Central Composite Designs - Axial Points

→ estimate → $[x^{*T}(X^TX)^{-1}x^*]\,\hat{\sigma}^2$

- A design is called **rotatable** if $Var(\hat{y}(\mathbf{x}))$ depends only on

  RSM interested in $\hat{y}$

  (1, $x_1, \cdots, x_k$, x_ix_j's, $x_1^2, \cdots, x_k^2$)

$$\|\mathbf{x}\| = (x_1^2 + \cdots + x_k^2)^{1/2},$$

  that is, if the accuracy of prediction of the response is the same on a sphere around the center of the design.

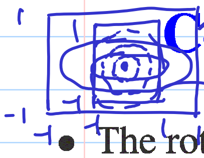
- For a central composite design whose factorial portion is a 2^{k-p} design of resolution V, it can be shown that rotatability is guaranteed by choosing

  It causes orthogonality between LME ↔ LME, 2fi ↔ 2fi, LME ↔ 2fi,

$$\alpha = \sqrt[4]{n_f}. \qquad (5)$$

  # of cube pts.

- Eqn. (5) serves as a useful guide even when the factorial portion does not have resolution V.



Central Composite Designs - Axial Points

- The rotatability criterion should not, however, be strictly followed.
  - Its definition depends on how the x_i variables are coded. This lack of invariance with respect to the coding scheme makes it less attractive as a theoretical criterion.
  - Because rotatability often requires that the factorial portion has resolution V, use of a smaller composite design whose factorial portion has a lower resolution has not been popular. However, some of the central composite designs whose factorial portions have resolution V or higher have excessive degrees of freedom.

    MA 2^{6-2} have resolution IV

    * For $k = 6$, the smallest design that satisfies the rotatability requirement is a 2^{6-1}_{VI} design for the factorial portion. → run size: $2^{6-1} + 2\times 6 + 1 = 45$
      * The total run size of the central composite design is 45, which has 17 additional degrees of freedom over the minimal run size.

- **Near rotatability** will be a more reasonable and practical criterion.

Central Composite Designs - Center Points

- The center points can $\widehat{Var}(\hat{y}_x) = [x^{*T}(X^TX)^{-1}x^*] \cdot \hat{\sigma}^2$
  - provide information on the pure error and → replicates
  - help stabilize the variance of the predicted response $\hat{y}$.
- For $\alpha = \sqrt{k}$, at least one center point is required for the estimability of the parameters in the second-order model. (Why?) Otherwise the variance of $\hat{y}(\mathbf{x})$ becomes infinite.
- To stabilize the prediction variance, the rule of thumb suggests
  - 3 to 5 runs at the center point when $\alpha \approx \sqrt{k}$, cube pts
  - 1 or 2 runs at the center point when $\alpha \approx 1$ axial pts
  - 2 to 4 runs should be considered between these two extremes
- To estimate the error variance, more than 4 or 5 runs may be required.

QME sum of those columns

v Reading: textbook, 10.7

Box-Behnken Designs

- A family of three-level second-order designs
- Combining two-level factorial designs with balanced (or partially balanced) incomplete block designs in a particular manner for $k=3,4,5$. for $k=6$.
- Illustration: A BIBD with 3 treatments and 3 blocks of size 2

1 within 1 between block comparison.

Block	Treatment 1	Treatment 2	Treatment 3
1	×	×	
2	×		×
3		×	×

	Factors x_1	x_2	x_3
1	±1	±1	0
2	±1	0	±1
3	0	±1	±1
4	0	0	0

2fi QME x_1x_2 x_1^2 x_2^2 x_3^2

*run size comparison

$k=$ 3, $12+n_c$ | $12+n_c$

4, $6\times2^2+n_c$ | $24+n_c$

5, $10\times2^2+n_c$ | $40+n_c$

- run size $= 3 \times 2^2 + n_c$
- Why is it a second-order design?

LME, 2fi, QME — why estimable? why not aliased?

Box-Behnken Designs - Some Properties

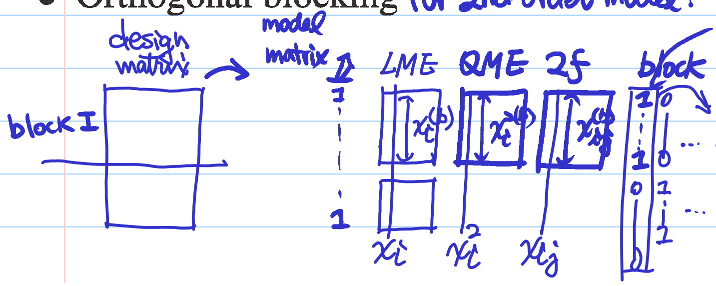
- Only require three levels of each factor (c.f., CCDs require 5 levels when $\alpha \neq 1$)
- All the design points (except the center) have length two, i.e., they all lie on the same sphere ← Spherical design.
  - These designs are particularly usited for spherical regions
  - Because of the spherical property, there should be at least three to five runs at the center point.
- The design for $k = 4$ is rotatable and the other designs are nearly rotatable
- Orthogonal blocking for 2nd-order model.

① The design pts in a block form a first order orthogonal design

$\sum x_i^{(b)} = 0.$

$0 = x_i^T(\mathbb{1}^{(b)} - \bar{b}\mathbb{1}) = x_i^T\mathbb{1}^{(b)} - \bar{b}\, x_i^T\mathbb{1}.$

$0 = x_{ij}^T(\mathbb{1}^{(b)} - \bar{b}\mathbb{1}) = x_{ij}^T\mathbb{1}^{(b)} - \bar{b}\, x_{ij}^T\mathbb{1}$, $\sum x_{ij}^{(b)} = 0$



$\mathbb{1}^{(b)} - \bar{b}\mathbb{1}$

$0 = x_i^{2T}(\mathbb{1}^{(b)} - \bar{b}\mathbb{1}) = x_i^{2T}\mathbb{1}^{(b)} - \bar{b}\, x_i^{2T}\mathbb{1} \Rightarrow x_i^{2T}\mathbb{1}^{(b)} = \bar{b}\, x_i^{2T}\mathbb{1}$

② ⇒ for each factor, sum of squares contribution from each block is proportional to run size.

Box-Behnken Designs - Orthogonal Blocking

- For $k = 4, 5$, the designs can be arranged in orthogonal blocks
- $k = 4$, can be arranged in 3 blocks

BIBD
1 2 3 4
6 block

$$
\begin{array}{c|c}
 & x_1^2 \\
\begin{array}{c} 4 \\ 4 \\ 1 \\ \\ \\ \\ \\ \\ \\ \end{array}
\left[\begin{array}{cccc}
\pm1 & \pm1 & 0 & 0 \\
0 & 0 & \pm1 & \pm1 \\
0 & 0 & 0 & 0 \\
\hline
\pm1 & 0 & 0 & \pm1 \\
0 & \pm1 & \pm1 & 0 \\
0 & 0 & 0 & 0 \\
\hline
\pm1 & 0 & \pm1 & 0 \\
0 & \pm1 & 0 & \pm1 \\
0 & 0 & 0 & 0
\end{array}\right]
&
\begin{array}{c} 1 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{array}
\end{array}
$$

LME → ok

2fi → $x_1 x_2^{(b)}$ ok. $x_1 x_3^{(b)} = 2$ ok.

QME → ok.

- $k = 5$, can be arranged in 2 blocks

BIBD
1 2 3 4 5

$$
\left[\begin{array}{ccccc}
\pm1 & \pm1 & 0 & 0 & 0 \\
0 & 0 & \pm1 & \pm1 & 0 \\
0 & \pm1 & 0 & 0 & \pm1 \\
\pm1 & 0 & \pm1 & 0 & 0 \\
0 & 0 & 0 & \pm1 & \pm1 \\
0 & 0 & 0 & 0 & 0 \\
\hline
0 & \pm1 & \pm1 & 0 & 0 \\
\pm1 & 0 & 0 & \pm1 & 0 \\
0 & 0 & \pm1 & 0 & \pm1 \\
\pm1 & 0 & 0 & 0 & \pm1 \\
0 & \pm1 & 0 & \pm1 & 0 \\
0 & 0 & 0 & 0 & 0
\end{array}\right]
$$

Check (exercise)

LME

2fi

QME

Uniform Shell Designs

- The designs have k^2+k+1 points, which consist of
  - k^2+k points uniformly spaced on the k-dimensional sphere, and
  - one center point
- For $k=2$, it can be described by a regular hexagon plus the center point

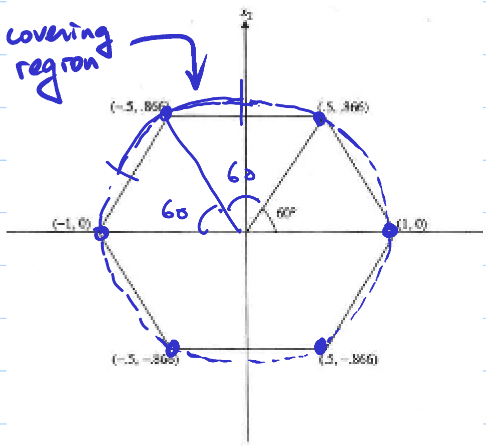
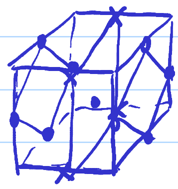


Figure 10: Uniform shell design, k=2



- For $k=3$, it is identical to the Box-Behnken design

Uniform Shell Designs

- Uniformity property
  - Covering region of a design point: collection of points on the sphere that are closer to this design point than to the other design points.
  - Uniformity ensures that the covering region of each design point has the *same* spherical area.
- Run size comparison

k	k^2+k+1	$(k+1)(k+2)/2$
2	7	6
3	13	10
4	21	15
5	31	21

  - For $k>5$, its run size is much larger than $(k+1)(k+2)/2$
- For $2 \le k \le 5$, the designs are given in Table 10C.1 (textbook)
  - These designs can be rotated ~~with~~ without affecting the uniformity property. However, rotation will likely increase the number of levels.
  - In the table, the design points minimize the number of the levels
- A disadvantage of spherical designs (CCD $\alpha=\sqrt{k}$, BBD, USD.): lack of coverage of the region between the origin and the spherical shell ← remedy: choose 2 concentric spherical shells of distinctly different radii.

v **Reading**: textbook, 10.8

RPD – location model, dispersion model

Analysis Strategies for Multiple Responses

e.g.

- Multiple response analysis starts with building a regression fitted model for each response separately
- Some analysis strategies
  study each response separately & find compromise solution.
  - Overlaid contour plots (if there are few responses and only two or three important input variables.)
  - Constrained optimization (if, among the responses, one is of primary importance) — max/min $\hat{y}_1$, subject to $a < \hat{y}_2 < b$, $c < \hat{y}_3$
  - Desirability function (if the goal is to find an optimal balance among several response characteristics)
- The desirability function approach transform each predicted response $\hat{y}_i$ to a desirability value d_i, where $0 \le d_i \le 1$
  - The value of the **desirability function** d increases as the "desirability" of the corresponding response increases.