

# On the Compounds of Hat Matrix for Six-Factor Central Composite Design with Fractional Replicates of the Factorial Portion

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**Abstract** The behaviours of the first compound of the hat matrix and the determinant-based loss criterion are examined for effects of a missing observation in three configurations of six-factor central composite design, varying in factorial portion. The hat matrix varies between one design configuration and another but remains unchanged within same design configuration with different defining relations. The diagonal entries of each corresponding hat matrix associated with a factorial point, an axial point and a center point respectively correspond to the losses computed using the determinant-based criterion. Loss due to missing center point in the three categories of design is very minimal when compared with loss due to either missing factorial point or missing axial point. The configuration with one-quarter fractional factorial portion attracts significantly higher losses to a missing observation of either factorial, axial or center portion when compared with either the configuration with one-half fractional factorial portion or the configuration with complete factorial portion. This is possibly because the configuration with one-quarter fractional factorial portion is near saturated. Variances associated with parameter estimates are minimum for the design category with complete factorial portion and maximum for the design category with one-quarter fractional factorial portion. Interestingly, the design category that minimizes the variances also minimizes the losses.

**Keywords** Missing observations, Compound of hat matrix, Fractional replicates, Loss criterion, Central composite design

## 1. Introduction

The concept of hat matrix plays a major role in modeling and is commonly encountered in regression and analysis of variance problems. Hoaglin and Welsch [11] linked its origin to John Tukey who is said to have introduced the matrix in the 1960s. Historically, the name takes its bearing from the fact that for a linear model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon} \quad (1)$$

the least squares estimate of  $\boldsymbol{\beta}$  is  $\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{y}$

Thus the fitted or estimated value is

$$\hat{\mathbf{y}} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{y} = \mathbf{H}\mathbf{y} \quad (2)$$

where  $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'$  is called the hat matrix and puts the “hat” on the vector of fitted or estimated value. Of course, as a projection matrix, the hat matrix projects  $\mathbf{y}$  into  $\hat{\mathbf{y}}$  in the model space. In a simpler language, the hat matrix converts values from the observed variable into estimates. In equation (1),  $\mathbf{y}$  denotes the vector of observations,  $\mathbf{X}$  denotes the model matrix,  $\boldsymbol{\beta}$  denotes the vector of unknown

parameters which are estimated on the basis of  $N$  uncorrelated observations and  $\boldsymbol{\varepsilon}$  denotes the random error component assumed normally and independently distributed with zero mean and constant variance.

One major role of the hat matrix in modeling problems is in identifying observations that have greater impacts on the estimation of model parameters and fitted values. Identifying and dealing with such observations help improve statistical inferences. The mention of hat matrix automatically directs one’s mind to leverage which according to Myung and Kahng [12] is one of the basic components of influence in linear regression models. Each diagonal element  $h_{ii}$  of the hat matrix is called leverage and measures the extent to which the fitted regression model  $\hat{y}_i$  is attracted by the given observation or data point  $y_i$ . In essence, the  $i^{th}$  leverage  $h_{ii}$  quantifies the influence that the observation  $y_i$  has on its predicted value  $\hat{y}_i$ . The diagonal elements of the hat matrix are such that  $0 \leq h_{ii} \leq 1$  and  $\sum_{i=1}^N h_{ii} = p$ ; where  $N$  is the number of data points and  $p$  is the number of model parameters, including the intercept. Aside investigating whether one or more observations excessively influence the estimated values, the hat matrix may also be used to quantify the effect of removing one or more observations from a design. Thus, the hat matrix (through its compounds) is useful in understanding effect of alterations to a complete data set.

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By the alterations, a removed observation is seen as a missing observation.

It is desirable to have the effect of missing observations as mild as possible. The term ‘‘Robust’’ first introduced by Box [9] is quite often encountered when studying the effects of missing observations. Akhtar [1] considered the effect of missing observations on the determinant of information matrix. Akhtar [6] considered the effect of missing observations on some configurations of five-factor central composite design and compared the variances of the parameter estimates as well as the sum of variances for each design configuration. Akram [7] assessed the effects of missing observation on the estimates of model parameters. Designs robust to missing observations have been considered by Ahmad and Gilmour [4] and Ahmad *et al.* [5] using minimax loss criterion. Chukwu *et al.* [10] considered the robustness of Split-plot central composite designs in the presence of a single missing observation. In their work, minimaxloss criterion, based on  $D$ -efficiency, and which accounts for the within-whole plot correlation among the observations, was presented for constructing split-plot response surface designs that are robust to missing a single observation of the various design points. Okon and Nsude [13] investigated alpha values for which the four-factor central composite designs are robust to a pair of missing observations under the minimaxloss criterion. Yakubu *et al.* [16] considered the impact of single missing observations of the various composite design points on estimation and predictive capability of central composite designs.

Some economical designs have been constructed and studied for their robustness to missing data by Ahmad and Akhtar [3]. In studying robust response surface designs against missing observations, Srisuradetchai [15] considered the sensitivity of small second-order designs through the loss of D-efficiency and established the impact of missing observations on predictive variances. Smucker *et al.* [14] considered the robustness of classical and optimal designs to missing observations using D- and I-efficiencies. Based on recommendation of Akhtar [6] to investigate models with more than five input variables, the effect of a missing observation in six-factor central composite design is considered in this paper. Particular interest is in robustness of fractional replicates of the factorial portion of the six-factor central composite design. Comparison of the effect of a missing observation shall be made using the first compound of the hat matrix.

## 2. Theoretical Background

For a symmetric matrix  $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$  of order  $N$ , the  $m^{\text{th}}$  compound of  $\mathbf{H}$  is a matrix of order  $\binom{N}{m}$ , where  $N$  is the number of data points in the complete design and  $m$  is the number of missing observations. The  $m^{\text{th}}$  compound of  $\mathbf{H}$  is formed by the elements of which are minors of  $|\mathbf{H}|$  of order  $m$ . All possible minors that are  $\binom{N}{m}$  from the same

combination of rows (or columns) of  $\mathbf{H}$  are placed in the same rows (or columns) of the  $m^{\text{th}}$  compound of  $\mathbf{H}$  say  $\mathbf{H}^{(m)}$ . The elements of  $\mathbf{H}^{(m)}$  are arranged in lexicographic (or lexical) order. The first compound of the hat matrix is the hat matrix itself. For more on compounds of the hat matrix, see Akram [7] and Atken and Rutherford [8].

In studying the effect of missing observations, Akbar and Prescott [2] defined loss as the relative reduction in the determinant of information matrix associated with the complete design. In this context, a complete design  $\xi_N$  is an  $N$ -point design constructed according to response surface model and having no missing data point. A six-factor central composite complete design with full replicate of factorial portion, full replicate of axial portion and four replicates of center portion constructed for a second-order complete model in twenty-eight parameters has eighty data points. The associated design matrix is a matrix of order (80x6). The associated model matrix  $\mathbf{X}$  is a matrix of order (80x28). The information matrix associated with the complete design is the matrix which is of order (28x28). Generally, an information matrix,  $\mathbf{X}'\mathbf{X}$ , of a design is a  $(pxp)$  matrix, where  $p$  represents the number of model parameters. When an observation or data point in the design is lost or missing, the matrix  $\mathbf{X}$  reduces by one row. Similarly, when  $m$  observations or data points in the design are lost or missing, the matrix  $\mathbf{X}$  reduces by  $m$  rows. As expected, the information matrix, say  $\mathbf{X}_r'\mathbf{X}_r$ , for the reduced design will be different from the information matrix,  $\mathbf{X}'\mathbf{X}$ , for the complete design. For  $(mxp)$  matrix of  $m$  missing rows,  $\mathbf{X}_m$ , corresponding to the  $m$  missing observations, the complete information matrix may be written as

$$\mathbf{X}'\mathbf{X} = \mathbf{X}_m'\mathbf{X}_m + \mathbf{X}_r'\mathbf{X}_r \quad (3)$$

By post multiplication,

$$(\mathbf{X}'\mathbf{X})(\mathbf{X}'\mathbf{X})^{-1} = [(\mathbf{X}_m'\mathbf{X}_m) + (\mathbf{X}_r'\mathbf{X}_r)](\mathbf{X}'\mathbf{X})^{-1} \quad (4)$$

This implies

$$\mathbf{I}_p = (\mathbf{X}_m'\mathbf{X}_m)(\mathbf{X}'\mathbf{X})^{-1} + (\mathbf{X}_r'\mathbf{X}_r)(\mathbf{X}'\mathbf{X})^{-1}; \mathbf{I}_p \text{ is an identity matrix of order } p.$$

By rearrangement we have

$$(\mathbf{X}_r'\mathbf{X}_r)(\mathbf{X}'\mathbf{X})^{-1} = \mathbf{I}_p - (\mathbf{X}_m'\mathbf{X}_m)(\mathbf{X}'\mathbf{X})^{-1} \quad (5)$$

Post multiplying by  $(\mathbf{X}'\mathbf{X})$  yields

$$(\mathbf{X}_r'\mathbf{X}_r)(\mathbf{X}'\mathbf{X})^{-1}(\mathbf{X}'\mathbf{X}) =$$

$$[\mathbf{I}_p - (\mathbf{X}_m'\mathbf{X}_m)(\mathbf{X}'\mathbf{X})^{-1}] (\mathbf{X}'\mathbf{X}) \quad (6)$$

$$\Rightarrow (\mathbf{X}_r'\mathbf{X}_r) = [\mathbf{I}_p - (\mathbf{X}_m'\mathbf{X}_m)(\mathbf{X}'\mathbf{X})^{-1}] (\mathbf{X}'\mathbf{X}) \quad (7)$$

$$|(\mathbf{X}_r'\mathbf{X}_r)| = |[\mathbf{I}_p - (\mathbf{X}_m'\mathbf{X}_m)(\mathbf{X}'\mathbf{X})^{-1}]| |(\mathbf{X}'\mathbf{X})| \quad (8)$$

This implies

$$\frac{|(\mathbf{X}_r'\mathbf{X}_r)|}{|(\mathbf{X}'\mathbf{X})|} = |[\mathbf{I}_p - (\mathbf{X}_m'\mathbf{X}_m)(\mathbf{X}'\mathbf{X})^{-1}]| \quad (9)$$

Akhtar [1] calls  $|[\mathbf{I}_p - (\mathbf{X}_m'\mathbf{X}_m)(\mathbf{X}'\mathbf{X})^{-1}]|$  the diagonal element of the  $m^{\text{th}}$  compound of  $(\mathbf{I}-\mathbf{H})$  where  $\mathbf{H}$  is the hat matrix according to the  $m$  missing points and  $\mathbf{I}$  is an identity matrix of same dimension as  $\mathbf{H}$ . The loss due to a single missing observation is defined as

$$l = 1 - \frac{|(X_r' X_r)|}{|(X' X)|} \quad (10)$$

and relates to the corresponding diagonal element of the first compound of the hat matrix  $\mathbf{H}$ .

### 3. Configurations of the Six-factor Central Composite Design

The loss due to missing observations of the six-factor central composite design shall be examined under three Configurations;

**Case 1:**  $k = 6$ , one replicate of factorial portion, one replicate of axial portion and four replicates of center portion.

**Case 2:**  $k = 6$ , one-half replicate of factorial portion, one replicate of axial portion and four replicates of center portion.

**Case 3:**  $k = 6$ , one-quarter replicate of factorial portion, one replicate of axial portion and four replicates of center portion.

By these three configurations, nonsingular information matrices may be obtained. Case 1 allows a complete design of size  $N = 80$  to be examined. The factorial portion comprises of design points associated with full  $2^6$  factorial design. The axial portion comprises of the design points  $\{(\pm 1,0,0,0,0,0), (0, \pm 1,0,0,0,0), (0,0, \pm 1,0,0,0), (0,0,0, \pm 1,0,0), (0,0,0,0, \pm 1,0)\}$ . The center portion comprises of the design point  $(0,0,0,0,0,0)$  repeated four times.

$1,0,0), (0,0,0,0, \pm 1,0), (0,0,0,0,0, \pm 1)\}$ . The center portion comprises of the design point  $(0,0,0,0,0,0)$  repeated four times.

Case 2 allows a complete design of size  $N = 48$  to be examined. The factorial portion comprises of design points associated with one-half fractional replicate of  $2^6$  factorial design. The factorial portion may be obtained using the defining relation  $I = +ABCDEF$  or  $I = -ABCDEF$ . The axial portion comprises of the design points  $\{(\pm 1,0,0,0,0,0), (0, \pm 1,0,0,0,0), (0,0, \pm 1,0,0,0), (0,0,0, \pm 1,0,0), (0,0,0,0, \pm 1,0)\}$ . The center portion comprises of the design point  $(0,0,0,0,0,0)$  repeated four times. Case 3 allows a complete design of size  $N = 32$  to be examined. The factorial portion comprises of design points associated with one-quarter fractional replicate of  $2^6$  factorial design. The factorial portion may be obtained using the defining relation  $I = +ABC$  and  $I = +DEF$  or  $I = +ABC$  and  $I = -DEF$  or  $I = -ABC$  and  $I = -DEF$  or  $I = -ABC$  and  $I = +DEF$ . The axial portion comprises of the design points  $\{(\pm 1,0,0,0,0,0), (0, \pm 1,0,0,0,0), (0,0, \pm 1,0,0,0), (0,0,0, \pm 1,0,0), (0,0,0,0, \pm 1,0)\}$ . The center portion comprises of the design point  $(0,0,0,0,0,0)$  repeated four times. The use of fractional factorials greatly reduces the required experimental runs. In fact, Case 3 brings the design to near-saturated.

Using the defining relations  $I = +ABCDEF$ , the aliases of effects under Case 2 are as follows;

A = BCDEF	AD = BCEF	CE = ABDF	ABF = CDE
B = ACDEF	AE = BCDF	CF = ABDE	ACD = BEF
C = ABDEF	AF = BCDE	DE = ABCF	ACE = BDF
D = ABCEF	BC = ADEF	DF = ABCE	ACF = BDE
E = ABCDF	BD = ACEF	EF = ABCD	ADE = BCF
F = ABCDE	BE = ACDF	ABC = DEF	ADF = BCE
AB = CDEF	BF = ACDE	ABD = CEF	AEF = BCD
AC = BDEF	CD = ABEF	ABE = CDF	

Using the defining relations  $I = +ABC$  and  $I = +DEF$  alongside the generalized interaction  $I = +ABCDEF$ , the aliases of effects under Case 3 are as follows;

A = BC = ADEF = BCDEF	AF = BCF = ADE = BCDE
B = AC = BDEF = ACDEF	BD = ACD = BEF = ACEF
C = AB = CDEF = ABDEF	BE = ACE = BDF = ACDF
D = ABCD = EF = ABCEF	BF = ACF = CDE = ACDE
E = ABCE = DF = ABCDF	CD = ABD = CEF = ABEF
F = ABCF = DE = ABCDE	CE = ABE = CDF = ABDF
AD = BCD = AEF = BCEF	CF = ABF = CDE = ABDE
AE = BCE = ADF = BCDF	

## 4. Results

### 4.1. Six-factor Central Composite Design with One Replicate of Factorial Portion, One Replicate of Axial Portion and Four Replicates of Center Portion

The hat matrix  $\mathbf{H} = \mathbf{X} (\mathbf{X}' \mathbf{X})^{-1} \mathbf{X}'$  associated with complete cuboidal six-factor central composite design having one

replicate of factorial portion, one replicate of axial portion and four replicates of center portion is as in Appendix A. The variances and covariances for the model parameter estimates are contained in the variance-covariance matrix  $(\mathbf{X}'\mathbf{X})^{-1}$  whose elements are as in the immediate.

Trace  $H = 28.0000$

$$\det(X'X) = 1.5533e+043$$

$$\det(X'X)^{-1} = 6.4379 \text{e-}044$$

For a missing observation, the 80-point design reduces by one observation. A row of the design matrix as well as the model matrix corresponding to the missing observation is deleted.

Associated with a missing vertex or factorial point is the determinant

$$\det(\mathbf{X}_f' \mathbf{X}_f) = 1.0238e+043$$

$$\det(X_f^T X_f)^{-1} = 9.7674 \text{e-}044$$

$$\frac{\det(X_f'X_f)}{\det(X'X)} = 0.6591$$

The loss due to missing vertex point is

$$l_f = 1 - \frac{\det(X'X_f)}{\det(X'X)} = 0.3409$$

This corresponds to the first entry, 0.3409, of the hat matrix in Appendix A.

Associated with a missing axial point is the determinant

$$\det(X_a'X_a) = 7.9503 \times 10^4$$

$$\det(X_a'X_a)^{-1} = 1.2578\text{e-}043$$

$$\frac{\det(X_a'X_a)}{\det(X'X)} = 0.5118$$

The loss due to missing axial point is

$$l_a = 1 - \frac{\det(X_a X_a)}{\det(X' X)} = 0.4882$$

This corresponds to the 65<sup>th</sup> entry, 0.4882, of the hat matrix in Appendix A.

Associated with a missing center point is the determinant

$$\det(\mathbf{X}_c' \mathbf{X}_c) = 1.4269 \times 10^4$$

$$\det(X_c'X_c)^{-1} = 7.0081\text{e-}044$$

$$\frac{\det(X'_c X_c)}{\det(X' X)} = 0.9186$$

The loss due to missing center point is

$$l_c = 1 - \frac{\det(X'_c X_c)}{\det(X' X)} = 0.0814$$

This corresponds to the 80<sup>th</sup> entry, 0.0814, of the hat matrix in Appendix A.

The variances of parameter estimates for the complete and reduced designs are as in Table 1.

**Table 1.** Variances of parameter estimates for the complete and reduced designs (one replicate of factorial portion)

Model term	Model parameter	Variance of parameter estimate associated with design with complete factorial point	Variance of parameter estimate associated with design with missing factorial point	Variance of parameter estimate associated with design with missing axial point	Variance of parameter estimate associated with design with missing center point
Intercept	$\beta_0$	0.0814	0.0814	0.0903	0.0886
$x_1$	$\beta_1$	0.0152	0.0155	0.0156	0.0152
$x_2$	$\beta_2$	0.0152	0.0155	0.0156	0.0152
$x_3$	$\beta_3$	0.0152	0.0155	0.0156	0.0152
$x_4$	$\beta_4$	0.0152	0.0155	0.0156	0.0152
$x_5$	$\beta_5$	0.0152	0.0155	0.0156	0.0152
$x_6$	$\beta_6$	0.0152	0.0155	0.0156	0.0152
$x_1 x_2$	$\beta_{12}$	0.0152	0.0160	0.0156	0.0152
$x_1 x_3$	$\beta_{13}$	0.0152	0.0160	0.0156	0.0152
$x_1 x_4$	$\beta_{14}$	0.0152	0.0160	0.0156	0.0152
$x_1 x_5$	$\beta_{15}$	0.0152	0.0160	0.0156	0.0152
$x_1 x_6$	$\beta_{16}$	0.0152	0.0160	0.0156	0.0152
$x_2 x_3$	$\beta_{23}$	0.0152	0.0160	0.0156	0.0152
$x_2 x_4$	$\beta_{24}$	0.0152	0.0160	0.0156	0.0152
$x_2 x_5$	$\beta_{25}$	0.0152	0.0160	0.0156	0.0152
$x_2 x_6$	$\beta_{26}$	0.0152	0.0160	0.0156	0.0152
$x_3 x_4$	$\beta_{34}$	0.0152	0.0160	0.0156	0.0152
$x_3 x_5$	$\beta_{35}$	0.0152	0.0160	0.0156	0.0152
$x_3 x_6$	$\beta_{36}$	0.0152	0.0160	0.0156	0.0152
$x_4 x_5$	$\beta_{45}$	0.0152	0.0160	0.0156	0.0152
$x_4 x_6$	$\beta_{46}$	0.0152	0.0160	0.0156	0.0152
$x_5 x_6$	$\beta_{56}$	0.0152	0.0160	0.0156	0.0152
$x_1^2$	$\beta_{11}$	0.4195	0.4195	0.7408	0.4197
$x_2^2$	$\beta_{22}$	0.4195	0.4195	0.4369	0.4197
$x_3^2$	$\beta_{33}$	0.4195	0.4195	0.4369	0.4197
$x_4^2$	$\beta_{44}$	0.4195	0.4195	0.4369	0.4197
$x_5^2$	$\beta_{55}$	0.4195	0.4195	0.4369	0.4197
$x_6^2$	$\beta_{66}$	0.4195	0.4195	0.4369	0.4197
Sum of variances		2.6614	2.9314	3.3432	2.926
Average variance		0.09505	0.104693	0.1194	0.1045

#### 4.2. Six-factor Central Composite Design with One-Half Replicate of Factorial Portion, One Replicate of Axial Portion and four Replicates of Center Portion

The hat matrix  $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$  associated with complete cuboidal six-factor central composite design having one-half replicate of factorial portion, one replicate of axial portion and four replicates of center portion is as in Appendix B. The variances and covariances for the model parameter estimates are contained in the variance-covariance matrix  $(\mathbf{X}'\mathbf{X})^{-1}$  whose elements are as in the immediate.

Trace  $\mathbf{H} = 28.0000$

$$\det(\mathbf{X}'\mathbf{X}) = 4.4373e+036$$

$$\det(\mathbf{X}'\mathbf{X})^{-1} = 2.2536e-037$$

For a missing observation, the 48-point design reduces by one observation. A row of the design matrix as well as the model matrix corresponding to the missing observation is deleted.

Associated with a missing vertex or factorial point is the determinant

$$\det(\mathbf{X}_f'\mathbf{X}_f) = 1.4361e+036$$

$$\det(\mathbf{X}_f'\mathbf{X}_f)^{-1} = 6.9635e-037$$

$$\frac{\det(\mathbf{X}_f'\mathbf{X}_f)}{\det(\mathbf{X}'\mathbf{X})} = 0.3236$$

The loss due to missing vertex point is

$$l_f = 1 - \frac{\det(\mathbf{X}_f'\mathbf{X}_f)}{\det(\mathbf{X}'\mathbf{X})} = 0.6764$$

This corresponds to the first entry, 0.6764, of the hat matrix in Appendix B.

Associated with a missing axial point is the determinant

$$\det(\mathbf{X}_a'\mathbf{X}_a) = 2.2077e+036$$

$$\det(\mathbf{X}_a'\mathbf{X}_a)^{-1} = 4.5297e-037$$

$$\frac{\det(\mathbf{X}_a'\mathbf{X}_a)}{\det(\mathbf{X}'\mathbf{X})} = 0.4975$$

The loss due to missing axial point is

$$l_a = 1 - \frac{\det(\mathbf{X}_a'\mathbf{X}_a)}{\det(\mathbf{X}'\mathbf{X})} = 0.5025$$

This corresponds to the 65<sup>th</sup> entry, 0.5025, of the hat matrix in Appendix B.

Associated with a missing center point is the determinant

$$\det(\mathbf{X}_c'\mathbf{X}_c) = 4.0750e+036$$

$$\det(\mathbf{X}_c'\mathbf{X}_c)^{-1} = 2.4540e-037$$

$$\frac{\det(\mathbf{X}_c'\mathbf{X}_c)}{\det(\mathbf{X}'\mathbf{X})} = 0.9184$$

The loss due to missing center point is

$$l_c = 1 - \frac{\det(\mathbf{X}_c'\mathbf{X}_c)}{\det(\mathbf{X}'\mathbf{X})} = 0.0816$$

This corresponds to the 80<sup>th</sup> entry, 0.0816, of the hat matrix in Appendix B.

The variances of parameter estimates for the complete and reduced designs are as in Table 2.

**Table 2.** Variances of parameter estimates for the complete and reduced designs (One-half replicate of factorial portion)

Model term	Model parameter	Variance of parameter estimate associated with design with complete factorial point	Variance of parameter estimate associated with design with missing factorial point	Variance of parameter estimate associated with design with missing axial point	Variance of parameter estimate associated with design with missing center point
Intercept	$\beta_0$	0.0816	0.0817	0.0908	0.0889
$x_1$	$\beta_1$	0.0294	0.0321	0.0312	0.0294
$x_2$	$\beta_2$	0.0294	0.0321	0.0294	0.0294
$x_3$	$\beta_3$	0.0294	0.0321	0.0294	0.0294
$x_4$	$\beta_4$	0.0294	0.0321	0.0294	0.0294
$x_5$	$\beta_5$	0.0294	0.0321	0.0294	0.0294
$x_6$	$\beta_6$	0.0294	0.0321	0.0294	0.0294
$x_1x_2$	$\beta_{12}$	0.0313	0.0343	0.0313	0.0313
$x_1x_3$	$\beta_{13}$	0.0313	0.0343	0.0313	0.0313
$x_1x_4$	$\beta_{14}$	0.0313	0.0343	0.0313	0.0313
$x_1x_5$	$\beta_{15}$	0.0313	0.0343	0.0313	0.0313
$x_1x_6$	$\beta_{16}$	0.0313	0.0343	0.0313	0.0313
$x_2x_3$	$\beta_{23}$	0.0313	0.0343	0.0313	0.0313
$x_2x_4$	$\beta_{24}$	0.0313	0.0343	0.0313	0.0313
$x_2x_5$	$\beta_{25}$	0.0313	0.0343	0.0313	0.0313
$x_2x_6$	$\beta_{26}$	0.0313	0.0343	0.0313	0.0313
$x_3x_4$	$\beta_{34}$	0.0313	0.0343	0.0313	0.0313
$x_3x_5$	$\beta_{35}$	0.0313	0.0343	0.0313	0.0313
$x_3x_6$	$\beta_{36}$	0.0313	0.0343	0.0313	0.0313
$x_4x_5$	$\beta_{45}$	0.0313	0.0343	0.0313	0.0313

$x_4 x_6$	$\beta_{46}$	0.0313	0.0343	0.0313	0.0313
$x_5 x_6$	$\beta_{56}$	0.0313	0.0343	0.0313	0.0313
$x_1^2$	$\beta_{11}$	0.4200	0.4201	0.7509	0.4203
$x_2^2$	$\beta_{22}$	0.4200	0.4201	0.4379	0.4203
$x_3^2$	$\beta_{33}$	0.4200	0.4201	0.4379	0.4203
$x_4^2$	$\beta_{44}$	0.4200	0.4201	0.4379	0.4203
$x_5^2$	$\beta_{55}$	0.4200	0.4201	0.4379	0.4203
$x_6^2$	$\beta_{66}$	0.4200	0.4201	0.4379	0.4203
Sum of variances		3.2475	3.3094	3.6789	3.2566
Average variance		0.115982	0.118193	0.131389	0.116307

#### **4.3. Six-Factor Central Composite Design with One-Quarter Replicate of Factorial Portion, One Replicate of Axial Portion and Four Replicates of Center Portion**

The hat matrix  $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$  associated with complete cuboidal six-factor central composite design having one-quarter replicate of factorial portion, one replicate of axial portion and four replicates of center portion is as in Appendix A. The variances and covariances for the model parameter estimates are contained in the variance-covariance matrix  $(\mathbf{X}'\mathbf{X})^{-1}$  whose elements are as in the immediate.

Trace  $H = 28.0000$

$$\det(\mathbf{X}'\mathbf{X}) = 2.8145 \times 10^{24}$$

$$\det(X'X)^{-1} = 3.5530\text{e-}025$$

For a missing observation, the 32-point design reduces by one observation. A row of the design matrix as well as the model matrix corresponding to the missing observation is deleted.

Associated with a missing vertex or factorial point is the determinant

$$\det(X_f^T X_f) = 1.1806 \times 10^{21}$$

$$\det(\mathbf{X}_f' \mathbf{X}_f)^{-1} = 8.4703 \times 10^{-22}$$

$$\frac{\det(\mathbf{X}_f' \mathbf{X}_f)}{\det(\mathbf{X}' \mathbf{X})} = 0.0004$$

The loss due to missing vertex point is

$$l_f = 1 - \frac{\det(X'_f X_f)}{\det(X' X)} = 0.9996$$

This corresponds to the first entry, 0.9996, of the hat matrix in Appendix C.

Associated with a missing axial point is the determinant

$$\det(X'_a X_a) = 7.5558e+022$$

$$\det(X'_a X_a)^{-1} = 1.3235e-023$$

$$\frac{\det(X'_a X_a)}{\det(X' X)} = 0.0268$$

The loss due to missing axial point is

$$l_a = 1 - \frac{\det(X'_a X_a)}{\det(X' X)} = 0.9732$$

This corresponds to the 65<sup>th</sup> entry, 0.9732, of the hat matrix in Appendix C.

Associated with a missing center point is the determinant

$$\det(X'_c X_c) = 2.5831e+024$$

$$\det(X'_c X_c)^{-1} = 3.8713e-025$$

$$\frac{\det(X'_c X_c)}{\det(X' X)} = 0.9178$$

The loss due to missing center point is

$$l_c = 1 - \frac{\det(X'_c X_c)}{\det(X' X)} = 0.0822$$

This corresponds to the 80<sup>th</sup> entry, 0.0822, of the hat matrix in Appendix C.

The variances of parameter estimates for the complete and reduced designs are as in Table 3.

**Table 3.** Variances of parameter estimates for the complete and reduced designs (One-quarter replicate)

Model term	Model parameter	Variance of parameter estimate associated with design with complete factorial point	Variance of parameter estimate associated with design with missing factorial point	Variance of parameter estimate associated with design with missing axial point	Variance of parameter estimate associated with design with missing center point
Intercept	$\beta_0$	0.0822	0.2500	0.2500	0.0896
$x_1$	$\beta_1$	0.5000	0.5000	9.8125	0.5000
$x_2$	$\beta_2$	0.5000	0.5000	0.5000	0.5000
$x_3$	$\beta_3$	0.5000	0.5000	0.5000	0.5000
$x_4$	$\beta_4$	0.5000	0.5000	0.5000	0.5000
$x_5$	$\beta_5$	0.5000	0.5000	0.5000	0.5000
$x_6$	$\beta_6$	0.5000	0.5000	0.5000	0.5000
$x_1 x_2$	$\beta_{12}$	0.5625	9.8750	0.5625	0.5625
$x_1 x_3$	$\beta_{13}$	0.5625	9.8750	0.5625	0.5625
$x_1 x_4$	$\beta_{14}$	0.0625	9.3750	0.0625	0.0625
$x_1 x_5$	$\beta_{15}$	0.0625	9.3750	0.0625	0.0625
$x_1 x_6$	$\beta_{16}$	0.0625	9.3750	0.0625	0.0625
$x_2 x_3$	$\beta_{23}$	0.5625	9.8750	9.8750	0.5625
$x_2 x_4$	$\beta_{24}$	0.0625	9.3750	0.0625	0.0625
$x_2 x_5$	$\beta_{25}$	0.0625	9.3750	0.0625	0.0625
$x_2 x_6$	$\beta_{26}$	0.0625	9.3750	0.0625	0.0625
$x_3 x_4$	$\beta_{34}$	0.0625	9.3750	0.0625	0.0625
$x_3 x_5$	$\beta_{35}$	0.0625	9.3750	0.0625	0.0625
$x_3 x_6$	$\beta_{36}$	0.0625	9.3750	0.0625	0.0625

$x_4x_5$	$\beta_{45}$	0.5625	9.8750	0.5625	0.5625
$x_4x_6$	$\beta_{46}$	0.5625	9.8750	0.5625	0.5625
$x_5x_6$	$\beta_{56}$	0.5625	9.8750	0.5625	0.5625
$x_1^2$	$\beta_{11}$	0.4211	0.7500	6.5625	0.4214
$x_2^2$	$\beta_{22}$	0.4211	0.7500	0.7500	0.4214
$x_3^2$	$\beta_{33}$	0.4211	0.7500	0.7500	0.4214
$x_4^2$	$\beta_{44}$	0.4211	0.7500	0.7500	0.4214
$x_5^2$	$\beta_{55}$	0.4211	0.7500	0.7500	0.4214
$x_6^2$	$\beta_{66}$	0.4211	0.7500	0.7500	0.4214
Sum of variances		9.5463	151.375	36.125	9.5555
Average variance		0.340939	5.40625	1.290179	0.341268

## 5. Discussion of Results

The behaviours of the hat matrix and the determinant-based loss criterion defined in Akhar and Prescott [2] have been examined for effect of missing observation of six factor central composite design having varying replicates of the factorial portion but fixed replicates of the axial and center portions. It is interesting to note that the hat matrix varies from one design configuration to another. For the design configuration with one complete replicate of factorial portion, the diagonal entries of the hat matrix associated with a factorial point, an axial point and a center point are respectively 0.3409, 0.4882 and 0.0814. For the design configuration with one-half fractional factorial replicate, the hat matrix remained the same for defining relations  $I = +ABCDEF$  and  $I = -ABCDEF$ . The diagonal entries of each corresponding hat matrix associated with a factorial point, an axial point and a center point are respectively 0.6764, 0.5025 and 0.0816. For the design configuration with one-quarter fractional factorial replicate, the hat matrix remained the same for defining relations  $I = +ABC$  and  $I = +DEF$ ,  $I = +ABC$  and  $I = -DEF$ ,  $I = -ABC$  and  $I = +DEF$  and  $I = -ABC$  and  $I = -DEF$ . The diagonal entries of each corresponding hat matrix associated with a factorial point, an axial point and a center point are respectively 0.9996, 0.9732 and 0.0822. Each of the computed loss value corresponds to the loss computed using the Akhar and Prescott [2] criterion. The loss function, as seen by the three categories of design, is affected by the number of design size, which in this research work is influenced by the number of design points in the factorial portion.

The loss due to missing factorial point is highest when one-quarter fractional factorial makes up the factorial portion of the central composite design and next highest for one-half fractional factorial. The minimum loss due to missing factorial point is attributed to the complete factorial design configuration. The loss due to missing axial point is highest when one-quarter fractional factorial makes up the factorial portion of the central composite design and next highest for one-half fractional factorial. The minimum loss due to missing axial point is attributed to the complete factorial design configuration. The loss due to missing center point is highest when one-quarter fractional factorial makes up the factorial portion of the central composite design and next highest for one-half fractional factorial. The minimum loss due to missing center point is attributed to the complete factorial design configuration. In fact, the loss due to missing center point in the three categories of design is very minimal when compared with loss due to either missing factorial point or missing axial point.

There is about 0.25% increase in loss of missing center point when using the design configuration with one-half fractional factorial and about 0.98% increase in loss of missing center point when using the design configuration with one-quarter fractional factorial. There is about 98.42% increase in loss of missing factorial point when using the design configuration with one-half fractional factorial and about 198.22% increase in loss of missing factorial point when using the design configuration with one-quarter fractional factorial. There is about 2.93% increase in loss of missing axial point when using the design configuration with one-half fractional factorial and about 99.34% increase in loss of missing axial point when using the design configuration with one-quarter fractional factorial. It is clearly seen that the configuration with one-quarter fractional factorial attracts higher losses to missing observations of either factorial, axial or center points when compared with either the configuration with one-half fractional factorial or the configuration with complete factorial portion. This result confirms the statement of Ahmad *et al.* [5] that the effect of missing observations can be much more serious when the design is saturated or near saturated. From characteristics of the design configurations outlined in Table 4, variances associated with parameter estimates are minimum for the design category with complete factorial portion and maximum for the design category with one-quarter fractional factorial. Interestingly, the design category that minimizes the variances also minimizes the losses.

**Table 4.** Some characteristics of the design configurations

Case 1 Configuration									
Design size	Minimum Variance	Maximum Variance	Sum of Variances	Average Variance	Det. of Information matrix	Det. of Variance-Covariance matrix	Loss due to missing observation		
							Factorial point	Axial point	Center point
80	0.0152	0.4195	2.9176	0.1042	1.5533e+043	6.4379e-044	-	-	-
79	0.0155	0.4195	2.9314	0.1047	1.0238e+043	9.7674e-044	0.3409	-	-
79	0.0156	0.7408	3.3432	0.1194	7.9503e+042	1.2578e-043	-	0.4882	-
79	0.0152	0.4197	2.9260	0.1045	1.4269e+043	7.0081e-044	-	-	0.0814
Case 2 Configuration									
Design size	Minimum Variance	Maximum Variance	Sum of Variances	Average Variance	Det. of Information matrix	Det. of Variance-Covariance matrix	Loss due to missing observation		
							Factorial point	Axial point	Center point
48	0.0294	0.4200	3.2475	0.1160	4.4373e+036	2.2536e-037	-	-	-
47	0.0321	0.4201	3.3094	0.1182	1.4361e+036	6.9635e-037	0.6764	-	-
47	0.0294	0.7509	3.6789	0.1314	2.2077e+036	4.5297e-037	-	0.5025	-
47	0.0294	0.4203	3.2566	0.1163	4.0750e+36	2.4540e-037	-	-	0.0816
Case 3 Configuration									
Design size	Minimum Variance	Maximum Variance	Sum of Variances	Average Variance	Det. of Information matrix	Det. of Variance-Covariance matrix	Loss due to missing observation		
							Factorial point	Axial point	Center point
32	0.0625	0.5625	9.5463	0.3409	2.8145e+024	3.5530e-025	-	-	-
31	0.2500	9.8750	151.375	5.4063	1.1806e+021	8.4703e-022	0.9996	-	-
31	0.0625	9.8750	36.125	1.2902	7.5558e+022	1.3235e-023	-	0.9732	-
31	0.0625	0.5625	9.5555	0.3413	2.5831e+024	3.8713e-025	-	-	0.0822

## Appendix A

Hat matrix associated with cuboidal six-factor central composite design with one replicate of factorial portion, one replicate of axial portion and four replicates of center portion

### Columns 1 through 20

0.3409	0.1543	0.1543	0.0303	0.1543	0.0303	0.0303	-0.0313	0.1543	0.0303	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313
0.1543	0.3409	0.0303	0.1543	0.0303	0.1543	-0.0313	0.0303	0.0303	0.1543	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313
0.1543	0.0303	0.3409	0.1543	0.0303	-0.0313	0.1543	0.0303	0.0303	-0.0313	0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303
0.0303	0.1543	0.1543	0.3409	-0.0313	0.0303	0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313
0.1543	0.0303	0.0303	-0.0313	0.3409	0.1543	0.1543	0.0303	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313
0.0303	0.1543	-0.0313	0.0303	0.1543	0.0303	0.3409	0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313
0.0303	-0.0313	0.1543	0.0303	0.1543	0.0303	0.3409	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303
-0.0313	0.0303	0.0303	0.1543	0.0303	0.1543	0.0303	0.3409	-0.0313	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303
0.1543	0.0303	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303
0.1543	0.0303	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303
0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313
0.1543	0.0303	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303
0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313
0.1543	0.0303	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303
0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	0.1543	-0.0313	0.0303	-0.0313
0.1543	0.0303	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	0.1543	-0.0313	0.0303
0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	0.1543	-0.0313
0.1543	0.0303	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	0.1543
0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303
0.1543	0.0303	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	0.1543
0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303
0.1543	0.0303	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	0.1543
0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303
0.1543	0.0303	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	0.1543
0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303
0.1543	0.0303	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	0.1543
0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303
0.1543	0.0303	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	0.1543
0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303
0.1543	0.0303	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	0.1543
0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303
0.1543	0.0303	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	0.1543
0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303
0.1543	0.0303	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	0.1543
0.0303	0.1543	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303
0.1543	0.0303	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0313	0.0303	-0.0										

**Columns 21 through 40**



### Columns 41 through 60

### **Columns 61 through 80**

## Appendix B

### **Hat matrix associated with cuboidal six-factor central composite design with one half replicate of factorial portion, one replicate of axial portion and four replicates of center portion**

## Columns 1 through 20

**Columns 21 through 40**

### Columns 41 through 48

## Appendix C

### **Hat matrix associated with cuboidal six-factor central composite design with one quarter replicate of factorial portion, one replicate of axial portion and four replicates of center portion**

### Columns 1 through 20

**Columns 21 through 32**

-0.0268	-0.0268	-0.0268	-0.0268	-0.0268	0.9732	-0.0268	-0.0268	0.0671	0.0671	0.0671	0.0671
-0.0268	-0.0268	-0.0268	-0.0268	-0.0268	0.9732	-0.0268	0.0671	0.0671	0.0671	0.0671	0.0671
-0.0268	-0.0268	-0.0268	-0.0268	-0.0268	0.9732	-0.0268	0.0671	0.0671	0.0671	0.0671	0.0671
0.0671	0.0671	0.0671	0.0671	0.0671	0.0671	0.0671	0.0671	0.0822	0.0822	0.0822	0.0822
0.0671	0.0671	0.0671	0.0671	0.0671	0.0671	0.0671	0.0671	0.0822	0.0822	0.0822	0.0822
0.0671	0.0671	0.0671	0.0671	0.0671	0.0671	0.0671	0.0671	0.0822	0.0822	0.0822	0.0822
0.0671	0.0671	0.0671	0.0671	0.0671	0.0671	0.0671	0.0671	0.0822	0.0822	0.0822	0.0822

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