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The Effects of Addition of n_c Center Points on the Optimality of Box-Benhken and Box-Wilson Second-Order Designs

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Abstract Relationships between optimal design properties and changing sizes of designs, by the addition of center points, are seen to be very strong between the Box-Benhken designs and the Box-Wilson designs defined at α = $\sqrt{K}$ and α = $F^{\frac{1}{4}}$. Variations seem to exist with Box-Wilson designs defined at α = 1.0. In particular, the determinant values of the information matrices of the Box-Benhken designs generally decrease as n_c increases. These are also true for all categories of the Box-Wilson designs. However, the minimum eigenvalue of the Box-Benhken design and the Box-Wilson design defined at α = $\sqrt{K}$ and α = $F^{\frac{1}{4}}$ is maximized when n_c= 5 and maximized when n_c= 1 for the Box-Wilson design defined at α = 1.0. For the Box-Benhken designs considered, the trace values of the variance-covariance matrices generally decrease as n_c increases. This is also true for the Box-Wilson designs defined at α = $\sqrt{K}$ and α = $F^{\frac{1}{4}}$. For the Box-Wilson designs defined at α = 1.0, the trace values of the variance-covariance matrices increase as n_c increases. The maximum scaled predictive variances associated with the Box-Benhken designs and the Box-Wilson designs generally increase as n_c increases and minimized when n_c= 1 for Box-Wilson design defined at α = 1.0 and when n_c= 2 for the Box-Benhken design and the Box-Wilson design defined at α = $\sqrt{K}$ and α = $F^{\frac{1}{4}}$. The trace of information matrix associated with all considered design types consistently decreases as n_c increases.

Keywords Box-Benhken designs, Box-Wilson designs, Center Point, Optimality constants

1. Introduction

Two popularly used Response Surface Methodology (RSM) designs in modeling second order effects are the Box-Benhken and Box-Wilson designs. Each of them has less number of experimental runs when compared with the three-level full factorial designs. The Box-Benhken design abbreviated BBD was introduced by Box and Benhken (1960) and constitutes an alternative to the Box-Wilson design (otherwise called Central Composite Design (CCD)) introduced by Box and Wilson (1951). Although some categories of the Box-Wilson designs are not rotatable, Box-Benhken designs are a class of rotatable or near-rotatable second-order designs based on three-level incomplete factorial designs. They are formed by combining two-level factorial designs with incomplete block design in a particular fashion. They are designs introduced for second-order models in order to limit the growing sample size as the number of model parameters increases. When compared with the CCDs, the BBDs have the advantage of reduced design points. In general, the number of design points of the BBDs is $2k(k-1)+n_c$, where k is the number of factors and n_c is the number of center points. On the other hand, the number of design points of the CCDs is 2^k+2k+n_c, where k remains the number of factors and n_c remains the number of center points.

The CCDs can be studied for $k \geq 2$ however, the BBDs do not exist for $k = 2$ and can be studied for $k \geq 3$. In the simplest case of $k = 3$, the number of design points of the Box-Benhken design is 12 plus n_c center points and the number of design points of the central composite design is 14 plus n_c center points. For $k = 4$, the number of design points of the Box-Benhken design is 24 plus n_c center points and the number of design points of the central composite design is 24 plus n_c center points. For $k = 5$, the number of design points of the Box-Benhken design is 40 plus n_c center points and the number of design points of the central composite design is 42 plus n_c center points. For $k = 6$, the number of design points of the Box-Benhken design is 60 plus n_c center points and the number of design points of the central composite design is 76 plus n_c center points. The advantage in reduced design size becomes more pronounced as k increases beyond seven. For instance, when $k = 10$, the number of design points of the Box-Benhken design is 180 plus n_c center points and the

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number of design points of the central composite design is 1,044 plus n_c center points.

Myres *et.al* (2009) observed that in many scientific studies that require Response Surface Methodology, researchers are inclined to require three evenly spaced factor levels of which Box-Benhken design is an efficient option and an important alternative to the central composite design Box-Benhken designs like some central composite designs are spherical and do not deviate substantially from being rotatable. Many standard ways of comparing designs, ranging from the use of numeric values to graphs, exist in Response Surface Methodolgy. Lucas (1976) compared Response Surface designs by their D- and G-efficiency values. A Box-Benhken design has been compared with a Uniform shell design of Doehlert (1970) in Crosier (1993). It was seen that the Box-Benhken design exhibited a very high G-efficiency value of 98.9% as against 59.7% of the Uniform shell design. Also, Box-Benhken design gave a better prediction at the perimeter of the design region while the Uniform shell design gave a better prediction near the center of the design region. Although the Uniform shell design generally requires fewer runs then CCDs and BBDs, they are not widely used in fitting second-order model. Crosier (1993) further compared the performance of three-factor central composite design having n_c =3 center points with the three-factor Box-Benhken design having n_c =3 center points. The Box-Benhken design performed better near the design center while the central composite design performed better near the perimeter.

Zolgharnein *et.al* (2013) carried out a comparative study of Box-Benhken, central composite and Doehlert matrix for multivariate optimization. Practical applications of Box-Benhken and Central Composite designs are numerous (see e.g Tekindal *et.al* (2012), Igder *et.al* (2012), Zolgharnein *et.al* (2013) and Sabela et.al (2014)). In this work, the effects of addition of n_c center points on the optimality of Box-Benhken and Box-Wilson second-order designs shall be the focus. The aim is to see how increasing the number of center runs added to Box-Benhken and Box-Wilson designs affects A-, D-, E-, G- and T-optimality values for the designs.

2. Methodology

For a *p* parameter polynomial in *k* factors, each *k*-factor, *N*-point Box-Benhken and Box-Wilson second-order response surface design, written as an *N*x*k* matrix, shall be studied for changes in A-, D-, E-, G- and T-optimality values when the center points, n_c , are increased. To estimate the parameters (coefficients) of the second-order polynomial, the matrix of the design shall be expanded into an *N*x*p* model matrix having one column for each parameter of the polynomial model. The moment matrix or information matrix of the design shall be obtained. In order to compare designs of varying sizes, the information matrix shall be normalized to remove the effect of the varying design sizes. Although Myres *et.al* (2009) recommends the use of three to five center runs, this study shall consider $1 \leq n_c \leq 5$. Three categories of the Box-Wilson design shall be investigated alongside the Box-Benhken design. The categories of Box-Wilson design are the central composite designs with respective axial distance α = 1, $\alpha = \sqrt{K}$ and $\alpha = F^{\frac{1}{4}}$, where $F = 2^k$. The designs shall be assessed with respect to statistical criteria, namely, A-, D-, E-, G- and T-optimality criteria, which are related to the variance-covariance matrix of the model parameter estimator. The chosen optimality criteria are commonly encountered in literatures on optimal design of experiment.

Rady *et al.* (2009) presented a survey on these optimality criteria as well as the relationships among them. As in literature, by A-optimality, a design in which the sum of the variances of the model coefficients is minimized is sought. It is defined as

$$\text{Min tr}\,(\mathrm{M}^{-1})$$

where Min implies that minimization is over all designs and tr represents trace.

By D-optimality, a design in which the determinant of the moment matrix

$$\mathrm{M} = \frac{X^T X}{\mathrm{N}}$$

is maximized over all designs is sought. Where X represents the model matrix associate with the D-optimal design and X^T represents its transpose. The criterion of D-optimality equivalently minimizes the determinant of M^{-1}.

By E-optimality criterion, a design which maximizes the minimum eigen value of M or equivalently minimizes the maximum eigen value of M^{-1} is sought. By E-optimality, a design which minimizes the maximum variance of all possible normalized linear combination of parameter estimates is sought. E-optimality criterion is defined by

$$\text{Max } \lambda_{min}(\mathrm{M}) \equiv \text{Min } \lambda_{max}(\mathrm{M}^{-1})$$

where λ_{min} and λ_{max} represent minimum eigen value and maximum eigen value, respectively. By G-optimality, a design which minimizes the maximum scaled prediction variance in the region of the design is sought. It is defined by

$$\text{Min}\{\max_{\underline{x} \in R} \mathrm{v}(\underline{x})\}$$

By T-optimality, a design which maximizes the trace of the information matrix is sought. It is defined as

$$\text{Max tr}\,(M)$$

where Max implies that maximization is over all designs and tr represents trace.

The second-order model to consider is the complete model having main effects, interaction effects and quadratic effects and is given as

$$\mathrm{y} = \beta_0 + \sum_{i=1}^{k} \beta_i\, x_i + \{\sum_{i=1}^{k-1} \sum_{j=i+1}^{k} \beta_{ij}\, (x_i\, x_j)\} + \sum_{i=1}^{k} \beta_{ii}\, x_i^2 + \varepsilon$$

To effectively compare the designs, the information matrix of any given design shall be normalized. By normalization, the effect of changing sample size shall be removed. In studying the effects of addition of n_c center points on the optimality of the BBDs and CCDs, we shall consider $n_c = 3, 4$ and 5, whose design sizes are moderately small and relatively close.

3. Results

The results of the investigation regarding the effects of center point on optimality of Box-Behnken and Box-Wilson designs are contained in Table 1. The first column entries on the table show the design type. The second column entries on the table show the number of controllable factors of experimentation. The third column entries on the table show the number of model parameters associated with the k variable model. The columns under Optimality Constant represent values obtained using A-, D-, E-, G- and T-optimality criteria. The design matrices are built from the designs and the models. For an illustration, assuming Box-Behnken design in k=3 variables, the associated 10-parameter model is

$$y = \beta_0 + \sum_{i=1}^{3} \beta_i x_i + \{\sum_{i=1}^{2} \sum_{j=i+1}^{3} \beta_{ij} (x_i x_j)\} + \sum_{i=1}^{3} \beta_{ii} x_i^2 + \varepsilon$$

The 16-point Box-Behnken design (with $n_c = 4$) is

$$\xi_{16} = \begin{pmatrix} -1 & -1 & 0 \\ -1 & 1 & 0 \\ 1 & -1 & 0 \\ 1 & 1 & 0 \\ -1 & 0 & -1 \\ -1 & 0 & 1 \\ 1 & 0 & -1 \\ 1 & 0 & 1 \\ 0 & -1 & -1 \\ 0 & -1 & 1 \\ 0 & 1 & -1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

With the model and the 16-point design, the associated model matrix is

$$X = \begin{pmatrix} 1 & -1 & -1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & -1 & 1 & 0 & -1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 1 & -1 & 0 & -1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & -1 & 0 & -1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & -1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & -1 & 0 & -1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & -1 & 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & -1 & 1 & 0 & 0 & -1 & 0 & 1 & 1 \\ 1 & 0 & 1 & -1 & 0 & 0 & -1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The corresponding normalized information matrix is

$$M = \frac{X'X}{N} = \begin{pmatrix} 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 & 0.5000 & 0.5000 & 0.5000 \\ 0 & 0.5000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.5000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.5000 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.2500 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.2500 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.2500 & 0 & 0 & 0 \\ 0.5000 & 0 & 0 & 0 & 0 & 0 & 0 & 0.5000 & 0.2500 & 0.2500 \\ 0.5000 & 0 & 0 & 0 & 0 & 0 & 0 & 0.2500 & 0.5000 & 0.2500 \\ 0.5000 & 0 & 0 & 0 & 0 & 0 & 0 & 0.2500 & 0.2500 & 0.5000 \end{pmatrix}$$

and its inverse matrix is

$$M^{-1} = \begin{pmatrix} 4 & 0 & 0 & 0 & 0 & 0 & 0 & -2 & -2 & -2 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 \\ -2 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 \\ -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 \end{pmatrix}$$

The determinant value of information matrix is 3.0518e-005.

The determinant value of its inverse matrix is 32768.

The trace of the information matrix is 4.7500.

The trace of its inverse matrix is 34.

The eigenvalues of the information matrix are

0.1340
0.2500
0.2500
0.2500
0.2500
0.2500
0.5000
0.5000
0.5000
1.8660

The eigenvalues of the inverse matrix are

0.5359
2.0000
2.0000
2.0000
4.0000
4.0000
4.0000
4.0000
4.0000
7.4641

Each point of the design, apart from the center point, has variance of predicted value of 12.0. The variance of predicted value at the center point is 4.0. Each design follows these unique presentations for defined k, p and N. MATLAB R2007b was used in all computations and the results are as presented in Table 1. The MATLAB outputs for BBD, k= 5, p=21, N=43, CCD, k = 3, α =1.682, N=15 and k = 3, p = 10, α = 1.7321, N = 15 have been included in the Appendix. Presentation for only three categories is purely for space management.

Table 1. Optimality Constants for the BBD and CCD

Design Type	No. of factors k	No. of parameters p	Design Size N	Optimality Constant							
				A-Optimality (Trace of M^{-1})	D-Optimality (Determinant of M)	D-Optimality (Determinant of M^{-1}	E-Optimality (min Eigen value of M)	E-Optimality (max Eigen value of M^{-1})	G-Optimality (maximum scaled predictive variance)	(minimum scaled predictive variance)	T-Optimality (Trace of M)
BBD	3	10	13	44.6875	6.0849e-005	1.6434e+004	0.0433	23.1054	13.0000	9.7500	5.6154
	3	10	14	35.8750	5.8002e-005	1.7241e+004	0.0791	12.6404	10.5000	7.0000	5.2857
	3	10	15	34.0625	4.3641e-005	2.2914e+004	0.1090	9.1767	11.2500	5.0000	5.0000
	3	10	16	34	3.0518e-005	32768	0.1340	7.4641	12	4	4.7500
	3	10	17	34.6375	2.0805e-005	4.8065e+004	0.1550	6.4527	12.7500	3.4000	4.5294
	4	15	25	106.2500	1.1206e-009	8.9235e+008	0.0198	50.5263	25.0000	14.5833	5.8000
	4	15	26	84.5000	1.2445e-009	8.0353e+008	0.0377	26.5529	15.1667	13.0000	5.6154
	4	15	27	78.7500	1.0598e-009	9.4356e+008	0.0538	18.5801	15.7500	9.0000	5.4444
	4	15	28	77.0000	8.1895e-010	1.2211e+009	0.0685	14.6076	16.3333	7.0000	5.2857
	4	15	29	76.8500	6.0474e-010	1.6536e+009	0.0817	12.2355	16.9167	5.8000	5.1379
	5	21	41	222.5104	9.8767e-017	1.0125e+016	0.0108	92.9662	41.0000	20.5000	5.8780
	5	21	42	180.6875	1.1909e-016	8.3971e+015	0.0208	47.9881	21.0000	21.0000	5.7619
	5	21	43	168.8646	1.0898e-016	9.1757e+015	0.0303	33.0103	21.5000	14.3333	5.6512
	5	21	44	164.5417	8.9666e-017	1.1152e+016	0.0392	25.5326	22.0000	11.0000	5.5455
	5	21	45	163.2188	6.9917e-017	1.4303e+016	0.0475	21.0552	22.5000	9.0000	5.4444
CCD $\alpha = 1$	3	10	15	31.9583	3.1964e-004	3.1285e+003	0.1333	7.5000	11.9583	4.3333	6.6000
	3	10	16	32.5931	2.1607e-004	4.6282e+003	0.1250	8.0000	12.7310	3.5862	6.2500
	3	10	17	33.6229	1.4425e-004	6.9322e+003	0.1176	8.5000	13.5102	3.1127	5.9412
	3	10	18	34.8643	9.6364e-005	1.0377e+004	0.1111	9.0000	14.2929	2.7857	5.6667
	3	10	19	36.2322	6.4803e-005	1.5431e+004	0.1053	9.5000	15.0776	2.5464	5.4211
	4	15	25	58.8571	5.3555e-006	1.8672e+005	0.0800	12.5000	16.4842	4.6610	10.6000
	4	15	26	60.2230	3.5282e-006	2.8343e+005	0.0769	13.0000	17.1373	4.0857	10.2308
	4	15	27	61.7917	2.3178e-006	4.3144e+005	0.0741	13.5000	17.7917	3.6667	9.8889
	4	15	28	63.4903	1.5257e-006	6.5544e+005	0.0714	14.0000	18.4469	3.3478	9.5714
	4	15	29	65.2774	1.0091e-006	9.9102e+005	0.0690	14.5000	19.1026	3.0971	9.2759
	5	21	43	113.1936	4.8335e-008	2.0689e+007	0.0465	21.5000	22.1846	5.8735	16.3488
	5	21	44	114.9446	3.3900e-008	2.9499e+007	0.0455	22.0000	22.2496	5.2878	16.0000
	5	21	45	116.8490	2.3688e-008	4.2215e+007	0.0444	22.5000	22.3931	4.8278	15.6667
	5	21	46	118.8622	1.6532e-008	6.0487e+007	0.0435	23.0000	22.5922	4.4569	15.3478
	5	21	47	120.9553	1.1544e-008	8.6625e+007	0.0426	23.5000	23.0600	4.1516	15.0426

Design Type	No. of factors k	No. of parameters p	Design Size N	Optimality Constant							
				A-Optimality	D-Optimality		E-Optimality		G-Optimality		T-Optimality
				(Trace of M^{-1})	(Determinant of M)	(Determinant of M^{-1})	(min Eigen value of M)	(max Eigen value of M^{-1})	(maximum scaled predictive variance)	(minimum scaled predictive variance)	(Trace of M)
CCD $\alpha = \sqrt{K}$	3	10	15	30.8625	0.0332	30.1510	0.0498	20.0902	15.0000	9.2859	10.6005
	3	10	16	22.2535	0.0348	28.7455	0.0929	10.7644	10.5713	8.0000	10.0004
	3	10	17	19.8666	0.0285	35.1373	0.1305	7.6608	11.2320	5.6667	9.4710
	3	10	18	19.0353	0.0214	46.6729	0.1636	6.1130	11.8927	4.5000	9.0004
	3	10	19	18.8262	0.0156	64.1160	0.1928	5.1876	12.5534	3.8000	8.5793
	4	15	25	47.3958	0.0188	53.1881	0.0319	31.3024	25.0000	14.5833	16.3600
	4	15	26	33.0417	0.0209	47.8943	0.0613	15.6778	15.1667	13.0000	15.7692
	4	15	27	28.6875	0.0178	56.2405	0.0884	11.3074	15.7500	9.0000	15.2222
	4	15	28	26.8333	0.0137	72.7821	0.1135	8.8099	16.3333	7.0000	14.7143
	4	15	29	25.9792	0.0101	98.5630	0.1368	7.3125	16.9167	5.8000	14.2414
	5	21	43	73.8010	0.0096	103.9613	0.0194	51.6341	43.0000	19.5803	22.8608
	5	21	44	49.1173	0.0119	84.2385	0.0378	26.4351	23.8859	20.0357	22.3640
	5	21	45	41.2336	0.0111	90.0276	0.0554	18.0360	24.4287	15.0000	21.8892
	5	21	46	37.5500	0.0093	107.1245	0.0723	13.8370	24.9716	11.5000	21.4351
	5	21	47	35.5463	0.0074	134.6230	0.0884	11.3179	25.5145	9.4000	21.0003
CCD $\alpha = F^{\frac{1}{4}}$	3	10	15	31.1796	0.0235	42.6197	0.0497	20.1094	14.8269	9.1247	10.1332
	3	10	16	22.6477	0.0245	40.8670	0.0922	10.8410	10.7188	7.9536	9.5624
	3	10	17	20.2762	0.0200	50.0510	0.1293	7.7331	11.3871	5.6447	9.0587
	3	10	18	19.4582	0.0150	66.5473	0.1618	6.1789	12.0560	4.4869	8.6110
	3	10	19	19.2637	0.0109	91.4712	0.1905	5.2485	12.7252	3.7911	8.2104
	4	15	25	47.3958	0.0188	53.1881	0.0319	31.3024	25.0000	14.5833	16.3600
	4	15	26	33.0417	0.0209	47.8943	0.0613	15.6778	15.1667	13.0000	15.7692
	4	15	27	28.6875	0.0178	56.2405	0.0884	11.3074	15.7500	9.0000	15.2222
	4	15	28	26.8333	0.0137	72.7821	0.1135	8.8099	16.3333	7.0000	14.7143
	4	15	29	25.9792	0.0101	98.5630	0.1368	7.3125	16.9167	5.8000	14.2414
	5	21	43	66.7195	0.0361	27.7216	0.0220	45.4690	38.2818	19.4033	24.6409
	5	21	44	46.3729	0.0421	23.7663	0.0406	24.6283	24.7860	19.8342	24.1036
	5	21	45	39.3723	0.0386	25.9008	0.0584	17.1336	25.2896	14.4081	23.5902
	5	21	46	36.0075	0.0321	31.1266	0.0753	13.2747	25.8201	11.1563	23.0991
	5	21	47	34.1494	0.0254	39.3520	0.0916	10.9225	26.3618	9.1739	22.6289

4. Discussion of Results

The results on the effects of addition of n_c center points on the optimality of Box-Benhken and Box-Wilson second-order designs show some interesting relationships. For the Box-Benhken designs considered, the trace of the variance-covariance matrix generally decreases as n_c increases, thus showing a negative linear relationship. This is also true for the central composite designs defined at α = $\sqrt{K}$ and α = $F^{\frac{1}{4}}$. For the central composite design defined at α = 1.0, the trace of the variance-covariance matrix increases as n_c increases, thus showing a positive linear relationship. Trace of the variance-covariance matrix for the three-variable Box-Benhken design is minimized when n_c= 4. For the four-variable Box-Benhken design, trace of the variance-covariance matrix is minimized when n_c= 5 and for the five-variable Box-Benhken design, trace of the variance-covariance matrix is minimized when n_c= 5. For the central composite design defined at α = 1.0, the trace of the variance-covariance matrix is minimized when n_c= 1. However, for the central composite design defined at α = $\sqrt{K}$ and α = $F^{\frac{1}{4}}$, the trace of the variance-covariance matrix is minimized when n_c= 5.

On D-optimality criterion, the determinant of the information matrix of the Box-Benhken design generally decreases as n_c increases. Equivalently, the determinant of the variance-covariance matrix of the Box-Benhken design generally increases as n_c increases. These are also true for all categories of the central composite design. For all cases considered, the determinant of information matrix is maximized at n_c = 2 except for the three-variable Box-Benhken design where the determinant of information matrix is maximized at n_c= 1. The minimum eigenvalue of the Box-Benhken design and the central composite design defined at α = $\sqrt{K}$ and α = $F^{\frac{1}{4}}$ is maximized when n_c= 5 and maximized when n_c= 1 for the central composite design defined at α = 1.0. The maximum scaled predictive variance associated with the Box-Benhken designs and the Box-Wilson designs generally increases as n_c increases and minimized when n_c= 1 for CCD defined at α = 1.0, when n_c= 2 for CCD defined at α = $\sqrt{K}$ and α = $F^{\frac{1}{4}}$ and the Box-Benhken design. For the three-variable 10-parameter Box-Benhken design, the minimum variance equals 10.5 which is approximately close to the number of model parameters. For the four-variable 15-parameter Box-Benhken design, the minimum variance equals 15.1667 which is approximately close to the number of model parameters. For the five-variable 21-parameter Box-Benhken design, the minimum variance equals 21.0 which is exactly the number of model parameters.

The closeness of the minimum variance of prediction to the number of model parameter associated with the CCDs defined at α = 1.0 was not obvious, however for CCDs defined at α = $\sqrt{K}$ and α = $F^{\frac{1}{4}}$ and for k=3 and k=4, near approximations exist. As in the literature, maximum value of the predictive variance equal tp or approximately equal to the number of model parameters show that the corresponding design is rotatable or near-rotatable. The trace of information matrix associated with all considered design types consistently decreases as n_c increases. Generally, the relationships between addition of center points and the optimality properties are very strong between the Box-Benhken designs and the central composite design defined at α = $\sqrt{K}$ and α = $F^{\frac{1}{4}}$. This is most likely due to the sphericity and rotatabilty properties of the three design types.

5. Conclusions

The effects of addition of n_c center points on the optimality of Box-Benhken and Box-Wilson second-order designs have been investigated. Relationships are seen to exist between optimal design properties and changing size of the designs by the addition of center points. The relationships are very strong between the Box-Benhken designs and the central composite design defined at α = $\sqrt{K}$ and α = $F^{\frac{1}{4}}$. Variations seem to exist with central composite designs defined at α = 1.0.

Appendix

MATLAB COMPUTATIONS FOR BBD

>> k= 5, p=21, N43.

>> det((A'*A)/43) = 1.0898e-016

>> (43*inv(A'*A))=

Columns 1 through 5

14.3333	0	0	0	0
0	2.6875	0	0	0
0	0	2.6875	0	0
0	0	0	2.6875	0
0	0	0	0	2.6875
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
-7.1667	0	0	0	0
-7.1667	0	0	0	0
-7.1667	0	0	0	0
-7.1667	0	0	0	0
-7.1667	0	0	0	0

Columns 6 through 10

0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
2.6875	0	0	0	0
0	10.7500	0	0	0
0	0	10.7500	0	0
0	0	0	10.7500	0
0	0	0	0	10.7500
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0

Columns 11 through 15

0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
10.7500	0	0	0	0
0	10.7500	0	0	0
0	0	10.7500	0	0
0	0	0	10.7500	0
0	0	0	0	10.7500
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0

Columns 16 through 20

0	-7.1667	-7.1667	-7.1667	-7.1667
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
10.7500	0	0	0	0
0	6.7187	3.1354	3.1354	3.1354
0	3.1354	6.7188	3.1354	3.1354
0	3.1354	3.1354	6.7188	3.1354
0	3.1354	3.1354	3.1354	6.7188
0	3.1354	3.1354	3.1354	3.1354

Column 21

-7.1667
0
0
0
0
0
0
0
0
0
0
0
0
0
0
0
3.1354
3.1354
3.1354
3.1354
6.7188

```
>> det(43*inv(A'*A)) = 9.1757e+015
>> ((A'*A)/43) =
```

Columns 1 through 5

1.0000	0	0	0	0
0	0.3721	0	0	0

0	0	0.3721	0	0
0	0	0	0.3721	0
0	0	0	0	0.3721
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0.3721	0	0	0	0
0.3721	0	0	0	0
0.3721	0	0	0	0
0.3721	0	0	0	0
0.3721	0	0	0	0

Columns 6 through 10

0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0.3721	0	0	0	0
0	0.0930	0	0	0
0	0	0.0930	0	0
0	0	0	0.0930	0
0	0	0	0	0.0930
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0

Columns 11 through 15

0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0.0930	0	0	0	0
0	0.0930	0	0	0
0	0	0.0930	0	0
0	0	0	0.0930	0
0	0	0	0	0.0930
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0

Columns 16 through 20

0	0.3721	0.3721	0.3721	0.3721
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0.0930	0	0	0	0
0	0.3721	0.0930	0.0930	0.0930
0	0.0930	0.3721	0.0930	0.0930
0	0.0930	0.0930	0.3721	0.0930
0	0.0930	0.0930	0.0930	0.3721
0	0.0930	0.0930	0.0930	0.0930

Column 21

0.3721
0
0
0
0
0
0
0

```
         0
         0
         0
         0
         0
         0
         0
         0
    0.0930
    0.0930
    0.0930
    0.0930
    0.3721
```

```
>> trace((A'*A)/43) = 5.6512
>> trace(43*inv(A'*A))=    168.8646
>> eig((A'*A)/43)
ans =

    0.0303
    0.0930
    0.0930
    0.0930
    0.0930
    0.0930
    0.0930
    0.0930
    0.0930
    0.0930
    0.0930
    0.2791
    0.2791
    0.2791
    0.2791
    0.3721
    0.3721
    0.3721
    0.3721
    0.3721
    1.7139

>> eig(43*inv(A'*A))
ans =

    0.5835
   33.0103
   3.5833
   3.5833
   3.5833
   3.5833
   2.6875
   2.6875
   2.6875
   2.6875
   2.6875
   10.7500
   10.7500
   10.7500
   10.7500
   10.7500
   10.7500
   10.7500
   10.7500
   10.7500
   10.7500

>> B*(43*inv(A'*A))*B'= 21.5000
>> C*(43*inv(A'*A))*C'= 21.5000
D*(43*inv(A'*A))*D'= 21.5000
E*(43*inv(A'*A))*E'= 21.5000
F*(43*inv(A'*A))*F'= 21.5000
G*(43*inv(A'*A))*G'= 21.5000
H*(43*inv(A'*A))*H'= 21.5000
I*(43*inv(A'*A))*I'= 21.5000
J*(43*inv(A'*A))*J'= 21.5000
K*(43*inv(A'*A))*K'= 21.5000
L*(43*inv(A'*A))*L'= 21.5000
M*(43*inv(A'*A))*M'= 21.5000
N*(43*inv(A'*A))*N'= 21.5000
O*(43*inv(A'*A))*O'= 21.5000
P*(43*inv(A'*A))*P'= 21.5000
Q*(43*inv(A'*A))*Q'= 21.5000
R*(43*inv(A'*A))*R'= 21.5000
S*(43*inv(A'*A))*S'= 21.5000
T*(43*inv(A'*A))*T'= 21.5000
U*(43*inv(A'*A))*U'= 21.5000
V*(43*inv(A'*A))*V'= 21.5000
W*(43*inv(A'*A))*W'= 21.5000
X*(43*inv(A'*A))*X'= 21.5000
Y*(43*inv(A'*A))*Y'= 21.5000
Z*(43*inv(A'*A))*Z'= 21.5000
(ZA)*(43*inv(A'*A))*(ZA)'= 21.5000
(ZB)*(43*inv(A'*A))*(ZB)'= 21.5000
ZC)*(43*inv(A'*A))*(ZC)'= 21.5000
(ZD)*(43*inv(A'*A))*(ZD)'= 21.5000
(ZE)*(43*inv(A'*A))*(ZE)'= 21.5000
(ZF)*(43*inv(A'*A))*(ZF)'= 21.5000
(ZG)*(43*inv(A'*A))*(ZG)'= 21.5000
```

(ZH)*(43*inv(A'*A))*(ZH)'= 21.5000
(ZI)*(43*inv(A'*A))*(ZI)'= 21.5000
(ZJ)*(43*inv(A'*A))*(ZJ)'= 21.5000
(ZK)*(43*inv(A'*A))*(ZK)'= 21.5000
(ZL)*(43*inv(A'*A))*(ZL)'= 21.5000
(ZM)*(43*inv(A'*A))*(ZM)'= 21.5000
(ZN)*(43*inv(A'*A))*(ZN)'= 21.5000
(ZO)*(43*inv(A'*A))*(ZO)'= 21.5000
(ZP)*(43*inv(A'*A))*(ZP)'= 14.3333

MATLAB COMPUTATIONS FOR CCD
>> k = 3, α=1.682, N=15

>> det((A'*A)/15)= 0.0235
>> (15*inv(A'*A))
ans =

Columns 1 through 5

14.8269	-0.0000	0	0	0
-0.0000	1.0982	0	0	0
0	0	1.0982	0	0
0	0	0	1.0982	0
0	0	0	0	1.8750
0	0	0	0	0
0	0	0	0	0
-5.0617	0.0000	0	0	0
-5.0617	0.0000	0	0	0
-5.0617	0.0000	0	0	0

Columns 6 through 10

0	0	-5.0617	-5.0617	-5.0617
0	0	0.0000	0.0000	0.0000
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
1.8750	0	0	0	0
0	1.8750	0	0	0
0	0	2.4777	1.5406	1.5406
0	0	1.5406	2.4777	1.5406
0	0	1.5406	1.5406	2.4777

>> det(15*inv(A'*A)) = 42.6189
>> trace((A'*A)/15) = 10.1332
>> trace(15*inv(A'*A)) = 31.1796
>> eig((A'*A)/15)
ans =

0.0497
0.5333
0.5333
0.5333
0.9105
0.9105
0.9105
1.0672
1.0672
3.6175

>> eig(15*inv(A'*A))
ans =

20.1094
0.2764
0.9370
1.0982
0.9370
1.0982
1.0982
1.8750
1.8750
1.8750

>> B*(15*inv(A'*A))*B'=10.0532
>> C*(15*inv(A'*A))*C'=10.0532
>> D*(15*inv(A'*A))*D'= 10.0532
>> E*(15*inv(A'*A))*E'=10.0532
>> F*(15*inv(A'*A))*F'=10.0532
>> G*(15*inv(A'*A))*G'=10.0532
>> H*(15*inv(A'*A))*H'=10.0532
>> I*(15*inv(A'*A))*I'=10.0532
>> J*(15*inv(A'*A))*J'= 9.1247
>> M*(15*inv(A'*A))*M'= 9.1247
>> K*(15*inv(A'*A))*K'= 9.1247
>> L*(15*inv(A'*A))*L'= 9.1247
>> M*(15*inv(A'*A))*M'= 9.1247
>> N*(15*inv(A'*A))*N'= 9.1247
>> O*(15*inv(A'*A))*O'= 9.1247
>> P*(15*inv(A'*A))*P'= 14.8269

MATLAB COMPUTATIONS FOR CCD
k = 3, p = 10, α = 1.7321, N = 15

>> det((A'*A)/15)
ans =
0.0332
>> (15*inv(A'*A))
ans =

Columns 1 through 5

15.0000	0	0	0	0
0	1.0714	0	0	0
0	0	1.0714	0	0
0	0	0	1.0714	0
0	0	0	0	1.8750
0	0	0	0	0
0	0	0	0	0
-4.9999	0	0	0	0
-4.9999	0	0	0	0
-4.9999	0	0	0	0

Columns 6 through 10

0	0	-4.9999	-4.9999	-4.9999
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
1.8750	0	0	0	0
0	1.8750	0	0	0
0	0	2.3411	1.5079	1.5079
0	0	1.5079	2.3411	1.5079
0	0	1.5079	1.5079	2.3411

```
>> det(15*inv(A'*A))
ans =
    30.1518
>> trace((A'*A)/15)
ans =
    10.6005
>> trace(15*inv(A'*A))
ans =
    30.8626
>> eig((A'*A)/15)
ans =

    0.0498
    0.5333
    0.5333
    0.5333
    0.9334
    0.9334
    0.9334
    1.2001
    1.2001
    3.7504

>> eig(15*inv(A'*A))
ans =
    20.0902
    0.2666
    0.8332
    0.8332
    1.0714
    1.0714
    1.0714
    1.8750
    1.8750
    1.8750

>> B*(15*inv(A'*A))*B' = 9.9106
>> C*(15*inv(A'*A))*C'= 9.9106
>> D*(15*inv(A'*A))*D'= 9.9106
>> E*(15*inv(A'*A))*E'= 9.9106
>> F*(15*inv(A'*A))*F'= 9.9106
>> G*(15*inv(A'*A))*G'= 9.9106
>> H*(15*inv(A'*A))*H'= 9.9106
>> I*(15*inv(A'*A))*I'= 9.9106
>> J*(15*inv(A'*A))*J'=9.2859
>> K*(15*inv(A'*A))*K'=9.2859
>> L*(15*inv(A'*A))*L'=9.2859
>> M*(15*inv(A'*A))*M'=9.2859
>> N*(15*inv(A'*A))*N'=9.2859
>> O*(15*inv(A'*A))*O'=9.2859
>> P*(15*inv(A'*A))*P'= 15.0000
```

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