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**SOME RESULTS ON THE CHOICE OF RUN ORDER  
FOR  
EXPERIMENTAL DESIGNS WITH CORRELATED ERRORS**

A THESIS PRESENTED IN PARTIAL FULFILMENT OF THE  
REQUIREMENTS FOR THE DEGREE OF  
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## **ABSTRACT**

This thesis examines the efficiency of some commonly used experimental designs in situations where the assumption of independent errors is violated. In particular this research mainly involves finding efficient run orders for various models of two level factorial experiments, three level factorial experiments and response surface designs when errors are assumed to follow either first order moving average model or first order autoregressive model. In this thesis, attention is given to systematic methods of allocating treatments based on various algorithms which provide more efficient designs and lead to good estimates of the parameters.

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## CHAPTER 1

### INTRODUCTION

In this chapter we discuss, in a preliminary way, some general philosophy necessary to the understanding of the theory and practice of experimental design, in particular factorial experiments.

#### 1.1 Factorial Experiments

In this section we introduce the concepts and notation used in our investigation such as design of experiments, factorial experiment,  $2^k$  design, design matrix, etc.

##### 1.1.1 Design of Experiments

The responses for the various conditions of the explanatory variables or treatments are customarily observed from an experiment. Each treatment is generally allocated to a single trial in an experiment. Such a trial is called an experimental unit or plot. Allocation of the treatments to the experimental units in an experiment is called the design of the experiment.

Estimates of the parameters are obtained by statistical methodology. The precision of estimates generally depend on the way of allocating treatments to the plots. In this thesis, attention is given to systematic methods of allocating treatments based on various algorithms. This is found to give more efficient designs which lead to good estimates of the parameters.

Certain standard types of design for certain types of problem and criteria for measuring the efficiency of a proposed design can be found by using

statistical theory. According to the Owen L.Davies view (Davies; 1978), the advantages of the statistical planning of experiments are:

- (i) We can take precautions before the research, that necessary steps are found to provide the required information.
- (ii) All possible sources of errors are investigated.
- (iii) An optimal number of observations may be found such that the experiment provides the required information with sufficient precision to avoid the unnecessary expense. It is very essential in industrial experiments.

Experimental design is heavily used not only in the biological field but also in the industrial field. Statistical theory gives standard designs such as Randomized Block Design, Latin Square, Split-Plot Design, Factorial Design, etc. This thesis is mainly focused on factorial design and its efficiency.

### **1.1.2 Factorial Design**

Many experimental situations need the investigation of the effects of varying two or more factors. For a complete exploration of such a situation it is not sufficient to vary one factor at a time, it may be necessary to examine all combinations of the different factor levels to explain the effect of each factor. Such an experiment is called a factorial experiment.

Any attribute of the experimental conditions which may be assigned in the experimental design, is called a factor. For example, temperature, pressure, spacing between plants, different operators, different batches of raw material and so on. There are two types of factors, namely qualitative and quantitative. If a factor can be measured numerically, it is called a

quantitative factor; otherwise, it is called a qualitative factor. The various values of a factor chosen in an experiment are known as factor levels.

Consider an experiment in which the effects of three factors are analyzed. Suppose the process can be carried out by each of two methods  $M_1$  and  $M_2$ ; the main stage can be carried out at each of three temperatures  $T_1$ ,  $T_2$  and  $T_3$ ; four batches of raw material  $B_1$ ,  $B_2$ ,  $B_3$  and  $B_4$  can be used.

Statistically, methods, temperatures and raw material are called factors. Since methods and raw material cannot be measured numerically, so these factors are called qualitative factors. Since temperature can be measured numerically, it is a quantitative factor. The "Method" factor has two levels due to the two different methods applied in this experiment. The "Temperature" and "Raw Material" have three levels and four levels respectively due to the three different temperatures and the four different raw materials used in this experiment. Thus  $2 \times 3 \times 4 = 24$  different sets of experimental conditions are available. Statistically it is known as  $2 \times 3 \times 4$  factorial design. The twenty four different sets of experimental conditions are the treatments and the 24 different experimental units are called runs.

In general, if there are  $\ell_1$  levels for the 1<sup>st</sup> factor,  $\ell_2$  levels for the 2<sup>nd</sup> factor, .....  $\ell_k$  levels for the k<sup>th</sup> factor then the experiment is called  $\ell_1 \times \ell_2 \times \dots \times \ell_k$  factorial design. Each combination of levels of different factors is a treatment in the factorial experiment. If  $\ell_1 = \ell_2 = \ell_3 = \dots = \ell_k = 2$  then the design is called a  $2^k$  factorial design. That means, k factors are involved in this design and each having 2 levels. If  $\ell_1 = \ell_2 = \dots = \ell_k = 3$  then the design is called  $3^k$  factorial design. That means, k factors are involved in this design and each having 3 levels.

The advantages of factorial design are :

- (i) To investigate a number of different factors simultaneously.

- (ii) If we need to investigate a large number of factors in an experiment, screening is needed to give a rough indication of which factors are important.
- (iii) If we investigate the interaction between different levels of several factors, it will give greater comprehensiveness.
- (iv) If the errors are independent and identically distributed, each main effect is estimated exactly with same degree of precision .

### 1.1.3 $2^k$ Design

Consider an experiment with  $k$  number of factors and each having 2 levels. The factors are denoted by capital letters A, B, C .....K. The high level(+) of the factor is denoted by corresponding small letters a, b, c, .....k. Further low level (-) is indicated by absence of the corresponding factor. Obviously, one level is higher than other level for a quantitative factor, but we arbitrarily call one level high and other level low for a qualitative factor. Let us now introduce the standard notation such as 1, a, b, ab, c ....., (abcd ..... k) in a  $2^k$  factorial design. '1' denotes that all  $k$  factors are at low level; 'a' denotes that only factor A is at high level and other factors B, C, .....K are at low level; 'ab' denotes that factors A and B are at high level and other factors C, D .....,K are at low level and so on. The mean responses at those treatment combinations are also indicated by the symbols 1, a, b, ab, ..... (abc .....k).

The term 'effect' of a factor, generally used in factorial design, is the change in response produced by a change in the level of the factor. That means, the effect is the difference between the average response of all trials carried out at the high level and the low level.

The main effect of a factor is an average effect. That means the main effect is the difference between the average response at high level and the average response at low level. If the effect of one factor is different at different levels of another then it is called a two factor interaction effect. Numerically the two factor interaction can be defined as half of the difference between the effect of one factor when other the factor is at higher level and the effect of corresponding one factor when other factor is at low level. Similarly, the three factor interaction is half of difference between the effect of a two factor interaction when other the factor is at higher level and the effect of the corresponding two factor interaction when the other factor is at low level. K-factor interactions may be obtained by this similar approach. All these definitions can be explained by the simple example of  $2^3$  factorial design.

Let A, B, C be three factors and each having 2 levels, so that  $2^3 = 8$  different treatment combinations are possible. They are low A, low B, low C; high A, low B, low C; low A, high B, low C; high A, high B, low C; low A low B, high C; high A, low B, high C low A, high B, high C; high A, high B, high C; which are statistically denoted by 1, a, b, ab, c, ac, bc, abc. These different treatment combinations are simply denoted in *Table 1.1*.

*Table1.1*

Run	Code	A	B	C
1	1	-	-	-
2	a	+	-	-
3	b	-	+	-
4	ab	+	+	-
5	c	-	-	+
6	ac	+	-	+
7	bc	-	+	+
8	abc	+	+	+



$$\begin{aligned}\text{Main effect A} &= (\text{Average of A at high level}) - (\text{Average of A at low level}) \\ &= \frac{1}{4} (a + ab + ac + abc) - \frac{1}{4} (1 + b + c + bc)\end{aligned}$$

Similarly,

$$\text{Main effect B} = \frac{1}{4} (b + ab + bc + abc) - \frac{1}{4} (1 + a + c + ac) \quad \text{and}$$

$$\text{Main effect C} = \frac{1}{4} (c + ac + bc + abc) - \frac{1}{4} (1 + a + b + ab)$$

$$\begin{aligned}\text{Interaction effect AB} &= \frac{1}{2} [(\text{effect of A when B is at high level}) \\ &\quad - (\text{effect of A when B is at low level})] \\ &= \frac{1}{2} \left\{ \frac{1}{2} ([abc + ab] - [bc + b]) - \frac{1}{2} ([ac + a] - [bc + b]) \right\} \\ &= \frac{1}{4} (abc + ab + c + 1) - \frac{1}{4} (ac + bc + a + b)\end{aligned}$$

Similarly,

$$\text{Interaction effect BC} = \frac{1}{4} (abc + bc + a + 1) - \frac{1}{4} (ab + ac + a + b),$$

$$\text{Interaction effect AC} = \frac{1}{4} (abc + ac + b + 1) - \frac{1}{4} (ab + bc + c + a) \quad \text{and}$$

$$\text{Interaction effect ABC} = \frac{1}{4} (abc + a + b + c) - \frac{1}{4} (ab + ac + bc + 1)$$

In general, for  $k$  factors and each having 2 levels, the interaction effect of  $ABCD \dots K = \left(\frac{1}{2}\right)^{k-1} (a - 1) (b - 1) \dots (k - 1)$  (1.1)

Table 1.2

Effect

Runs	Code	A	B	C	AB	AC	BC	ABC
1	1	-	-	-	+	+	+	-
2	a	+	-	-	-	-	+	+
3	b	-	+	-	-	+	-	+
4	ab	+	+	-	+	-	-	-
5	c	-	-	+	+	-	-	+
6	ac	+	-	+	-	+	-	-
7	bc	-	+	+	-	-	+	-
8	abc	+	+	+	+	+	+	+

We can easily see that in the expansion of the main effect A, all treatment combinations containing 'a' have the plus sign and not containing 'a'

have the minus sign. All other main effects can be written in similar manner. The signs for any interaction are equal to those obtained by multiplying together the signs for the main effects corresponding to the letters in the interaction. For example, if factor A is at high level(+1) and factor B is at low level(-1) then interaction between A and B is negative one. That is  $(-1) \times (+1) = (-1)$ . Thus, the signs for all the effects in a  $2^3$  experiment may be given in *Table 1.2*.

#### 1.1.4 Parametrization

The general model for a  $2^3$  experiment is

$$Y_{ijk} = \mu + \alpha_i + \beta_j + \gamma_k + \alpha_i \beta_j + \beta_j \gamma_k + \alpha_i \gamma_k + \alpha_i \beta_j \gamma_k + \epsilon_{ijk} \quad (1.2)$$

where  $Y_{ijk}$  : The response in a trial with factor A, at the  $i^{\text{th}}$  level, factor B at the  $j^{\text{th}}$  level and factor C at the  $k^{\text{th}}$  level.

$\mu$  : True mean of all trials

$\alpha_i$  :  $i^{\text{th}}$  level of main effect of A

$\beta_j$  :  $j^{\text{th}}$  level of main effect of B

$\gamma_k$  :  $k^{\text{th}}$  level of main effect of C

$\alpha_i \beta_j$  : interaction effect of A and B

$\beta_j \gamma_k$  : interaction effect of B and C

$\alpha_i \gamma_k$  : interaction effect of A and C

$\alpha_i \beta_j \gamma_k$  : interaction effect of A, B and C

and  $\epsilon_{ijk}$ 's (for all  $i, j, k$ ) are independent identical normally distributed with mean zero and common variance  $\sigma^2$ .

Since the factor A has two levels, therefore the low level and the high level of the factor A effect can be written as  $-\alpha$  and  $\alpha$  respectively. Hence,  $2\alpha$  is the main effect of factor A. Similarly other main effects of factor B and C are  $2\beta$  and  $2\gamma$  respectively. As far as interactions are concerned,  $2(\alpha \times \beta)$ ,  $2(\beta \times \gamma)$ ,  $2(\alpha \times \gamma)$  and  $2(\alpha \times \beta \times \gamma)$  are interaction effects of AB, BC, AC

and ABC respectively. That means, the estimated values of  $\mu$ ,  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\alpha\beta$ ,  $\beta\gamma$ ,  $\alpha\gamma$  and  $\alpha\beta\gamma$  are given as follows.

$$\begin{aligned}\mu &= \frac{1}{8}(abc + ab + ac + bc + a + b + c + 1) \\ \alpha &= \frac{1}{8}(abc + ab + ac + a) - \frac{1}{8}(bc + b + c + 1) \\ \beta &= \frac{1}{8}(abc + ab + bc + b) - \frac{1}{8}(ac + a + c + 1) \\ \gamma &= \frac{1}{8}(abc + ac + bc + c) - \frac{1}{8}(ab + a + b + 1) \\ \alpha\beta &= \frac{1}{8}(abc + ab + c + 1) - \frac{1}{8}(ac + bc + a + b) \\ \beta\gamma &= \frac{1}{8}(abc + bc + a + 1) - \frac{1}{8}(ab + ac + b + c) \\ \alpha\gamma &= \frac{1}{8}(abc + ac + b + 1) - \frac{1}{8}(ab + bc + a + c) \\ \alpha\beta\gamma &= \frac{1}{8}(abc + a + b + c) - \frac{1}{8}(ab + bc + ca + 1)\end{aligned}$$

We can use dummy variables  $X_1, X_2, X_3, \dots, X_k$  to represent the factors A, B, .....K. If factors are two level then  $X_i$  ( $i = 1, 2, \dots, k$ ) is defined as follows.

$$X_i = \begin{cases} -1 & \text{if corresponding factor at low level} \\ +1 & \text{if corresponding factor at high level} \end{cases}$$

Therefore, in the  $2^3$  factorial experiment, the eight treatment combinations can be written as  $(-1, -1, -1); (+1, -1, -1); (-1, +1, -1); (+1, +1, -1); (-1, -1, +1); (+1, -1, +1); (-1, +1, +1); (+1, +1, +1)$ . The model can then be written as:

$$\begin{aligned}Y_j &= \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_4 X_1 X_2 + \beta_5 X_2 X_3 + \beta_6 X_1 X_3 + \\ &\quad \beta_7 X_1 X_2 X_3 + \epsilon_j \quad j = 1, 2, \dots, n. \quad (1.3)\end{aligned}$$

where  $\beta_0 = \mu$ ,  $\beta_1 = \alpha$ ,  $\beta_2 = \beta$ ,  $\beta_3 = \gamma$ ,  $\beta_4 = \alpha\beta$ ,  $\beta_5 = \beta\gamma$ ,  $\beta_6 = \alpha\gamma$ , and  $\beta_7 = \alpha\beta\gamma$  Equation (1.3) can be represented in matrix form. That is,

$$Y = X\beta + \epsilon; \quad \epsilon \sim N(0, \sigma^2 I_n) \quad (1.4)$$

$X$  is the  $(n \times 8)$  design matrix whose elements are plus one and negative one,  $\beta$  is a  $(8 \times 1)$  parameter vector and  $n$  is the number of observations.

### 1.1.5 Design Matrix

If the model is 'main effects only' ( that is, no interaction in the model,  $\alpha\beta = \beta\gamma = \alpha\gamma = \alpha\beta\gamma = 0$  ) in the  $2^3$  factorial design, then the design matrix  $X$ , using the run order on page 3, will be given as follows.

$$X = \begin{bmatrix} +1 & -1 & -1 & -1 \\ +1 & +1 & -1 & -1 \\ +1 & -1 & +1 & -1 \\ +1 & +1 & +1 & -1 \\ +1 & -1 & -1 & +1 \\ +1 & +1 & -1 & +1 \\ +1 & -1 & +1 & +1 \\ +1 & +1 & +1 & +1 \end{bmatrix} \quad (1.5)$$

If the model is a full model (including all main effects and all possible interactions) in the  $2^3$  factorial design, the design matrix  $X$  will be given as follows.

$$X = \begin{bmatrix} +1 & -1 & -1 & -1 & +1 & +1 & +1 & -1 \\ +1 & -1 & -1 & +1 & +1 & -1 & -1 & +1 \\ +1 & -1 & +1 & -1 & -1 & +1 & -1 & +1 \\ +1 & -1 & +1 & +1 & -1 & -1 & +1 & -1 \\ +1 & +1 & -1 & -1 & -1 & -1 & +1 & +1 \\ +1 & +1 & -1 & +1 & -1 & +1 & -1 & -1 \\ +1 & +1 & +1 & -1 & +1 & -1 & -1 & -1 \\ +1 & +1 & +1 & +1 & +1 & +1 & +1 & +1 \end{bmatrix} \quad (1.6)$$

We can get different designs by permuting the rows of the above design matrix. Since the matrix has 8 rows, so it can be arranged in  $8!$  ways. Because of the arbitrary allocation of high(+)/low(-) levels, the above

arrangements can be reduced by  $2^3 = 8$  times. That is, only  $\frac{8!}{8} = 7!$  arrangements are necessary. Further due to the arbitrary assignment of factors A, B and C,  $7!$  arrangements are reduced by  $3! = 6$  times. That is, there are  $\frac{7!}{6} = 5! \times 7 = 840$  possible designs available.

Another procedure for obtaining a design matrix X is given below.

Step1: We have to keep all elements of the first column as +1 to include the overall mean.

Step2: An arbitrary choice of main effects of factor A, B, C are represented by three orthogonal columns in which each column contains four +1s and four -1s.

Step3: All possible multiplication of these orthogonal columns will provide all interactions of AB, BC, AC and ABC.

For step 2 we use a matrix whose columns consist of all possible arrangements of four +1s and four -1s. As far as arbitrary high(+)/low(-) levels of factor is concerned, we can keep last number as +1. Therefore,  ${}^7C_3 = 35$  different arrangements are possible. We denote this matrix as M and it is given in the *Appendix 1*. Note that for step 2 a full factorial is obtained only if the third chosen column is not the product of the other two; otherwise we get a repeated half-factorial.

### 1.1.6 Analysis

The model is

$$Y = X\beta + \epsilon \quad \epsilon \sim NII(0, \sigma^2 I_n)$$

Total error =  $\Omega = \epsilon^t \epsilon$

$$= Y^t Y - 2\beta^t X^t Y + \beta^t X^t X \beta \text{ and the matrix } X \text{ is full column}$$

rank. The least squares estimator of  $\beta$ , minimizing  $\Omega$ , is given by

$$\begin{aligned}
\hat{\beta} &= (X^t X)^{-1} X^t Y \\
&\text{and} \\
\text{Cov}(\hat{\beta}) &= \text{Cov}\left[(X^t X)^{-1} X^t Y\right] \\
&= (X^t X)^{-1} X^t \text{Cov}(Y) \left[(X^t X)^{-1} X^t\right]^t \\
&= (X^t X)^{-1} \sigma^2.
\end{aligned} \tag{1.7}$$

Let  $C = (X^t X)$  then the matrix  $C$  is called the information matrix. Let  $D = C^{-1}$  then the matrix  $D$  is called the dispersion matrix of the parameters. Therefore,

$$\text{Cov}(\hat{\beta}) = (X^t X)^{-1} \sigma^2 = C^{-1} \sigma^2 = D \sigma^2 \tag{1.8}$$

Here  $(X^t X) = n I_k$  where  $n$  is the number of observations,  $k$  is the number of parameters involved in the model and  $I$  is a  $(k \times k)$  identity matrix. Therefore  $C = n I_k$  and  $D = \frac{1}{n} I_k$ .

### 1.1.7 Orthogonality

We have seen that the information matrix  $C$  is a diagonal matrix with respect to design matrix  $X$ . That means, off-diagonal elements of the  $C$  matrix are zero. Therefore the inverse matrix of  $C$  is also diagonal. That means, the estimator of one parameter is independent of the other parameter estimators. That is, orthogonality provides that all the main effects and interaction effects of the factorial design can be independently estimated without entanglement.

Mathematically, the two linear functions of the observations  $x_1, \dots, x_n$  such that  $L_1 = a_1 x_1 + a_2 x_2 + \dots + a_n x_n$  and  $L_2 = b_1 x_1 + b_2 x_2 + \dots + b_n x_n$  are said to be orthogonal if  $\sum a_i b_i = 0$  provided not all  $a_i, b_i$  are zero. From Equation (1.7), we can see that if the columns of the design matrix

are orthogonal the corresponding parameter estimates will be independent.

Generally, fully orthogonal experiments are more efficient. That is, for a given number of trials they estimate the effects with greater precision.

## 1.2 Correlated Models

We have assumed in the previous sections that all  $\epsilon_i$ 's are independent in the model, but errors may be serially correlated in a real experiment. The estimation of the model may therefore be influenced by the above mentioned correlation. Thus, this type of difficult situation needs to be analysed in the real experiment. This is also one of the main interests in my research.

If the  $i^{\text{th}}$  observation error  $\epsilon_i$  is associated with either  $(i-1)^{\text{th}}$  observation error  $\epsilon_{i-1}$  or  $(i+1)^{\text{th}}$  observation error  $\epsilon_{i+1}$  then the errors are said to be serially correlated. If  $\epsilon_i$  is high and  $\epsilon_{i+1}$  tends to be high then it is said to be a positive serial correlation. If  $\epsilon_i$  is high and  $\epsilon_{i+1}$  tends to be low, then it is said to be negatively serially correlated. If observations are serially correlated, the standard error for estimated values of the model parameters may be dramatically wrong. Therefore, this may lead to incorrect interpretation of the result of the experiment.

For example, the responses might be affected by hidden variables. Such a variable is called a lurking variable. Examples of lurking variable are slight variations in quality of starting material, slight changes in techniques by operators in different shifts, weather conditions, etc. The lurking variable causes serial correlation. In most practical situations we might expect observations to be positively serially correlated.

This correlation needs to be allowed for in order to use regression analysis. In practice this is attempted by one of two ways namely,

- (i) Breaking the links by using randomization.
- (ii) Selecting the appropriate design for the model dependence like MA(1) or AR(1) or etc. and using an appropriate analysis.

From this analysis, we conclude that the independence assumption is commonly violated in the practical experiment so that our model needs to be modified to a general linear model.

That is

$$Y = X\beta + \epsilon \quad \epsilon \sim N(0, \sigma^2 V) \quad (1.9)$$

where  $V$  is  $(n \times n)$  positive definite covariance-variance matrix. We can find a non singular matrix  $K$  such that  $V = K^t K$  and write  $K = V^{\frac{1}{2}}$ .

$$\therefore K^{-1}Y = K^{-1}Xb + K^{-1}\epsilon \quad (1.10)$$

Let  $Y^* = K^{-1}Y$ ,  $X^* = K^{-1}X$  and  $\epsilon^* = K^{-1}\epsilon$

$$\begin{aligned} \text{then } \text{Cov}(\epsilon^*) &= \text{Cov}(K^{-1}\epsilon) \\ &= (K^{-1})^t \text{Cov}(\epsilon) K^{-1} \\ &= (K^{-1})^t K^t K K^{-1} \sigma^2 \\ &= I_n \sigma^2. \end{aligned} \quad (1.11)$$

It shows that the errors( $\epsilon^*$ ) are uncorrelated. Therefore, we finally get,

$$Y^* = X^*\beta + \epsilon^* \quad \epsilon^* \sim N(0, I_n \sigma^2) \quad (1.12)$$

This is look like a our original model with independent errors. Therefore, as usual the least squares estimate of  $\beta$  is given by

$$\begin{aligned} \hat{\beta} &= [(X^*)^t X^*]^{-1} (X^*)^t Y^* \\ &= (X^t V^{-1} X)^{-1} (X^t V^{-1} Y) \quad \text{and} \end{aligned} \quad (1.13)$$

$$\text{Cov}(\hat{\beta}) = (X^t V^{-1} X)^{-1} \sigma^2 \quad (1.14)$$

It is noticeable that the information matrix  $C = X^t V^{-1} X$  is no longer a diagonal matrix. Therefore the estimator of one parameter is not independent of other parameters. That means, we have lost the orthogonal property.

If the errors in successive observations are assumed to follow a first order moving average MA(1) process with  $\epsilon_i = a_i + \delta a_{i-1}$  where  $a_i$ 's are



independent, zero mean random shocks with variance  $\sigma^2$  and  $-1 < \delta < 1$ , then  $\text{Cov}(\epsilon_i, \epsilon_{i-1}) = E(\epsilon_i \epsilon_{i-1}) = \delta \sigma^2$

$$\text{Var}(\epsilon_i) = E(\epsilon_i^2) = (1 + \delta^2) \sigma^2$$

Hence, correlation coefficient between  $\epsilon_i$  and  $\epsilon_{i-1} = \rho = \frac{\delta}{1 + \delta^2}$  ;  $-0.5 < \rho < 0.5$

and the error covariance matrix  $V$  has the form:

$$V = \begin{bmatrix} 1 & \rho & 0 & . & . & . & . & . & 0 \\ \rho & 1 & \rho & 0 & . & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & . & . & . & . & \rho & 1 & \rho \\ 0 & 0 & 0 & . & . & . & . & . & \rho & 1 \end{bmatrix} \quad (1.15)$$

The  $(i,j)^{\text{th}}$  element of  $V^{-1}$  can be written as

$$(V^{-1})_{ij} = (1 + \delta^2)(-\delta)^{j-i} \frac{D_{i-1} D_{n-j}}{D_n} \quad \text{for } i \leq j \quad (1.16)$$

where  $D_n = \frac{1 - \delta^{2n+2}}{1 - \delta^2}$

Alternatively, consider a first order auto regressive process with  $\epsilon_i = \rho \epsilon_{i-1} + a_i$ , where the  $a_i$ 's are independent, mean zero random shocks

and variance  $\sigma^2$  and  $1 < \rho < 1$ . Thus,  $\epsilon_i = \rho^{i-j} \epsilon_j + \sum_{k=j}^i a_k$  for  $i > j$  and

therefore  $\text{Cov}(\epsilon_i, \epsilon_j) = \rho^{i-j} \sigma^2$  for  $i > j$ . Hence the correlation between any two observations is  $\rho^{|i-j|}$ . Thus, the  $V$  matrix has the form:

$$V = \begin{bmatrix} 1 & \rho & \rho^2 & . & . & . & . & . & \rho^{n-1} \\ \rho & 1 & \rho & \rho^2 & . & . & . & . & \rho^{n-2} \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ \rho^{n-1} & \rho^{n-2} & \rho^{n-3} & . & . & . & . & \rho & 1 \end{bmatrix} \quad (1.17)$$

Therefore,  $V^{-1} = (1 - \rho^2)^{-1} S$  (1.18)

Where  $S_{11} = S_{nn} = 1$ ,  $S_{ii} = 1 + \rho^2$  for  $i=2,3,\dots,(n-1)$  and

$$S_{ij} = \begin{cases} -\rho & \text{if } |i - j| = 1 \\ 0 & \text{if } |i - j| > 1 \end{cases}$$

[Cheng & Steinberg, 1991].

### 1.3 Efficiency

Efficiency measures how good the estimators of the parameters are for a specific design. A good design will give a 'small' dispersion matrix  $D$  or 'large' information matrix  $C$ . It is possible that, at the stage of planning the experiment can be improved by considering efficiency.

#### 1.3.1 Definition of the Efficiency

Three different measures of efficiency are considered here. These measures are defined in terms of the covariance matrix of the estimators in the generalized linear model. They are

- (i) D-efficiency: Determinant  $|C|^{1/\alpha}$  where  $\alpha$  is the number of parameters involved in the model. For example, using the information matrix  $C$  defined on page 11, the D-efficiency for the main effects  $2^3$  factorial experiment with independent errors is  $|8^4|^{1/4} = 8$ .
- (ii) A-efficiency: Sum of the eigenvalues of matrix  $C^{-1}$ . That is, it is equivalently  $\text{tr}(C^{-1})$ . The A-efficiency for same example considered above, is  $4/8 = 1/2$ .
- (iii) E-efficiency: Maximum of the eigenvalues of matrix  $C^{-1}$ . The E-efficiency for the same example is  $1/8$ .

It is noticeable that if the errors are correlated,  $C = X^t V^{-1} X$  and the efficiency of the design depends on the run order. One of the intentions of

this research is that we need to choose a run order which will be efficient for a given correlation model.

### 1.3.2 Some Results on Partitioned Matrices

If we are only concerned about a subset of the parameter vector such as main effects only or excluding the overall mean, then the  $(n \times k)$  design matrix  $X$  and the parameter vector  $\beta$  can be partitioned as  $X = (X_1 | X_2)$  and  $\beta = \begin{bmatrix} \beta_0 \\ \beta^* \end{bmatrix}$  respectively, where  $X_1$  and  $X_2$  are  $(n \times p)$  and  $(n \times q)$  matrices respectively ( $k = p + q$ ).  $\beta_0$  and  $\beta^*$  are  $(p \times 1)$  and  $(q \times 1)$  parameter vectors respectively. Therefore our original model Equation(1.9) can be written as

$$Y = [X_1 | X_2] \begin{bmatrix} \beta_0 \\ \beta^* \end{bmatrix} + \epsilon \quad (1.19)$$

According to the above partition, the information matrix  $C$  and dispersion matrix  $D$  can be written as

$$C = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} \quad \text{and} \quad D = \begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix} \quad (1.20)$$

where  $C_{11}$  and  $D_{11}$  are  $(p \times p)$  matrices,  $C_{12}$  and  $D_{12}$  are  $(p \times q)$  matrices,  $C_{21}$  and  $D_{21}$  are  $(q \times p)$  matrices,  $C_{22}$  and  $D_{22}$  are  $(q \times q)$  matrices. Since  $C = D^{-1}$ , Therefore

$$\begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} \begin{bmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{bmatrix} = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} \quad (1.21)$$

We can get from Equation (1.21),

$$D_{22} = [C_{22} - C_{21}C_{11}^{-1}C_{12}]^{-1} \quad (1.22)$$

The usefulness of the above partition is explained by following examples.

- (1) Calculate the efficiency when the overall mean is not of interest, but it is in the model. Therefore  $X_1$  is the first column of the design matrix  $X$  and  $\beta_0$  is called a nuisance parameter, in otherwords  $\beta_0$  is the mean

and  $\beta^*$  is the vector of parameters of real interest. Hence  $C_{11} = \underline{1}^t V^{-1} \underline{1}$   
 $= \sum_i \sum_j v_{ij}$ , where  $v_{ij}$  is the  $(i,j)^{th}$  element of matrix  $V$ .

$$\begin{aligned}
 \text{From Equation (1.20),} \quad |C| &= |C_{11}C_{22} - C_{12}C_{21}| \\
 &= |C_{11}[C_{22} - C_{11}^{-1}C_{12}C_{21}]| \\
 &= |C_{11}D_{22}^{-1}| \\
 &= |C_{11}| |D_{22}^{-1}|
 \end{aligned} \tag{1.23}$$

$D_{22}^{-1}$  is the adjusted information matrix. Efficiency measures excluding the mean should use this. But since  $C_{11}$  is a constant single element, therefore the order of D-efficiency for different designs will be the same including or excluding the mean.

- (2) Find the efficiency when higher order interactions are not in the model. That is, the model is reduced ( $\beta^* = \underline{0}$ ). This implies that matrices  $C_{12}$ ,  $C_{21}$ ,  $C_{22}$  and  $D_{12}$ ,  $D_{21}$ ,  $D_{22}$  are dropped out from the matrix  $C$  and  $D$  respectively. Therefore  $C = C_{11}$  and  $|C| = |C_{11}|$ . In the case of a reduced model the information matrix  $C_{11}$  can be easily obtained from the full model because the design matrix  $X$  for the full model is invertible, making the full model dispersion matrix easy to calculate.

That is, we can get from Equation(1.21),

$$C_{11}^{-1} = D_{11} - D_{12}D_{22}^{-1}D_{21} \tag{1.24}$$

Here  $C_{11}^{-1}$  is the actual dispersion matrix, and  $D$  is obtained by partitioning the dispersion matrix we would get from using the full model.

## 1.4 $3^k$ Design

Sometimes the effects of several factors are investigated in which one or more of the factors are investigated at three levels. If there are  $k$  factors with each having 3 levels then it is called  $3^k$  design.

$3^k$  design abbreviations are different from the  $2^k$  design. Consider as an example the  $3^2$  design. It is common to represent the factors by capital letters and the three levels by 0, 1, 2. Alternatively  $a_0, a_1$  and  $a_2$  are levels of the factor A and  $b_0, b_1$  and  $b_2$  are levels of the factor B. Therefore various representation of the treatment combinations of a  $3^2$  factorial design are given below.

1st Method of abbreviation	00	10	20	01	11	21	02	12	22
2nd Method of abbreviation	$a_0b_0$	$a_1b_0$	$a_2b_0$	$a_0b_1$	$a_1b_1$	$a_2b_1$	$a_0b_2$	$a_1b_2$	$a_2b_2$

A treatment  $(0, 0)$  or  $(a_0, b_0)$  indicates that factors A and B are at zero level; A treatment  $(1, 0)$  or  $(a_1, b_0)$  indicates that factor A is at first level and factor B is at zero level and so on.

### 1.4.1 Effects for $3^k$ Design

It has already been shown that when a factor is investigated at two levels, its main effect is uniquely defined. Note that the effects for factors with two levels cannot be simply extended to factors with three levels. When a factor is examined at three levels, its main effect is defined as differences between the means corresponding to different levels of the factors. For example [Davies, 1978] let  $\bar{y}_1, \bar{y}_2$  and  $\bar{y}_3$  be the mean of three levels respectively. The possible difference are  $\bar{y}_1 - \bar{y}_2, \bar{y}_2 - \bar{y}_3,$

$\bar{y}_1 - \bar{y}_3, \bar{y}_1 - \frac{1}{2}(\bar{y}_2 + \bar{y}_3), \bar{y}_2 - \frac{1}{2}(\bar{y}_1 + \bar{y}_3)$  and so on. The comparisons of interest will depend on the nature of the factors, in particular whether they are qualitative or quantitative. For qualitative factors in which one level denotes a control with mean  $\bar{y}_1$  and other two denote treatments, the comparisons of interest are either  $\bar{y}_2 - \bar{y}_1$  and  $\bar{y}_3 - \bar{y}_1$  or  $\bar{y}_3 - \bar{y}_2$  and  $\bar{y}_1 - \frac{1}{2}(\bar{y}_2 + \bar{y}_3)$ . For quantitative factors, comparisons of interest will be

those giving the most information on this regard such as linear and quadratic. For example, the comparisons  $\bar{y}_3 - \bar{y}_1$  or  $(-1, 0, 1)$  and

$\bar{y}_3 - 2\bar{y}_2 + \bar{y}_1$  or (1, -2, 1) represent the linear and quadratic regression effects of the quantitative factor.

#### 1.4.2 Parametrization

Consider the  $3^2$  factorial structure when factors are quantitative. The possible combination of treatments are interpreted by the following table.

Table 1.3

		Factor B		
		$b_0 (-1)$	$b_1 (0)$	$b_2 (1)$
Factor A	$a_0 (-1)$	$T_1$	$T_4$	$T_7$
	$a_1 (0)$	$T_2$	$T_5$	$T_8$
	$a_2 (1)$	$T_3$	$T_6$	$T_9$

where  $T_k = a_i \times b_j$  ( $i, j = 0, 1, 2$  and  $k = 1, 2, \dots, 9$ ) is the  $k^{\text{th}}$  treatment combination. The effect of the factors A and B are represented and calculated in the following manner.

A possible model of  $3^2$  factorial experiment is given below.

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_{11} X_1^2 + \beta_{22} X_2^2 + \beta_{12} X_1 X_2 + \beta_{112} X_1^2 X_2 + \beta_{122} X_1 X_2^2 + \beta_{1122} X_1^2 X_2^2 + \epsilon \quad (1.25)$$

where  $X_1$  and  $X_2$  are two factors,  $\underline{\beta} = (\beta_0, \beta_1, \beta_2, \beta_{11}, \beta_{22}, \beta_{12}, \beta_{112}, \beta_{122}, \beta_{1122})^t$  is a parameter vector and  $\epsilon \sim NII(0, \sigma^2 I_9)$ .

According to the parametrization and allocation of the treatment, design will be set up in the following manner.

	Mean	Linear		Quadratic			3		4
	$X_0$	$X_1$	$X_2$	$X_1^2$	$X_2^2$	$X_1 X_2$	$X_1^2 X_2$	$X_1 X_2^2$	$X_1^2 X_2^2$
$T_1$	1	-1	-1	1	1	1	-1	-1	1
$T_2$	1	0	-1	0	1	0	0	0	0
$T_3$	1	1	-1	1	1	-1	-1	1	1
$T_4$	1	-1	0	1	0	0	0	0	0
$T_5$	1	0	0	0	0	0	0	0	0
$T_6$	1	1	0	1	0	0	0	0	0
$T_7$	1	-1	1	1	1	-1	1	-1	1
$T_8$	1	0	1	0	1	0	0	0	0
$T_9$	1	1	1	1	1	1	1	1	1

(1.26)

abbreviation:  $3 = 3^{\text{rd}}$  order = Linear  $\times$  Quadratic.  
 $4 = 4^{\text{th}}$  order = Quadratic  $\times$  Quadratic.

We can easily see that some columns are not orthogonal to other columns. For example column  $X_0$  is not orthogonal to column  $X_1^2$ ,  $X_2^2$ , etc. Note that it is algebraically easy to work with set of orthogonal variables rather than original variables such as  $X_0$ ,  $X_1^2$ ,  $\dots$ , etc. Orthogonal variables may be obtained by considering a reparametrization. That means, the model needs to be reparametrized in order to make orthogonal variables and give easy interpretation. As far as reparametrization is concerned, the new design matrix is given below.

Mean	Lin A	Lin B	Qud A	Qud B	Lin A $\times$ Lin B	Qud A $\times$ Lin B	Lin A $\times$ Qud B	Qud A $\times$ Qud B
1	-1	-1	1	1	1	-1	-1	1
1	0	-1	-2	1	0	2	0	-2
1	1	-1	1	1	-1	-1	1	1
1	-1	0	1	-2	-1	0	2	-2
1	0	0	-2	-2	0	0	0	4
1	1	0	1	-2	1	0	-2	-2
1	-1	1	1	1	-1	1	-1	1
1	0	1	-2	1	0	-2	0	-2
1	1	1	1	1	1	1	1	1

(1.27)

It is observed that the contrasts corresponding to the linear, quadratic, interaction effects, etc. have different variances. Since measures of the efficiency are defined in terms of covariance matrix, therefore efficiency for the  $3^2$  factorial experiment cannot be measured jointly. To enable them to be jointly assessed, they need to be rescaled to have the same variance. That is, unscaled effects need to be rescaled to have common

variance. Because the unscaled effect  $a_i = \frac{z_i^t Y}{z_i^t z_i}$  has variance  $\frac{\sigma^2}{z_i^t z_i}$ , where

$Y = (Y_1, Y_2, Y_3, Y_4, Y_5, Y_6, Y_7, Y_8, Y_9)^t$  is the vector of response observations and  $z_i$  is the  $i^{\text{th}}$  column of the above design matrix (1.27), a standardized effect

$A_i = (z_i^t z_i)^{1/2} a_i = \frac{z_i^t Y}{(z_i^t z_i)^{1/2}}$  has common variance  $\sigma^2$ . Therefore the

appropriate design for a  $3^2$  factorial design is given below.

Mean	Lin A	Lin B	Qud A	Qud B	Lin A x Lin B	Qud A x Lin B	Lin A x Qud B	Qud A x Qud B
$1/\sqrt{9}$	$-1/\sqrt{6}$	$-1/\sqrt{6}$	$1/\sqrt{18}$	$1/\sqrt{18}$	$1/\sqrt{6}$	$-1/\sqrt{12}$	$-1/\sqrt{12}$	$1/\sqrt{36}$
$1/\sqrt{9}$	0	$-1/\sqrt{6}$	$-2/\sqrt{18}$	$1/\sqrt{18}$	0	$2/\sqrt{12}$	0	$-2/\sqrt{36}$
$1/\sqrt{9}$	$1/\sqrt{6}$	$-1/\sqrt{6}$	$1/\sqrt{18}$	$1/\sqrt{18}$	$-1/\sqrt{6}$	$-1/\sqrt{12}$	$1/\sqrt{12}$	$1/\sqrt{36}$
$1/\sqrt{9}$	$-1/\sqrt{6}$	0	$1/\sqrt{18}$	$-2/\sqrt{18}$	$-1/\sqrt{6}$	0	$2/\sqrt{12}$	$-2/\sqrt{36}$
$1/\sqrt{9}$	0	0	$-2/\sqrt{18}$	$-2/\sqrt{18}$	0	0	0	$4/\sqrt{36}$
$1/\sqrt{9}$	$1/\sqrt{6}$	0	$1/\sqrt{18}$	$-2/\sqrt{18}$	$1/\sqrt{6}$	0	$-2/\sqrt{12}$	$-2/\sqrt{36}$
$1/\sqrt{9}$	$-1/\sqrt{6}$	$1/\sqrt{6}$	$1/\sqrt{18}$	$1/\sqrt{18}$	$-1/\sqrt{6}$	$1/\sqrt{12}$	$-1/\sqrt{12}$	$1/\sqrt{36}$
$1/\sqrt{9}$	0	$1/\sqrt{6}$	$-2/\sqrt{18}$	$1/\sqrt{18}$	0	$-2/\sqrt{12}$	0	$-2/\sqrt{36}$
$1/\sqrt{9}$	$1/\sqrt{6}$	$1/\sqrt{6}$	$1/\sqrt{18}$	$1/\sqrt{18}$	$1/\sqrt{6}$	$1/\sqrt{12}$	$1/\sqrt{12}$	$1/\sqrt{36}$

(1.28)

Therefore, the effects such as linear, quadratic and interaction for a  $3^2$  factorial experiment are given as follows.

Main effect :

$$\begin{aligned}\text{Linear A} &= \frac{1}{3} (a_2 - a_0)(b_2 + b_1 + b_0) \\ \text{Quadratic A} &= \frac{1}{6} (a_2 - 2a_1 + a_0)(b_2 + b_1 + b_0) \\ \text{Linear B} &= \frac{1}{3} (a_2 + a_1 + a_0)(b_2 - b_0) \\ \text{Quadratic B} &= \frac{1}{6} (a_2 + a_1 + a_0)(b_2 - 2b_1 + b_0)\end{aligned}$$

Interaction effect:

$$\begin{aligned}\text{Lin A} \times \text{Lin B} &= \frac{1}{2} (a_2 - a_0)(b_2 - b_0) \\ \text{Lin A} \times \text{Qud B} &= \frac{1}{4} (a_2 - a_0)(b_2 - 2b_1 + b_0) \\ \text{Qud A} \times \text{Lin B} &= \frac{1}{4} (a_2 - 2a_1 + a_0)(b_2 - b_0) \\ \text{Qud A} \times \text{Qud B} &= \frac{1}{8} (a_2 - 2a_1 + a_0)(b_2 - 2b_1 + b_0)\end{aligned}$$

$$\text{Over all mean effect} = \frac{1}{9} (a_2 + a_1 + a_0)(b_2 + b_1 + b_0)$$

(1.29)



## 1.5 Response Surface Design

The general purpose of the response surface experiment is given below.

- (i) To identify which variables are relevant.
- (ii) To get some inside information about the variables, such as whether variables act linearly or not, which variables interact with each other, etc.
- (iii) To seek an optimum “mixture” of the levels of the factors involved.

It is commonly observed that a response (or output) variable of the factorial experiment depends on the levels of a number of quantitative predictors (or input) variable. This type of situation can be written in mathematical form. That is, response variable  $Y$  is a function of level of these variables  $X_1, X_2, \dots, X_k$ . It can be written as

$$Y = f(X_1, X_2, \dots, X_k) + \epsilon \quad (1.30)$$

where  $X_1, X_2, \dots, X_k$  are factors involved or  $(X_1, X_2, \dots, X_k)$  is called factor space or region of interest,  $\epsilon$  is a random error which satisfied our usual assumption and  $\eta = f(X_1, X_2, \dots, X_k)$  which is not only a polynomial pattern but also unknown, is called the response surface. Note that if there is only one input variable, we can visualize the response variable as curve. It is known as response curve.

Further, it is convenient to work with coded variables  $\zeta_i$  instead of the actual numerical measures of the variables  $X_i$ . Let  $X_c$  be the center of the region and  $d$  be the difference between  $X_c$  and actual level of interest for  $X_i$ . Therefore, coded variable  $\zeta_i$  is defined as follows.

$$\zeta_i = \frac{X_i - X_c}{d}$$

Note that it is actually linear transformations of the original  $X_i$ .

For example, response in a chemical investigation might be yield( $Y$ ) of sulfuric acid and the input variables affecting this yield might be the

pressure( $X_1$ ) and temperature( $X_2$ ) of the reaction. The mathematical pattern is

$$Y = f(X_1, X_2) + \epsilon$$

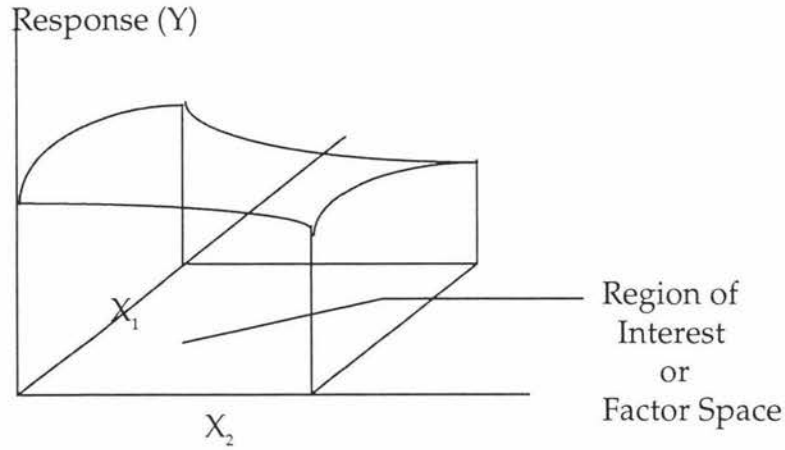


Figure 1.5.1

It can be drawn in three dimensional space. That is, response surface can be obtained in three dimensional space. It is shown in the Figure(1.5.1).

In general, if function  $f$  is approximated by a polynomial of degree  $d$ , the model is called a  $d^{\text{th}}$  order model and at least one of the factors level should be  $d+1$ . For example, if function  $f$  is approximated by a polynomial of degree 1, this level of the factor is 2 and a 1<sup>st</sup> order model of the function  $f$  has the form :

$$f(X_1, X_2, \dots, X_k) = \beta_0 + \sum_{i=1}^k \beta_i X_i \quad (1.31)$$

where  $\beta$  is a parameter vector,  $\beta^t = (\beta_0, \beta_1, \dots, \beta_k)$

If function  $f$  is approximated by a polynomial of degree 2, then at least one of the factors level is 3 and a 2<sup>nd</sup> order model of the function  $f$  has the form :

$$f(X_1, X_2, \dots, X_k) = \beta_0 + \sum_{i=1}^k \beta_i X_i + \sum_{i=1}^k \beta_{ii} X_i^2 + \sum_{j(<i)} \sum_i \beta_{ij} X_i X_j \quad (1.32)$$

where  $\beta$  is a parameter vector and

$$\beta^t = (\beta_0, \beta_1, \dots, \beta_k, \beta_{11}, \dots, \beta_{kk}, \beta_{12}, \dots, \beta_{(k-1)k})$$

Since a lot of responses are observed when factors are more than three, so it is very difficult to investigate these situations. This difficulty is overcome by using fractional replication in the response surface design.

## **1.6 Aim of the Research**

The main aim of this research is to find an efficient run order for various models of two level factorial experiments, three level factorial experiments, etc. when errors are assumed to follow either first order moving average model or first order autoregressive model. Further, we are trying to get a general procedure for various model to obtain an efficient design. For this, Chapter 2 and Chapter 3 cover 2-level and 3-level factorial experiments respectively and Chapter 4 deals with response surface estimation.

## CHAPTER 2

### RESULTS FOR 2-LEVEL FACTORIAL EXPERIMENTS

In this chapter, we discuss the results for the 2-level factorial experiment and find the statistical and mathematical reasons for these results when successive observations are serially correlated. Finally suggestions will be given how to get most efficient design for various situations.

#### 2.1 MA(1) Correlated Models in the $2^3$ Factorial Experiment

The aim of this section is to discuss the efficiency of the design of a  $2^3$  factorial experiment when the errors are assumed to follow MA(1) correlated model. Three cases will be considered:

- (i) Main effects only.
- (ii) Full model.
- (iii) No highest order interaction in the model.

##### 2.1.1 Main Effects Only

Constantine [1989] investigated the efficiency of designs for the main effects model of the  $2^3$  factorial experiment when the errors are assumed to follow MA(1) correlated models. The D-efficiency criterion, explained in section 1.3.1, was initially used to find the most efficient design. He showed theoretically that a 1<sup>st</sup> order linear approximation  $V^{-1}$  may be used to find the efficient run order of the experiment. To confirm this, the basic definition of the D-efficiency and a value based on his linear approximation of  $V^{-1}$  approach were compared for finding the efficient design. Finally he showed numerically that the same design is obtained as most efficient in both cases.

From his analysis, he concluded that having maximum or minimum number of sign changes in each column of the design is most efficient with respect to positive or negative association respectively between successive observations. In 2-level factorial experiment, a transition from either -1 to 1 or 1 to -1 is a one sign change and it is explained below by a simple example. Consider the design, *Equation (1.5)* in page 9, the number of sign changes in the 1<sup>st</sup>, 2<sup>nd</sup>, 3<sup>rd</sup> and 4<sup>th</sup> column of the design matrix are 0, 7, 3, 1 respectively.

The following shortcomings were found in his approach:

- (i) When he calculate the D-efficiency, he included the overall mean column in the design matrix. Since this is a nuisance parameter, it is not an appropriate method to take this parameter into account. Efficiency should be calculated using the adjusted information matrix however it does not affect the ordering of the designs (see section 1.3.2 ).
- (ii) Only 35 different designs are considered for a  $2^3$  factorial experiment by Constantine, but actually 840 different designs are possible for a  $2^3$  factorial experiment (see section 1.1.5). Further, some of his designs were not full factorial design.
- (iii) D-efficiencies for  $\rho = 0.25$ , as given in table format in his paper [Constantine 1989], are wrongly calculated.

Let  $ijkl$  denote the main effects design matrix consisting of the  $i^{\text{th}}$ ,  $j^{\text{th}}$ ,  $k^{\text{th}}$  and  $l^{\text{th}}$  columns of the matrix  $X$  *Equation(1.6)* given in the section 1.1.5. where  $1 \leq i, j, k, l \leq 8$  . That means, columns  $i, j, k, l$  are considered as columns of the main effect design matrix. This notation was used by Constantine. For example, 1468 means 1<sup>st</sup>, 4<sup>th</sup>, 6<sup>th</sup> and 8<sup>th</sup> column of the said design matrix  $X$ . Using his notation D-efficiencies are correctly calculated for his designs and given in *Table 2.1*.

Table 2.1

Design	D-efficiency	Design	D-efficiency
1468	10.053	1247	8.1652
1467	9.6125	1268	8.1263
1478	9.2092	1356	7.7134
1346	9.3290	1578	7.7028
1678	8.8306	1267	7.8237
1348	8.9139	1234	7.9067
1456	9.0609	1358	7.4706
1347	8.5460	1278	7.4443
1368	8.5699	1236	7.5954
1458	8.7635	1357	7.1379
1367	8.1830	1245	7.7700
1246	8.9133	1238	7.2123
1457	8.3848	1256	7.3747
1568	8.3238	1258	7.0840
1378	7.8506	1237	6.9578
1248	8.4552	1257	6.8245
1567	7.9311	1235	6.6211
1345	8.1323		

We use another notation to produce all 840 full factorial  $2^3$  designs. That is  $i, j, k$  denotes  $i^{\text{th}}, j^{\text{th}}$  and  $k^{\text{th}}$  column of matrix  $M$  given in *Appendix 1*, where  $1 \leq i, j, k \leq 35$ . That means, if an overall mean column is included in the design matrix, columns  $1^*, i, j, k$  are considered as columns of the main effect design, where  $1^*$  is a  $(8 \times 1)$  column vector which contains all plus. It is known as the nuisance parameter column.

We find that the design with columns  $1^*, 8, 17, 21$  of the  $M$  matrix provides the highest D-efficiency value 10.053 for  $\rho = 0.25$  among the 840 designs. Therefore column  $1^*, 8, 17, 21$  is the main effect design matrix which is most efficient too. This design is the same as design 1468 which was selected as the most efficient design by Constantine. The design matrix is given below.

$$\begin{bmatrix} +1 & +1 & -1 & -1 \\ +1 & -1 & +1 & +1 \\ +1 & +1 & +1 & -1 \\ +1 & -1 & -1 & +1 \\ +1 & -1 & +1 & -1 \\ +1 & +1 & -1 & +1 \\ +1 & -1 & -1 & -1 \\ +1 & +1 & +1 & +1 \end{bmatrix}$$

It is observed from this design that sign changes of column 2, 3, and 4 of this design are 6, 5 and 7 respectively. This is the maximum possible number of sign changes in the  $2^3$  main effect factorial design. Therefore, maximum number of sign changes in each column of the design matrix is the most efficient design when successive observations are positively correlated. The dispersion matrix  $\mathbf{D}$  is given below with respect to the design with column 1\*, 8, 17, 21 of the matrix.

$$\mathbf{D} = \begin{pmatrix} 0.1787 & -0.007 & 0.0000 & 0.0000 \\ -0.007 & 0.0818 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0976 & 0.0084 \\ 0.0000 & 0.0000 & 0.0084 & 0.0695 \end{pmatrix}$$

The variances for estimates of the parameters are given by diagonal elements of the  $\mathbf{D}$  matrix, in which the first diagonal element of the  $\mathbf{D}$  matrix represent the variance of the nuisance parameter. Therefore, the (3x3) lower part of the  $\mathbf{D}$  matrix, called here the  $\mathbf{D}^*$  matrix, is appropriate for efficiency measures. Since, variance for the estimates of the parameters are 0.082, 0.098, 0.069 which are quit small, so that it is preferable to estimate the parameters. In addition, the covariance of the estimates of the first parameter and second parameter, and first parameter and third parameter are zero. That means, there is no correlation between those estimates. Since correlation coefficient between the second and third parameter estimates is 0.102, therefore those two parameter estimates are weakly correlated. We may conclude from these argument that parameters are estimated effectively.

A histogram of D-efficiency values for all 840 design is given in *Appendix 2*. The alternative measures of A-efficiency and E-efficiency are also considered, but these measures give the same efficient design as we found earlier. That means, any one of the efficiency measures is enough to find the efficient design under this situation. Thus, we concentrate only D-efficiency alone. We have discussed up to this point efficiency for a single value  $\rho = 0.25$ . Next we are trying to find efficient designs among the 840 designs for various values of  $\rho$  ( $-0.5 < \rho < 0.5$ ). Results are given in *Table 2.2* and *Figure 2.1*.

Table 2.2

$\rho$ values	Maximum D-efficiency	Design from M matrix	Sign Changes
-0.4	12.375	1, 15, 28	} 2, 2, 3
-0.3	10.558	1, 15, 28	
-0.2	9.379	1, 15, 28	
-0.1	8.567	1, 15, 28	
0.0	8.000	Any one	
0.1	9.198	8, 17, 21	} 6, 5, 7
0.2	10.969	8, 17, 21	
0.3	13.827	8, 17, 21	
0.4	19.342	8, 17, 21	

It is possible to get the sign changes for the main effect columns of the  $2^3$  factorial experiment design matrix as 1, 2, 3 when  $\rho$  is negative, but it is not a full factorial design. Therefore minimum sign changes for the main effect columns of the  $2^3$  full factorial experiment design matrix are 2, 2, 3. This corresponding design is found as most efficient design when  $\rho$  is negative. That means, minimum number of sign changes for the main effect columns of the  $2^3$  full factorial experiment design matrix' is most efficient design when  $\rho$  is negative.



Note that  $\rho = 0$  means successive observations are not correlated.

That is,  $V = \sigma^2 I_8$

Therefore  $C = X^T V^{-1} X = 8I_4$  [ $\because X$  is a  $(8 \times 4)$  orthogonal matrix]

Hence D-efficiency  $= |C|^{1/4} = [8^4]^{1/4} = 8$  (2.1)

Thus, in the uncorrelated case we can say that D-efficiency does not depends on the design matrix. Therefore any design may be chosen as the most efficient design for this case.

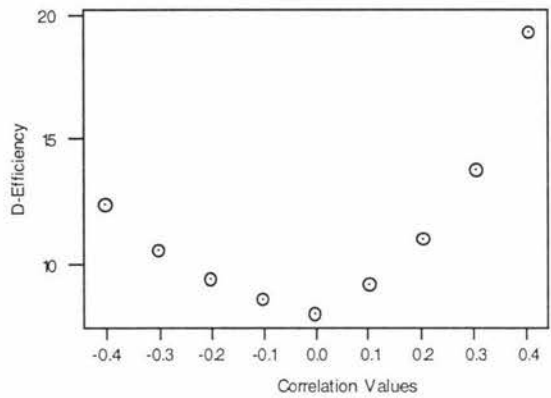


Figure 2.1

We can see from the Figure(2.1), large positive correlation or small negative correlation appears to give a large gain in D-efficiency. Therefore D-efficiency of the design not only depends on the sign changes of the design matrix but also depends on the value of the correlation between successive observations.

However, we can see from Table 2.2 that the same design with column 1\*, 8, 17, 21 from M matrix is the most efficient for various positive correlation between successive observations, and same design with column 1\*, 1, 15, 28 from M matrix is the most efficient for various negative correlation between successive observations. Therefore, since positive correlation is more likely in practice, in our future analysis the correlation between successive observations is kept as positive constant ( $\rho = 0.25$ ).

### 2.1.2 Full Model

The full model of two level factorial experiment includes both all main effects and all interaction effects of the factors. In some situations under this model, all the effects can be calculated, but it cannot be tested due to the unknown error term. It is known as a saturated design.

If we consider the full model of the  $2^3$  factorial, the design matrix  $X$  is a  $(8 \times 8)$  full orthogonal matrix. An example is given in the *Equation(1.6)*, section 1.1.5. Thus,  $X^t X = 8 I_8$

$$\text{Therefore, } X^{-1} = \frac{1}{8} X^t \quad (2.2)$$

Hence, the dispersion matrix can be written as follows.

$$\begin{aligned} D &= (X^t V^{-1} X)^{-1} \\ &= X^{-1} V (X^t)^{-1} \\ &= \frac{1}{8^2} X^t V X \quad [\because X \text{ is a } (8 \times 8) \text{ orthogonal matrix}] \end{aligned} \quad (2.3)$$

We can algebraically prove that D-efficiency or A-efficiency or E-efficiency for various full designs has always same value. The mathematical proof for these results is considered in two cases, given below.

- (i) The nuisance parameter (overall mean) is included in the design matrix.

$$\begin{aligned} \text{D-efficiency} &= |C|^{1/\alpha} \\ &= |D|^{-1/\alpha} \\ &= \left| \frac{1}{8^2} X^t V X \right|^{-1/\alpha} \\ &= \left[ \frac{1}{8^2} |X^t \|V\| X| \right]^{-1/\alpha} \\ &= \left[ \frac{1}{8^2} |X^t X \|V\| \right]^{-1/\alpha} \end{aligned}$$

$$= \left[ \frac{1}{8} |V| \right]^{-1/\alpha} \quad [\because X \text{ is a } (8 \times 8) \text{ orthogonal matrix}] \quad (2.4)$$

We can easily say from *Equation(2.4)* that D-efficiency is not dependent on the design matrix  $X$  and only depends on the covariance matrix  $V$  which is a constant matrix. Therefore, D-efficiency is a constant value for any orthogonal full design matrix.

$$\begin{aligned} \text{trace}(D) &= \text{trace}\left(\frac{1}{8^2} X^t V X\right) \\ &= \frac{1}{8^2} \text{trace}(X^t X V) \quad [\because \text{Trace property}] \\ &= \frac{1}{8^2} \text{trace}(8I_8 V) \quad [\because X \text{ is a } (8 \times 8) \text{ orthogonal matrix}] \\ \text{trace}(D) &= \frac{1}{8} \text{trace}(V). \end{aligned} \quad (2.5)$$

$$\begin{aligned} \text{A-efficiency} &= \text{sum of the eigenvalues of } C^{-1} \\ &= \text{trace}(D) \\ &= \frac{1}{8} \text{trace}(V). \end{aligned} \quad (2.6)$$

According to the *Equation(2.5)*, the trace of the  $D$  matrix is also constant. Therefore A-efficiency for various designs of full model is constant.

Let  $\lambda$  be an eigenvalue of matrix  $D$ . Thus  $|D - \lambda I| = 0$ . By using the *Equation(2.2)*, it is equivalent to  $\left| \frac{1}{8} V - \lambda I \right| = 0$ . Hence eigenvalues  $\lambda$  of  $D$  are eigenvalues of  $\frac{1}{8} V$  and vice versa. Therefore E-efficiency for any orthogonal full design matrix is constant.

(ii) Nuisance parameter is not included in the efficiency measure, but is in the model.

The partition of the information matrix  $C$  provided from *Equation(1.23)* that,  $|C| = |C_{11}| |C_{22.1}|$  where  $C_{11} = \underline{1}^t V^{-1} \underline{1}$  is a single element and  $\underline{1}$  is a  $(8 \times 1)$

column matrix whose elements are one. Hence  $|C_{22.1}| = \frac{|C|}{|C_{11}|}$ . Since  $|C|$  is a constant for the full model case, so  $|C_{22.1}|$  is also a constant. From section 1.3.2, D-efficiency =  $|C_{22.1}|^{1/(\alpha-1)}$ . Therefore D-efficiency for this case is a constant too.

$\text{trace}(\mathbf{D})$  = sum of the diagonal element of  $\mathbf{D}$ .

$$= d_{11} + \text{trace}(\mathbf{D}_{22}).$$

Since  $\text{trace}(\mathbf{D})$  is a constant in the full model case and  $d_{11} = \frac{1}{8^2} \mathbf{1}^t \mathbf{V} \mathbf{1}$  is a constant, so that  $\text{trace}(\mathbf{D}_{22})$  is a constant. Therefore A-efficiency =  $\text{trace}(\mathbf{D}_{22})$  is also a constant.

Under this situation, the E-efficiency is the largest eigenvalue of  $C_{22.1}$ . The matrix  $C$  can be partitioned as follows.

$C = \begin{bmatrix} \mathbf{1}^t \\ \mathbf{X}^t \end{bmatrix} V^{-1} [\mathbf{1} \mid \mathbf{X}]$ , where  $\mathbf{X}$  is a  $n \times (n-1)$  matrix whose columns are orthogonal to  $\mathbf{1}$ . (2.7)

$$C = \begin{bmatrix} \mathbf{1}^t V^{-1} \mathbf{1} & \mathbf{1}^t V^{-1} \mathbf{X} \\ \mathbf{X}^t V^{-1} \mathbf{1} & \mathbf{X}^t V^{-1} \mathbf{X} \end{bmatrix}$$

$$\text{Hence, } C_{22.1} = \mathbf{X}^t \left[ V^{-1} - \frac{V^{-1} \mathbf{1} \mathbf{1}^t V^{-1}}{\mathbf{1}^t V^{-1} \mathbf{1}} \right] \mathbf{X}. \quad (2.8)$$

Let  $V^* = \left[ V^{-1} - \frac{V^{-1} \mathbf{1} \mathbf{1}^t V^{-1}}{\mathbf{1}^t V^{-1} \mathbf{1}} \right]$  then  $C_{22.1} = \mathbf{X}^t V^* \mathbf{X}$ . The dimension of the matrices  $C_{22.1}$  and  $V^*$  are  $(n-1) \times (n-1)$  and  $(n \times n)$  respectively, and one eigenvalue of  $V^*$  matrix is zero with corresponding eigenvector  $\mathbf{1}^t$ . Suppose the non zero eigenvalues of the  $V^*$  matrix are namely  $\lambda_1, \lambda_2, \dots, \lambda_{n-1}$  which are constant due to the constant  $V^*$  matrix, and corresponding eigenvectors are namely  $\underline{v}_1, \underline{v}_2, \dots, \underline{v}_{n-1}$ . Because of the orthogonality property of eigenvectors, these are all orthogonal to  $\mathbf{1}$ , so are basis for the column space of  $\mathbf{X}$ .

Therefore, they can be represented as  $X\underline{u}_1, X\underline{u}_2, \dots, X\underline{u}_{n-1}$ , where  $\underline{u}_j$ 's are (n-1) column vectors for  $j = 1, 2, \dots, n-1$ .

Consider  $C_{22.1}\underline{u}_j = X^t V^* X \underline{u}_j ; j = 1, 2, \dots, n-1$ .

$$\begin{aligned} &= X^t V^* \underline{v}_j \\ &= X^t \lambda_j \underline{v}_j \quad [\because \underline{v}_j \text{ is the eigen vector of } V^* \text{ matrix}] \\ &= \lambda_j \underline{u}_j \quad [\because \underline{v}_j = X \underline{u}_j \text{ and } X^t X = I_{n-1}]. \end{aligned} \quad (2.9)$$

Since this is true for all  $j = 1, 2, \dots, (n-1)$ , so that constant values of  $\lambda_1, \lambda_2, \dots, \lambda_{n-1}$  are the eigenvalues of the matrix  $C_{22.1}$ . Therefore the maximum eigenvalue of the matrix  $C_{22.1}$  is a constant. That is, E-efficiency is also constant under this situation.

Hence, the measures of D-efficiency, A-efficiency and E-efficiency are no longer useful for the full model due to the constant measure. Note that it is explained only for three factors case, but this result is true for any number of factors.

Measures of efficiency need thus to be redefined for the full model case. For this, a new E'-efficiency is defined as the maximum value of the diagonal elements of D matrix excluding the first diagonal element. That is, E'-efficiency is the maximum variance for the estimates of the parameter except nuisance parameter. Smaller variation is commonly desired in an experiment. Therefore the minimum value of E'-efficiency is the most efficient design. That means, this criterion looks like a minimax criterion which is used to find the most efficient design in the full model case.

By considering the  $2^3$  factorial experiment for the full model, the E'-efficiency of various designs is investigated when the correlation between successive observations is 0.25. Note that only three different E'-efficiencies namely 0.1328, 0.1484, 0.1641 are obtained among the 840 designs. That means, three different groups of designs are available. Sign

changes for full design matrix of different groups are 3, 3, 4, 4, 4, 5, 5; 2, 3, 3, 4, 5, 6 and 1, 3, 3, 4, 4, 6, 7. Therefore, these groups are distinguished by minimum number sign changes of the full design matrix being either 3, 2 or 1. Maximum of the minimum number of sign changes of the full design matrix gives best E'-efficiency. Therefore, we can conclude that maximising the minimum number of sign changes of the full design matrix provides an efficient design for the full model.

The diagonal elements of the  $D = \frac{1}{n^2} X^t V X$  matrix, which give the variance of the parameter estimates, for full model of the  $2^n$  factorial experiment can be given as follows.

$$d_{jj} = \frac{1}{8^2} \begin{pmatrix} x_{1j} & x_{2j} & \dots & x_{nj} \end{pmatrix} \begin{pmatrix} 1 & \rho & 0 & \dots & 0 \\ \rho & 1 & \rho & 0 & \dots & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \rho & 1 \end{pmatrix} \begin{pmatrix} x_{1j} \\ x_{2j} \\ \cdot \\ \cdot \\ x_{nj} \end{pmatrix}$$

$$d_{jj} = \frac{1}{64} \left( \sum_{i=1}^n x_{ij}^2 + 2\rho \sum_{i=1}^{n-1} x_{ij} x_{i+1j} \right) \text{ for } j = 1 \dots n. \quad (2.10)$$

where  $x_{ij}$  is the  $(i,j)^{th}$  element of  $(n \times n)$  design matrix  $X$  and takes the value +1 or -1. Note that there is a relationship between the expression

$\sum_{i=1}^{n-1} x_{ij} x_{i+1j}$  and number of sign changes of the particular column. That is,  
 $\sum_{i=1}^{n-1} x_{ij} x_{i+1j} = (n-1) - 2S_j$  for all  $j = 1, \dots, n$ , where  $S_j$  is the total number of sign changes for  $j^{th}$  column.

Since  $\sum_{i=1}^n x_{ij}^2 = n$  is always constant, thus it is indicated that  $d_{jj}$  is small if either  $\sum_{i=1}^{n-1} x_{ij} x_{i+1j}$  is negative when  $\rho$  is positive or  $\sum_{i=1}^{n-1} x_{ij} x_{i+1j}$  is positive when  $\rho$  is negative. Since smaller variance of the parameters estimates gives a more efficient design, the sequence  $\{x_{ij}\}_{i=1}^n$  for the  $j^{th}$  column of the

design matrix  $X$  should be either  $-1, 1, -1, 1, \dots$  when  $\rho$  is positive or  $-1, -1, \dots, -1, 1, \dots, 1, 1, 1$  when  $\rho$  is negative. We can therefore mathematically say that having maximum/minimum number of sign changes of the single column when correlation between successive observations is positive/negative leads to the smallest possible variance for the corresponding parameter estimate. For the full model with MA(1) errors, the variance of the estimator depends only on the number of sign changes in the corresponding column.

A model which is reduced from the full model by equating some parameters to zero, is defined as a reduced model. The design matrix for the reduce model is obtained by deleting some columns from the full design matrix. The actual covariance matrix  $D_R$  for the reduced model is given below.

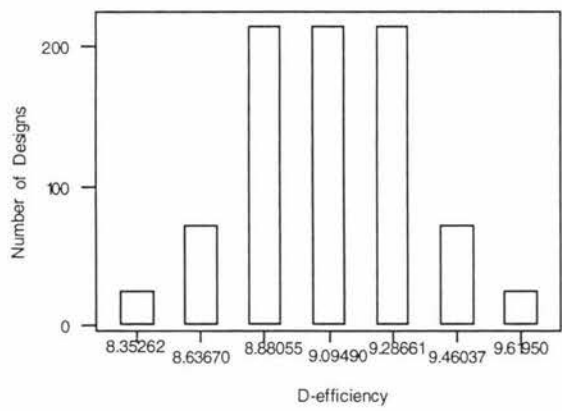
$$\begin{aligned} D_R &= [X^t V^{-1} X]^{-1} \quad [\because X \text{ is not a full design matrix}] \\ &= C_{11}^{-1} \quad [\because \text{According to the partition notation}] \\ &= D_{11} - D_{12} D_{22}^{-1} D_{21} \quad [\because \text{From Equation(1.25)}]. \end{aligned}$$

Due to orthogonal property and MA(1) correlation model, the off diagonal elements of the dispersion matrix  $D$  are relatively small. That is, the elements of the matrices  $D_{12}$  and  $D_{21}$  are small which are negligible. That means,  $D_R$  is approximately same as  $D_{11}$ . This gives a strategy for suggesting designs which should be efficient for the reduced model. An example is given in the next section.

### 2.1.3 No Highest Order Interaction in the Model

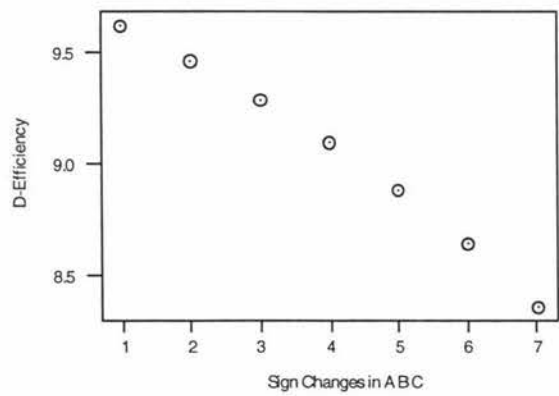
The higher order interactions are often assumed to be negligible in real life factorial experiments. For example, due to the lack of replication sometimes it may be used as an error term. We now consider the case when the highest order interaction is not in the model. That means, this is not a full model, so the D-efficiency criterion can be used to evaluate the efficient design.

All 840 different designs of the  $2^3$  factorial experiment are considered to investigate this situation practically when  $\rho = 0.25$ . Only seven different D-efficiency values are obtained for the various 840 different designs. This information is clearly given in the *Figure(2.2)*.



*Figure 2.2*

Since the minimum and maximum number of sign changes for any column, except the nuisance parameter column, of the design matrix which is obtained from  $2^3$  factorial experiment are one and seven respectively, so that seven different numbers of sign changes are possible for the interaction  $A \times B \times C$  column. This may be the reason for seven different values of D-efficiency. The *Figure(2.3)* confirms that the D-efficiency of the model is determined by the number of sign changes of the interaction  $A \times B \times C$  which is not in the model.



*Figure 2.3*



It is indicated that the minimum sign change of interaction  $AxBxC$ , which is one, gives the highest D-efficiency for the said model. That is, an efficient design for this model is generally obtained when the number of sign changes in the highest order interaction  $AxBxC$  is one. Next this result is to be proved algebraically.

$$\begin{aligned}
|D| &= \begin{vmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{vmatrix} \quad [\because \text{From Equation(1.20)}] \\
&= |D_{11}D_{22} - D_{12}D_{21}| \\
&\equiv |D_{11}D_{22}| \quad [\because \text{correlated model and orthogonal} \Rightarrow D_{12} \equiv 0 \equiv D_{21}] \\
&= |D_{11}|d_{88} \quad [\because \text{particularly this case } D_{22} = d_{88}]. \tag{2.11}
\end{aligned}$$

The interaction  $AxBxC$  is the highest order interaction in the  $2^3$  factorial experiment and  $d_{88}$  is the variance of the interaction  $AxBxC$  effect. It is desired to have a small variance for the other parameters. That means, a small determinant of  $D_{11}$  is wanted. But the determinant of  $D$  is constant, so that  $d_{88}$  needs to be large. With reference to the *Equation(2.10)*, it can be made by considering the situation either minimum number of sign changes in the 8<sup>th</sup> column of the design matrix  $X$  when  $\rho$  is positive or maximum number of sign changes in the 8<sup>th</sup> column of the design matrix  $X$  when  $\rho$  is negative. That is, to provide an efficient design, the column corresponding to the interaction  $AxBxC$  for the full design matrix  $X$  may be allocated as either  $-1, -1, -1, -1, 1, 1, 1, 1$  when  $\rho$  is positive or  $-1, 1, -1, 1, -1, 1, -1, 1$  when  $\rho$  is negative. We can see that this result coincides with our practical results.

But *Figure(2.2)* tell us only twenty-four different designs are available as most efficient among the 840 designs. That is, twenty-four different efficient designs are obtained when the number of sign changes at the higher order interaction  $Ax BxC$  of the  $2^3$  factorial experiment is one.

A general procedure to obtain an efficient design for 2 level factorial experiments when the highest order interaction is not in the model, is given below.

Step 1: Define the odd set and even set.

If the number of factors is an odd number, odd set = {1, 2factor interaction, 4factor interaction, . . . . } and even set = {longest string in the design, main effects, 3factor interaction, 5factor interaction, . . . . . }.

If the number of factors is an even number, odd set = {main effects, 3factor interaction, 5factor interaction, . . . . } and even set = {1, longest string in the design, 2factor interaction, 4factor interaction, . . . . . }.

Step 2: To get the design, write down the odd set followed by the even set or vice versa.

For example, odd set and even set for the  $2^3$  factorial experiment are {1, ab, ac, bc} and {abc, a, b, c} respectively. Therefore a suitable run order for an efficient design when the highest order interaction is not in the model is 1, ab, ac, bc, abc, a, b, c and corresponding design matrix is given below.

$$\begin{bmatrix} +1 & -1 & -1 & -1 & +1 & +1 & +1 \\ +1 & +1 & +1 & -1 & +1 & -1 & -1 \\ +1 & +1 & -1 & +1 & -1 & +1 & -1 \\ +1 & -1 & +1 & +1 & -1 & -1 & +1 \\ +1 & +1 & +1 & +1 & +1 & +1 & +1 \\ +1 & +1 & -1 & -1 & -1 & -1 & +1 \\ +1 & -1 & +1 & -1 & -1 & +1 & -1 \\ +1 & -1 & -1 & +1 & +1 & -1 & -1 \end{bmatrix} \quad (2.12)$$

The sign changes for  $2^{\text{nd}}, 3^{\text{th}}, 4^{\text{th}}, 5^{\text{th}}, 6^{\text{th}}, 7^{\text{th}}$  columns of this design matrix are 4, 5, 3, 3, 7, 4 respectively.

Consider an other example when the number of factors is even. The odd set and even set for the  $2^4$  factorial experiment are {a, b, c, d, abc, abd, acd, bcd} and {1, abcd, ab, ac, ad, bc, bd, cd } respectively. Therefore a suitable run order for an efficient design when the highest order interaction(ABCD) is not in the model, is a, b, c, d, abc, abd, acd, bcd, 1, abcd, ab, ac, ad, bc, bd, cd and corresponding design matrix is given below.

+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	-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	-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	+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	+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	+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	-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	-1
+1	-1	-1	+1	+1	+1	-1	-1	-1	-1	+1	+1	+1	-1	-1

The sign changes for  $2^{nd}$ ,  $3^{th}$ ,  $4^{th}$ ,  $5^{th}$ ,  $6^{th}$ ,  $7^{th}$ ,  $8^{th}$ ,  $9^{th}$ ,  $10^{th}$ ,  $11^{th}$ ,  $12^{th}$ ,  $13^{th}$ ,  $14^{th}$ ,  $15^{th}$  columns of this design matrix are 5, 10, 13, 9, 5, 12, 8, 7, 11, 4, 8, 12, 9, 6 respectively.

In both case, we can see from the above designs that the number of sign changes for highest order interaction is one. That means, the above mentioned procedure gives an efficient run order for 2-level factorial experiment when the highest order interaction is not in the model.

## 2.2 AR(1) Correlated Models in the $2^3$ Factorial Experiment

This section is similar to section 2.1. The only difference is that successive observations are assumed to follow an AR(1) correlated model. Three cases of the  $2^3$  factorial experiment will be considered under this situation:

- (i) Main effects only
- (ii) Full model
- (iii) No highest order interaction in the model.

### 2.2.1 Main Effects Only

Ching-Shui Cheng and David M. Steinberg [Cheng & Steinberg, 1991] investigated the effect of different run orders on the efficiency of the design for the main effects model of the 2-level factorial experiment when observations are correlated by a first order autoregressive error model. The D-efficiency criterion is used to find the efficient design. Results of this situation were found to be similar to Constantine's results. That is, run orders with many sign changes will be efficient when observations are positively correlated. According to this result, they provided an algorithm to find the efficient run order for any number of factors. It is known as the reverse foldover algorithm. According to their algorithm [Cheng & Steinberg, 1991], the following steps are needed to find the most efficient run order.

- “ (1) Select as the first generator the longest string in the design. If there are several such strings, any may be selected.
- (2) Select the remaining generators, choosing at each step the longest string in the design that preserves a generator set. Ties may be broken arbitrarily.
- (3) Choose any run as the first run in the design.
- (4) Having written down the first  $2^u$  runs,  $0 \leq u \leq k - p$ , generate the next  $2^u$  as follows: write down the  $2^u$  runs in reverse order and multiply each of the new runs by the  $(u+1)^{\text{st}}$  generator.
- (5) Repeat step 4 until the entire design has been generated.”

They used the  $2^4$  factorial experiment for illustration. Here we consider the  $2^3$  factorial experiment which makes it easier to check their algorithm due to the possibility of examining all 840 designs. Therefore we are trying to confirm this algorithm via the  $2^3$  factorial experiment systematically rather than using randomized run orders of the  $2^4$  experiment.

Consider the  $2^3$  factorial experiment to find the efficient run order with respect to the reverse foldover algorithm. The run order 'abc' is the first generator. Any two runs with two factors at high level can be used as remaining generators, say 'ab' and 'bc'. Let 'a' be the first run. According to step 4, the first two runs are 'a' and 'bc' [ $\because a \times abc = bc$ ]. Reversing the order and multiplying by 'ab', third and fourth run orders will be 'ac' [ $\because bc \times ab = ac$ ] and 'b' [ $\because a \times ab = b$ ] respectively. Again reversing the order and multiplying by 'bc' provides the complete run order: a, bc, ac, b, c, ab, 1, abc and the design matrix given below according to this run order.

$$\begin{bmatrix} +1 & +1 & -1 & -1 \\ +1 & -1 & +1 & +1 \\ +1 & +1 & -1 & +1 \\ +1 & -1 & +1 & -1 \\ +1 & -1 & -1 & +1 \\ +1 & +1 & +1 & -1 \\ +1 & -1 & -1 & -1 \\ +1 & +1 & +1 & +1 \end{bmatrix} \quad (2.13)$$

This run order has the 18 sign changes which is the total maximum possible. According to our notation of section 2.1.1, representation of this design is columns 1\*, 8, 21, 17 of the M matrix. This design is the same as Constantine's efficient design.

Note that the algorithm gives different run orders depending on the selection of first run order. For example, if we select the first run order as '1' and generator as 'abc', 'ab' and 'bc' then the final run order will be 1, abc, c, ab, ac, b, a, bc. However, the total number of sign changes for this

design is eighteen and D-efficiency of the new design will be the same as the earlier design *Equation(2.13)* due to the arbitrary allocation of high/low levels. That means, the D-efficiency value does not change if we interchange all plus one and all negative one for particular column.

We find that the design with columns 1\*, 8, 17, 21 of the M matrix provides the highest D-efficiency value 11.5441 for  $\rho = 0.25$  among the 840 designs. Therefore column 1\*, 8, 17, 21 is the main effects design matrix which is most efficient. That is, the most efficient design of the  $2^3$  factorial experiment, which is obtained by an exhaustive search, coincides with the efficient design of 2-level factorial experiment which is obtained by the foldover algorithm.

The dispersion matrix D is given below with respect to the design with column 1\*, 8, 17, 21 of matrix M when  $\rho = 0.25$ .

$$D = \begin{bmatrix} 0.1923 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.1233 & 0.0199 & -0.0017 \\ 0.0000 & 0.0199 & 0.1015 & 0.0199 \\ 0.0000 & -0.0017 & 0.0199 & 0.1233 \end{bmatrix}$$

We can see that variances of the parameter estimates are very small and off diagonal elements of the D matrix are almost zero. It indicates that parameters will be effectively estimated by the above mentioned design matrix. A histogram of D-efficiency values for 840 design under this situation is given in *Appendix 3*. The alternative measures of A-efficiency and E-efficiency were considered to find different efficient designs, but these measures also give same efficient design as we found earlier.

Since this is an AR(1) model, theoretically  $\rho$  lies between negative one to positive one. Therefore we need to consider the D-efficiency for various values of  $\rho$ . Results are given in *Table(2.3)* and *Figure(2.4)*.

Table 2.3

$\rho$ values	Maximum D-efficiency	Design from M matrix	Sign Changes
-0.9	86.4043	1, 15, 28	2, 2, 3
-0.8	41.8552	1, 15, 28	
-0.7	27.1016	1, 15, 28	
-0.6	19.8109	1, 15, 28	
-0.5	15.5193	1, 15, 28	
-0.4	12.7424	1, 15, 28	
-0.3	10.8478	1, 15, 28	
-0.2	9.5242	1, 15, 28	
-0.1	8.6053	1, 15, 28	
0.0	8	Any one	6, 5, 7
0.1	9.1421	8, 17, 21	
0.2	10.6305	8, 17, 21	
0.3	12.6011	8, 17, 21	
0.4	15.2838	8, 17, 21	
0.5	19.0957	8, 17, 21	
0.6	24.8742	8, 17, 21	
0.7	34.5774	8, 17, 21	
0.8	54.0859	8, 17, 21	
0.9	112.8235	8, 17, 21	

Note that  $\rho = 0$  situation is similar to section 2.1.1 (see Equation 2.1). We can say from Table 2.3 that the efficient design depends only on the correlation sign. We can see from the Table 2.2 and Table 2.3 that D-efficiency values for both cases are almost same when  $\rho$  values are small and same efficient design is found whether the MA(1) or AR(1) model is assumed.

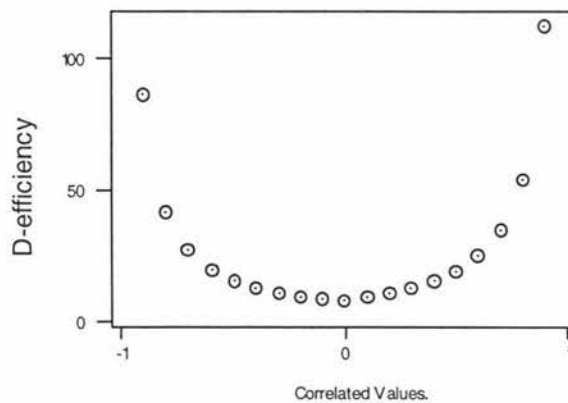


Figure 2.4

We wish to know how D-efficiency is affected by the total number of sign changes of the design matrix  $X$  when  $\rho$  is either large or small. 840 designs

were considered for this when  $\rho = 0.25$  and  $\rho = 0.9$ . D-efficiency versus total number of sign changes of the design matrix  $X$  were plotted in both cases. These are given in *Appendix 4 & 5*. We can see from *Appendix 4 & 5* that D-efficiency is gradually increased as the total number of sign changes of the design matrix  $X$  increases. However the maximum D-efficiency value for a given number of total sign changes is in general greater than the minimum D-efficiency value obtained where there is one more sign change. We can observe that very few designs overlapped when  $\rho = 0.25$ , but lot of designs overlapped when  $\rho = 0.9$ . That is, the amount of overlap of the range of D-efficiency values in successive numbers of sign changes is increased as  $\rho$  value increase. This will be discussed in section 2.2.3 algebraically.

### 2.2.2 Algorithm for Minimum Number of Sign Changes of Design Matrix

We have already mentioned that the minimum/maximum number of sign changes of the design matrix is most efficient when the correlation coefficient is negative/ positive. But Cheng and Steinberg only gave an algorithm to get the maximum number sign changes in the run order. We are providing below an algorithm which gives the minimum number of sign changes in the run order. Steps for the algorithm are given below.

- Step 1: Select the first run order as longest string in the design.
- Step 2: Select as generators the main effects high level. Viz.  $a, b, c, \dots$ , etc.
- Step 3: Having written down the first  $2^u$  runs,  $0 \leq u \leq k - p$ , generate the next  $2^u$  as follows: write down the  $2^u$  runs in order and multiply reversibly each of the new runs by the  $(u+1)^{st}$  generator.
- Step 4: Repeat step 3 until the entire design has been generated.
- Step 5: After obtaining the entire design, move the first run to the end.



Consider a  $2^3$  experiment as an example.

Step 1: abc is a first run order because it is the longest string in the design.

Step 2: a, b, c are the generators, being the high level of the main effects.

Step 3&4: Since  $(abc) \times (a) = bc$ , so first two run orders are abc, bc. Further,  $(abc, bc) \times (b) = c, ac$ , so first four run orders are abc, bc, c, ac. If we apply the same procedure, run orders of the design matrix will be abc, bc, c, ac, a, 1, b, ab.

Step 5: Final run orders of the design are bc, c, ac, a, 1, b, ab, abc.

The design matrix is obtained by algorithm and given below.

$$\begin{bmatrix} +1 & -1 & +1 & +1 \\ +1 & -1 & -1 & +1 \\ +1 & +1 & -1 & +1 \\ +1 & +1 & -1 & -1 \\ +1 & -1 & -1 & -1 \\ +1 & -1 & +1 & -1 \\ +1 & +1 & +1 & -1 \\ +1 & +1 & +1 & +1 \end{bmatrix} \quad (2.14)$$

Using our notation, this design matrix is denoted by columns 1', 1,15, 28 of the M matrix which is same as we found earlier. This algorithm is now tested only three factors case. It will be tested for four factors in section 2.3.

### 2.2.3 Full Model

In this section, all possible effects of a  $2^3$  factorial experiment are considered when errors are assumed to follow AR(1) correlated models. In the  $2^3$  factorial experiment, an  $(8 \times 8)$  orthogonal design matrix can be obtained for full model case. Hence, D-efficiency, A-efficiency and E-efficiency are no longer useful here too to find an efficient design (see section 2.1.2). According to the same argument of section 2.1.2, E'-efficiency is again used to find the efficient design.

considered separately. We now try to find the reason for this algebraically.

If  $\rho$  is small then  $\rho^2, \dots, \rho^7$  are negligible. Therefore, the V Equation(1.17) matrix under the AR(1) situation looks like a MA(1) situation V matrix Equation(1.15). Hence, the dispersion matrix  $D = \frac{1}{8^2} X' V X$  (see Equation (2.15)) for the full model when errors are assumed to follow an AR(1) correlated model is approximately the same as the dispersion matrix  $D$  of full model when errors are assumed to follow an MA(1) correlated model. It indicates that  $E^*$ -efficiencies are theoretically approximately the same in both cases when  $\rho$  is small. That means, our earlier result is theoretically confirmed for full model case when  $\rho$  is small. Next, we discuss about the main effect model case.

$$D = \frac{1}{8^2} \begin{bmatrix} x_{11} & x_{21} & \dots & x_{71} & x_{81} \\ x_{12} & x_{22} & \dots & x_{72} & x_{82} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ x_{17} & x_{27} & \dots & x_{77} & x_{87} \\ x_{18} & x_{28} & \dots & x_{78} & x_{88} \end{bmatrix} \begin{bmatrix} 1 & \rho & \rho^2 & \dots & \rho^6 & \rho^7 \\ \rho & 1 & \rho & \rho^2 & \dots & \rho^5 & \rho^6 \\ \rho^2 & \rho & 1 & \rho & \dots & \rho^4 & \rho^5 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \rho^6 & \rho^5 & \rho^4 & \dots & \rho & 1 & \rho \\ \rho^7 & \rho^6 & \rho^5 & \dots & \rho & 1 & 1 \end{bmatrix} \begin{bmatrix} x_{11} & x_{12} & \dots & x_{17} & x_{18} \\ x_{21} & x_{22} & \dots & x_{27} & x_{28} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ x_{71} & x_{72} & \dots & x_{77} & x_{78} \\ x_{81} & x_{82} & \dots & x_{87} & x_{88} \end{bmatrix} \quad (2.15)$$

Since we are considering about the main effects model, the D-efficiency criterion can be used to find the efficient design rather than  $E^*$ -efficiency. By using the partition concept of the full model,  $C_{11}$  is enough to calculate the D-efficiency for main effects model and is defined as  $[D_{11} - D_{12}D_{22}^{-1}D_{21}]^{-1}$  (see Equation(1.24)). Remember Equation(2.3) for full model that,  $D = \frac{1}{8^2} X' V X$ .

Since if  $\rho$  is small then  $\rho^2, \dots, \rho^7$  are negligible, therefore we can easily understand from Equation(2.15) that the elements of the partition matrix  $D_{12}$  and  $D_{21}$  are small. That is,  $C_{11} \cong D_{11}^{-1}$  and the  $j^{\text{th}}$  diagonal element of the

D matrix is  $\lambda_{jj} = \frac{1}{64}(\sum_{i=1}^8 x_{ij}^2 + 2\rho \sum_{i=1}^7 x_{ij}x_{i+1,j})$  if  $\rho$  is small. That means, the main effects model with AR(1) correlated errors will give similar results to the main effects model with MA(1) errors if  $\rho$  is small. Therefore, we can generally say that we don't need to think about the error correlated models such as MA(1) or AR(1) if  $\rho$  is small.

Returning to the full model when errors are assumed to follow an AR(1) correlated model, the  $j^{\text{th}}$  diagonal element( $\lambda_{jj}$ ) of the **D** matrix (Equation(2.15)) is given below.

$$\lambda_{jj} = \frac{1}{64}(\sum_{i=1}^8 x_{ij}^2 + 2\rho \sum_{i=1}^7 x_{ij}x_{i+1,j} + 2\rho^2 \sum_{i=1}^6 x_{ij}x_{i+2,j} + 2\rho^3 \sum_{i=1}^5 x_{ij}x_{i+3,j} + \dots + 2\rho^6 \sum_{i=1}^2 x_{ij}x_{i+6,j} + 2\rho^7 x_{ij}x_{i+7,j}) \quad (2.16)$$

Due to the different lags, the product of the  $x_{ij}$  and  $x_{i+k,j}$  may be either positive or negative. For example, if we want more sign changes in the  $j^{\text{th}}$  column (viz. lag one), the product of the  $x_{ij}$  and  $x_{i+2,j}$  (viz. lag two) will tend to be positive and so on.

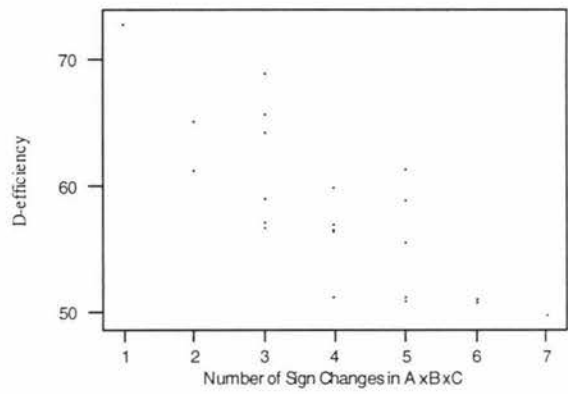
We can easily see from Equation(2.16) that a diagonal element of the **D** matrix highly depends on the sign changes at different lags in the corresponding column if  $\rho$  is large. That means,  $E^*$ -efficiency depends on other lags too. Due to the different patterns of sign changes, we have got five different  $E^*$ -efficiency values for full model when  $\rho$  is large.

#### 2.2.4 No Highest Order Interaction in the Model

We can obviously see from the previous section that this situation is similar to the same model pattern with MA(1) correlated errors when  $\rho$  is small. Therefore, this case is investigated here only for large  $\rho$  value.

All 840 different designs of  $2^3$  factorial experiment are considered to investigate this situation practically when  $\rho = 0.9$ . Seven different groups

of D-efficiency values are obtained for the various 840 different designs due to the seven possible sign changes of interaction  $A \times B \times C$  column. Within a group, different D-efficiency values are obtained due to the different pattern in the corresponding column. This information is clearly given in the *Figure(2.5)*.



*Figure 2.5*

The *Figure(2.5)* clearly indicates that the D-efficiency for the model is determined largely by the number of lag-one sign changes of interaction  $A \times B \times C$  which is not in the model. It is indicated that the minimum sign change of interaction  $A \times B \times C$  which is one, gives highest D-efficiency for the said model. That is, an efficient design for this model is generally obtained when the number of lag one sign changes of the higher order interaction  $A \times B \times C$  is one. Algebraic proof and method of approach to obtain the efficient design, given in section 2.1.3, are still valid for this situation too.

### 2.3 $2^4$ Factorial Experiment

The purpose of this section is to investigate whether results of the  $2^3$  factorial experiment are relevant to the  $2^4$  factorial experiment or not. We have already mentioned in the previous section that the first order autoregressive error correlated model is approximately the same as the first order moving average correlated model unless  $\rho$  is large. Therefore, two cases of the first order autoregressive error correlated model are

sufficient to satisfy the both error correlated model such as AR(1) and MA(1). They are (i)  $\rho$  is small  
(ii)  $\rho$  is large.

Cheng and Steinberg [Cheng & Steinberg, 1991] suggested by using reverse foldover algorithm that the same efficient design will be obtained for the main effects  $2^4$  factorial experiment, if  $\rho$  is either small or large.

By using the reverse foldover algorithm for the  $2^4$  factorial experiment, this run order will be: 1, abcd, d, abc, cd, ab, c, abd, ad, bc, acd, b, ad, bc, a, bcd. According to this run order, sign changes for the main effect columns of the design matrix are 14, 15, 13 and 11 respectively. According to the Constantine method, 15, 14, 13 and 12 sign changes for main effects columns of the design are possible for  $2^4$  factorial experiment. However those designs are not full factorial design. It is explained by following simple example.

$$\begin{bmatrix} +1 & -1 & +1 & -1 & +1 \\ +1 & +1 & -1 & +1 & -1 \\ +1 & -1 & +1 & -1 & +1 \\ +1 & +1 & -1 & +1 & -1 \\ +1 & -1 & +1 & +1 & -1 \\ +1 & +1 & -1 & -1 & +1 \\ +1 & -1 & +1 & +1 & -1 \\ +1 & +1 & -1 & -1 & +1 \\ +1 & -1 & -1 & +1 & +1 \\ +1 & +1 & +1 & -1 & -1 \\ +1 & -1 & -1 & +1 & +1 \\ +1 & +1 & +1 & -1 & -1 \\ +1 & -1 & -1 & -1 & -1 \\ +1 & +1 & +1 & +1 & +1 \\ +1 & -1 & -1 & -1 & -1 \\ +1 & +1 & +1 & +1 & +1 \end{bmatrix}$$

The sign changes for the second, third, fourth and fifth columns of the above design are 15, 14, 13 and 12 respectively. This is an orthogonal design but not full factorial design.

Following the discussion in section 1.1.5, the number for different run orders of the  $2^4$  factorial experiment is  $54486432000 \left[ \frac{16!}{16 * 4!} \right]$ . Due to the huge number of designs, it is infeasible to examine all possible designs of the  $2^4$  factorial experiment. Instead, different designs are obtained by randomly changing the run orders of the  $2^4$  factorial experiment. Different run orders are randomly taken from standard run order (1, a, b, ab, c, ac, bc, abc, d, ad, bd, abd, cd, acd, bcd, abcd) of the  $2^4$  factorial experiment.

Table 2.4

	D-efficiency for foldover algorithm	501 Designs D-efficiency Five Number Summary				
		Min	L. Quartile	Median	U. Quartile	Max
$\rho = 0.25$	24.062	15.359	17.547	18.247	18.798	21.867
Main effect Sign changes	14, 15, 13, 11	6, 6, 3, 6	7, 9, 8, 5	9, 6, 10, 7	8, 7, 12, 7	13, 9, 11,12
$\rho = 0.9$	250.036	90.389	130.014	141.6765	153.878	189.994
Main effect Sign changes	14, 15, 13, 11	7, 4, 5, 6	10, 8, 6, 5	8, 6, 7, 10	9, 8, 8, 8	11, 9, 11,10

Five hundred and one random designs are taken to test our uncertainty. For this, we find the D-efficiency when errors are assumed to follow a first order auto regressive model and the number of sign changes for main effects of the above mentioned five hundred and one designs.

We found that all five hundred and one design D-efficiency values are smaller than the reverse foldover algorithm design D-efficiency, for both small(0.25) and large(0.9) values of  $\rho$ . The results are given in Table 2.4. From this, we can say that the reverse foldover algorithm may be used for four factors.

Next, consider the case of negatively correlated errors. We gave an algorithm for negative correlation in the section 2.2.3. It was examined only for three factors. Next, we verify this algorithm for four factors.

Table 2.5

	D-efficiency for foldover algorithm	501 Designs D-efficiency Five Number Summary				
		Min	L. Quartile	Median	U. Quartile	Max
$\rho = -0.25$	21.859	14.349	16.497	17.124	17.767	19.973
Main effect Sign changes	7, 4, 2, 2	11, 13, 9, 10	10, 7, 5, 12	7, 11, 7, 7	7, 5, 10, 8	5, 4, 8, 5
$\rho = -0.9$	209.1702	68.278	107.029	119.297	133.244	175.871
Main effect Sign changes	7, 4, 2, 2	13, 11, 9, 9	6, 10, 9, 9	11, 8, 7, 6	6, 6, 7, 10	7, 5, 4, 6

By using this algorithm for the  $2^4$  factorial experiment, the chosen run order will be: bcd, cd, acd, ad, d, bd, abd, ab, b, 1, a, ac, c, bc, abc, abcd. If  $\rho = -0.25$ , D-efficiency for this run order is 21.8592 and sign changes for main effect columns of the design matrix are 7, 4, 2 and 2 respectively. Five hundred and one random designs, which are obtained by the

procedure described earlier, are taken to test this algorithm. We found that D-efficiency using the algorithm is higher than all five hundred and one random D-efficiency values. The results are given in *Table 2.5*.

Therefore, this algorithm appears to be useful for any number of factors to find the most efficient design when correlation between successive observations is negative.



## CHAPTER 3

### RESULTS FOR 3-LEVEL FACTORIAL EXPERIMENTS

#### 3.1 Preface

The structure and notation for a 3-level factorial experiment have already been discussed in sections 1.4.1 & 1.4.2. Since this is a 3-level factorial experiment, both linear and quadratic effects need to be considered when we are going to investigate the efficient run order for a 3-level experiment, and a very huge number of designs is available in this situation. Therefore, efficient designs will be found by using a random sample as was done for the  $2^4$  factorial experiment. Three different models will be considered:

- (i) Linear effects only
- (ii) Main effects only
- (iii) Main effects and Linear interactions.

Since none of these situations comprise a full model, the D-efficiency criterion will not be constant, so can be used to find the efficient run order for the 3-level factorial experiment.

#### 3.2 Linear Effects Only

Initially, we are considering the linear effects of the  $3^2$  factorial experiment when errors are assumed to follow a first order moving average model. We have taken one thousand random designs from the standard form (see *Equation 1.26*) for this investigation when the correlation coefficient is 0.25. The highest D-efficiency value among the thousand random designs was

9.0267. Therefore, the most efficient design among the said designs and corresponding dispersion matrix  $\mathbf{D}$  are given below.

$$\mathbf{D} = \begin{bmatrix} 0.1593 & -0.0035 & 0.0008 \\ -0.0035 & 0.1196 & 0.0108 \\ 0.0008 & 0.0108 & 0.10356 \end{bmatrix}$$

Since the variances of the parameters, which are the diagonal elements of the  $\mathbf{D}$  matrix, are small and the off diagonal elements are very small too, this suggests that the parameters are estimated effectively.

$$\begin{bmatrix} +1 & +1 & +1 \\ +1 & 0 & 0 \\ +1 & +1 & 0 \\ +1 & -1 & 0 \\ +1 & +1 & -1 \\ +1 & -1 & +1 \\ +1 & -1 & -1 \\ +1 & 0 & +1 \\ +1 & 0 & -1 \end{bmatrix}$$

Note that this is an orthogonal full factorial design matrix, and number of sign changes in the second and third columns of the above design matrix are three and four respectively.

We have found from the results of the 2-level main effect factorial experiment that maximum possible sign changes for the each column of the design matrix will provide good estimators for the parameters. We have difficulty to use this concept for the 3-level factorial experiment, because the second level of the 3-level factorial experiment is denoted as zero. That means, it is not clear how to define sign changes for each linear effect column in such a way that it relates to the variance of the parameter. Therefore, we have to get some information about the zero algebraically.

With reference to the full model and the reduced model on page 31 and page 36 respectively, the actual covariance matrix  $D_R$  can be represented as  $D_{11} - D_{12}D_{22}^{-1}D_{21}$ . Due to the very small values of the  $D_{12}$  and  $D_{21}$ ,  $D_R$  is approximately same as  $D_{11}$  and the  $j^{th}$  diagonal element of  $D_{11}$  is given as follows.

$$d_{jj} = \frac{1}{81} \begin{pmatrix} x_{1j} & x_{2j} & . & . & . & . & . & x_{8j} & x_{9j} \end{pmatrix} \begin{pmatrix} 1 & \rho & 0 & . & . & . & . & . & 0 \\ \rho & 1 & \rho & 0 & . & . & . & . & 0 \\ 0 & \rho & 1 & \rho & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ 0 & 0 & . & . & . & 0 & \rho & 1 & \rho \\ 0 & 0 & . & . & . & 0 & 0 & \rho & 1 \end{pmatrix} \begin{pmatrix} x_{1j} \\ x_{2j} \\ . \\ . \\ . \\ . \\ . \\ x_{8j} \\ x_{9j} \end{pmatrix} \quad (3.1)$$

where  $x_{ij}$  takes the values either -1 or 0 or 1 for all  $i = 1 \dots 9$ .

$$d_{jj} = \frac{1}{81} \left( \sum_{i=1}^9 x_{ij}^2 + 2\rho \sum_{i=1}^8 x_{ij}x_{i+1,j} \right) \text{ for } j = 1 \dots 9 \quad (3.2)$$

Since small variance is more desirable to estimate the parameters effectively, we want  $d_{jj}$  to be small. If zero comes in between the negative one and positive one, the product will be zero. In fact, if the product is negative one, the diagonal element  $d_{jj}$  will be small. To make  $d_{jj}$  smaller we can arrange the column in the following manner. First write down the alternative numbers except zero then fill the rest of the column by zero. For example, one of the linear effect columns for  $3^2$  design should be 1, -1, 1, -1, 1, -1, 0, 0, 0 and the number of sign changes of this column is five, where only transition either from -1 to 1 or from 1 to -1 are counted as sign changes here.

These results suggest that it may be possible to get the efficient run order by maximising the sign changes. In the next section, an algorithm is suggested for getting the efficient run order for the linear effect of the 3-level factorial experiment when errors are assumed to follow the MA(1) model.

### 3.2.1 Algorithm for the Linear Effects of the 3-Level Factorial Experiment

Before giving the algorithm steps, we have to keep some mathematical operations in mind which are explained below.

Let  $a_0 = -1, a_1 = 0$  and  $a_2 = +1$

then  $a_i \times a_i = a_2$  for  $i = 0, 2$ ;

$a_i \times a_1 = a_i$  for  $i = 0, 2$ ;

$a_1 \times a_1 = a_1$  ;

and  $a_1 \times a_2 = a_0$  ;

where  $a_0, a_1$  and  $a_2$  are called first, second and third level of the factor A.

Step 1: Select the first run order as the third level of each factor.

Step 2: Select the first generator as the first level of each factor.

Step 3: Generate the new run order as follows. Having written down the runs in order, multiply by generators in reverse order and add to form the new run order. If the same run is produced again, it is to be ignored at that position

Step 4: Select the other generators sequentially by increasing the level for one factor when other factor levels are constant. [Example for  $3^2$  factorial experiment :  $a_0b_0, a_1b_0, a_2b_0, a_0b_1, a_1b_1, a_2b_1, \dots$  etc.]

Step 5: Repeat from step 3 until the entire design has been generated.

Consider a  $3^2$  factorial experiment as an example.

Step 1: Since  $a_2$  and  $b_2$  are the third levels of the factors A and B respectively,  $a_2b_2$  is the first run order.

Step 2: Since  $a_0$  and  $b_0$  are the first level of the factors A and B respectively,  $a_0b_0$  is the first generator.

Step 3: The second run order is  $a_2b_2 \times a_0b_0 = a_0b_0$ . [Considered as an order pair multiplication].

Step 4: The second generator is  $a_1b_0$ . Therefore, the run orders will be  $a_0b_0 \times a_1b_0 = a_1b_2$  and  $a_2b_2 \times a_1b_0 = a_1b_0$ . That is, the first four run orders are  $a_2b_2$ ,  $a_0b_0$ ,  $a_1b_2$  and  $a_1b_0$ . The third generator is  $a_2b_0$ . Since  $a_1b_0 \times a_2b_0 = a_1b_2$  and  $a_1b_2 \times a_2b_0 = a_1b_0$  are already in the run order, so these two run orders are ignored at this point. Therefore the new runs will be  $a_0b_0 \times a_2b_0 = a_0b_2$  and  $a_2b_2 \times a_2b_0 = a_2b_0$ . The first six run orders are  $a_2b_2$ ,  $a_0b_0$ ,  $a_1b_2$ ,  $a_1b_0$ ,  $a_0b_2$  and  $a_2b_0$ . The fourth generator is  $a_0b_1$ . According to the similar manner, runs are  $a_0b_1$ ,  $a_2b_1$  and  $a_1b_1$ ; other runs, which are repeated again, are ignored.

Step 5: The final run order is  $a_2b_2$ ,  $a_0b_0$ ,  $a_1b_2$ ,  $a_1b_0$ ,  $a_0b_2$ ,  $a_2b_0$ ,  $a_0b_1$ ,  $a_2b_1$  and  $a_1b_1$ .

$$\begin{bmatrix} +1 & +1 & +1 \\ +1 & -1 & -1 \\ +1 & 0 & +1 \\ +1 & 0 & -1 \\ +1 & -1 & +1 \\ +1 & +1 & -1 \\ +1 & -1 & 0 \\ +1 & +1 & 0 \\ +1 & 0 & 0 \end{bmatrix} \quad (3.3)$$

The design matrix obtained by the algorithm is given in *Equation(3.3)*. Sign changes for the second and third column of this design matrix are 4 and 5 respectively. D-efficiency for this design matrix is 10.0797 which is higher than the D-efficiency values for all thousand random designs when  $\rho = 0.25$ . Therefore, this design seems to be a most efficient design. That means, this method is useful to find the efficient design under this situation. However, we next examine this method for three factors in order to test the algorithm.

According to the given algorithm, the run orders for the linear effect of  $3^3$  factorial design are  $a_2 b_2 c_2, a_0 b_0 c_0, a_1 b_2 c_2, a_1 b_0 c_0, a_0 b_2 c_2, a_2 b_0 c_0, a_0 b_1 c_2, a_2 b_1 c_0, a_1 b_1 c_2, a_1 b_1 c_0, a_2 b_1 c_2, a_0 b_1 c_0, a_0 b_0 c_2, a_2 b_2 c_0, a_1 b_0 c_2, a_1 b_2 c_0, a_2 b_0 c_2, a_0 b_2 c_0, a_2 b_0 c_1, a_0 b_2 c_1, a_1 b_0 c_1, a_1 b_2 c_1, a_0 b_0 c_1, a_2 b_2 c_1, a_2 b_1 c_1, a_0 b_1 c_1, a_1 b_1 c_1$ . The design matrix of these run orders is given in *Equation(3.4)*.

The sign changes of the second, third, fourth columns of this design matrix are 9, 16 and 17 respectively. The D-efficiency for this design matrix is 31.0177 when  $\rho = 0.25$  and the dispersion matrix  $\mathbf{D}$  is given below.

$$\mathbf{D} = \begin{bmatrix} 0.0547 & -0.0006 & -0.0005 & -0.0004 \\ -0.0006 & 0.0389 & 0.0033 & 0.0008 \\ -0.0005 & 0.0033 & 0.0301 & 0.0007 \\ -0.0004 & 0.0008 & 0.0007 & 0.02886 \end{bmatrix}$$

Five hundred random designs are taken for testing purpose. The highest D-efficiency among the five hundred design matrix is 24.691 when  $\rho = 0.25$ . Thus the D-efficiency which is obtained by the algorithm is much higher than all five hundred random designs D-efficiency. That suggest

that the algorithm is still useful to find an efficient design for the linear effect of the 3-level factorial experiment.

$$\begin{bmatrix}
 +1 & +1 & +1 & +1 \\
 +1 & -1 & -1 & -1 \\
 +1 & 0 & +1 & +1 \\
 +1 & 0 & -1 & -1 \\
 +1 & -1 & +1 & +1 \\
 +1 & +1 & -1 & -1 \\
 +1 & -1 & 0 & +1 \\
 +1 & +1 & 0 & -1 \\
 +1 & 0 & 0 & +1 \\
 +1 & 0 & 0 & -1 \\
 +1 & +1 & 0 & +1 \\
 +1 & -1 & 0 & -1 \\
 +1 & -1 & -1 & +1 \\
 +1 & +1 & +1 & -1 \\
 +1 & 0 & -1 & +1 \\
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 +1 & +1 & -1 & +1 \\
 +1 & -1 & +1 & -1 \\
 +1 & +1 & -1 & 0 \\
 +1 & -1 & +1 & 0 \\
 +1 & 0 & -1 & 0 \\
 +1 & 0 & +1 & 0 \\
 +1 & -1 & -1 & 0 \\
 +1 & +1 & +1 & 0 \\
 +1 & +1 & 0 & 0 \\
 +1 & -1 & 0 & 0 \\
 +1 & 0 & 0 & 0
 \end{bmatrix}
 \tag{3.4}$$

Next, we need to consider the linear effects of the  $3^2$  factorial experiment when errors are assumed to follow a first order auto regressive model. Since if  $\rho$  is small then  $\rho^2, \rho^3, \dots, \rho^8$  are small, so the error covariance

matrix which is defined as first order auto regressive pattern, is approximately the same as the error covariance matrix for a first order moving average pattern. Therefore, it is enough to consider this situation only for large  $\rho$ .

One thousand designs for the linear effect of the  $3^2$  factorial experiment are chosen randomly to investigate this situation when errors are assumed to follow a first order auto regressive model ( $\rho = 0.90$ ). The highest D-efficiency among the thousand designs is 92.6948, but the D-efficiency which is obtained by the algorithm is 94.8094. That is, the algorithm will provide the efficient design here too.

Five hundred designs for the linear effect of the  $3^3$  factorial experiment are chosen randomly to investigate this situation when errors are assumed to follow first order auto regressive model ( $\rho = 0.90$ ). A histogram of D-efficiency values for all five hundred designs is given in *Appendix 6*. The highest D-efficiency among the five hundred designs is 233.2113, but the D-efficiency which is obtained by the algorithm is 296.5731. That means, the highest D-efficiency is obtained by the algorithm. Therefore, the algorithm provide an efficient design here too. Note that variance of the parameters is the sum of product terms at 1<sup>st</sup>, 2<sup>nd</sup>, .., 8<sup>th</sup> lag. The large value of D-efficiency is obtained due to this reason.

We can conclude that the design which has the maximum possible number of sign changes and maximum possible zero's pooled together in each linear effect column of the design, is a most efficient design when correlation between successive observation is positive, whether the MA(1) or AR(1) model is assumed. The above algorithm give an efficient run order in both cases.



### 3.3 Main Effects Only

Main effects of three level factorial experiment include both linear and quadratic effects of the main factors. In the design matrix, the three levels for the linear and quadratic effect are denoted by -1, 0, 1 and 1, -2, 1 respectively. That is, negative one and zero in the linear effect column convert to the quadratic effect column as positive one and negative two respectively in order to get an orthogonal full factorial design. In this situation, we need to use the standardised orthogonal design matrix in order to compare the variance of the parameters (see section 1.4.2).

Note that, maximum or minimum number of sign changes in the linear effect columns will provide poor sign changes in the quadratic effect column. For example, the maximum number of sign changes in the linear effect column of the  $3^2$  factorial experiment is achieved with 1, -1, 1, -1, 1, -1, 0, 0, 0 and the corresponding quadratic effect column is 1, 1, 1, 1, 1, 1, -2, -2, -2. The sign changes of the linear and quadratic effect columns are 5 and 1 respectively. On the other hand, the minimum number of sign changes in the linear effect column of the  $3^2$  factorial experiment is achieved with 1, 1, 1, 0, 0, 0, -1, -1, -1 and the corresponding quadratic effect column is again 1, 1, 1, -2, -2, -2, 1, 1, 1. The sign changes of the linear and quadratic effect columns are 0 and 2 respectively. Therefore, we cannot simply extend the above mentioned algorithm (linear effect algorithm) here. Instead, we try to analyze this situation the other way around. That is, the sign changes for quadratic effect column are first considered then we can set up the linear effect column with respect to the quadratic effect column.

If the design has an orthogonal design matrix, the total minimum and maximum number of sign changes for the quadratic main effect columns of

the  $3^2$  factorial experiment are 3 and 12 respectively. That means, there are ten different groups of designs available according to the sign changes for the quadratic main effect columns of the  $3^2$  factorial experiment. One design from each group is arbitrarily chosen for this study and the run orders are given below.

Group 1:  $(a_2 b_2) (a_0 b_0) (a_2 b_0) (a_0 b_2) (a_2 b_1) (a_0 b_1) (a_1 b_1) (a_1 b_2) (a_1 b_0)$ .

Group 2:  $(a_0 b_0) (a_2 b_2) (a_2 b_0) (a_1 b_2) (a_1 b_0) (a_1 b_1) (a_0 b_1) (a_2 b_1) (a_0 b_2)$ .

Group 3:  $(a_0 b_2) (a_0 b_0) (a_2 b_0) (a_0 b_1) (a_2 b_2) (a_2 b_1) (a_1 b_1) (a_1 b_2) (a_1 b_0)$ .

Group 4:  $(a_2 b_0) (a_1 b_0) (a_2 b_2) (a_0 b_0) (a_1 b_2) (a_1 b_1) (a_0 b_1) (a_2 b_1) (a_0 b_2)$ .

Group 5:  $(a_2 b_2) (a_0 b_2) (a_2 b_1) (a_2 b_0) (a_0 b_1) (a_0 b_0) (a_1 b_1) (a_1 b_2) (a_1 b_0)$ .

Group 6:  $(a_0 b_2) (a_1 b_0) (a_2 b_2) (a_0 b_1) (a_1 b_2) (a_1 b_1) (a_2 b_1) (a_0 b_0) (a_2 b_0)$ .

Group 7:  $(a_2 b_2) (a_0 b_0) (a_2 b_1) (a_0 b_2) (a_1 b_1) (a_2 b_0) (a_0 b_1) (a_1 b_2) (a_1 b_0)$ .

Group 8:  $(a_0 b_0) (a_1 b_2) (a_0 b_1) (a_2 b_2) (a_1 b_1) (a_1 b_0) (a_2 b_1) (a_0 b_2) (a_2 b_0)$ .

Group 9:  $(a_0 b_1) (a_2 b_0) (a_0 b_2) (a_1 b_1) (a_0 b_0) (a_1 b_2) (a_2 b_1) (a_1 b_0) (a_2 b_2)$ .

Group 10:  $(a_2 b_2) (a_1 b_2) (a_2 b_1) (a_0 b_2) (a_1 b_1) (a_0 b_0) (a_0 b_1) (a_1 b_0) (a_2 b_0)$ .

### 3.3.1 MA(1) Correlated Model

D-efficiencies for the main effect of the  $3^2$  factorial experiment according to the above mentioned run orders are calculated when errors are assumed to follow an MA(1) correlated model ( $\rho = 0.25$ ). Results are given in *Table 3.1*.

We can see from *Table 3.1* that the total number of sign changes for groups 1, 2 and 5 are constant which is ten. But corresponding D-efficiencies are slightly increased, at the same time the total number of sign changes for the quadratic effect columns of the above mentioned groups are increased and total number of sign changes for the linear effect columns of the above mentioned groups are decreased. The slight increase of the D-efficiency

seems to depend more on the total sign changes of the quadratic effect columns. The same situation is applicable for groups 7 and 8.

Table 3.1

Groups	Sign Changes			D-efficiency
	Linear	Quadratic	Total	
Group 1	7	3	10	1.1022
Group 2	6	4	10	1.1121
Group 3	3	5	09	1.0473
Group 4	5	6	11	1.1615
Group 5	3	7	10	1.1146
Group 6	4	8	12	1.2003
Group 7	6	9	15	1.3096
Group 8	5	10	15	1.3267
Group 9	5	11	16	1.3879
Group 10	4	12	16	1.3711

However, D-efficiency for the groups 4 and 5 are 1.1615 and 1.1146, and the total number of sign changes for the quadratic effect columns of the group 4 and 5 are six and seven, but the total number of sign changes for the design of the groups 4 and 5 are eleven and ten respectively. That is, D-efficiency seems to depend not only on the total number of sign changes for the quadratic effect columns but also depends on the total number of sign changes for the design.

Further, the total number of sign changes for the groups 9 and 10 are constant which is sixteen. But corresponding D-efficiencies are slightly decreased, at the same time total number of sign changes for the quadratic

effect columns of the groups 9 and 10 are increased and total number of sign changes for the linear effect columns of the above mentioned groups are decreased. Thus D-efficiency seems to depend mostly on the sign changes for the quadratic effect columns; although group 9 has the highest D-efficiency among the ten groups and has the highest total sign changes of the design, but not the highest number of quadratic sign changes.

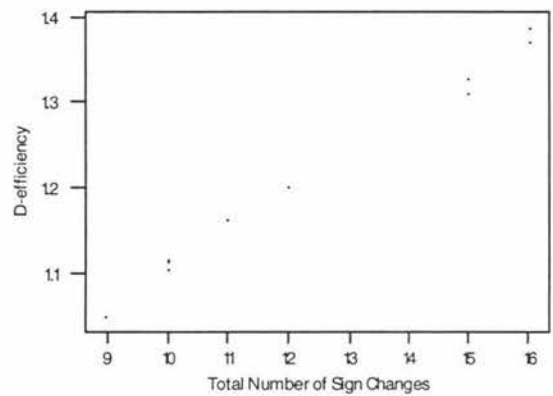


Figure 3.1

D-efficiency versus total number of sign changes is plotted and given in Figure 3.1. From this, we can easily see that D-efficiency increased as total number of sign changes increase.

We may conclude from the above arguments that maximum possible sign changes within the main effect columns of the orthogonal full factorial design is an efficient design.

According to the above result, an efficient run order may be obtained by the following procedure.

Step 1: Try to make the maximum possible total sign changes for the quadratic effect columns of the main effects. This can be done

by keeping the -2s apart as much as possible subject to orthogonality.

Step 2: Maximise the sign changes for the linear effect columns of the main effects subject to chosen quadratic effect columns and full factorial.

Since we arrived at this procedure by only examining ten arbitrary designs, one thousand random designs are taken from standard run order of the  $3^2$  factorial experiment in order to test the procedure. Necessary results are given in the *Table 3.2*.

Table 3.2

	D-efficiency		
	Minimum	Median	Maximum
Values	0.9588	1.1495	1.3822
Corresponding Design	1 -1 1 1 1	1 0 1 -2 1	1 -1 -1 1 1
	1 1 1 1 1	1 -1 1 1 1	1 0 0 -2 -2
	1 1 0 1 -2	1 1 -1 1 1	1 -1 1 1 1
	1 -1 0 1 -2	1 -1 0 1 -2	1 1 -1 1 1
	1 0 0 -2 -2	1 1 0 1 -2	1 0 1 -2 1
	1 0 1 -2 1	1 1 1 1 1	1 1 0 1 -2
	1 0 -1 -2 1	1 -1 -1 1 1	1 0 -1 -2 1
	1 -1 -1 1 1	1 0 0 -2 -2	1 1 1 1 1
	1 1 -1 1 1	1 0 -1 -2 1	1 -1 0 1 -2
Sign Changes	2 1 2 2	3 1 2 4	2 3 6 5
Total	7	10	16

The highest D-efficiency among the thousand random designs is 1.3822 and corresponding total sign changes for linear, quadratic and design are 5, 11 and 16 respectively. This suggest that the procedure is valid.

Since we have discussed up to this point two factors only, next we are considering the three level factorial experiment for three factors when errors are assumed to follow the MA(1) correlated ( $\rho = 0.25$ ) model. For this, five hundred  $3^3$  full factorial designs are taken. Histogram of the D-efficiency is given in the *Appendix 7*. Results are given in the *Table 3.3*.

*Table 3.3*

	D-efficiency	Sign Changes		
		Linear	Quadratic	Total
<b>Minimum</b>	1.0374	14	30	44
<b>Median</b>	1.1416	18	35	53
<b>Maximum</b>	1.2901	26	38	64

We can see from *Table 3.3* that minimum D-efficiency is 1.0374 and maximum D-efficiency is 1.2901. Note that the difference between these two values is quite small, but the difference between the total sign changes for linear effect columns when D-efficiency is minimum and the total sign changes for linear effect columns when D-efficiency is maximum, is high compared with quadratic effect columns. This suggest that, D-efficiency does not much depend on the sign changes for the linear effect columns of the  $3^3$  main effect factorial experiment. Next we find the run order according to the our earlier suggestion and corresponding design is given in *Equation(3.5)*. The sign changes of second, third, fourth, fifth, sixth and seventh columns of this design matrix are 6, 7, 8, 18, 18 and 18 respectively. D-efficiency for this design is 1.3979 which is higher than maximum D-

efficiency of the five hundred designs. That means, our suggestion is useful to find the efficient run order.

$$\begin{bmatrix}
 1 & -1 & -1 & -1 & 1 & 1 & 1 \\
 1 & 0 & 1 & 0 & -2 & 1 & -2 \\
 1 & 1 & 0 & -1 & 1 & -2 & 1 \\
 1 & 0 & -1 & 0 & -2 & 1 & -2 \\
 1 & -1 & -1 & 1 & 1 & 1 & 1 \\
 1 & 0 & 1 & -1 & -2 & 1 & 1 \\
 1 & 1 & 0 & 1 & 1 & -2 & 1 \\
 1 & 0 & -1 & -1 & -2 & 1 & 1 \\
 1 & -1 & 1 & 0 & 1 & 1 & -2 \\
 1 & 0 & 0 & -1 & -2 & -2 & 1 \\
 1 & 1 & 1 & 0 & 1 & 1 & -2 \\
 1 & 0 & -1 & 1 & -2 & 1 & 1 \\
 1 & -1 & 1 & -1 & 1 & 1 & 1 \\
 1 & 0 & 0 & 0 & -2 & -2 & -2 \\
 1 & 1 & -1 & -1 & 1 & 1 & 1 \\
 1 & 0 & 1 & 1 & -2 & 1 & 1 \\
 1 & -1 & -1 & 0 & 1 & 1 & -2 \\
 1 & 0 & 0 & 1 & -2 & -2 & 1 \\
 1 & 1 & 1 & -1 & 1 & 1 & 1 \\
 1 & -1 & 0 & 1 & 1 & -2 & 1 \\
 1 & 1 & -1 & 0 & 1 & 1 & -2 \\
 1 & -1 & 0 & -1 & 1 & -2 & 1 \\
 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
 1 & 1 & 0 & 0 & 1 & -2 & -2 \\
 1 & -1 & 1 & -1 & 1 & 1 & 1 \\
 1 & -1 & 0 & 0 & 1 & -2 & -2 \\
 1 & 1 & -1 & 1 & 1 & 1 & 1
 \end{bmatrix} \tag{3.5}$$

### 3.3.2 AR(1) Correlated Model

If  $\rho$  is small, the first order autoregressive error correlated model is similar to the first order moving average error correlated model. Therefore, we

now investigate the main effect of the  $3^2$  factorial experiment only for large  $\rho$  (0.9) when errors are assumed to follow the AR(1) correlated model.

One thousand random designs are taken from standard run order of the  $3^2$  factorial experiment in order to investigate this situation. Necessary results are given in the *Table 3.4*.

*Table 3.4*

	D-efficiency		
	Minimum	Median	Maximum
<b>Values</b>	4.9994	8.2028	12.4513
<b>Corresponding Design</b>	1 -1 0 1 -2	1 1 0 1 -2	1 1 0 1 -2
	1 -1 -1 1 1	1 1 1 1 1	1 -1 -1 1 1
	1 -1 1 1 1	1 1 0 1 -2	1 1 1 1 1
	1 0 1 -2 1	1 -1 -1 1 1	1 -1 0 1 -2
	1 0 -1 -2 1	1 0 -1 -2 1	1 0 -1 -2 1
	1 0 0 -2 -2	1 0 1 -2 1	1 -1 1 1 1
	1 1 1 1 1	1 0 0 -2 -2	1 0 0 -2 -2
	1 1 -1 1 1	1 -1 1 1 1	1 1 -1 1 1
	1 1 0 1 -2	1 1 -1 1 1	1 0 1 -2 1
<b>Sign Changes</b>	0 3 2 4	2 2 2 5	3 3 5 5
<b>Total</b>	9	11	16

We can say from the *Table 3.4* that D-efficiency is increased as total number of sign changes for the design increases. Maximum D-efficiency is obtained when the total number of sign changes is sixteen which is the maximum total number of possible sign changes for a  $3^2$  orthogonal full factorial experiment. That is, maximum sign changes for each columns of the design which is an orthogonal full factorial design, is an efficient design here too. Thus, our earlier suggestion is useful to obtain the efficient design here too.



Next we are investigating this result for the main effects of the  $3^3$  factorial experiment when errors are assumed to follow AR(1) correlated model. For this, five hundred  $3^3$  full factorial designs are taken. Results are given in the *Table 3.5*

*Table 3.5*

	D-efficiency	Sign Changes		
		Linear	Quadratic	Total
<b>Minimum</b>	6.9822	08	37	45
<b>Median</b>	8.8213	19	34	53
<b>Maximum</b>	11.7356	23	45	68

We can see from the *Table 3.5* that D-efficiency is increased as total number of sign changes increases, especially total number of sign changes increases for quadratic effect columns. However, substantial total sign changes for the linear effect columns is needed to obtain large D-efficiency.

According to the *Equation(3.5)* design, D-efficiency for AR(1) correlated model ( $\rho = 0.9$ ) is 12.8939 which is higher than maximum D-efficiency of the five hundred random designs. That means, our procedure is very useful to obtain efficient run order either MA(1) or AR(1) correlated model.

### 3.4 Main Effects and Linear Interactions

In this case, all possible main effects and linear interactions are considered as a model. This model corresponds to quadratic response surface (see section 1.5). However, this is not a full model. Therefore, we can use D-efficiency criterion to find the efficient design. We found the efficient design among the thousand random designs of the  $3^2$  factorial design

whether the MA(1) or AR(1) model is assumed. However, we were unable to find a reliable method to obtain the efficient run order. In this situation, we may suggest that before planning the design, efficient run orders need to be found from random designs by using a computer program such as Splus. This program is given in the *Appendix 8*.

It is noticeable that for 3-level factorial experiment, there is a compromise between estimating the linear effects efficiently and estimating the quadratic effects and interactions. It is not clear how to weight the contributions of these different types of effects. The standardization used in this Chapter is only one possible method. In order to overcome this situation, the problem of choosing an efficient run order for the estimation of a quadratic response surface will be considered more carefully in Chapter 4.

## CHAPTER 4

### RESPONSE SURFACES

#### 4.1 Preface

This section is entirely different from earlier Chapters. Response surface experiments are often used to find an optimum setting. It is explained in section 1.5. Our main interest of research is to find the efficient design. Unfortunately, the measure of efficiency used earlier may not be relevant here. Therefore, we are going to use a different criterion specifically for this type of experiment [12].

Let  $Y_0$  be the true mean response at the optimal setting of  $X_0$  and  $Y_{\hat{0}}$  be the true mean response at the estimated optimal setting of  $X_{\hat{0}}$ . Therefore, 'Loss' is given as  $Y_0 - Y_{\hat{0}}$  when the optimum is a maximum or  $Y_{\hat{0}} - Y_0$  for a minimum, which represent the difference between the mean response at the true optimum setting and the mean response at the estimated optimum setting. We can assume without loss of generality that the optimum is a minimum. Note that the expected 'Loss' function is a risk function. Therefore, our criterion is that optimal setting for response experiments will be obtained when risk is minimized.

We will use the usual quadratic response function and assume this is exact rather than an approximation. The one factor case will be studied first to illustrate the approach.

#### 4.2 One Factor

In this situation, responses are taken to find the optimum solution for one factor with three levels. We shall assume that responses are given by the following formula.

$$Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \epsilon \quad (4.1)$$

where  $Y$  and  $X$  are response and explanatory variable respectively,  $\epsilon$  is a random error term and  $\beta_0$ ,  $\beta_1$  and  $\beta_2$  are parameters. Algebraically, the mean response can be written as follows.

$$Y = \text{constant} + \beta_2 \left(X + \frac{\beta_1}{2\beta_2}\right)^2 \quad (4.2)$$

This equation indicates that responses will be provided by a parabola. For

turning point,  $\frac{dY}{dX} = 0$

$$\Rightarrow 2\beta_2 \left(X + \frac{\beta_1}{2\beta_2}\right) = 0$$

$$\Rightarrow X_0 = \frac{-\beta_1}{2\beta_2} \quad (4.3)$$

Therefore, the response at the turning point is given below.

$$Y_0 = \text{constant} + \beta_2 \left(X_0 + \frac{\beta_1}{2\beta_2}\right)^2$$

$$Y_0 = \text{constant} \left[ \because X_0 = \frac{-\beta_1}{2\beta_2} \right] \quad (4.4)$$

Similarly,  $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X + \hat{\beta}_2 X^2$  is the estimated response curve and

$X_0 = \frac{-\hat{\beta}_1}{2\hat{\beta}_2}$  is the turning point for the estimated response curve,

where  $\hat{\beta}_0 = \beta_0 + \pi_0$ ,  $\hat{\beta}_1 = \beta_1 + \pi_1$  and  $\hat{\beta}_2 = \beta_2 + \pi_2$ ,  $\hat{\beta}_0$ ,  $\hat{\beta}_1$  and  $\hat{\beta}_2$  are estimators for the parameters  $\beta_0$ ,  $\beta_1$  and  $\beta_2$  respectively, and  $\pi_0$ ,  $\pi_1$  and  $\pi_2$  are errors for the parameter estimates. The joint distribution of these errors will depend on the design of the experiment. Therefore the response at this estimated turning point is given below.

$$Y_{\hat{0}} = \text{constant} + \beta_2 \left(X_{\hat{0}} + \frac{\beta_1}{2\beta_2}\right)^2 \quad (4.5)$$

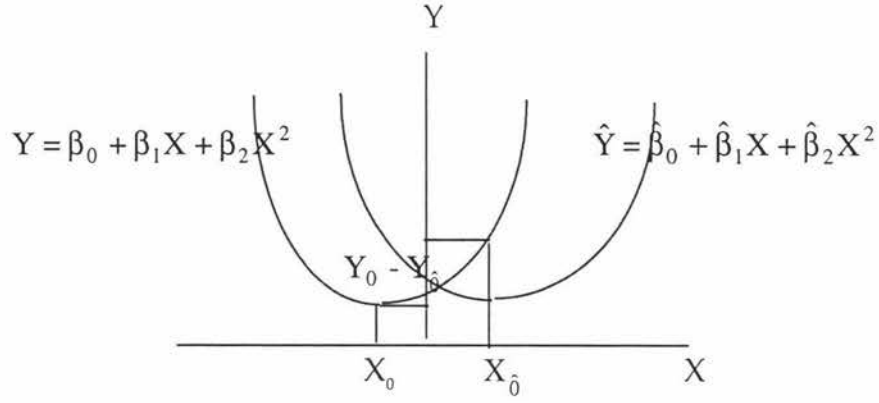


Figure 4.1

All above mentioned quantities are clearly described by the Figure 4.1. Our basic idea for finding the optimum design is that the optimum design should make the expected loss  $(Y_{\hat{0}} - Y_0)$  a minimum. In what follows, we are considering an algebraic approach to find the minimum expected loss.

Loss for the response =  $Y_{\hat{0}} - Y_0$

$$\begin{aligned}
 &= \beta_2 \left[ \frac{-\hat{\beta}_1}{2\hat{\beta}_2} + \frac{\beta_1}{2\beta_2} \right]^2 \\
 &= \frac{\beta_2}{4} \left[ \frac{1}{\beta_2} (\beta_1 + \pi_1) \left(1 + \frac{\pi_2}{\beta_2}\right)^{-1} - \frac{\beta_1}{\beta_2} \right]^2 \\
 &= \frac{1}{4\beta_2} \left[ (\beta_1 + \pi_1) \left(1 - \frac{\pi_2}{\beta_2} + \frac{\pi_2^2}{\beta_2^2} - \dots\right) - \beta_1 \right]^2 \\
 &= \frac{1}{4\beta_2} \left[ \pi_1^2 - 2 \frac{\beta_1}{\beta_2} \pi_1 \pi_2 + \frac{\beta_1^2}{\beta_2^2} \pi_2^2 \right] \quad (4.6)
 \end{aligned}$$

$[\because 2^{\text{nd}} \text{ order approximation}]$ .

Expected values for this loss =  $E[Y_{\hat{0}} - Y_0]$

$$\begin{aligned}
 &= \frac{1}{4\beta_2} \left[ \text{Var}(\pi_1) - 2 \frac{\beta_1}{\beta_2} \text{Cov}(\pi_1 \pi_2) + \frac{\beta_1^2}{\beta_2^2} \text{Var}(\pi_2) \right] \\
 &\quad [\because E(\pi_i) = 0 \text{ for all } i]
 \end{aligned}$$

$$\begin{aligned}
E[Y_{\hat{0}} - Y_0] &= \frac{1}{4\beta_2} \begin{bmatrix} 1 & \frac{-\beta_1}{\beta_2} \end{bmatrix} \begin{bmatrix} \text{Var}(\pi_1) & \text{Cov}(\pi_1\pi_2) \\ \text{Cov}(\pi_1\pi_2) & \text{Var}(\pi_1) \end{bmatrix} \begin{bmatrix} \frac{1}{\beta_2} \\ \frac{-\beta_1}{\beta_2} \end{bmatrix} \\
&= \frac{1}{4\beta_2} Z^t \Pi Z
\end{aligned} \tag{4.7}$$

where  $Z^t = \begin{bmatrix} 1 & \frac{-\beta_1}{\beta_2} \end{bmatrix} = [1 \quad 2X_0]$  and

$$\begin{aligned}
\Pi &= \begin{bmatrix} \text{Var}(\pi_1) & \text{Cov}(\pi_1\pi_2) \\ \text{Cov}(\pi_1\pi_2) & \text{Var}(\pi_2) \end{bmatrix} \\
&= \text{dispersion matrix of parameters} \\
&= [X^t V^{-1} X]^{-1}; X \text{ is a design matrix and } V \text{ is the error covariance}
\end{aligned}$$

matrix.

Now we use this result to find the optimum solution for the  $3^1$  factorial experiment when errors are assumed to follow MA(1) correlated models ( $\rho = 0.25$ ). In this situation, we have only two different designs available. Because, we do not need to consider 1, -1, 0 as the correlation model is time

reversible. That is, the design matrix  $X$  is either  $X_a = \begin{bmatrix} 1 & -1 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \end{bmatrix}$  or

$X_b = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & -1 & 1 \end{bmatrix}$  and the  $V$  matrix is given below

$$V = \begin{bmatrix} 1 & 0.25 & 0 \\ 0.25 & 1 & 0.25 \\ 0 & 0.25 & 1 \end{bmatrix}$$

If  $X = X_a$

then  $X^t V^{-1} X = \begin{bmatrix} 1 & 0 & -0.75 \\ 0 & 0.5 & 0 \\ -0.75 & 0 & 1 \end{bmatrix}$ . Hence  $\Pi = \begin{bmatrix} 0.5 & 0 \\ 0 & 1 \end{bmatrix}$ .

From Equation(4.7) therefore,  $E_1 [Y_{\hat{0}} - Y_0] = \frac{1}{4\beta_2} \begin{bmatrix} 1 & 2X_0 \end{bmatrix} \begin{bmatrix} 0.5 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 2X_0 \end{bmatrix}$

$$= \frac{1}{4\beta_2} [0.5 + 4X_0^2].$$

Similarly, if  $X=X_b$  then  $\Pi = \begin{bmatrix} 0.375 & -0.125 \\ -0.125 & 1.375 \end{bmatrix}$ .

$$E_2[Y_0 - Y_{\hat{0}}] = \frac{1}{4\beta_2} [0.375 - 0.5X_0 + 5.5X_0^2].$$

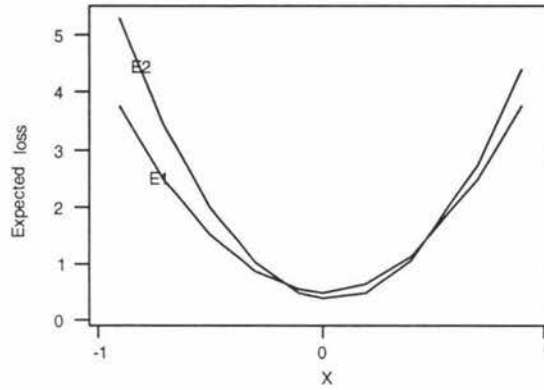


Figure 4.2

Since we need the minimum of the  $E_1$  and  $E_2$ , we don't need to be concerned about the quantity  $\frac{1}{4\beta_2}$ . Therefore, we can draw a graph

$E[Y_{\hat{0}} - Y_0]$  (without  $\frac{1}{4\beta_2}$ ) versus  $X_0$ . It is given in the Figure 4.2. We can see

from Figure 4.2 that if  $X_0$  is closer to zero,  $E_2[Y_{\hat{0}} - Y_0]$  is smaller; otherwise  $E_1[Y_{\hat{0}} - Y_0]$  is smaller. Note that since the difference between  $E_1[Y_{\hat{0}} - Y_0]$  and  $E_2[Y_{\hat{0}} - Y_0]$  is very small when  $X_0$  is closer to zero, we could argue that  $E_1[Y_{\hat{0}} - Y_0]$  is minimum almost everywhere, and that the best efficient

design for the  $3^1$  factorial experiment, when errors are assumed to follow

$$\text{MA(1) model, is } X = X_a = \begin{bmatrix} 1 & -1 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \end{bmatrix}$$

Anyway we can algebraically interpret the situation more accurately as is given below.

$$\text{Minimum Expected loss} = \begin{cases} E_2[Y_0 - Y_{\hat{0}}] & \text{if } -0.16 < X_0 < 0.5 \\ E_1[Y_0 - Y_{\hat{0}}] & \text{if otherwise.} \end{cases}$$

$$\text{That is, efficient design } X = \begin{cases} X_b & \text{if } -0.16 < X_0 < 0.5 \\ X_a & \text{if otherwise.} \end{cases}$$

Here, we have uncertainty because we don't know anything about the  $X_0$  before the experiment. In this situation, one approach is that a prior distribution for  $X_0$  can be assumed, for example a normal distribution with mean zero and variance  $\sigma^2$ . This is a reasonable assumption, because zero mean and normal distribution gives a symmetrical pattern for the prior, and standard deviation  $\sigma$  provides a measure of the uncertainty about the location of the optimum.

In this view  $E[Y_{\hat{0}} - Y_0]$  can be denoted as the conditional expectation of loss ( $L = Y_{\hat{0}} - Y_0$ ) given  $X_0$  ( $E[L/X_0]$ ).

That is,  $E[L_i/X_0] = E_i[Y_0 - Y_{\hat{0}}]$  for all  $i = 1, 2$ .

and  $E[L_i] = E[E[L_i/X_0]]$  (4.8)

Therefore,  $E[L_1] = E\left[\frac{1}{4\beta_2}[0.5 + 4X_0^2]\right]$



$$\begin{aligned}
&= \frac{1}{4\beta_2} [0.5 + 4\sigma^2] \quad [\because E[X_0] = 0] \\
E[L_2] &= E\left[\frac{1}{4\beta_2} [0.375 - 0.5X_0 + 5.5X_0^2]\right] \\
&= \frac{1}{4\beta_2} [0.375 + 5.5\sigma^2]
\end{aligned}$$

Hence, if  $\sigma^2 > 0.08$  then  $E[L_1] < E[L_2]$ ; otherwise  $E[L_2] < E[L_1]$ . That means, if  $\sigma^2 > 0.08$ , the best design  $X$  is  $X_a$ ; otherwise choose the design  $X_b$ .

## 4.2 More Than One Factor

First, we are considering the quadratic response surface in two variables, when errors are assumed to follow MA(1) correlated models. Therefore, the mean response of the experiment is measured by the following equation.

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + b_{11} X_1^2 + b_{22} X_2^2 + 2b_{12} X_1 X_2 \quad (4.9)$$

It can be explained by matrix form. That is,

$$\begin{aligned}
Y &= \beta_0 + (X_1 \ X_2) \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} + (X_1 \ X_2) \begin{pmatrix} b_{11} & b_{12} \\ b_{12} & b_{22} \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \\
Y &= \beta_0 + \underline{X}^t \underline{\beta} + \underline{X}^t \underline{B} \underline{X} \quad (4.10)
\end{aligned}$$

where  $\underline{X} = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix}$ ,  $\underline{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix}$  and  $\underline{B} = \begin{pmatrix} b_{11} & b_{12} \\ b_{12} & b_{22} \end{pmatrix}$ .

Note that it can be similarly written in the matrix form for more than two explanatory variables under the above mentioned situation.

For turning point of the Equation(4.10),  $\frac{dY}{d\underline{X}} = 0$ . Since this is a matrix

differentiation, finally we get  $\underline{\beta} + 2\underline{B}\underline{X} = \underline{0}$

$$\Rightarrow \underline{X}_0 = -\frac{1}{2} \underline{B}^{-1} \underline{\beta}$$

That is, 
$$\underline{X}_0 = \begin{pmatrix} X_{01} \\ X_{02} \end{pmatrix} = -\frac{1}{2|B|} \begin{pmatrix} b_{22} & -b_{12} \\ -b_{12} & b_{11} \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} \quad (4.11)$$

Similarly the estimated optimal factor levels are given by  $\underline{X}_{\hat{0}} = -\frac{1}{2}\hat{B}^{-1}\hat{\underline{\beta}}$ ,

where 
$$\hat{B} = \begin{pmatrix} B_{11} + \phi_{11} & B_{12} + \phi_{12} \\ B_{12} + \phi_{12} & B_{22} + \phi_{22} \end{pmatrix} = B + \Phi, \quad \hat{\underline{\beta}} = \begin{pmatrix} \beta_1 + \pi_1 \\ \beta_2 + \pi_2 \end{pmatrix} = \underline{\beta} + \underline{\pi}, \quad \text{and}$$

$\pi_1, \pi_2, \phi_{11}, \phi_{22}$  and  $\phi_{12}$  are the errors in the estimates of the parameter.

The responses at the turning point and estimated turning point are given below.

$$Y_0 = \beta_0 + \underline{X}_0^t \underline{\beta} + \underline{X}_0^t B \underline{X}_0$$

and

$$Y_{\hat{0}} = \beta_0 + \underline{X}_{\hat{0}}^t \underline{\beta} + \underline{X}_{\hat{0}}^t B \underline{X}_{\hat{0}} \quad (4.12)$$

Loss for the response =  $Y_{\hat{0}} - Y_0$

$$\begin{aligned} &= \underline{X}_{\hat{0}}^t \underline{\beta} - \underline{X}_0^t \underline{\beta} + \underline{X}_{\hat{0}}^t B \underline{X}_{\hat{0}} - \underline{X}_0^t B \underline{X}_0 \\ &= \underline{X}_{\hat{0}}^t B \underline{X}_{\hat{0}} - 2\underline{X}_0^t B \underline{X}_0 + \underline{X}_0^t B \underline{X}_0 \quad [\because \underline{\beta} = -2B\underline{X}_0] \\ &= [\underline{X}_{\hat{0}} - \underline{X}_0]^t B [\underline{X}_{\hat{0}} - \underline{X}_0] \end{aligned} \quad (4.13)$$

Let us consider  $\underline{X}_{\hat{0}} = -\frac{1}{2}\hat{B}^{-1}\hat{\underline{\beta}}$

$$\begin{aligned} &= -\frac{1}{2}[B + \Phi]^{-1}[\underline{\beta} + \underline{\pi}] \\ &= -\frac{1}{2}[I + B^{-1}\Phi]^{-1}[B^{-1}\underline{\beta} + B^{-1}\underline{\pi}] \\ &= [I - B^{-1}\Phi][\underline{X}_0 - \frac{1}{2}B^{-1}\underline{\pi}] \quad [\because \underline{X}_0 = -\frac{1}{2}B^{-1}\underline{\beta}] \end{aligned} \quad (4.14)$$

Hence,

$$\underline{X}_{\hat{0}} - \underline{X}_0 = -B^{-1} \left[ \frac{1}{2} \underline{\pi} + \Phi \underline{X}_0 \right] \quad [\because \text{First order approximation in the error terms}]$$

$$\text{Therefore, } Y_{\hat{0}} - Y_0 = \left[ \frac{1}{2} \underline{\pi} + \Phi \underline{X}_0 \right]^t B^{-1} \left[ \frac{1}{2} \underline{\pi} + \Phi \underline{X}_0 \right] \quad (4.15)$$

Expected values for this error =  $E[Y_{\hat{0}} - Y_0]$

$$= E[\text{trace}(B^{-1} \left[ \frac{1}{2} \underline{\pi} + \Phi \underline{X}_0 \right] \left[ \frac{1}{2} \underline{\pi} + \Phi \underline{X}_0 \right]^t)]$$

Hence

$$\begin{aligned} E[Y_{\hat{0}} - Y_0] &= E[\text{trace}(\frac{1}{4} B^{-1} \underline{\pi} \underline{\pi}^t + \frac{1}{2} B^{-1} \Phi \underline{X}_0 \underline{\pi}^t + \frac{1}{2} B^{-1} \underline{\pi} \underline{X}_0^t \Phi^t + B^{-1} \Phi \underline{X}_0 \underline{X}_0^t \Phi^t)] \\ &= \frac{1}{|B|} [\eta_0 + \eta_1 X_{01} + \eta_2 X_{02} + \eta_{11} X_{01}^2 + \eta_{22} X_{02}^2 + \eta_{12} X_{01} X_{02}] \quad (4.16) \end{aligned}$$

$$\text{where } \eta_0 = \frac{1}{4} [d_{1,1} b_{22} - 2d_{1,2} b_{12} + d_{2,2} b_{11}]$$

$$\eta_1 = d_{1,11} b_{22} - (d_{2,11} + d_{1,12}) b_{12} + d_{2,12} b_{11}$$

$$\eta_2 = d_{1,12} b_{22} - (d_{1,22} + d_{2,12}) b_{12} + d_{2,22} b_{11}$$

$$\eta_{11} = d_{11,11} b_{22} - 2d_{11,12} b_{12} + d_{12,12} b_{11}$$

$$\eta_{22} = d_{12,12} b_{22} - 2d_{22,12} b_{12} + d_{22,22} b_{11}$$

$$\eta_{12} = 2d_{11,12} b_{22} - 2(d_{11,22} + d_{12,12}) b_{12} + 2d_{22,12} b_{11}$$

and

$$d_{i,j} = E[\pi_i \pi_j] = E[\pi_j \pi_i] \quad \text{for all } i, j = 1, 2$$

$$d_{i,jk} = E[\pi_i \phi_{jk}] = E[\phi_{jk} \pi_i] \quad \text{for all } i, j, k = 1, 2$$

$$d_{ij,kl} = E[\phi_{ij} \phi_{kl}] = E[\phi_{kl} \phi_{ij}] \quad \text{for all } i, j, k, l = 1, 2 \quad (4.17)$$

The parameter error dispersion matrix  $D = (X^t V^{-1} X)^{-1}$ , where  $V$  assumed to follow either MA(1) or AR(1) correlated models, is given below.

$$D = \begin{matrix} & \pi_1 & \pi_2 & \phi_{11} & \phi_{22} & \phi_{12} \\ \begin{matrix} \pi_1 \\ \pi_2 \\ \phi_{11} \\ \phi_{22} \\ \phi_{12} \end{matrix} & \begin{bmatrix} d_{1,1} & d_{1,2} & d_{1,11} & d_{1,22} & d_{1,12} \\ d_{1,2} & d_{2,2} & d_{2,11} & d_{2,22} & d_{2,12} \\ d_{1,11} & d_{2,11} & d_{11,11} & d_{11,22} & d_{11,12} \\ d_{1,22} & d_{2,22} & d_{11,22} & d_{22,22} & d_{22,12} \\ d_{1,12} & d_{2,12} & d_{11,12} & d_{22,12} & d_{12,12} \end{bmatrix} \end{matrix} \quad (4.18)$$

Since we don't know  $X_{01}$  and  $X_{02}$ , we assume a prior distribution for  $\underline{X}_0$ . Here we take  $\underline{X}_0$  to be bivariate normally distributed with mean  $(0, 0)^t$  and covariance matrix  $\sigma^2 I_2$ . That is, the joint probability density function  $f(x_{01}, x_{02})$  is given below.

$$f(x_{01}, x_{02}) = \frac{1}{2\pi\sigma^2} \exp\left[-\frac{x_{01}^2 + x_{02}^2}{2\sigma^2}\right] \quad (4.19)$$

In this view,  $E[Y_{\hat{0}} - Y_0]$  can be written as the conditional expectation of loss  $L = Y_{\hat{0}} - Y_0$  given  $X_{01}$  and  $X_{02}$  and denoted by  $E[L | X_{01}, X_{02}]$ .

Therefore,  $E[L] = E[E[L | X_{01}, X_{02}]]$

$$\text{Thus, } E[L] = E\left[\frac{1}{|B|} [\eta_0 + \eta_{11}X_{10} + \eta_{22}X_{20} + \eta_{11}X_{10}^2 + \eta_{22}X_{20}^2 + \eta_{12}X_{10}X_{20}]\right]$$

$$= \frac{1}{|B|} [\eta_0 + \eta_{11}\sigma^2 + \eta_{22}\sigma^2] \quad (4.20)$$

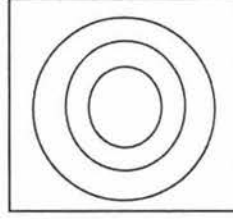
$$[\because E[X_{01}] = E[X_{02}] = 0 \text{ and independence}]$$

Unfortunately, the minimum expected loss for the overall design still can not be calculated, because  $\eta_0, \eta_{11}$  and  $\eta_{22}$  depend on the B matrix elements. That means, we can not apply our criterion directly. Hence, we have to analyse this situation by cases.

Note that since  $|B|$  is a constant and we need the minimum value of the expected optimum for the various design, we don't need to be concerned

about the scaling constant  $|B|$ . We will consider three cases for the contours of the true response surface, as given below.

Case 1: True contour pattern is a circle.



If the contours are circular,  $b_{11} = b_{22}$  and  $b_{12} = 0$ .

$$\text{Thus, } \eta_0 = \frac{1}{4}(d_{1,1} + d_{2,2})b_{11}$$

$$\eta_{11} = (d_{11,11} + d_{12,12})b_{11}$$

$$\eta_{22} = (d_{12,12} + d_{22,22})b_{11}$$

Since  $b_{11}$  now factors out of our criterion, we are arbitrarily choosing  $b_{11} = 1$ .

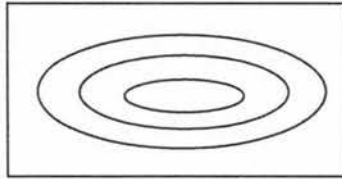
$$\text{Therefore, } \eta_0 = \frac{1}{4}(d_{1,1} + d_{2,2})$$

$$\eta_{11} = d_{11,11} + d_{12,12}$$

$$\eta_{22} = d_{12,12} + d_{22,22}$$

$$\text{Hence, } E[L] = \frac{1}{4}(d_{1,1} + d_{2,2}) + (d_{11,11} + 2d_{12,12} + d_{22,22})\sigma^2 [\because |B| = 1] \quad (4.21)$$

Case 2: True contour pattern is an ellipse



If the contours are like this type of ellipse,  $b_{22} = \alpha b_{11}$  and  $b_{12} = 0$ .

$$\text{Thus, } \eta_0 = \frac{1}{4}(\alpha d_{1,1} + d_{2,2})b_{11}$$

$$\eta_{11} = (\alpha d_{11,11} + d_{12,12})b_{11}$$

$$\eta_{22} = (\alpha d_{12,12} + d_{22,22})b_{11}$$

In this case, we are arbitrarily choosing  $b_{11} = 1$  and  $\alpha = 2$ .

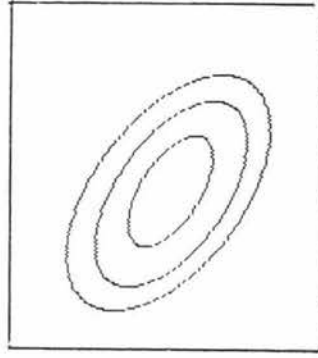
$$\text{Hence, } \eta_0 = \frac{1}{4}(2d_{1,1} + d_{2,2})$$

$$\eta_{11} = 2d_{11,11} + d_{12,12}$$

$$\eta_{22} = 2d_{12,12} + d_{22,22}$$

$$\text{Therefore, } E[L] = \frac{1}{2} \left[ \frac{1}{4}(2d_{1,1} + d_{2,2}) + (2d_{11,11} + 3d_{12,12} + d_{22,22})\sigma^2 \right] [\because |B| = 2] \quad (4.22)$$

Case 3: True contour pattern is an ellipse which is in some direction.



If the contour like this type of ellipse,  $b_{22} = \alpha b_{11}$  and  $b_{12}$  not equal to zero. In this case, expected optimum is defined by the Equation(4.20) and  $\eta_0, \eta_{11}$  and  $\eta_{22}$  are also defined by the Equation(4.17). For numerical investigation, we are choosing  $b_{11} = 1, b_{12} = 1, b_{22} = 2$ .

$$\text{Thus, } \eta_0 = \frac{1}{4}(2d_{1,1} + d_{2,2} - 2d_{1,2})$$

$$\eta_{11} = 2d_{11,11} + d_{12,12} - 2d_{11,12}$$

$$\eta_{22} = 2d_{12,12} + d_{22,22} - 2d_{22,12}$$

Therefore,

$$E[L] = \frac{1}{4} [(2d_{1,1} + d_{2,2} - 2d_{1,2}) + (2d_{11,11} + 3d_{12,12} + d_{22,22} - 2d_{11,12} - 2d_{22,12})\sigma^2] \quad [\because |B| = 1] \quad (4.23)$$

Next, we want to find an efficient run order for a central composite design via this criterion when errors are assumed to follow MA(1) model ( $\rho = 0.25$ ). It is infeasible to examine all possible run orders for two factor central composite designs for all mentioned cases. Therefore, five hundred run orders are randomly taken to find an efficient central composite design.

In order to make random central composite design, the following steps are needed. Fourteen central composite points, as generated for two factors by the Minitab, are considered as the standard run order and given below. Random designs will be made by randomly reordering the rows. This type of approach will be made for all cases.

$$\begin{bmatrix} -1 & -1 \\ 1 & -1 \\ -1 & 1 \\ 1 & 1 \\ -1.414 & 0 \\ 1.414 & 0 \\ 0 & -1.414 \\ 0 & 1.414 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \quad (4.24)$$

Since the expected loss depends on the  $\sigma^2$  for all three cases (see *Equations (4.21), (4.22) & (4.23)*) and  $\sigma$  provides a measure of the uncertainty about the location of the optimum, we choose two values of  $s$ , one “large” and other one “small” related to the size of the factor space. Now consider the prior probability that the optimum is inside the experimental region, that

is,  $P(R) = \iint_R f(x_{01}, x_{02}) dx_{01} dx_{02}$ , where  $f(x_{01}, x_{02})$  is a joint probability density function of variables  $X_{01}$  and  $X_{02}$  and  $R$  is a region which we are interest. Therefore,

$$P(R) = \iint_R \left[ \frac{1}{\sqrt{2\pi\sigma^2}} \right]^2 \exp\left(-\frac{x_{01}^2 + x_{02}^2}{2\sigma^2}\right) dx_{01} dx_{02} [\because \text{using Equation (4.19)}]$$

The coordinate  $(x_{01}, x_{02})$  can be written as a poolar coordinate. That is,

$$x_{01} = r \cos \theta \text{ and } x_{02} = r \sin \theta, \quad 0 \leq \theta \leq 2\pi \text{ and } 0 \leq r \leq \sqrt{2}$$

$$\begin{aligned} \text{Hence, } P(R) &= \int_0^{\sqrt{2}} \int_0^{2\pi} \frac{1}{2\pi\sigma^2} \exp\left(-\frac{r^2}{2\sigma^2}\right) r d\theta dr [\because \text{change of variables}] \\ &= \left[ -\exp\left(-\frac{r^2}{2\sigma^2}\right) \right]_0^{\sqrt{2}} \\ &= 1 - \exp\left(-\frac{1}{\sigma^2}\right) \end{aligned}$$

If  $\sigma = 0.3$  then  $P(R) \cong 1$  and if  $\sigma = 0.8$  then  $P(R) \cong 0.80$ . so these two values are used in the investigation representing a concentrated and a diffuse prior respectively. Least expected losses among the five hundred random designs for case1, case2 and case3 are 0.1029, 0.07669 and 0.1499 respectively when  $\sigma = 0.3$ , and 0.4017, 0.2948 and 0.5685 respectively when  $\sigma = 0.8$ .

A histogram for the expected loss calculated for five hundred random designs, is given in *Appendix 9*, 10 and 11 for all three cases when  $\sigma = 0.3$ , and in *Appendix 12*, 13 and 14 for all three cases when  $\sigma = 0.8$ . This is very useful to see how the minimum expected loss compares with other expected losses.

By considering the dispersion matrix and corresponding design, we found that maximum sign changes for the linear effect columns and linear



interaction column provide small variance of the parameter estimates. Note that the linear interaction effect column contains only four values which are 1 and -1 and rest of this column are filled by zero. That means, maximum sign changes for the linear interaction column is three. As far as 1 and -1 are concerned in the liner effect columns, maximum possible sign changes for these columns are two and one if we want to make three sign changes in the linear interaction column. That means, we can not make the maximum sign changes for the linear effect columns and the linear interaction column simultaneously.

$$\begin{bmatrix}
 1 & 0 & 0 & 0 & 0 & 0 \\
 1 & 0 & -1.414 & 0 & 1.999 & 0 \\
 1 & 0 & 0 & 0 & 0 & 0 \\
 1 & 0 & 0 & 0 & 0 & 0 \\
 1 & -1.414 & 0 & 1.999 & 0 & 0 \\
 1 & 1 & 1 & 1 & 1 & 1 \\
 1 & 1 & -1 & 1 & 1 & -1 \\
 1 & -1 & -1 & 1 & 1 & 1 \\
 1 & -1 & 1 & 1 & 1 & -1 \\
 1 & 1.414 & 0 & 1.999 & 0 & 0 \\
 1 & 0 & 0 & 0 & 0 & 0 \\
 1 & 0 & 0 & 0 & 0 & 0 \\
 1 & 0 & 1.414 & 0 & 1.999 & 0 \\
 1 & 0 & 0 & 0 & 0 & 0
 \end{bmatrix} \quad (4.25)$$

Further, we found that if the values -1.414 and 1.414 are widely separated in the linear effect columns, the variance of the quadratic estimates is small. Since we have to make the maximum sign changes in the linear effect columns, the pattern of the one linear effect column should be 0, 0, 0, 0, -1.414, 1, 1, -1, -1, 1.414, 0, 0, 0, 0 and other one should be 0, -1.416, 0, 0, 0, 1, -1, -1, 1, 0, 0, 0, 1.416, 0 to make small variance for the estimates of the

parameter when  $\rho$  is positive. Therefore, the recommended two factor central composite design for our model is given in *Equation(4.25)*.

The sign changes for the linear effect columns and the linear interaction column are 3, 2 and 3 respectively. The expected losses for this design are given in the *Table 4.1*.

*Table 4.1*

	Expected Loss		
	Case 1	Case 2	Case 3
$\sigma = 0.3$	0.1017 *	0.0769 **	0.1533 **
$\sigma = 0.8$	0.3982 *	0.3037 **	0.6068 **

The single star ‘\*’ indicates that these expected losses are less than minimum expected loss among the five hundred random designs under the similar situation.

The double star ‘\*\*’ indicates that these expected losses are little bit higher than minimum expected loss among the five hundred random designs under the similar situation, but the expected loss for this design is less than the expected loss for the most of the random designs. This statement is confirmed by the histograms which are given in the *Appendix 11, 12, 13, 14, 15 and 16*.

That means, the expected loss for the particular design is less than expected loss for the most of the random designs. Therefore, we can say that our earlier argument is useful to make an efficient run order for this central composite design.

Finally, we can conclude that maximum sign changes in the linear effect columns subject to produce the maximum sign changes in the linear interaction column, and -1.414 and 1.414 are largely separated in the linear effect columns, is an efficient central composite design when errors are positively correlated with MA(1) model.

# Appendix 1

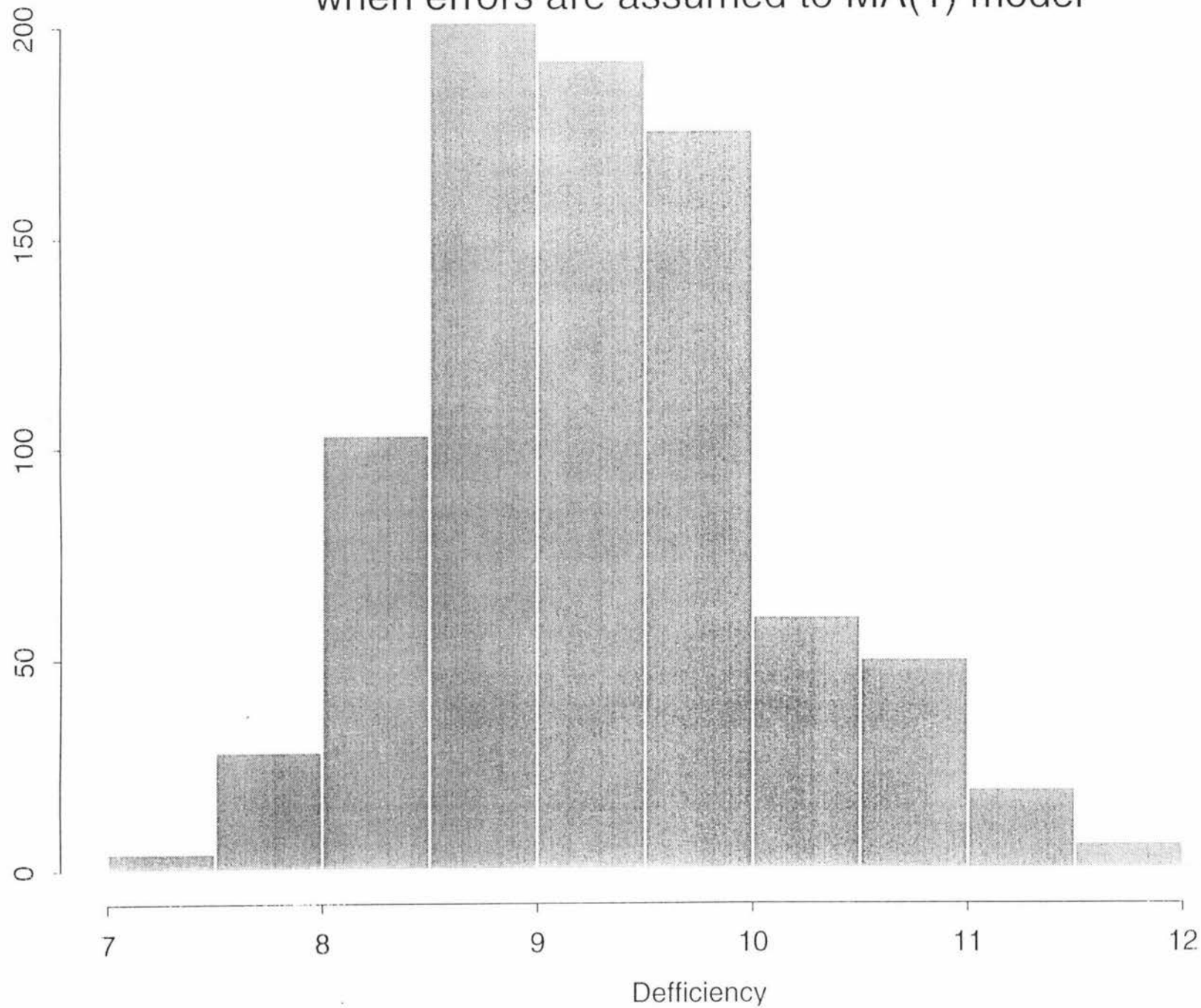
## M matrix

1	1	2	3	4	5	6	7	8	9	10	11
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	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	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

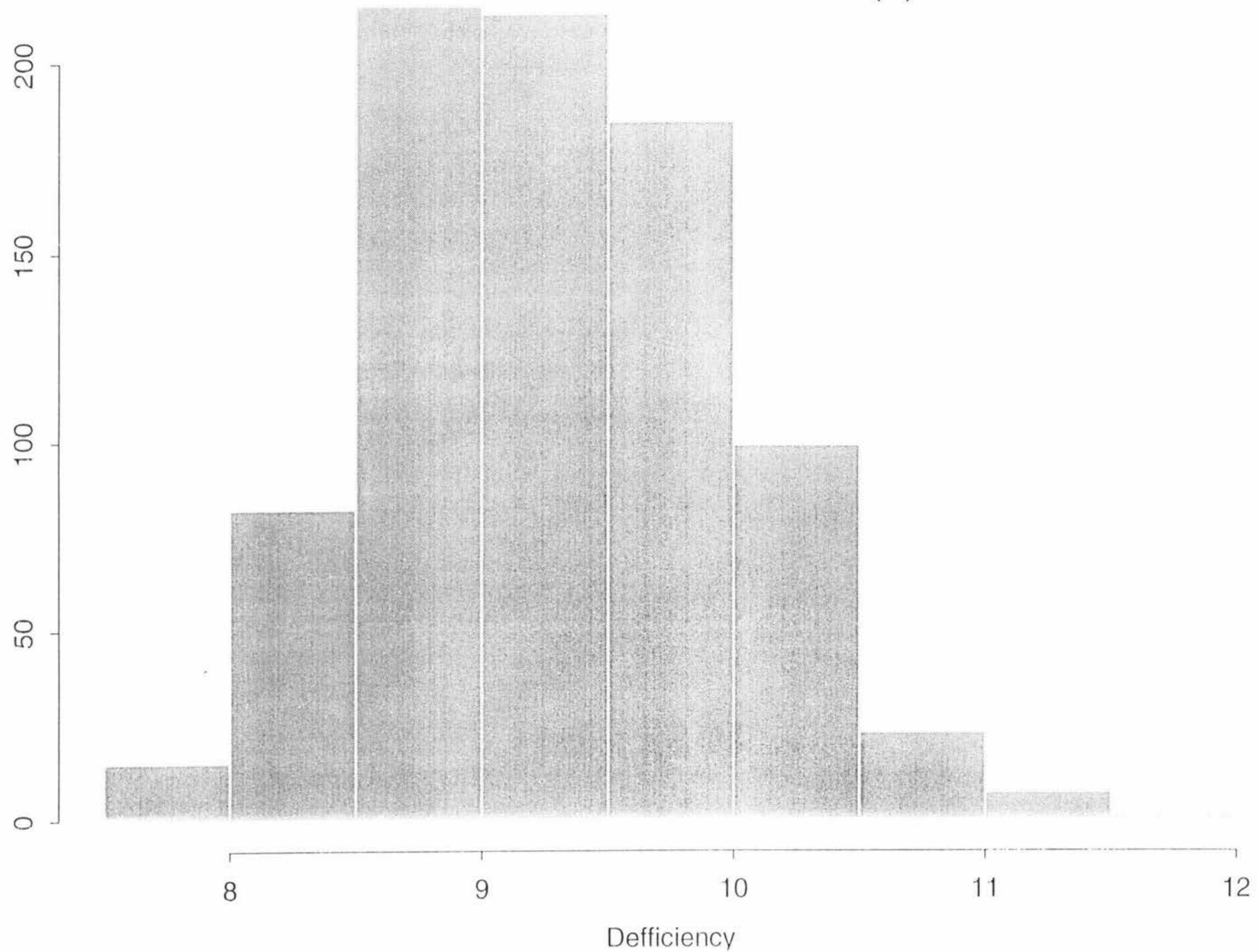
12	13	14	15	16	17	18	19	20	21	22	23
1	1	1	1	-1	-1	-1	-1	-1	-1	-1	-1
-1	-1	-1	-1	1	1	1	1	1	1	1	1
-1	-1	-1	-1	1	1	1	1	-1	-1	-1	-1
1	-1	-1	-1	1	-1	-1	-1	1	1	1	-1
-1	1	1	-1	-1	1	-1	-1	1	-1	-1	1
-1	1	-1	1	-1	-1	1	-1	-1	1	-1	1
1	-1	1	1	-1	-1	-1	1	-1	-1	1	-1
1	1	1	1	1	1	1	1	1	1	1	1

24	25	26	27	28	29	30	31	32	33	34	35
-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	-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	-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

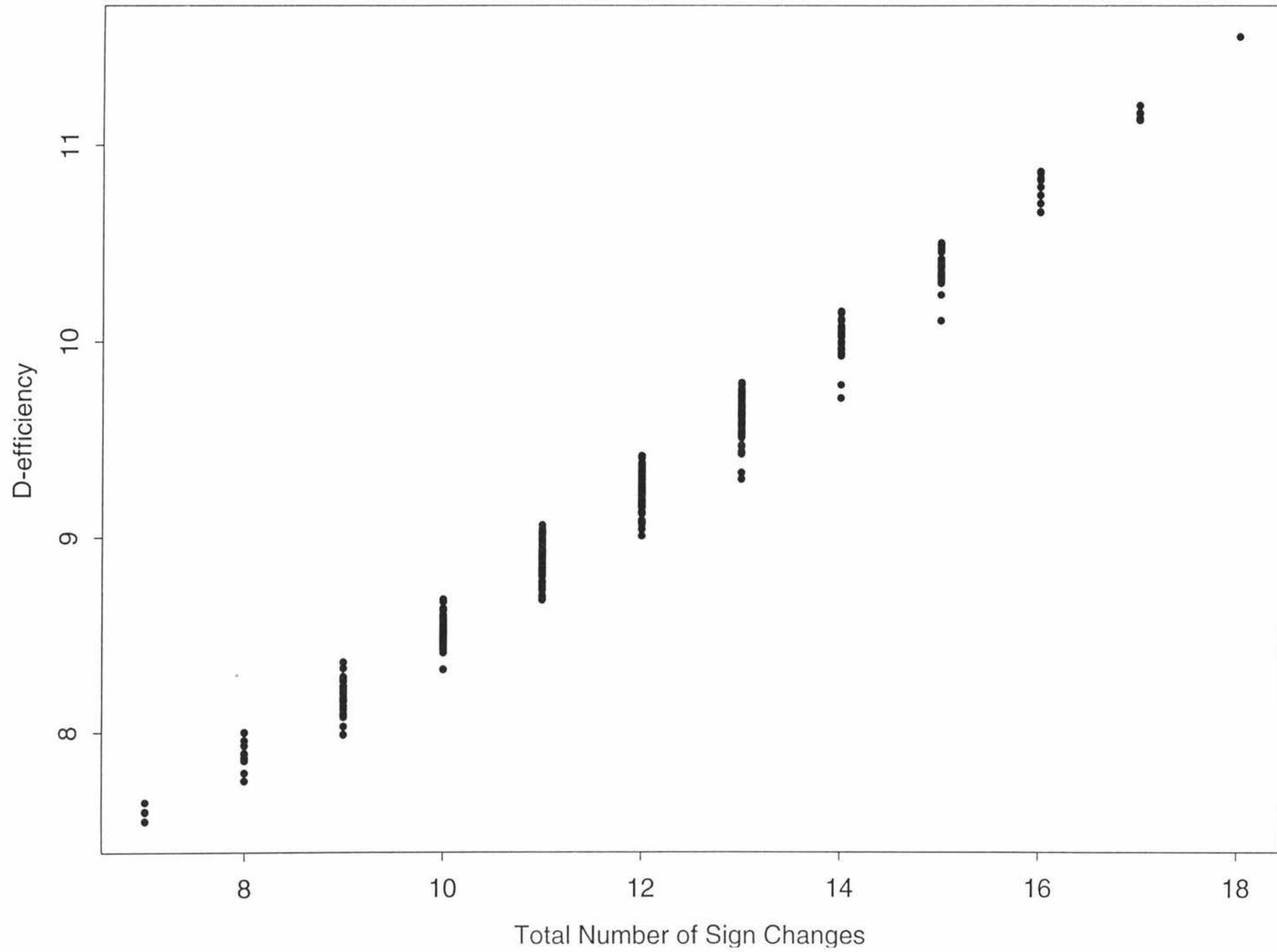
Appendix 2  
Histogram for the D-efficiency of the (2x2x2) factorial Design  
when errors are assumed to MA(1) model



Appendix 3  
Histogram for the D-efficiency of the (2x2x2) factorial Design  
when errors are assumed to AR(1) model

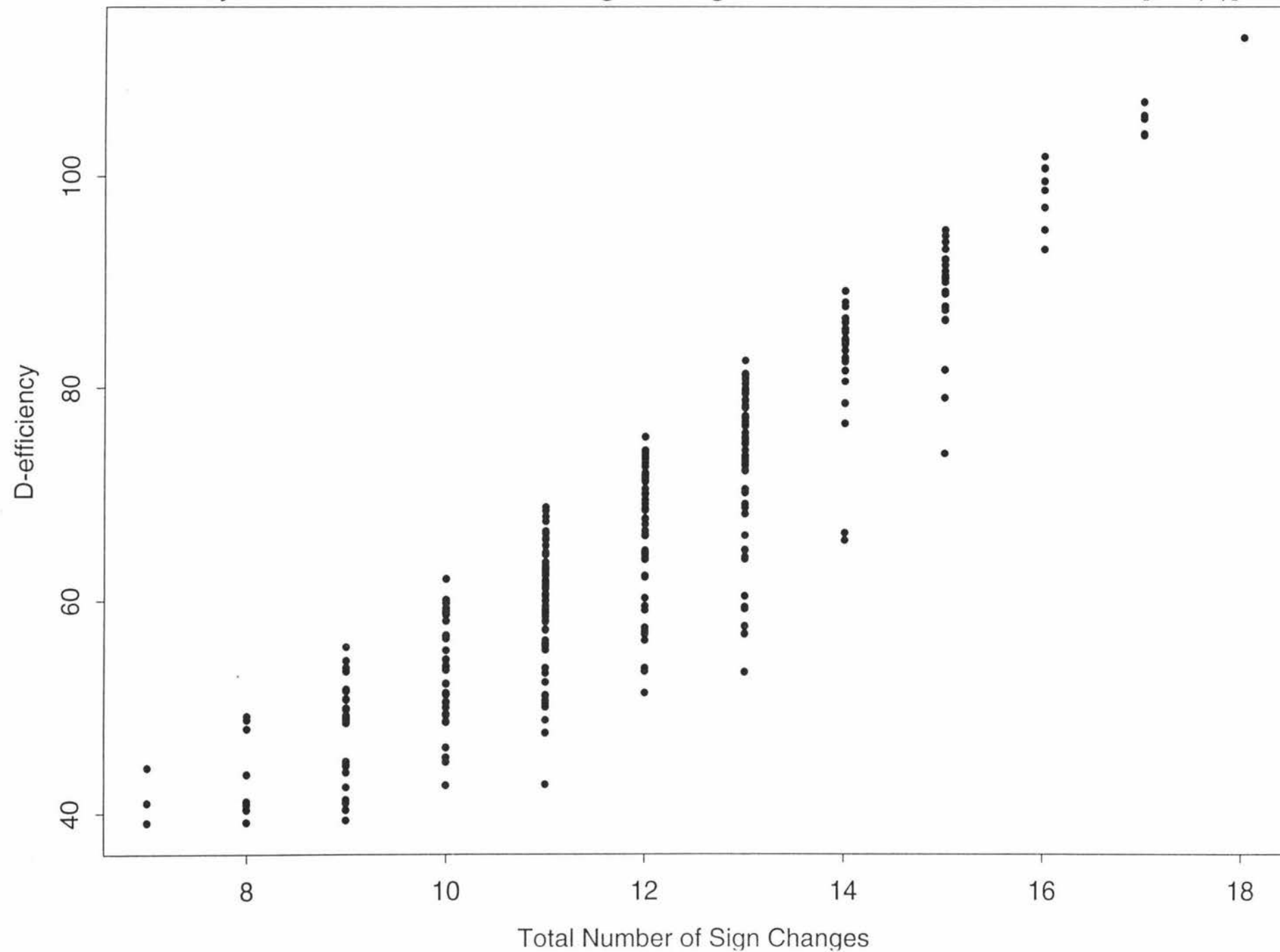


D-efficiency versus Total Number of Sign changes when correlation coefficient[AR(1)] is 0.25

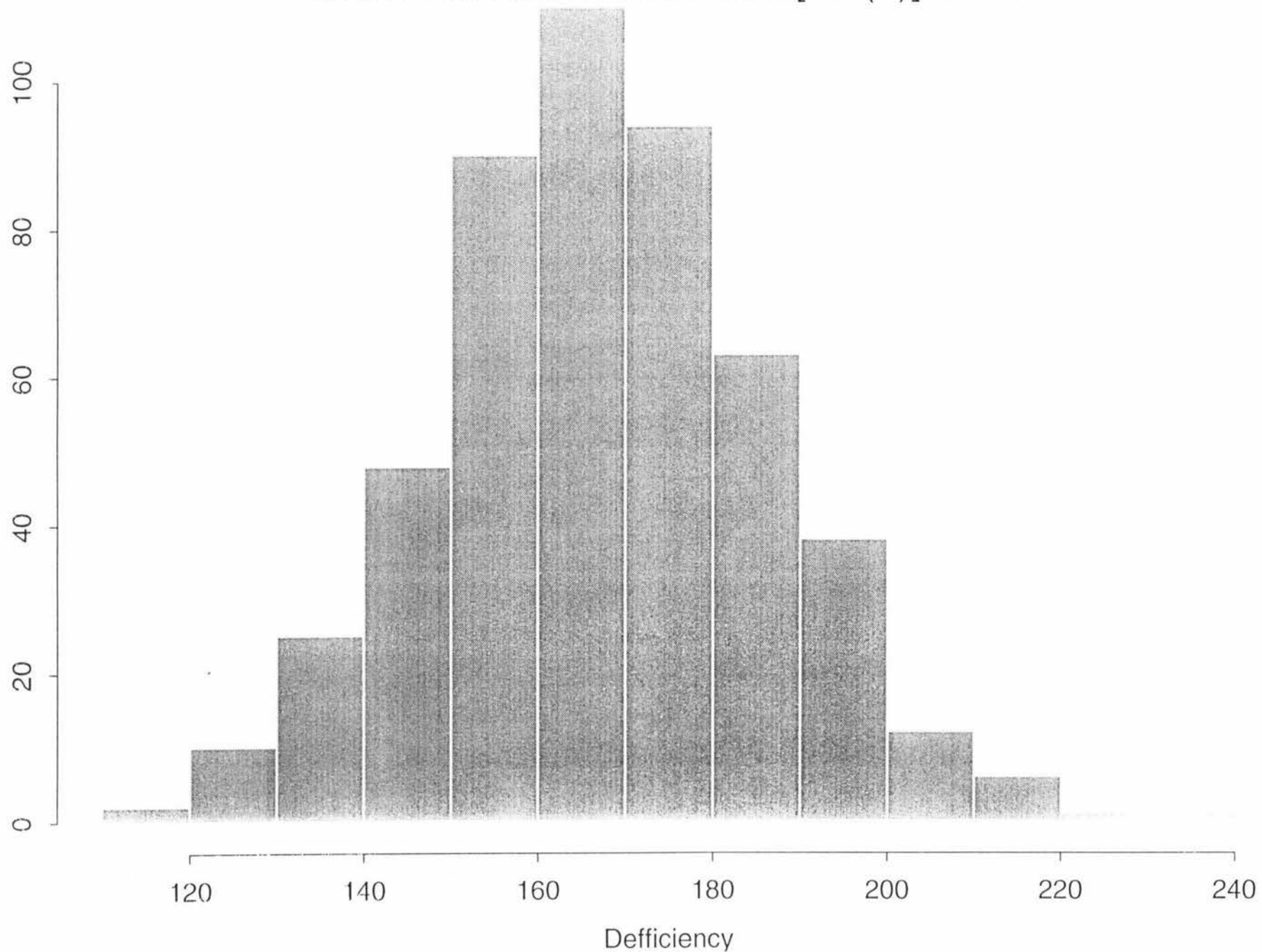




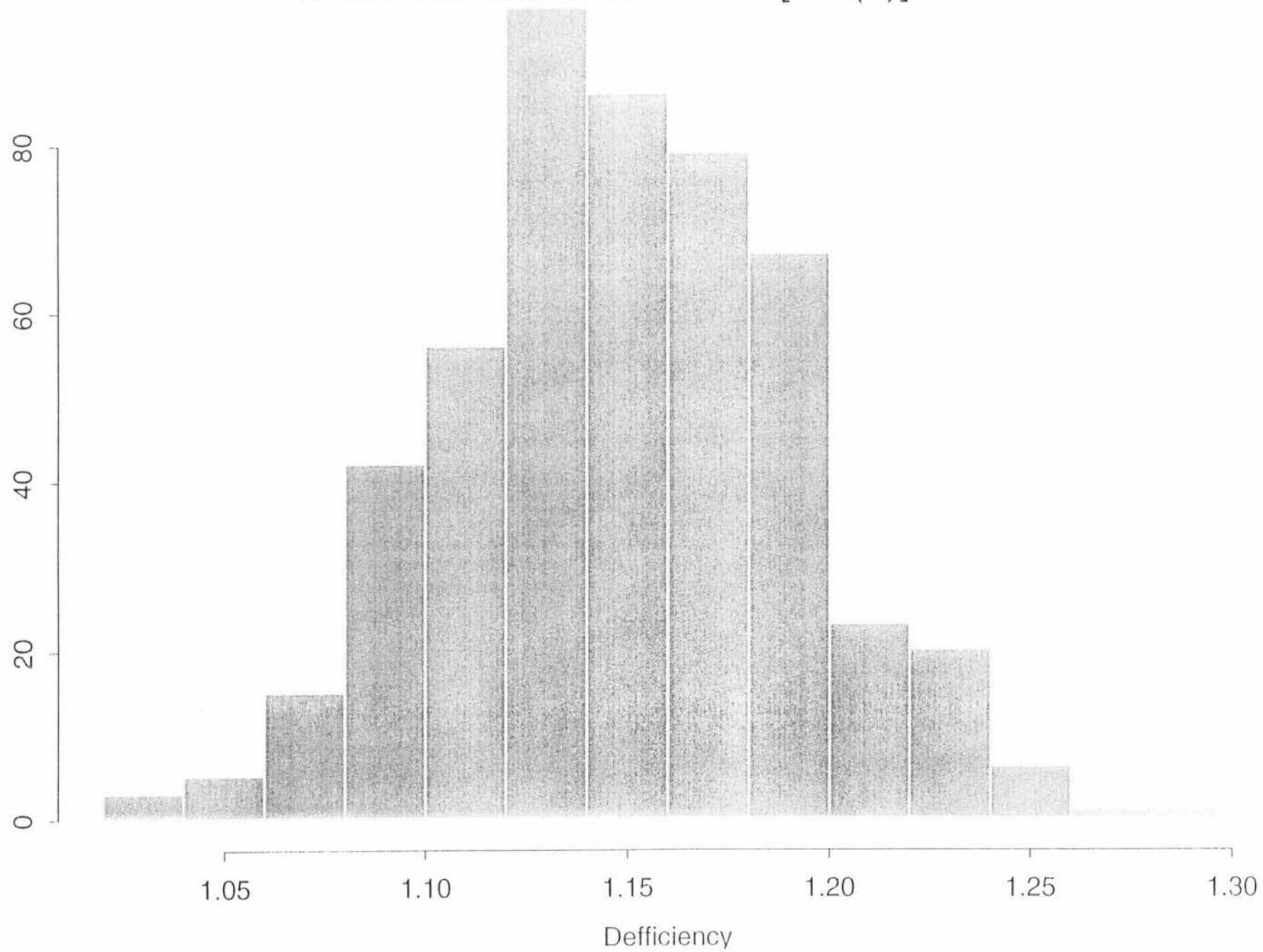
D-efficiency versus Total Number of Sign changes when correlation coefficient[AR(1)] is 0.9



Appendix 6  
Histogram for the D-efficiency of the (3x3x3) factorial Design  
when correlation coefficient[AR(1)] is 0.9



Appendix ,  
Histogram for the D-efficiency of the (3x3x3) factorial Design  
when correlation coefficient[MA(1)] is 0.25



# APPENDIX 8

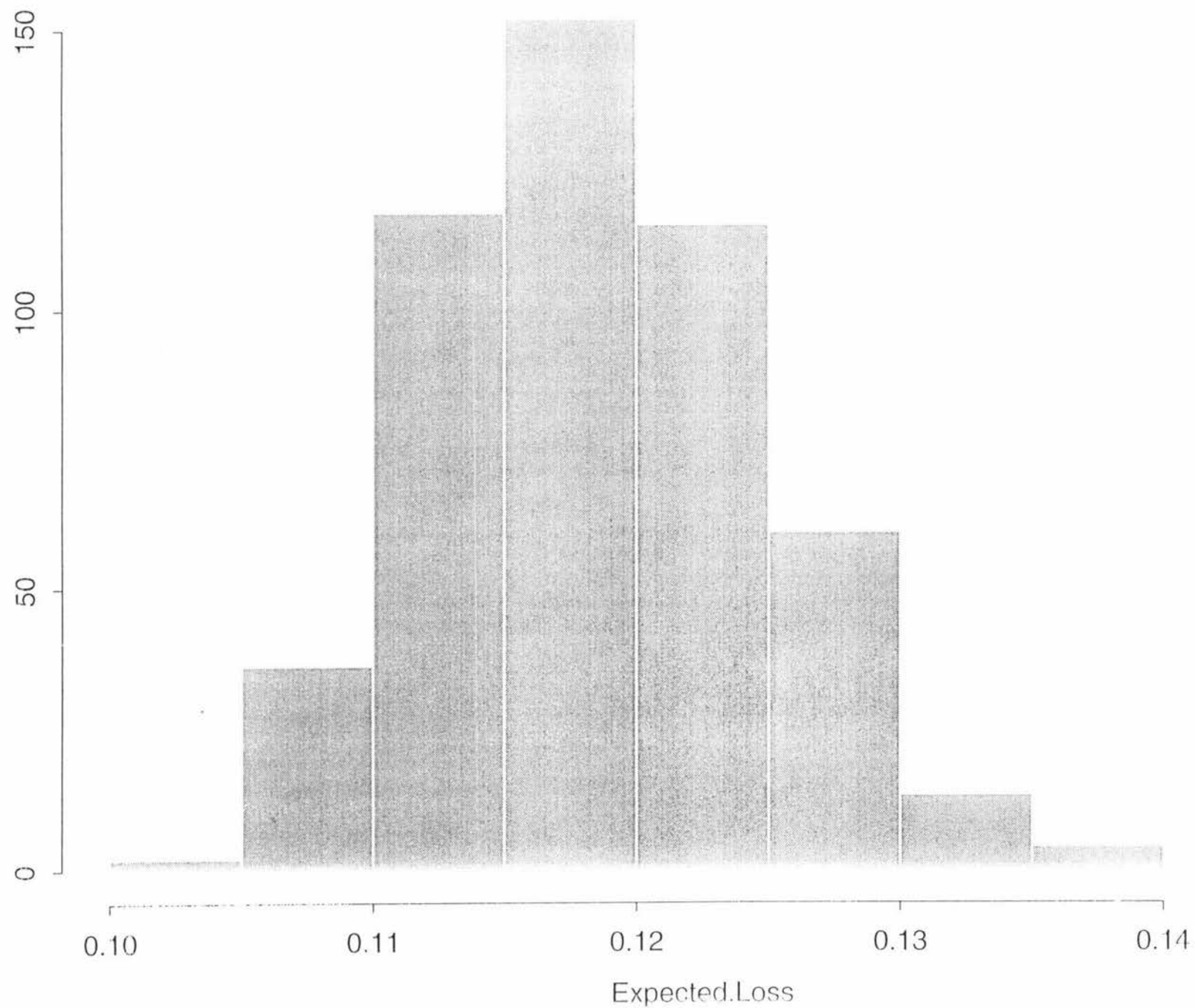
```
rr<-0.25
{MAV32mat<-MAV32mat(rr)
MA32mat<-c(0,0,0,0,0,0,0,0,0,0,0,0)
for (k in 0:1000)
{ it<-k+1
if(it<1001)
{samp<-sample(1:9,9)
sl32samp<-ssl32[samp,]
sl32samp.tra<-t(sl32samp)
MAV32matinv<-solve(MAV32mat)
MA32Exa<-sl32samp.tra**MAV32matinv**sl32samp
MA32re<-det(MA32Exa)^(1/6)
InvMA32Exa<-solve(MA32Exa)
MA32Dstar<-InvMA32Exa[2:6,2:6]
MA32Deff<-det(MA32Dstar)^(-1/5)
MA32mat<-rbind(MA32mat,c(samp,MA32re,MA32Deff))}}
```

```
rr<-0.25
{ARV32mat<-ARV32mat(rr)
AR32mat<-c(0,0,0,0,0,0,0,0,0,0,0,0)
for (k in 0:1000)
{ it<-k+1
if(it<1001)
{samp<-sample(1:9,9)
sl32samp<-ssl32[samp,]
sl32samp.tra<-t(sl32samp)
ARV32matinv<-solve(ARV32mat)
AR32Exa<-sl32samp.tra**ARV32matinv**sl32samp
AR32re<-det(AR32Exa)^(1/6)
InvAR32Exa<-solve(AR32Exa)
AR32Dstar<-InvAR32Exa[2:6,2:6]
AR32Deff<-det(AR32Dstar)^(-1/5)
AR32mat<-rbind(AR32mat,c(samp,AR32re,AR32Deff))}}
```

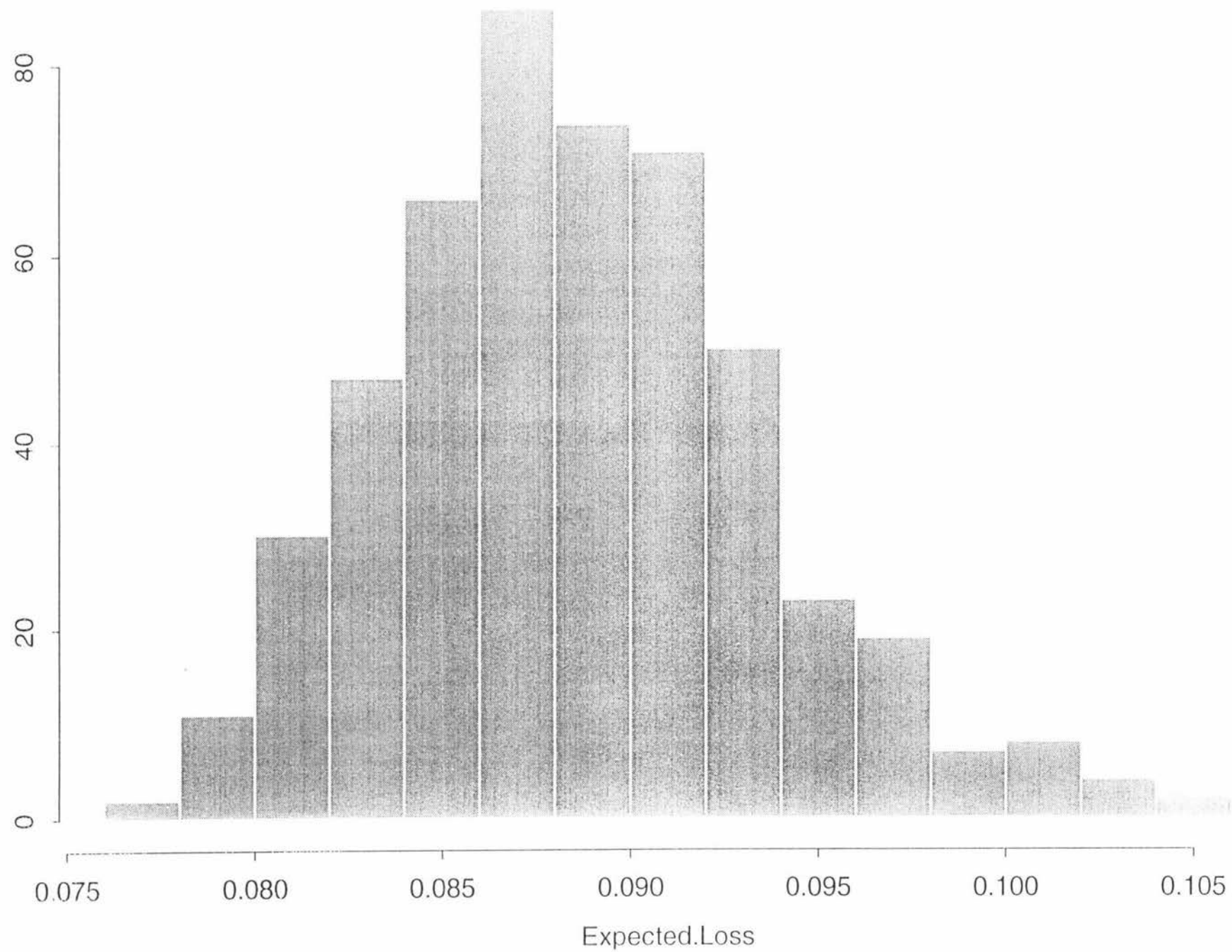
```
> ssl32
```

	sme	sl1	sl2	sq1	sq2	sq3
[1,]	0.3333333	-0.4082483	-0.4082483	0.2357023	0.2357023	0.5
[2,]	0.3333333	0.0000000	-0.4082483	-0.4714045	0.2357023	0.0
[3,]	0.3333333	0.4082483	-0.4082483	0.2357023	0.2357023	-0.5
[4,]	0.3333333	-0.4082483	0.0000000	0.2357023	-0.4714045	0.0
[5,]	0.3333333	0.0000000	0.0000000	-0.4714045	-0.4714045	0.0
[6,]	0.3333333	0.4082483	0.0000000	0.2357023	-0.4714045	0.0
[7,]	0.3333333	-0.4082483	0.4082483	0.2357023	0.2357023	-0.5
[8,]	0.3333333	0.0000000	0.4082483	-0.4714045	0.2357023	0.0
[9,]	0.3333333	0.4082483	0.4082483	0.2357023	0.2357023	0.5

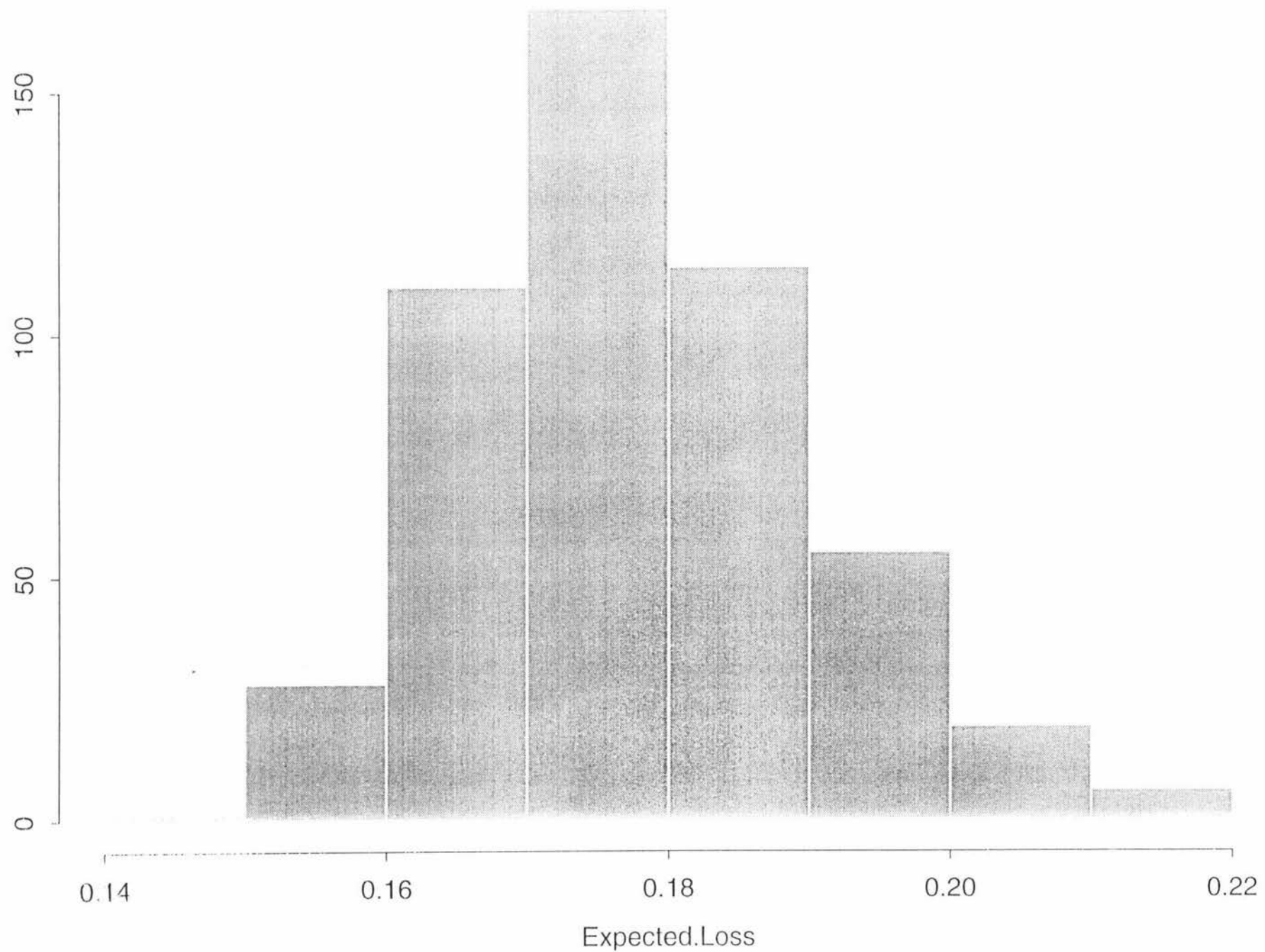
Appendix 9  
Histogram for the Expected Loss case 1 when  $s = 0.3$



Appendix 10  
Histogram for the Expected Loss case 2 when  $s = 0.3$

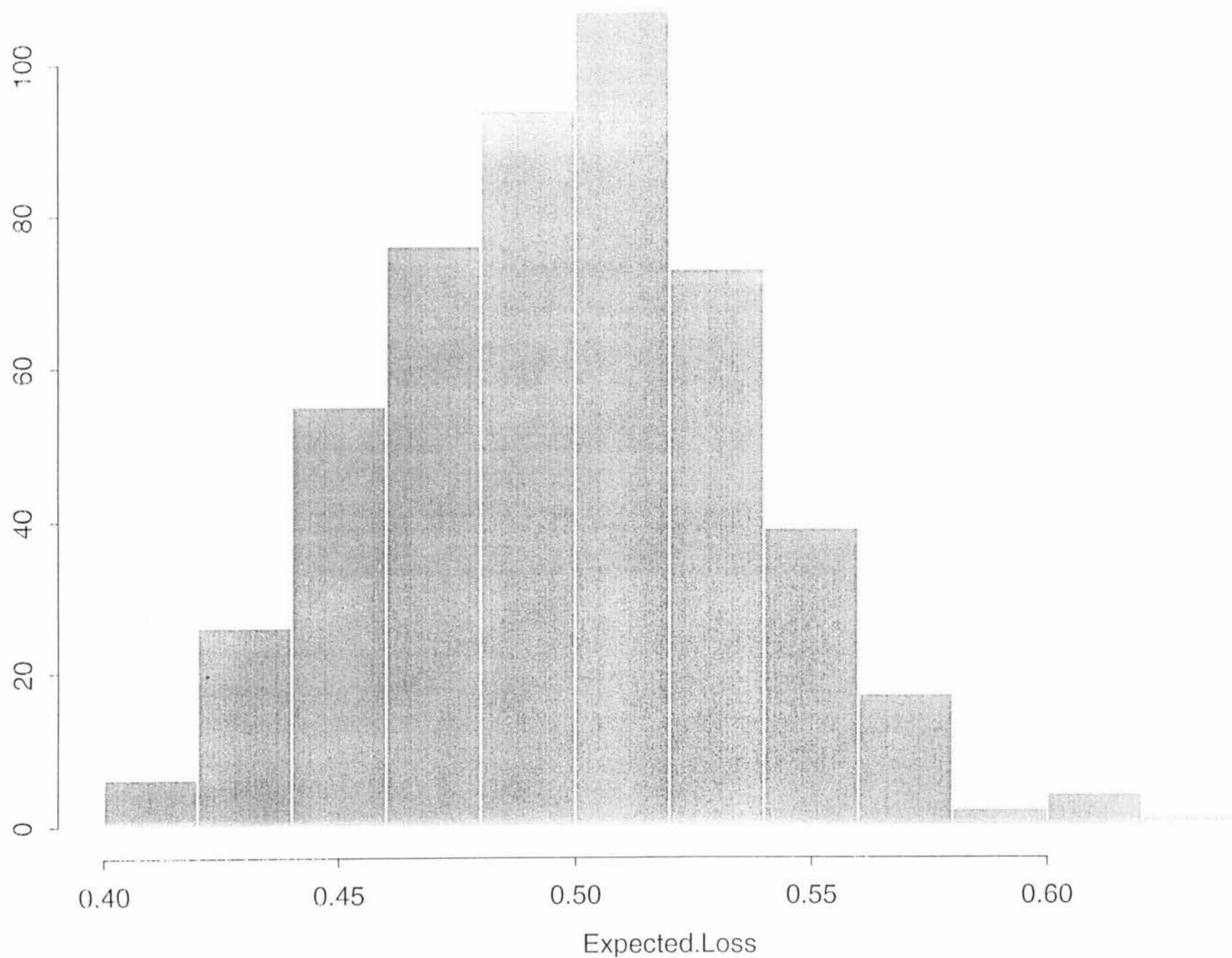


Appendix 11  
Histogram for the Expected Loss case 3 when  $s = 0.3$





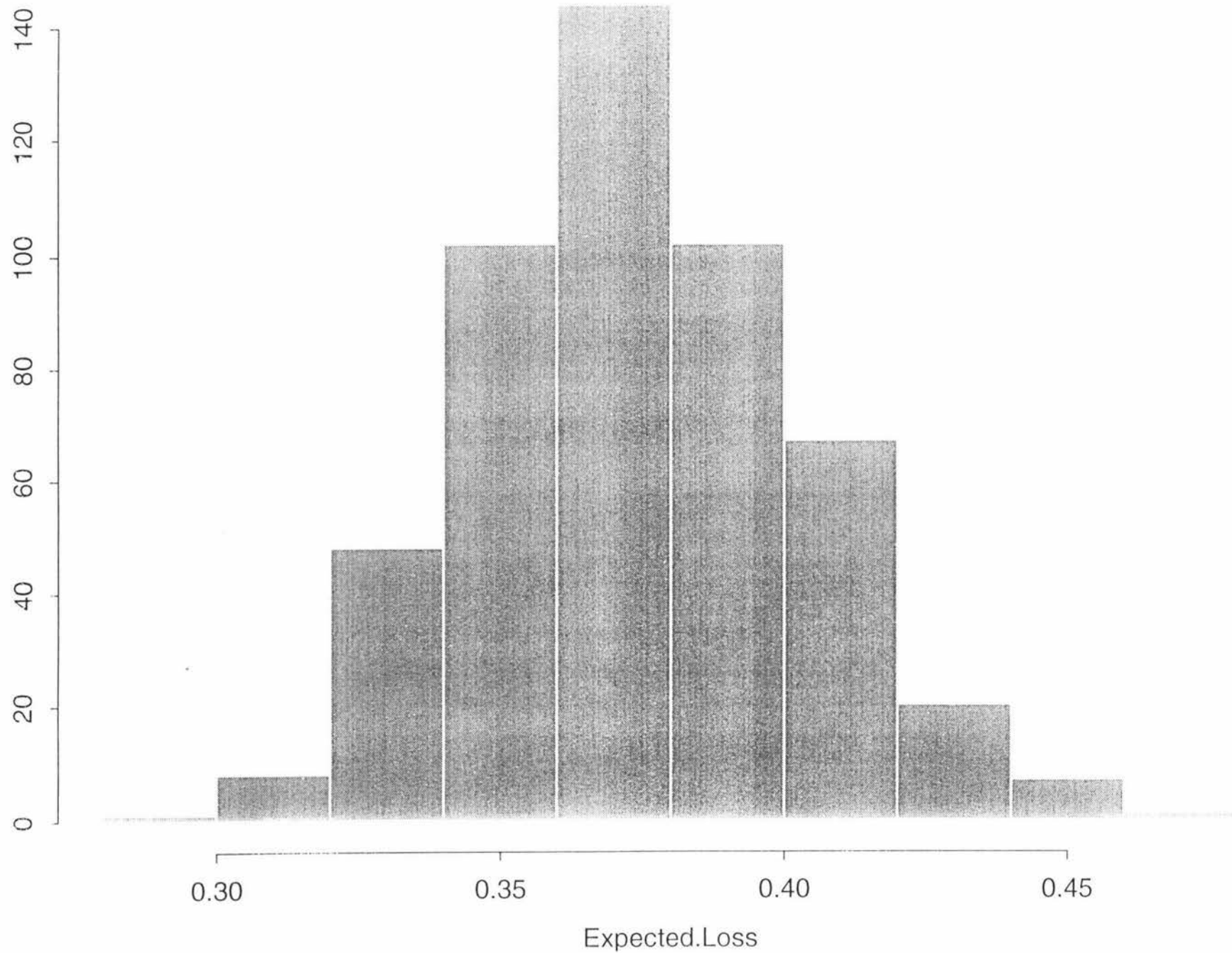
Appendix 12  
Histogram for the Expected Loss case 1 when  $s = 0.8$



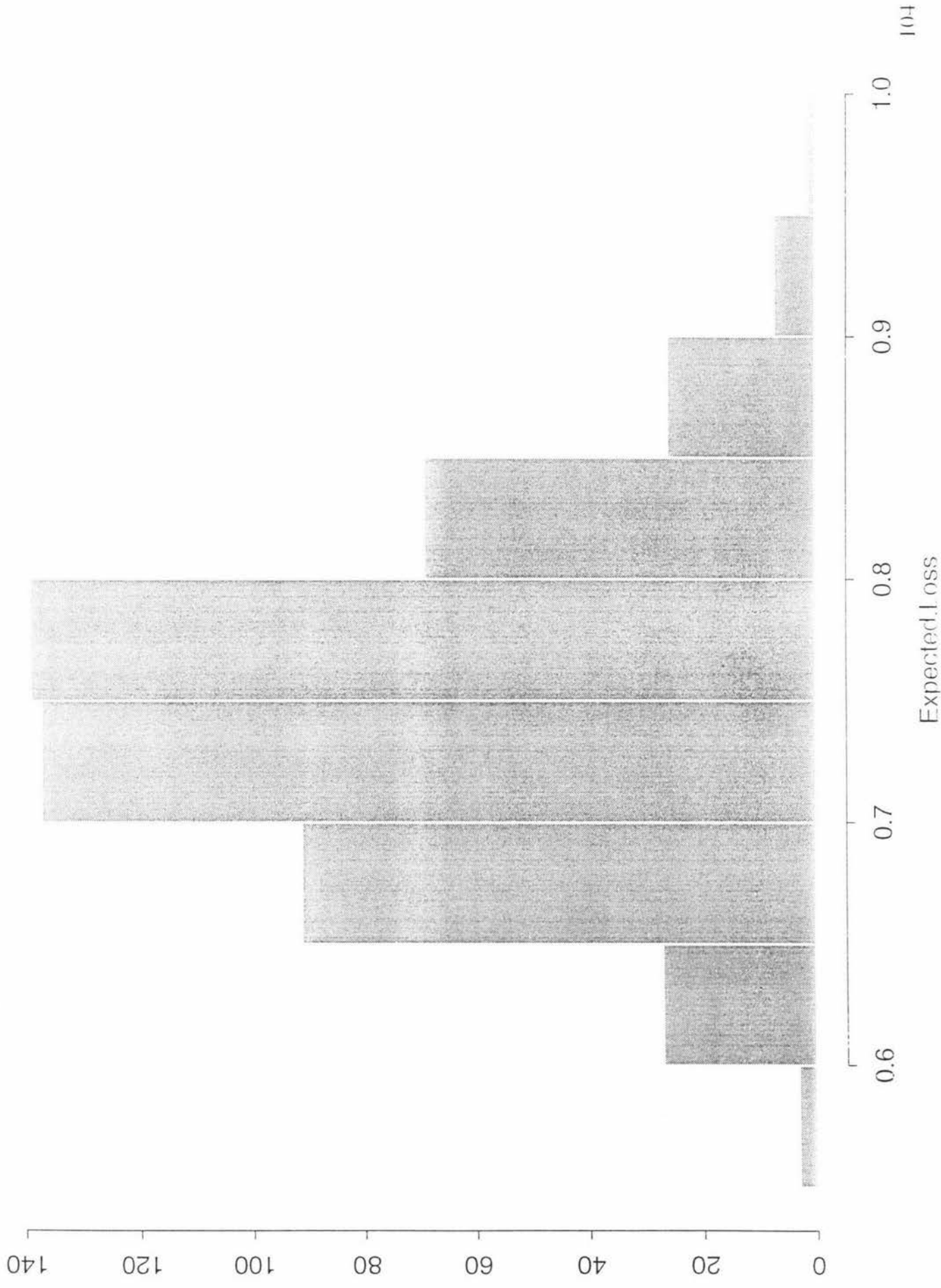


# Appendix 13

## Histogram for the Expected Loss case 2 when $s = 0.8$



Appendix 14  
Histogram for the Expected Loss case 3 when  $s = 0.8$



## Bibliography

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