8.5 Rotatability

- Recall: $\text{Var}[\hat{y}(\mathbf{x})] = \sigma^2 \mathbf{x}^{(m)'}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}^{(m)}$ is the prediction variance and $N\text{Var}[\hat{y}(\mathbf{x})]/\sigma^2 = N\mathbf{x}^{(m)'}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}^{(m)}$ is the scaled prediction variance.

- A design is **rotatable** if the prediction variance $\text{Var}[\hat{y}(\mathbf{x})]$ (or, equivalently, the scaled prediction variance $N\text{Var}[\hat{y}(\mathbf{x})]/\sigma^2$) is a function only of the distance ρ from the point $\mathbf{x} = (x_1, x_2, \ldots, x_k)$ to the center of the design (where $\rho^2 = \sum x_i^2$).

- Thus, with a rotatable design, the prediction variance $\text{Var}[\hat{y}(\mathbf{x})]$ is the same at all points $\mathbf{x}$ that are equidistant from the design center.

- In the earlier two-factor CCD example of deriving the prediction variance, we showed that the prediction variance was a function only of ρ. Therefore, that CCD is rotatable.

- Consequently, the prediction variance $\text{Var}[\hat{y}(\mathbf{x})]$ is constant on spheres centered at the design center. This constant variance property is appealing when the experimenter does not initially know where in the design space the most accurate and precise predictions are needed.

- Note that rotatability does not ensure stable or near-stable predictions throughout the design region. It only ensures the constant variance property on spheres.

- However, rotatability or near-rotatability is often easy to achieve without sacrificing other important design properties (such as allowing a test for lack of fit).

Design Moments

- Many properties of experimental designs are quantified by **design moments**. Given a model matrix

$$\mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{21} & \cdots & x_{k1} \\ 1 & x_{12} & x_{22} & \cdots & x_{k2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{1N} & x_{2N} & \cdots & x_{kN} \end{bmatrix}$$

The relevant design moments are:

$$[i] = \qquad\qquad\qquad i = 1, \ldots, k$$

$$[ii] = \qquad\qquad\qquad i = 1, \ldots, k$$

$$[ij] = \qquad\qquad\qquad i, j = 1, \ldots, k \quad i \neq j$$

Therefore, for a <u>first-order model</u> design

$$\frac{\mathbf{X}'\mathbf{X}}{N} = \begin{bmatrix} 1 & [1] & [2] & [3] & \cdots & [k] \\ & [11] & [12] & [13] & \cdots & [1k] \\ & & [22] & [23] & \cdots & [2k] \\ & & & \ddots & \cdots & \vdots \\ & & & & & [kk] \end{bmatrix}$$

- For an orthogonal first-order design

$$\frac{\mathbf{X}'\mathbf{X}}{N} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ & [11] & 0 & \cdots & 0 \\ & & [22] & \cdots & 0 \\ & & & \ddots & \vdots \\ & & & & [kk] \end{bmatrix}$$

Examples include the 2^k, 2^{k-p}, and Plackett-Burman designs.

- An **odd moment** is any moment for which at least one design variable has an odd power. For example, $[i], [ij], [ijj], [iii]$ are odd moments. All other moments are called **even moments**.

- For a <u>second-order model</u>, the model matrix will include columns for the intercept, first-order term, squared terms, and cross-product terms. Therefore, in addition to the first-order model moments, the relevant design moments for the second-order model are:

$[iii] =$ $\qquad$ $i = 1, \ldots, k$ $\qquad$ $[iiii] =$ $\qquad$ $i = 1, \ldots, k$

$[ijk] =$ $\qquad$ $i, j, k = 1, \ldots, k \;\; i, j, k$ not equal

$[ijj] =$ $\qquad$ $i, j = 1, \ldots, k \;\; i \neq j$

$[iijj] =$ $\qquad$ $i, j = 1, \ldots, k \;\; i \neq j$

$[iiij] =$ $\qquad$ $i, j = 1, \ldots, k \;\; i \neq j$

- For example, when $k = 3$

$$\mathbf{X} = \left[\begin{array}{c|ccc|ccc|ccc} 1 & x_{11} & x_{21} & x_{31} & x_{11}^2 & x_{21}^2 & x_{31}^2 & x_{11}x_{21} & x_{11}x_{31} & x_{21}x_{31} \\ 1 & x_{12} & x_{22} & x_{32} & x_{12}^2 & x_{22}^2 & x_{32}^2 & x_{12}x_{22} & x_{12}x_{32} & x_{22}x_{32} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{1N} & x_{2N} & x_{3N} & x_{1N}^2 & x_{2N}^2 & x_{3N}^2 & x_{1N}x_{2N} & x_{1N}x_{3N} & x_{2N}x_{3N} \end{array}\right]$$

and

$$\frac{\mathbf{X}'\mathbf{X}}{N} = \left[\begin{array}{c|ccc|ccc|ccc} 1 & [1] & [2] & [3] & [11] & [22] & [33] & [12] & [13] & [23] \\ \cline{2-10} & [11] & [12] & [13] & [111] & [122] & [133] & [112] & [113] & [123] \\ & & [22] & [23] & [112] & [222] & [233] & [122] & [123] & [223] \\ & & & [33] & [113] & [223] & [333] & [123] & [133] & [233] \\ \cline{2-10} & & & & [1111] & [1122] & [1133] & [1112] & [1113] & [1123] \\ & & & & & [2222] & [2233] & [1222] & [1223] & [2223] \\ & & & & & & [3333] & [1233] & [1333] & [2333] \\ \cline{2-10} & & & & & & & [1122] & [1123] & [1223] \\ & & & & & & & & [1133] & [1233] \\ & & & & & & & & & [2233] \end{array}\right]$$

Moment Matrix Conditions for Rotatability

- A first-order design is rotatable if and only if all odd moments are zero and all even second order moments are equal. That is, $[i] = 0$, $[ij] = 0$, and $[ii] = \lambda_2$. The quantity λ_2 is determined by the scaling of the design variables.

- For example, a 2^{k-p} design of at least resolution III which uses a ± 1 coding is rotatable with $[i] = 0$, $[ij] = 0$, and $[ii] = \lambda_2 = 1.0$.

The necessary form of $\mathbf{X}'\mathbf{X}/N$ of a rotatable k-variable second-order design:

$$\frac{\mathbf{X}'\mathbf{X}}{N} = \left[\begin{array}{cc|c|c} 1 & \mathbf{0}_{1\times k} & \mathbf{0}_{1\times k*} & \lambda_2 \mathbf{J}'_k \\ \mathbf{0}_{k\times 1} & \lambda_2 \mathbf{I}_k & \mathbf{0}_{k\times k*} & \mathbf{0}_{k\times k} \\ \hline \mathbf{0}_{k*\times 1} & \mathbf{0}_{k*\times k} & \lambda_4 \mathbf{I}_{k*} & \mathbf{0}_{k*\times k} \\ \hline \lambda_2 \mathbf{J}_k & \mathbf{0}_{k\times k} & \mathbf{0}_{k\times k*} & \lambda_4(2\mathbf{I}_k + \mathbf{J}'_k\mathbf{J}_k) \end{array}\right]$$

- Thus, a second-order design is rotatable if and only if

  1. All odd moments are zero.
  2. $[ii] =$
  3. $[iiii] =$
  4. $[iijj] =$

  where the quantities λ_2 and λ_4 are determined by the scaling of the design variables.

- Note: Conditions (3) and (4) can be combined into a single condition $[iiii]/[iijj] = 3$ for $i \neq j$. This is what is stated in the Myers, Montgomery, and Anderson-Cook text.

8.5.1 Rotatability and the CCD

- For any central composite design (CCD), all odd moments are zero due to the orthogonality among the x_i, x_ix_j, and x_i^2 columns. Nonorthoganality occurs (i) between the column of ones and the x_i^2 columns and (ii) between the x_i^2 and x_j^2 columns ($i \neq j$).

- Therefore, to make a rotatable CCD, we must find the appropriate choice of α so that $\mathbf{X}'\mathbf{X}/N$ satisfies the rotatability criterion $[iiii]/[iijj] = 3$ where $[iiii]$ and $[iijj]$ are the moments corresponding to the products among the x_i^2 columns.

- For any CCD, $[iiii] = F + 2\alpha^4$ and $[iijj] = F$ where F is the number of factorial points. Thus, for rotatability,

$$\frac{[iiii]}{[iijj]} = \frac{F + 2\alpha^4}{F} = 3$$

  Solving for α yields $\alpha = \sqrt[4]{F}$. *For a CCD to be rotatable,* $\alpha = \sqrt[4]{F}$.

- If $\alpha = \sqrt{k}$ is used, then at least one center point is required for the CCD. Otherwise, $(\mathbf{X}'\mathbf{X})^{-1}$ does not exist, and hence, $\text{Var}[\widehat{y}(\mathbf{x})]$, does not exist.

- If the design region is spherical, the best CCD with $k = 3$ based on $\text{Var}[\widehat{y}(\mathbf{x})]$ throughout the spherical region uses $\alpha = \sqrt{3}$ (with 3-5 center points). This design is near-rotatable.

ROTATABLE 2-FACTOR CCD

$$
X = \begin{array}{c}
\begin{array}{cccccc} & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \end{array} \\
\begin{bmatrix}
1 & -1 & -1 & 1 & 1 & 1 \\
1 & -1 & 1 & 1 & 1 & 1 \\
1 & 1 & -1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 \\
1 & \sqrt{2} & 0 & 2 & 0 & 0 \\
1 & -\sqrt{2} & 0 & 2 & 0 & 0 \\
1 & 0 & \sqrt{2} & 0 & 2 & 0 \\
1 & 0 & -\sqrt{2} & 0 & 2 & 0 \\
1 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\end{array}
\Rightarrow X'X = \left[\begin{array}{ccc|cc|c}
9 & 0 & 0 & 8 & 8 & 0 \\
0 & 8 & 0 & 0 & 0 & 0 \\
0 & 0 & 8 & 0 & 0 & 0 \\
\hline
8 & 0 & 0 & 12 & 4 & 0 \\
8 & 0 & 0 & 4 & 12 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & 4
\end{array}\right]
$$

LET $\lambda_2 = 8/9 \quad \lambda_4 = 4/9$

THEN

$$
\frac{X'X}{N} = \frac{X'X}{9} = \left[\begin{array}{ccc|cc|c}
1 & 0 & 0 & 8/9 & 8/9 & 0 \\
0 & 8/9 & 0 & 0 & 0 & 0 \\
0 & 0 & 8/9 & 0 & 0 & 0 \\
\hline
8/9 & 0 & 0 & 4/9(3) & 4/9 & 0 \\
8/9 & 0 & 0 & 4/9 & 4/9(3) & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & 4/9
\end{array}\right]
= \left[\begin{array}{cc|c|c}
1 & \emptyset & \lambda_2 \quad \lambda_2 & \emptyset \\
\emptyset & \lambda_2 I_2 & \emptyset \quad \emptyset & \emptyset \\
\hline
\begin{matrix}\lambda_2 \\ \lambda_2\end{matrix} & \begin{matrix}\emptyset \\ \emptyset\end{matrix} & \lambda_4(2I_2 + J_2J_2') & \emptyset \\
\hline
0 & \emptyset & \emptyset & \lambda_4 I
\end{array}\right]
$$

$\Rightarrow$ THE DESIGN IS ROTATABLE

NOTE: $\dfrac{F + 2\alpha^4}{F} = \dfrac{4 + 2(\sqrt{2})^4}{4} = \dfrac{4+8}{4} = 3$

$$\alpha = \sqrt[4]{F} = \sqrt[4]{4} = \sqrt{2}$$

ROTATABILITY AND THE FOUR FACTOR BBD (NO BLOCKS)

$$
X = \begin{array}{c}
\begin{array}{cccccccccccccccc}
 & x_1 & x_2 & x_3 & x_4 & x_1x_2 & x_1x_3 & x_1x_4 & x_2x_3 & x_2x_4 & x_3x_4 & x_1^2 & x_2^2 & x_3^2 & x_4^2
\end{array} \\
\left[\begin{array}{c|cccc|cccccc|cccc}
1 & \pm1 & \pm1 & 0 & 0 & \pm1 & 0 & 0 & 0 & 0 & 0 & J_4 & J_4 & 0 & 0 \\
1 & 0 & 0 & \pm1 & \pm1 & 0 & 0 & 0 & 0 & 0 & \pm1 & 0 & 0 & J_4 & J_4 \\
1 & \pm1 & 0 & 0 & \pm1 & 0 & 0 & \pm1 & 0 & 0 & 0 & J_4 & 0 & J_4 & J_4 \\
1 & 0 & \pm1 & \pm1 & 0 & 0 & 0 & 0 & \pm1 & 0 & 0 & 0 & J_4 & J_4 & 0 \\
1 & \pm1 & 0 & \pm1 & 0 & 0 & \pm1 & 0 & 0 & 0 & 0 & J_4 & 0 & J_4 & 0 \\
1 & 0 & \pm1 & 0 & \pm1 & 0 & 0 & 0 & 0 & \pm1 & 0 & 0 & J_4 & 0 & J_4 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}\right]
\end{array}
\begin{array}{c}
\text{PTS} \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ 4 \\ \left.\begin{array}{c} \\ \\ \\ \end{array}\right\} 3 \\ \hline 27
\end{array}
$$

WHERE $0 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}_{4\times1}$ AND $J_4 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$ IN $X_{(27\times12)}$

$$
\frac{X'X}{N} = \left[\begin{array}{c|cccc|cccccc|cccc}
27 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 12 & 12 & 12 & 12 \\ \hline
0 & 12 & 0 & 0 & 0 & & & & & & & & & & \\
0 & 0 & 12 & 0 & 0 & & & 0_{4\times6} & & & & & 0_{4\times4} & & \\
0 & 0 & 0 & 12 & 0 & & & & & & & & & & \\
0 & 0 & 0 & 0 & 12 & & & & & & & & & & \\ \hline
0 & & & & & 4 & 0 & 0 & 0 & 0 & 0 & & & & \\
0 & & & & & 0 & 4 & 0 & 0 & 0 & 0 & & & & \\
0 & & 0_{6\times4} & & & 0 & 0 & 4 & 0 & 0 & 0 & & 0_{6\times4} & & \\
0 & & & & & 0 & 0 & 0 & 4 & 0 & 0 & & & & \\
0 & & & & & 0 & 0 & 0 & 0 & 4 & 0 & & & & \\
0 & & & & & 0 & 0 & 0 & 0 & 0 & 4 & & & & \\ \hline
12 & & & & & & & & & & & 12 & 4 & 4 & 4 \\
12 & & 0_{4\times4} & & & & & 0_{4\times6} & & & & 4 & 12 & 4 & 4 \\
12 & & & & & & & & & & & 4 & 4 & 12 & 4 \\
12 & & & & & & & & & & & 4 & 4 & 4 & 12
\end{array}\right] \Big/ 27
$$

ALL ODD MOMENTS ARE 0, AND

$$\lambda_2 = \frac{12}{27} \qquad \lambda_4 = \frac{4}{27} \quad \Rightarrow \lambda_4\left(2I_4 + J_4J_4'\right)$$

$$= \frac{4}{27}\begin{bmatrix} 3 & 1 & 1 & 1 \\ 1 & 3 & 1 & 1 \\ 1 & 1 & 3 & 1 \\ 1 & 1 & 1 & 3 \end{bmatrix} = \begin{bmatrix} 12 & 4 & 4 & 4 \\ 4 & 12 & 4 & 4 \\ 4 & 4 & 12 & 4 \\ 4 & 4 & 4 & 12 \end{bmatrix} \Big/ 27$$

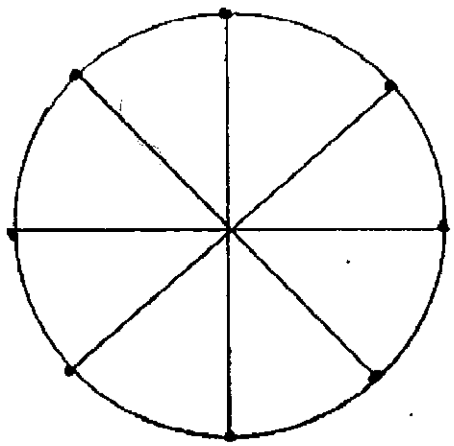
8.5.2 Cuboidal vs Spherical Design Regions

- It is common for the experimenter to specify a minimum and maximum setting on each of the k design variables. In such cases, the experimental region is a k-dimensional hypercube.
- The CCD with $\alpha = 1$ corresponds to this situation and is called a **face-centered cube design**. It is called a face-centered cube design because the axial points occur at the center of the faces of the k-dimensional cube (rather than extend the axial points beyond the faces of the cube ($\alpha > 1$), as in a spherical region).
- The face-centered cube CCD possesses several desirable features:
  - The factorial and axial points are on the boundary of the design region (on the cube).
  - The design is symmetric in the experimental region and as a result 'covers' or 'fills in' the design region is a symmetric fashion.
- The face-centered cube CCD is not rotatable. However, rotatability or near-rotatability is not an important design property in a cuboidal design region. Rotatability is a property to be considered for spherical design regions.
- The face-centered cube CCD does not require center points because $(\mathbf{X}'\mathbf{X})^{-1}$ exists. $\mathrm{Var}[\widehat{y}(\mathbf{x})]$ is relatively insensitive to the number of center points. Center points are included for testing for lack of fit.
- Whether or not a design should contain axial points with $\alpha > 1$ should depend on whether or not the axial values are scientifically permissible or feasible.

8.6 Equiradial Designs

- An **equiradial set** of points consists of a set of points such that all points are equidistant from the origin.
- An **equiradial design** is a design which consists of two or more equiradial sets of points.
- Consider a single equiradial set of points of distance ρ from the origin. That is, $\sum_{i=1}^{k} x_i^2 = \rho^2$. Then the column of ones and the columns corresponding to the $x_1^2, \ldots, x_k^2$ in the design matrix are linearly dependent which results in a singular $\mathbf{X}'\mathbf{X}$ matrix. Specifically, for each row of $\mathbf{X}$, the sum of the x_i^2 columns $= \rho^2$. Thus, the intercept column of ones $= (1/\rho^2)\sum_{i=1}^{k} x_i^2$ making $\mathbf{X}$ less than full column rank (and $\mathbf{X}'\mathbf{X}$ singular).
- Therefore, a single equiradial set cannot provide a design for fitting a second-order model.
- Inclusion of one or more center points to any single equiradial set of points results in a nonsingular $\mathbf{X}'\mathbf{X}$. Therefore, a second-order model can be fit by a single equiradial set plus center points.
- Examples of second-order equiradial designs that are rotatable include those designs whose equiradial sets of points are characterized as being equally spaced points on a circle ($k = 2$), a sphere ($k = 3$), or a hypersphere ($k \geq 4$). These points will form the vertices of a regular polygon, polyhedron, or polytope.
- Rotatable CCDs are equiradial designs.

8 POINT EQUIRADIAL DESIGN EXAMPLE



$$X = \begin{array}{c} \begin{array}{cccccc} & x_1 & x_2 & x_1x_2 & x_1^2 & x_2^2 \end{array} \\ \begin{bmatrix} 1 & 1 & 0 & 0 & 1 & 0 \\ 1 & -1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & -1 & 0 & 0 & 1 \\ 1 & \sqrt{2}/2 & \sqrt{2}/2 & 1/2 & 1/2 & 1/2 \\ 1 & \sqrt{2}/2 & -\sqrt{2}/2 & -1/2 & 1/2 & 1/2 \\ 1 & -\sqrt{2}/2 & \sqrt{2}/2 & -1/2 & 1/2 & 1/2 \\ 1 & -\sqrt{2}/2 & -\sqrt{2}/2 & 1/2 & 1/2 & 1/2 \end{bmatrix} \end{array}$$

$$X'X = \begin{bmatrix} 8 & 0 & 0 & 0 & 4 & 4 \\ 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 4 & 0 & 0 & 0 & 3 & 1 \\ 4 & 0 & 0 & 0 & 1 & 3 \end{bmatrix}$$

NOTE: COLUMN 1 (INTERCEPT) = SUM OF COLUMNS 5 AND 6

$\Rightarrow (X'X)^{-1}$ DOES NOT EXIST

$\Rightarrow$ WE CANNOT FIT THE SECOND-ORDER MODEL

IF WE ADD 1 CENTERPOINT $[1\ 0\ 0\ 0\ 0\ 0]$ TO X WE HAVE

$$X^* = \begin{bmatrix} X \\ \hline 1\ 0\ 0\ 0\ 0\ 0 \end{bmatrix}.$$ THEN

$$X^{*\prime}X^* = \begin{bmatrix} 9 & 0 & 0 & 0 & 4 & 4 \\ 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 4 & 0 & 0 & 0 & 3 & 1 \\ 4 & 0 & 0 & 0 & 1 & 3 \end{bmatrix}$$

NOTE: $(X^{*\prime}X^*)^{-1}$ EXISTS

$\Rightarrow$ WE CAN FIT THE SECOND-ORDER MODEL