TWO FACTOR CENTRAL COMPOSITE DESIGNS ROBUST TO A PAIR OF MISSING OBSERVATIONS

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ABSTRACT

The losses due to a pair of missing observations are studied for two factor central composite designs of different configurations of factorial or axial parts. The designs robust to a pair of missing observations are developed under minimaxloss criterion. These minimaxloss-2 designs are then compared with other central composite designs of the same configuration.

Key Words & Phrases: *Central composite designs; minimaxloss criterion; robust designs; loss of efficiency.*

1. INTRODUCTION

A two factor central composite design (c.c.d.) consists of

(i) 2^2 factorial points with co-ordinates $(\pm 1,\ \pm 1)$,

(ii) 4 axial points at $\pm\alpha$ distance from the centre of the design with co-ordinates $(\pm, 0)$ and $(0,\ \pm\alpha)$ and

(iii) One or more points at the centre of the design.

Factorial and axial parts may be replicated and the total design points $n=n_f+n_a+n_c$ where n_f, n_a and n_c are numer of factorial, axial and centre points respectively.

Box (1954) developed orthogonal central composite designs. Box and Hunter (1957) developed rotatable designs. Herzberg (1966) introduced cylindrically rotatable designs. S. Huda (1988, 1989) also studied cylindrically rotatable design. Box and Draper (1959) developed designs robust to inadequate model. Box and Draper (1975) investigated designs robust to outliers.

Herzberg and Andrews (1975, 1976) and Andrews and Herzberg (1979) studied designs robust to missing values. They took different probability of missing for each observation in optimal designs. McKee and Kashirsagar (1982) investigated effect of missing observations on parameter estimates and their variances, for central composite designs. For recent review of robust designs see Akhtar and Prescott (1987).

Akhtar and Prescott (1986) developed a minimaxloss criterion to find the designs for which the maximum loss of efficiency due to a single and a pair of missing observations is minimum. Akhtar (1987(a), 1987(b), 1988, 1991(a), 1991(b)) developed central composite designs robust to a single missing observations. Here we develop two factor central composite designs of different configurations of factorial and axial part for which the maximum loss of efficiency due to a pair of missing observations is minimum. These 'minimaxloss-2' designs are robust to a pair of missing observations. These deisgns are compared with other designs of the same configuration.

2-MINIMAXLOSS CRITERION

Let the postulated response surface model is a second order polynomial of the form

$$\underline{y} = \underline{X}\underline{\beta} + \underline{\varepsilon} \qquad\qquad \underline{E}(\underline{\varepsilon}) = 0,\ \underline{E}(\underline{\varepsilon}\underline{\varepsilon}') = \underline{\sigma}^2\underline{I}$$

where $\underline{y}$ is an nx1 vector of response, $\underline{X}$ is an n x p matrix formed from the design matrix according to terms in the response surface model, $\underline{\beta}$ is a p x 1 vector of coefficients and $\underline{\varepsilon}$ is an n x 1 vector of errors. The least square estimates are

$$\hat{\underline{\beta}} = (\underline{X}'\underline{X})^{-1}\underline{X}'\underline{Y}$$
$$\hat{\underline{y}} = \underline{X}\hat{\underline{\beta}} = \underline{X}(\underline{X}'\underline{X})^{-1}\underline{X}'\underline{Y} = \underline{R}\underline{y}$$

where $\underline{R} = \underline{X}(\underline{X}'\underline{X})^{-1}\underline{X}'$ is a matrix of order $n \times n$.

In c.c.d. the D-optimal criterion $|\underline{X}'\underline{X}|$ is an increasing function of α and is maximum for $\alpha = \infty$. For ith missing observation $|\underline{X}'\underline{X}|$ reduces to ${}_i|\underline{X}'\underline{X}|$. For ith and jth missing observations $|\underline{X}'\underline{X}|$ reduces to ${}_{ij}|\underline{X}'\underline{X}|$. It may be shown that

$${}_i|\underline{X}'\underline{X}| = |\underline{X}'\underline{X}|\,(1-r_{ii})$$

and $${}_{ij}|\underline{X}'\underline{X}| = |\underline{X}'\underline{X}|\,[(1-r_{ii})(1-r_{jj})-r^2_{ij}]$$

where r_{ii}, r_{jj} and r_{ij} are the elements of $\underline{R}$ corresponding to i and jth design points. The above equations may also be written as

$${}_i|\underline{X}'\underline{X}| = |\underline{X}'\underline{X}| \,.\, A_i$$

and $${}_{ij}|\underline{X}'\underline{X}| = |\underline{X}'\underline{X}| \,.\, A_{ij}$$

where A_i is the ith diagonal element of the first compound of $(\underline{I}-\underline{R})$ and A_{ij} is the diagonal elemnt of the second compound of $(\underline{I}-\underline{R})$ corresponding to (i,j)th pair of observations (for compounds of matrix see Aitken & Rutherford (1964) P.90.

For a design with particular $|\underline{X}'\underline{X}|$ we want ${}_{ij}|\underline{X}'\underline{X}|$ for reduced design to be as near to $|\underline{X}'\underline{X}|$ as possible. Let us define the 'loss' in terms of $|\underline{X}'\underline{X}|$ due to (i,j)th pair of missing observations as

$$L_{ij} = \frac{|\underline{X}'\underline{X}| - {}_{ij}|\underline{X}'\underline{X}|}{|\underline{X}'\underline{X}|} = 1 - A_{ij}.$$

After some algebra it may be shown that

$$\overline{L}_{ij} = 1 - \overline{A}_{ij}$$

remains constant for a particular n and p. Thus the loss for particular (i,j) pair is reduced at the cost of increase in the losses due to other pairs. For a particular n and p we select a design for which the maximum loss due to a pair of missing observaions is minimum. This design is called minimaxloss-2 design and is robust to two missing observations.

The two missing observations may be any of the $\binom{n}{2}$ pairs of n observations in a design. In two factor central composite design the possible pairs of factorial observations may be grouped as ff0, ff1 and ff2. These are pairs of factorial observations with 0, 1 and 2 signs different in co-ordinates. The examples of ff1 are

$$\begin{pmatrix} +1 & +1 \\ -1 & +1 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} +1 & -1 \\ -1 & -1 \end{pmatrix}$$

ff0 is empty unless factorial part is replicated. In axial part aa0, aa1 and aa2 represent the pairs of observations at the same axial point, at the same axis and at different axes respectivly. aa0 is empty unless axial part is replicated. fa1 is the pair of a factorial point and an axial point on the same side of the square and fa2 is the pair of a factorial point and an axial point on other sides of the square. These are pairs of factorial or axial points with centre point fc or ac and pair of two centre points cc. The losses due to pairs falling in the same group are same. If we take 3 or more centre points then the maximum loss due to a pair of missing observations does not correspond to pairs involving one or two centre points.

3-SINGLE REPLICATION OF FACTORIAL AND AXIAL PARTS

This two factor c.c.d. consists of 4 factorial, 4 axial and 3 or more centre points. Pairs ff0 and aa0 are empty. The losses due to all possible pairs of missing observations are studied for three centre points and a range of α from 1.0 to 2.0. Over a range of α, max(L_{ff1}, L_{ff2}) corresponds to either L_{ff1} or L_{ff2}, max(L_{aa1},L_{aa2}) corresponds to either L_{aa1} or L_{aa2} and max(L_{fa1}, L_{fa2}) = L_{fa1}. Max(L_{ff1}, L_{ff2}), max(L_{aa1}, L_{aa2}) and L_{fa1} for this design are plotted against α in Figure 1. Max (L_{ff1}, L_{ff2}) decreases and max(L_{aa1}, L_{aa2}) increases with the increase in α. L_{fa1} decreases and then increases with the increase in α. Maximumloss is computed to be minimum for α=1.4142. L_{fa1} > max(L_{ff1}, L_{ff2}) = max(L_{aa1}, L_{aa2}) at this point. Thus the design with n_f=4, n_a=4, n_c=3 and α=1.4142 is the minimaxloss design robust to a pair of missing observations. The losses and variances of parameter estimates of this minimaxloss2 design are compared with those of other designs of the same configuration in Table 1 and 2 respectively.

TABLE - 1

Losses due to different pairs of missing observations.

No. of variables $k = 2$ Total design points $n = 11$
No. of parameters $p = 6$ No. of centre points $= 3$

Design.	Alpha	|X'X| for complete design.	Maxloss due to two fact. obs. missing.	Maxloss due to two. axial obs. missing.	Maxloss due to one axial & one fact. obs. missing.	Overall maxloss due to a pair of obs. missing.	Maxloss due to a single obs. missing.
Alpha=1.0	1.0000	0.1094E+05	0.9737	0.7895	0.9591	0.9737	0.7939
Orthogonal	1.1472	0.2324E+05	0.9459	0.8142	0.9541	0.9541	0.7334
Minimaxloss 1&2 (Rotatable, Outlier robust & Alpha = √k)	1.4142	0.9830E+05	0.8750	0.8750	0.9504	0.9504**	0.6250*

* Minimaxloss due to one missing observation.

** Minimaxloss due to two missing observations.

4-FACTORIAL PART REPLICATED TWICE

This design consists of $n_f=8$, $n_a=4$ and $n_c \geq 3$. Total design points are 15 or more. From the groups of possible pairs of obserations, ff0 is non empty and aa0 is empty. The losses corresponding to different missing pairs ar studied for 3 centre points and α from 1.0 to 2.0. Computations over a range of α have shown that

$$\max(L_{ff0}, L_{ff1}, L_{ff2}) = L_{ff0}$$

$$\max(L_{fa1}, L_{fa2}) = L_{fa1}$$

and

$$\max(L_{aa1}, L_{aa2}) = L_{aa1} \text{ or } L_{aa2}.$$

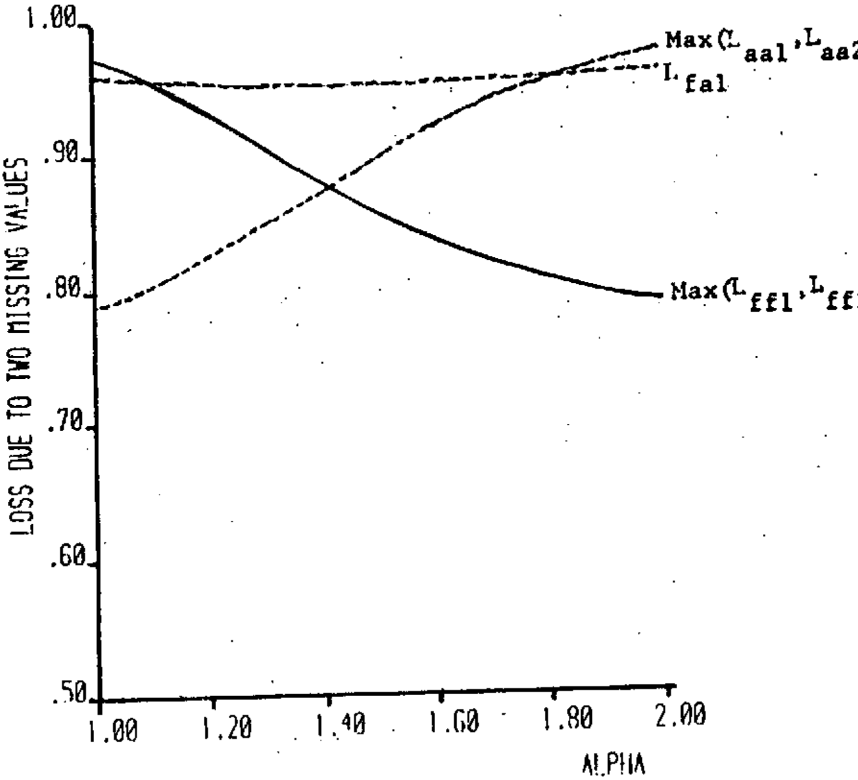


Figure 1 Losses due to a pair of missing observati

for design with $k = 2$, $n_f = n_a = 4$ and n_c =

plotted against α .

TABLE - 2

Variances of parameter estimates for complete design and for designs with a pair of observation missing.

No. of variables	k = 2	Total design points	n = 11
No. of parameters	p = 6	No. of centre points	= 3

Alpha	n	Variance of parameter estimates. Intercept.	Linear (min)	Linear (max)	Quadratic. (min)	Quadratic. (max)	Interaction,	Sum of variances.
1.0000	11	0.2632	0.1667	0.1667	0.3947	0.3947	0.2500	1.6360
	9ff	0.3333	0.3333	0.3333	0.8333	0.8333	1.8333	4.5000
	9aa	0.3333	0.1667	0.2500	0.7500	0.8333	0.2500	2.5833
	9fa	0.2857	0.5000	0.9732	0.5357	1.2589	1.0000	4.5536
1.1472	11	0.3006	0.1508	0.1508	0.2886	0.2886	0.2500	1.4293
	9ff	0.3333	0.2654	0.2654	0.4811	0.4811	1.1674	2.9937
	9aa	0.3333	0.1508	0.2500	0.4811	0.5579	0.2500	2.0231
	9fa	0.3120	0.3782	0.8666	0.3555	0.9504	0.9753	3.7379
1.4142	11	0.3333	0.1250	0.1250	0.1771	0.1771	0.2500	1.1875
	9ff	0.3333	0.1975	0.1875	0.2083	0.2083	0.7500	1.8750
	9aa	0.3333	0.1250	0.2500	0.2083	0.4583	0.2500	1.6250
	9fa	0.3333	0.2432	0.7488	0.1886	0.6154	0.7230	2.8524

ff - A pair of factorial obs. on far corners of cube missing.

aa - A pair of axial obs. on the same axis missing.

fa - A factorial obs. and a nearest axial obs. missing.

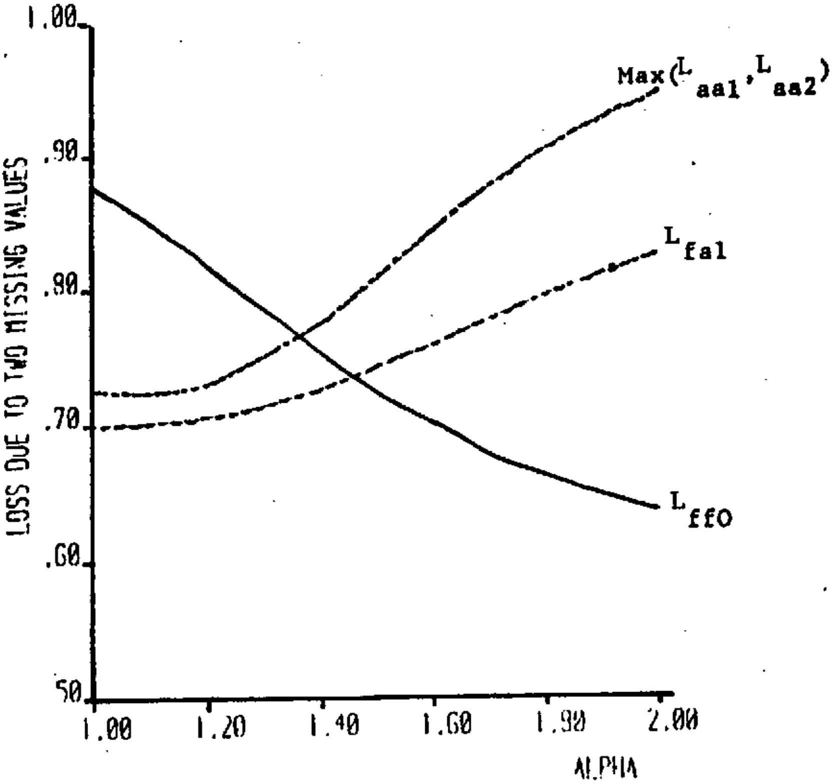
TABLE - 3

Losses due to different pairs of missing observations.

No. of variables k = 2 Total design points n = 15
No. of parameters p = 6 No. of centre points = 3
Factorial observations replicated twice.

Design.	Alpha	X' X. for complete design.	Maxloss due to two fact. obs. missing.	Maxloss due to two axial obs. missing.	Maxloss due to one axial & one fact. obs. missing.	Overall maxloss due to a pair of obs. missing.	Maxloss due to a single obs. missing.
Alpha=1.0	1.0000	0.1120E+06	0.8786	0.7257	0.7000	0.8786	0.4393
Minimaxloss1	1.0530	0.1398E+06	0.8644	0.7240	0.7007	0.8644	0.4323*
Orthogonal	1.2154	0.2743E+06	0.8152	0.7328	0.7070	0.8152	0.4515
Outlier robust	1.2523	0.3208E+06	0.8031	0.7399	0.7097	0.8031	0.4583
Minimaxloss2	1.3660	0.5304E+06	0.7655	0.7655	0.7214	0.7655**	0.4856
Alpha=√k	1.4142	0.6635E+06	0.7500	0.7778	0.7280	0.7778	0.5000
Rotatable	1.6818	0.2554E+07	0.6807	0.8686	0.7738	0.8686	0.5949

* Minimaxloss due to one missing observation.
** Minimaxloss due to two missing observations.



igure: 2

Losses due to a pair of missing observations for design with
k = 2, n_f = 3, n_a = 4 and n_c =3, plotted against α .

TABLE - 4

Variances of parameter estimates for complete design and for designs with a pair of observation missing.

No. of variables k = 2   Total design points n = 15
No. of parameters p = 6   No. of centre points = 3
Factorial observations replicated twice.

Alpha	n	Variance of parameter estimates.						
		Inter-cept.	Linear (min)	Linear (max)	Quadr-atic. (min)	Quadr-atic. (max)	Inter-action,	Sum of variances.
1.0000	15	0.2571	0.1000	0.1000	0.3571	0.3571	0.1250	1.2964
	13ff	0.2706	0.2647	0.2647	0.4412	0.4412	0.3824	2.0647
	13aa	0.3333	0.1000	0.1250	0.6250	0.8333	0.1250	2.1417
	13fa	0.2800	0.1190	0.1473	0.4673	0.5000	0.1548	1.6683
1.0530	15	0.2711	0.0979	0.0979	0.3135	0.3135	0.1250	1.2189
	13ff	0.2835	0.2391	0.2391	0.3863	0.3863	0.3554	1.8898
	13aa	0.3333	0.0979	0.1250	0.5349	0.6778	0.1250	1.8939
	13fa	0.2904	0.1160	0.1464	0.4110	0.4266	0.1546	1.5451
1.2154	15	0.3111	0.0913	0.0913	0.2291	0.2291	0.1250	1.0769
	13ff	0.3171	0.1815	0.1815	0.2705	0.2705	0.2941	1.5150
	13aa	0.3333	0.0913	0.1250	0.3819	0.3889	0.1250	1.4454
	13fa	0.3185	0.1069	0.1441	0.2803	0.3084	0.1542	1.3125
1.2523	15	0.3182	0.0898	0.0898	0.2157	0.2157	0.1250	1.0543
	13ff	0.3225	0.1717	0.1717	0.2508	0.2508	0.2837	1.4512
	13aa	0.3333	0.0898	0.1250	0.3388	0.3721	0.1250	1.3840
	13fa	0.3233	0.1048	0.1437	0.2573	0.2936	0.1542	1.2769
1.3660	15	0.3319	0.0852	0.0852	0.1802	0.1802	0.1250	0.9879
	13ff	0.3324	0.1472	0.1472	0.1992	0.1992	0.2582	1.2835
	13aa	0.3333	0.0852	0.1250	0.2393	0.3404	0.1250	1.2483
	13fa	0.3324	0.0987	0.1428	0.2003	0.2571	0.1539	1.1850
1.4142	15	0.3333	0.0833	0.0833	0.1667	0.1667	0.1250	0.9583
	13ff	0.3333	0.1389	0.1389	0.1806	0.1806	0.2500	1.2222
	13aa	0.3833	0.0833	0.1250	0.2083	0.3333	0.1250	1.2083
	13fa	0.3333	0.0961	0.1425	0.1807	0.2440	0.1537	1.1503
1.6818	15	0.2991	0.0732	0.0732	0.1014	0.1014	0.1250	0.7733
	13ff	0.3111	0.1068	0.1068	0.1023	0.1023	0.2229	0.9523
	13aa	0.3333	0.0732	0.1250	0.1042	0.3269	0.1250	1.0875
	13fa	0.3089	0.0828	0.1432	0.1022	0.1790	0.1530	0.9690

ff - A pair of obs. on the same factorial point missing.
aa - A pair of axial obs. on the same axis missing.
fa - A factorial obs. and a nearest axial obs. missing.

TABLE - 5

Losses due to different pairs of missing observations.

No. of variables k = 2 Total design points n = 15
No. of parameters p = 6 No. of centre points = 3
Axial observations replicated twice?

Design.	Alpha	|X'X| for complete design.	Maxloss due to two fact. obs. missing.	Maxloss due to two. axial obs. missing.	Maxloss due to one axial & one fact. obs. missing.	Overall maxloss due to a pair of obs. missing.	Maxloss due to a single obs. missing.
Alpha=1.0	1.0000	0.5325E+05	0.9423	0.6346	0.8233	0.9423	0.6923
Orthogonal	0.9677	0.4430E+05	0.9516	0.6278	0.8316	0.9516	0.7082
Rotatable	1.1892	0.1596E+06	0.8686	0.6807	0.7738	0.8686	0.5949
Alpha=√k	1.4142	0.6635E+06	0.7778	0.7500	0.7280	0.7778	0.5000
Minimaxloss2	1.4641	0.9238E+06	0.7655	0.7654	0.7214	0.7655**	0.4856
Outlier robust	1.5971	0.2245E+07	0.7399	0.8031	0.7097	0.8031	0.4583
Minimaxloss1	2.0861	0.4718E+08	0.7280	0.8889	0.6997	0.8889	0.4445*

* Minimaxloss due to one missing observation.
** Minimaxloss due to two missing observations.

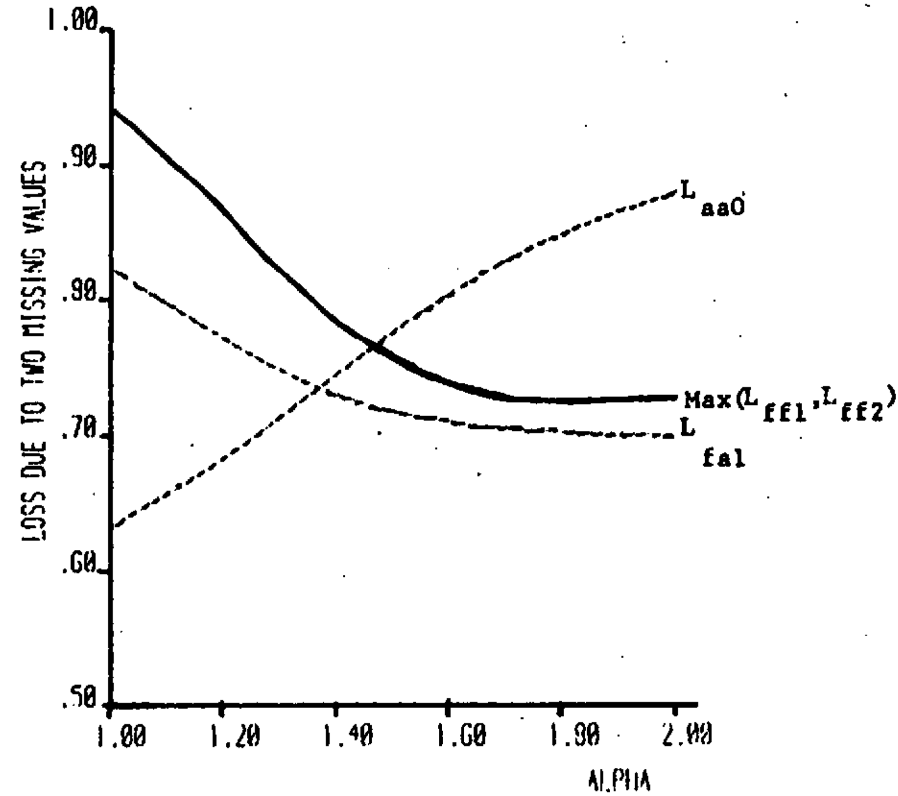


Figure : 3

Losses due to a pair of missing observations for design with $k = 2$, $n_f = 4$, $n_a = 8$ and $n_c = 3$, plotted against α .

TABLE - 6

Variances of parameter estimates for complete design and for designs with a pair of observation missing.

No. of variables k = 2 Total design points n = 15
No. of parameters p = 6 No. of centre points = 3
Axial observations replicated twice.

Alpha	n	Variance of parameter estimates						Sum of variances.
		Inter-cept.	Linear (min)	Linear (max)	Quadr-atic. (min)	Quadr-atic. (max)	Inter-action,	
1.0000	15	0.2308	0.1250	0.1250	0.2692	0.2692	0.2500	1.2692
	13ff	0.3333	0.1875	0.1875	0.5833	0.5833	1.3333	3.2093
	13aa	0.2468	0.1481	0.1481	0.3195	0.3195	0.2500	1.4318
	13fa	0.2517	0.1854	0.2449	0.3333	0.3946	0.4915	1.9014
0.9677	15	0.2187	0.1291	0.1291	0.2851	0.2851	0.2500	1.2970
	13ff	0.3333	0.1980	0.1980	0.6652	0.6652	1.5001	3.5600
	13aa	0.2363	0.1520	0.1520	0.3422	0.3422	0.2500	1.4747
	13fa	0.2404	0.1970	0.2582	0.3571	0.4223	0.5046	1.9796
1.1892	15	0.2991	0.1036	0.1036	0.2027	0.2027	0.2500	1.1617
	13ff	0.3333	0.1402	0.1402	0.2917	0.2917	0.8072	2.0042
	13aa	0.3045	0.1267	0.1267	0.2296	0.2295	0.2500	1.2669
	13fa	0.3089	0.1348	0.1848	0.2281	0.2710	0.4323	1.5599
1.4142	15	0.3333	0.0833	0.0833	0.1354	0.1354	0.2500	1.0208
	13ff	0.3333	0.1042	0.1042	0.1458	0.1458	0.6250	1.4584
	13aa	0.3333	0.1057	0.1057	0.1540	0.1540	0.2500	1.1027
	13fa	0.3333	0.0993	0.1393	0.1389	0.1658	0.3936	1.2703
1.4641	15	0.3319	0.0795	0.0795	0.1216	0.1216	0.2500	0.9842
	13ff	0.3333	0.0981	0.0981	0.1270	0.1270	0.6103	1.3937
	13aa	0.3321	0.1016	0.1016	0.1392	0.1392	0.2500	1.0637
	13fa	0.3324	0.0935	0.1317	0.1234	0.1474	0.3885	1.2170
1.5971	15	0.3182	0.0704	0.0704	0.0894	0.0894	0.2500	0.8877
	13ff	0.3333	0.0842	0.0842	0.0897	0.0897	0.5924	1.2735
	13aa	0.3196	0.0916	0.0916	0.1046	0.1046	0.2500	0.9618
	13fa	0.3233	0.0806	0.1143	0.0895	0.1072	0.3788	1.0937
2.0861	15	0.2465	0.0467	0.0467	0.0287	0.0287	0.2500	0.6473
	13ff	0.3333	0.0521	0.0521	0.0308	0.0308	0.6238	1.1229
	13aa	0.2492	0.0638	0.0638	0.0356	0.0356	0.2500	0.6980
	13fa	0.2718	0.0507	0.0730	0.0293	0.0356	0.3656	0.8261

ff - A pair of factorial obs. on far corners of cube missing.
aa - A pair of obs. on the same axial point missing.
fa - A factorial obs. and a nearest axial obs. missing.

For design with 3 centre points L_{ff0}, L_{fa1} and max (L_{aa1}, L_{aa2}) are plotted against α in Figure 2. The maximum loss is computed to be minimum for α = 1.366. Thus design with n_f=8, n_a=4, n_c=3 and α=1.366 is the minimaxloss-2 design. This design is compared, for its losses and variances of parameter estimates, with other designs of the same configurations in Table 3 and Table 4 respectively.

5- AXIAL PART REPLICATED TWICE

A two factor c.c.d. with axial part replicated twice consists of n_f=4, n_a=8 and n_c=3 or more. In this configuration ff0 is empty and aa0 is non empty. The losses corresponding to different missing pairs are studied over a range of α from 1.0 to 2.5. Computations have shown that for the range of α, max (L_{ff1},L_{ff2}) corresponds to either L_{ff1} or L_{ff2}.

$$\max(L_{aa0}, L_{aa1}, L_{aa2}) = L_{aa0}$$

and

$$\max(L_{fa1}, L_{fa2}) = L_{fa1}.$$

max(L_{ff1}, L_{ff2}), L_{aa0} and L_{fa1} are plotted against α in Figure 3. The maximum loss is computed to be minimum for α=1.4641. Thus the two factor design with n_f=4, n_a=8, n_c=3 and α=1.4641 is a minimaxloss2 design robust to a pair of missing observations. The losses and variances of this design are compared to those of other designs of the same configuration in Table 5 and Table 6 respectively.

CONCLUSIONS

It has been found that wo factor c.c.d. robust to a pair of missing observations with single replicate of factorial and axial parts has α=1.4142. This design is also robust to a single missing observation. When factorial part is replicated twice the design robust to a pair of missing observations has α=1.366. For this design with axial part replicated twice α=1.4641. All the above designs have 3 centre points each. The maximum losses due to a pair of missing observations are minimum for these designs. Thus these designs are named as Minimaxloss2 designs. These designs also have small variances of parameter estimates for complete as well as reduced designs with a pair of missing observations.

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