Response Surface Methodology, Stat 579 | Homework 08 | Name: Answer Key
Fall 2014 | | Prof. Erik B. Erhardt

Part I. (50 points) I recommend reading through all the parts of the HW (with my adjustments) before starting; this may save you some work.
MMA-RSM Chapter 8: 8.8 (a),(b),(d), 8.12, 8.14, 8.15.

- For 8.12, (c) refer to 8.15.
- For 8.14, add 7 rather than 6 additional design points. Make your list of candidates a sensible one with all points within the unit cube. Use D-efficiency as the criterion. Is the resulting augmented design a standard design? If so, tell what it is.
- For 8.15, do this just for D-optimality. The formula near the middle of page 387 may be useful to you.

General: Try to do all calculations in R. All R code for the assignment should be included with the part of the problem it addresses (for code and output use a fixed-width font, such as Courier). Code is used to calculate result; text is used to report and interpret results – do not report or interpret results in the code.

(15pts) **1. 8.8**

Consider the following first-order design

$$\mathbf{D} = \begin{bmatrix} -1 & -1 & -1 \\ 1 & 1 & -1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & 1 & 1 \\ -1 & -1 & 1 \end{bmatrix}.$$

(a) (5 pts) Is the design first-order orthogonal? Explain?

Solution: Note that $\mathbf{D}$ has two replicated rows: (2,3) and (5,8). Because $\mathbf{D}^\top\mathbf{D}$ is not diagonal, the first-order design $\mathbf{D}$ is not orthogonal,

$$\mathbf{D}^\top\mathbf{D} = \begin{bmatrix} 8 & 0 & 0 & 0 \\ 0 & 8 & 4 & 0 \\ 0 & 4 & 8 & -4 \\ 0 & 0 & -4 & 8 \end{bmatrix}.$$

```
# function to determine whether a matrix is orthogonal
f.is.orth <- function(X) {
  return(all(diag(diag(t(X) %*% X)) == (t(X) %*% X)))
}

D <- matrix(c(
        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,  1,  1,  1
      , 1, -1, -1,  1
      )
      , byrow = TRUE, ncol = 4)

f.is.orth(D)
## [1] FALSE
```

(b) (5 pts) Give the D-efficiency of this design.

Solution: A variance-optimal design is the 2^3 full factorial, which has $\mathbf{M} = N^{-1}\mathbf{X}^\top\mathbf{X} = \mathbf{I}_p$, thus $\max_\zeta |\mathbf{M}(\zeta)| = 1$ for the optimal design. The D_{eff} for this design is

$$D_{\text{eff}} = \left(|N^{-1}\mathbf{X}^\top\mathbf{X}|/1\right)^{1/4} = 0.8408964.$$

```r
# compute D-efficiency manually
X <- D;
N <- dim(X)[1];
p <- dim(X)[2];
M <- t(X) %*% X / N;
optM <- 1;
D.eff <- (det(M)/optM)^{1/p};
D.eff
## [1] 0.8409
# compute efficiencies using AlgDesign package
library(AlgDesign)

### linear, but calculation doesn't work when design is singular
# eff.8.8 <- eval.design(~ ., as.data.frame(D))
# D.eff.lin <- eval.design(~ ., desDE£design)£determinant
# A.eff.lin <- 1/eval.design(~ ., desDE£design)£A
```

(c) (0 pts) Give the I-efficiency of the design.
Skip (c)

Solution: Skip (c)

(d) (5 pts) Give the A-efficiency of the design. Hint: The A-efficiency of a design is given by $\frac{\min_\zeta \operatorname{tr}\left([\mathbf{M}(\zeta)]^{-1}\right)}{N\operatorname{tr}[(\mathbf{X}^\top\mathbf{X})^{-1}]}$. Now, of course, for a first-order model with range $[-1,+1]$ on each design variable we have $\min_\zeta \operatorname{tr}\left([\mathbf{M}(\zeta)]^{-1}\right) = p$.

Solution: A variance-optimal design is the 2^3 full factorial, which has $\min_\zeta |N\operatorname{tr}[(\mathbf{M}(\zeta))^{-1}]| = p$ for the optimal design. The A_{eff} for this design is

$$A_{\text{eff}} = p/\left(N\operatorname{tr}[(\mathbf{X}^\top\mathbf{X})^{-1}]\right) = 2/3.$$

```r
A.eff <- p / (N * (sum(diag(solve(t(X) %*% X)))))
A.eff
## [1] 0.6667
```

(20^{pts}) **2. 8.12** Often a standard second-order design is planned because the practitioner expects that the fitted model will, indeed, be second-order. However, when the analysis is conducted, it is determined that the model is considerably less than order 2. As an example, suppose a $k = 2$ CCD with $a = 1.0$ and two center runs is used and all second-order effects (quadratic and interaction) are very insignificant. The design is used eventually for a first-order model.
For (c) refer to 8.15.
This is a 3^2 design with two center runs, for $n = 10$.

(a) (5 pts) What is the D-efficiency for a $k = 2$ CCD with $a = 1.0$ and two center runs for a first-order model? Comment.

Solution: $D_{\text{eff}} = 0.711379$.

```r
library(AlgDesign)
D <- rbind(gen.factorial(3,2), c(0,0))
D
```

```
##    X1 X2
## 1  -1 -1
## 2   0 -1
## 3   1 -1
## 4  -1  0
## 5   0  0
## 6   1  0
## 7  -1  1
## 8   0  1
## 9   1  1
## 10  0  0
```

```
#desDE <- optFederov(~quad(.), D, nTrials=10, evaluateI=TRUE)
#
#desDE[1:5]
#eval.design(~ ., desDE£design)   #£

# linear
# eval.design(~ ., D)
D.eff.lin <- eval.design(~ ., D)$determinant
A.eff.lin <- 1/eval.design(~ ., D)$A
c(D.eff.lin, A.eff.lin)
```

```
## [1] 0.7114 0.6923
```

(b) (5 pts) How does the D-efficiency change if there are no center runs?

Solution: $D_{\text{eff}} = 0.8255$.

```
# remove center runs
D2 <- D[!(rowSums(abs(D)) == 0),]
# linear
# eval.design(~ ., D2)
D.eff.lin <- eval.design(~ ., D2)$determinant
A.eff.lin <- 1/eval.design(~ ., D2)$A
c(D.eff.lin, A.eff.lin)
```

```
## [1] 0.8255 0.8182
```

(c) (5 pts) Is the difference between the results in (a) and (b) expected?

Solution: The D_{eff} increases without the center runs because center runs do not increase the determinant of $\mathbf{X}^\top\mathbf{X}$.

(d) (5 pts) Give the A-efficiency for both designs.

Solution: The A_{eff} for the model with center runs is 0.692308, and without is 0.818182.

(10pts) **3. 8.14** Consider the following experimental design:

$$\mathbf{D} = \begin{bmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

A second stage is used, as it becomes obvious that the model is quadratic. Use a computer-generated design package to augment the above design with six more design points in order to accommodate a complete second-order model.

Add 7 rather than 6 additional design points. Make your list of candidates a sensible one with all points within the unit cube. Use D-efficiency as the criterion. Is the resulting augmented design a standard design? If so, tell what it is.

Solution: I'll consider possible augmented points on a grid of points over each variable with levels $(-1, -0.5, 0, 0.5, 1)$.

```
#### 8.14
# original design points
D <- as.data.frame(
        matrix(c(
          -1, -1, -1
        ,  1, -1, -1
        , -1,  1, -1
        , -1, -1,  1
        ,  1,  1, -1
        ,  1, -1,  1
        , -1,  1,  1
        ,  0,  0,  0
        ,  0,  0,  0
        )
        , byrow = TRUE, ncol = 3)
      )

# augment design candidate values
D.candidate.values <-  data.frame(V1 = seq(-1, 1, by = 0.5)
                                , V2 = seq(-1, 1, by = 0.5)
                                , V3 = seq(-1, 1, by = 0.5))
D.candidate.points <- expand.grid(D.candidate.values)

# combine original points with candidate points
D.all <- rbind(D, D.candidate.points)

# keep the original points and augment the design with 7 points
library(AlgDesign)
D.aug <- optFederov(~ quad(.), D.all, nTrials = dim(D)[1] + 7, rows = 1:dim(D)[1]
                    , augment = TRUE, criterion = "D", maxIteration = 1e4, nRepeats = 1e2)

# Added points
D.aug$design[(dim(D)[1]+1):dim(D.aug$design)[1],]

##     V1 V2 V3
## 24   1  0 -1
## 64   1 -1  0
## 84   1  1  0
## 112  0 -1  1
## 124  1  0  1
## 132  0  1  1
## 134  1  1  1

library(AlgDesign)
# quadratic
#rm(D.eff.lin, A.eff.lin)
D.eff.lin <-     eval.design(~ quad(.), D.aug$design)$determinant
A.eff.lin <- 1 / eval.design(~ quad(.), D.aug$design)$A
c(D.eff.lin, A.eff.lin)

## [1] 0.4459 0.2631
```

The 7 added points above using $D_{\text{eff}} = 0.445916$ results in a design we don't have a name for. It adds 1 corner point to complete the cube, and 6 "mid-edge" points of the cube.
It is slightly more efficient than the face-centered CCD with $D_{\text{eff}} = 0.429990$.

```
# face-centered CCD
D.face <- as.data.frame(
        matrix(c(
          -1, -1, -1
        ,  1, -1, -1
```

```
        , -1,  1, -1
        , -1, -1,  1
        ,  1,  1, -1
        ,  1, -1,  1
        , -1,  1,  1
        ,  1,  1,  1
        ,  0,  0,  0
        ,  0,  0,  0
        ,  1,  0,  0
        , -1,  0,  0
        ,  0,  1,  0
        ,  0, -1,  0
        ,  0,  0,  1
        ,  0,  0, -1
        )
        , byrow = TRUE, ncol = 3)
      )
library(AlgDesign)
# quadratic
#rm(D.eff.lin, A.eff.lin)
D.eff.lin <-     eval.design(~ quad(.), D.face)$determinant
A.eff.lin <- 1 / eval.design(~ quad(.), D.face)$A
c(D.eff.lin, A.eff.lin)

## [1] 0.4300 0.3068
```

It is slightly less efficient than a free design with 16 points with $D_{\text{eff}} = 0.4583448$.

```
# free design
library(AlgDesign)
D.free <- optFederov(~ quad(.), D.candidate.points, nTrials = 9 + 7
                    , criterion = "D", maxIteration = 1e4, nRepeats = 1e2)
# Added points
D.free$design

##     V1 V2 V3
## 1   -1 -1 -1
## 5    1 -1 -1
## 13   0  0 -1
## 15   1  0 -1
## 21  -1  1 -1
## 25   1  1 -1
## 53   0 -1  0
## 55   1 -1  0
## 61  -1  0  0
## 75   1  1  0
## 101 -1 -1  1
## 105  1 -1  1
## 115  1  0  1
## 121 -1  1  1
## 123  0  1  1
## 125  1  1  1

# quadratic
#rm(D.eff.lin, A.eff.lin)
D.eff.lin <-     eval.design(~ quad(.), D.free$design)$determinant
A.eff.lin <- 1 / eval.design(~ quad(.), D.free$design)$A
c(D.eff.lin, A.eff.lin)

## [1] 0.4583 0.2636
```

(5^{pts}) **4. 8.15** Consider a first-order orthogonal design with ±1 levels. Show that the addition of center runs must lower the D-efficiency. Show that the same is true for A-efficiency and for G-efficiency.
Do this just for D-optimality. The formula near the middle of page 387 may be useful to you.

Solution: With center runs

$$
\begin{aligned}
\mathbf{X}^\top \mathbf{X} &= \begin{bmatrix} N+n_c & 0 & \cdots & 0 \\ 0 & N & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & N \end{bmatrix} \qquad \text{giving} \\
(\mathbf{X}^\top \mathbf{X})^{-1} &= \operatorname{diag}\left(\frac{1}{N+n_c}, \frac{1}{N}, \dots, \frac{1}{N}\right).
\end{aligned}
$$

Thus,

$$
\begin{aligned}
\mathbf{M} &= \operatorname{diag}\left(1, \frac{N}{N+n_c}, \dots, \frac{N}{N+n_c}\right) \qquad \text{and} \\
|\mathbf{M}| &= \left(\frac{N}{N+n_c}\right)^k \le 1.
\end{aligned}
$$

The last expression equals 1 if $n_c = 0$ and is strictly less than 1 if $n_c > 0$. Therefore, after adding center points, $D_{\text{eff}} < 1$.