Advanced Experimental Design
Homework 6

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Problem: Write down the design matrix for a two-variable experimental layout which displays seven points equally spaced on a circle and contains a sufficient number of center points to be approximately a uniform precision design.

Is this design rotatable as a second order model? Orthogonal as a second order model?

Solution: For a second order model the criteria for rotatability are, under the assumption that $\sum_{u=1}^{n} x_{iu} = 0$,

$$\sum_{u=1}^{n} x_{iu} x_{ju} = 0, \qquad i \neq j = 1, \ldots, n \tag{1}$$

$$\sum_{u=1}^{n} x_{iu} x_{ju} x_{ku} = 0, \qquad i, j, k = 1, \ldots, n \tag{2}$$

$$\sum_{u=1}^{n} {x_{iu}}^4 = 3 \sum_{u=1}^{n} {x_{iu}}^2 {x_{ju}}^2, \qquad i \neq j \tag{3}$$

Now more generally, let there be n points equally spaced on a circle, and N total points (including $N - n$ center points).

Without loss of generality we may assume that the radius of the circle is 1, and that one of these points is $(0, 1)$.

Let $\theta = \frac{2\pi}{n}$ and $\alpha = \frac{n}{N}$. Our design matrix is then

$$X = \begin{array}{c} \\ 0 \\ \vdots \\ i \\ \vdots \\ n \\ \vdots \\ N-1 \end{array} \begin{array}{c} \begin{array}{cccccc} x_0 & x_1 & x_2 & x_1x_2 & {x_1}^2 - \frac{\alpha}{2} & {x_2}^2 - \frac{\alpha}{2} \end{array} \\ \begin{pmatrix} 1 & \cos(0\cdot\theta) & \sin(0\cdot\theta) & \cos(0\cdot\theta)\sin(0\cdot\theta) & \cos(0\cdot\theta)^2 - \frac{\alpha}{2} & \sin(0\cdot\theta)^2 - \frac{\alpha}{2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \cos(i\cdot\theta) & \sin(i\cdot\theta) & \cos(i\cdot\theta)\sin(i\cdot\theta) & \cos(i\cdot\theta)^2 - \frac{\alpha}{2} & \sin(i\cdot\theta)^2 - \frac{\alpha}{2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 0 & 0 & -\frac{\alpha}{2} & -\frac{\alpha}{2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 0 & 0 & -\frac{\alpha}{2} & -\frac{\alpha}{2} \end{pmatrix} \end{array}.$$

We need to assume that $n \geq 5$ and $N - n \geq 1$ so the design matrix has rank 6 (and so $X'X$ is non-singular), and the central point has finite variance.

To compute $X'X$ we need the following identities (which follow from Euler's Identity or DeMoivre's Theorem):

$$\sum_{m=0}^{n-1} \cos^2(m\cdot\theta) = \frac{n}{2} \tag{4}$$

$$\sum_{m=0}^{n-1} \cos^4(m\cdot\theta) = \frac{3n}{8} \tag{5}$$

$$\sum_{m=0}^{n-1} \cos^{2k+1}(m\cdot\theta) = 0, \tag{6}$$

and likewise with sin replacing cos.

Note that from these identities the rotatability of the design follows immediately.

It now follows that

$$\begin{aligned} X'X &= \begin{pmatrix} \frac{n}{\alpha} & & & & & \\ & \frac{n}{2} & & & & \\ & & \frac{n}{2} & & & \\ & & & \frac{n}{4} & & \\ & & & & V & C \\ & & & & C & V \end{pmatrix} \\ (X'X)^{-1} &= \begin{pmatrix} \frac{\alpha}{n} & & & & & \\ & \frac{2}{n} & & & & \\ & & \frac{2}{n} & & & \\ & & & \frac{4}{n} & & \\ & & & & V' & C' \\ & & & & C' & V' \end{pmatrix}, \end{aligned}$$

where

$$\begin{aligned} V &= \frac{3n}{8} - \frac{\alpha n}{4}, \\ C &= \frac{n}{8} - \frac{\alpha n}{4} \\ V' &= \frac{V}{V^2 - C^2} \\ C' &= -\frac{C}{V^2 - C^2}. \end{aligned}$$

Note that this design will be orthogonal if and only if $\alpha = \frac{1}{2}$, i.e. the number of central and non-central points is the same.

One way of deciding how many central points to include in order to have approximately uniform precision is to choose α in such a way that the variance for $(0,0)$ (the center) and $(1,0)$ (a point on the circle) is approximately the same.

Computing, the variance for $(0,0)$ is

$$\frac{\alpha}{n} + \frac{\alpha^2}{2}(V' + C')$$

and the variance for $(0,1)$ is

$$\frac{\alpha}{n} + \frac{2}{n} + \left(\left(1 - \frac{\alpha}{2}\right)^2 + \left(\frac{\alpha}{2}\right)^2\right) V' - \alpha\left(1 - \frac{\alpha}{2}\right) C'.$$

Setting these equal and solving for α, we get the somewhat surprising result that $\alpha = \frac{5}{6}$, independent of n.

Following this criterion for choosing the number of central points for an approximately uniform precision design, the number of central points should be about $\frac{1}{5}$th of the number of non-central points.

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