t \in \mathscr{T} . \tag{7.21}$$

This means that, relative to the inner product $\langle A, B \rangle = \operatorname{trace} AB$, the matrix $Q'_R M Q_R - M$ is orthogonal to all matrices $f(t)f(t)'$ with $t \in \mathscr{T}$. Denoting by $\mathscr{L}$ the subspace of symmetric matrices that is generated by $f(t)f(t)'$ with $t \in \mathscr{T}$, we get

$$Q'_R M Q_R - M \perp \mathscr{L} . \tag{7.22}$$

On the other hand there is a design τ which has M for its moment matrix, leading to

$$M \quad = \sum_{i=1}^{l} \tau(t_i) f(t_i) f(t_i)' \in \mathscr{L}\,,$$

$$Q_R' M Q_R = \sum_{i=1}^{l} \tau(t_i) f(R' t_i) f(R' t_i)' \in \mathscr{L}\,.$$

Hence $Q_R' M Q_R - M$ itself is a member of $\mathscr{L}$. Because of (7.22) then $Q_R' M Q_R = M$. Since $R \in \text{Orth}\,(m)$ is arbitrary, M is invariant. □

8 Second Order Rotatability of Experimental Designs

Can one actually obtain second order rotatable experimental designs? The answer is yes, and there are many published examples available. First of all, it is always possible to find measure designs (designs whose support does not necessarily consist of finitely many points, but of measure allocated to points or regions). For a discussion see, for example, Neumaier and Seidel (1990), or Kiefer (1985). Discrete point designs can be achieved by combining sets of points on concentric spheres. For a general discussion, see Seymour and Zaslavsky (1984). In practical experimental work, the emphasis is on designs with a relatively small number of points; for point sets, see Coxeter (1963, pp. 292–295). For specific designs see, for example, Box and Carter (1959), Box and Draper (1959), Box and Behnken (1960a, b), Box and Hunter (1957), Draper (1960), Draper and Herzberg (1968), Herzberg (1967), Huda (1981), Nigam (1977), Nigam and Das (1966), Nigam and Dey (1970), Raghavarao (1963), and Singh (1979). In general, any specified rotatable matrix can be achieved by a design consisting of a combination of symmetric sets of design points on concentric spheres.

9 Equivalence of Second Order Regression Functions

In models for a second order polynomial fit the regression function $f: \mathbb{R}^m \mapsto \mathbb{R}^k$ can be expressed in at least three distinct ways, using the Kronecker product notation, the Schläflian notation, or the Box-Hunter minimal set of monomials:

$$f_K(t) = \begin{pmatrix} 1 \\ t \\ t \otimes t \end{pmatrix}, \quad k = 1 + m + m^2$$

$$f_S(t) = \begin{pmatrix} 1 \\ t \\ t^{[2]} \end{pmatrix} , \quad k = \tfrac{1}{2}(m+1)(m+2)$$

$$f_{BH}(t) = (1, t_1, \ldots, t_m, t_1^2, \ldots, t_m^2, t_1 t_2, \ldots, t_{m-1} t_m)' , \quad k = \tfrac{1}{2}(m+1)(m+2) . \tag{9.1}$$

Let the corresponding moment matrices be $M_J = \sum_{t \in \text{supp}\, \tau} \tau(t) f_J(t) f_J(t)'$, for $J = K, S, BH$.

Lemma 9.1. We have rank $M_K = (m+1)(m+2)/2$ if and only if M_S is positive definite if and only if M_{BH} is positive definite. In this case the three corresponding variance surfaces all coincide:

$$f_K(t)' M_K^- f_K(t) = f_{BH}(t)' M_{BH}^{-1} f_{BH}(t) = f_S(t)' M_S^{-1} f_S(t) , \tag{9.2}$$

as do the three corresponding information surfaces.

Proof: The three different expressions for the regression functions in (9.1) lead to the following respective differences in the portions of (9.2) related to the intersection of cross-product columns and rows in the moment matrices:

$$(t_i t_j, t_i t_j) \begin{pmatrix} \lambda_4 & \lambda_4 \\ \lambda_4 & \lambda_4 \end{pmatrix}^- \begin{pmatrix} t_i t_j \\ t_i t_j \end{pmatrix} , \quad t_1 t_2 \sqrt{2} (2\lambda_4)^{-1} t_1 t_2 \sqrt{2} , \quad t_1 t_2 (\lambda_4)^{-1} t_1 t_2 .$$

These portions are orthogonal to all other pieces of (9.2) and the other pieces are identical for all representations. The second and third portions of (9.3) are obviously identical, and equal to $t_1^2 t_2^2/\lambda_4$. By Lemma 7.3, any generalized inverse can be used in the first portion. Two obvious choices are

$$\frac{1}{4\lambda_4} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \quad \text{and} \quad \frac{1}{\lambda_4} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} ,$$

both of which, again, give $t_1^2 t_2^2/\lambda_4$. □

The implication of Lemma 9.1 is that rotatability is the same whether defined in the Kronecker calculus using M_K, in the Schläflian calculus M_S, or in the Box-Hunter calculus M_{BH}. Another way of establishing Lemma 9.1 is furnished by reparametrization arguments as in Gaffke (1987), re-expressing f_K, f_S, and f_{BH} as linear transformations of one another.

As an aside we mention that the origin of the term "Schläflian matrix" remains unclear to us. Reference to Schläfli's work may originate with Muir (1911, pp. 52–53) who quotes Schläfli (1851) with a theorem on determinants that relate to polynomials of degree *r*. The term "Schläflian matrix" is used in Aitken (1949, p. 60), but not in Aitken (1951, p. 137f).

In matrix algebra other names prevail. Wedderburn (1934, p. 75) speaks of "induced or power matrices". Marcus and Minc (1964, p. 20) and Minc (1978, p. 87) use the term "induced matrix". The approach in those books does not readily reveal the properties that are needed in our statistical context; the closest we could find is the formula on the top of page 90 in Minc (1978).

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