OPTIMALITY PREDICTION OF SECOND ORDER BOX-BEHNKEN DESIGN ROBUST TO MISSING OBSERVATION

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Abstract

The study of robust missing observations has gained prominence in statistical research. In particular, the Response Surface Methodology (RSM), a widely applied approach in experimental design, faces challenges when dealing with missing data. This paper investigates two design variants: the three-level second-order Box-Behnken design (BBD) with one missing observation and the Small Box-Behnken Design (SBBD), which involves fewer experimental runs than the standard BBD. We evaluate prediction performance using a fraction of design space (FDS) plot, revealing the distribution of scaled prediction variance (SPV) values across the design space. Additionally, we assess the efficiency of design model parameters using information-based criteria (A, D, and G relative efficiency). Our analysis spans k factors, ranging from k = 3 to 9. The findings guide practitioners in selecting optimal design points for efficient parameter estimation and accurate prediction within the context of missing observations. This comparative study sheds light on the trade-offs between BBD and SBBD, providing valuable insights for experimental design practitioners.

Keywords: Box-Behnken Design, Fraction of Design Space, Scaled Prediction Variance, Optimality, Small Box-Behnken Design

I. Introduction

Response Surface Methodology is a powerful statistical and mathematical model construction technique blend. It's designed to assess the impact of multiple independent variables and find their optimal values to yield the most desirable outcomes. This methodology benefits scenarios that aim to optimize a product or process. The empirical model is based on data observed from the system or process. *RSM* involves building empirical models using multiple regression and statistical techniques [19]. The second-order model is commonly used in *RSM*, particularly in Central Composite Designs (*CCD*) and *BBD*. Robust missing observation is a critical research area in all statistical methodologies. Even in well-planned experiments, there may be a chaos of missing observations that becomes challenging for estimating parameters in a model. Much of the robust missing observation research in the literature review is performed in different Central Composite Design types using various alpha (α) values rather than second-order Box-Behnken Designs. Draper [7] reviews the research on robust missing observation methods in response surface design and credits the first researcher to develop a parameter estimation formula. Akhtar and Prescott

[2]proposed a minimax loss criterion for handling missing observations, which is now the most used in response surface designs. Akhtar [1] examines a five-factor *CCD* with two missing observations in three different settings. Smucker et al. [20] gave empirical results for the effect of missing observations on various classical and optimal designs and a new type of missing-robust design in screening and response surface settings. Alrweili et al. [4] use the minimax loss criterion to create more robust designs for missing observations by combining the latest *CCDs* from *GSA* and *AEK*, which are new designs. Hayat et al. [8]explore designs from regular and irregular structure subsets, assess how they dealt with missing design points using the minimax loss criterion, and investigate their alphabetic optimality and prediction performance with *FDS* plots of the response difference variance. Alanazi et al.[3] present closed-form expressions for missing two observations as a function of α, the axial value used in *CCDs* with up to 10 factors. Whittinghill [22] explores how Box-Behnken Designs can handle missing observations without losing the ability to estimate all the parameters of interest and the article defines tmax as the maximum number of rows that can be arbitrarily deleted from the design matrix and keep the parameters estimable. Tanco et al.[21] used tmax and D-Efficiency criteria to evaluate three-level second-order polynomial designs, such as Box-Behnken, Face Centered, and other smaller and intermediate designs. Rashid et al.[18] investigate how to deal with one missing observation in Augmented *BBD* (*ABBD*) and Augmented Fractional *BBD* (*AFBBD*) using the minimax loss criterion and relative *D* and *G* efficiency. Rashid et al. [17] examine how a missing observation affects the estimation and prediction abilities of the *ABBD'S* relative *A*-, *D*-, and *G*-efficiencies. Hemavathi et al. [9] explore how sequential third-order rotatable design can handle missing observations without losing much information. Also, the paper measures the information loss due to one or two missing experimental runs at different distances from the center of the design. Park et al. [16] use graphical methods such as variance dispersion graphs, a fraction of the design space plot, and *G*-, *I*- optimality criteria to examine how different experimental designs perform in spherical and cuboidal regions for three to seven factors. Chigbu et al. [13] compare *CCD*, Small Composite Design (*SCD*), and MinResV designs for spherical regions with $k = 3$ to 7 factors based on the optimality criteria and the Variance Dispersion Graph (*VDG*), and the results show that none of these designs is consistently better for themselves. Li et al. [12] evaluate different *CCD*, *SCD*, and *MinResV* designs for spherical and cuboidal regions with various axial values, and they utilize *FDS* plots and box plots to analyze the prediction variance properties of the designs. Onwuameze et al. [14] use graphical methods such as *VDG* and *FDS* plots to evaluate the prediction variance performance of *CCD*, *SCD*, and *MinResV* in the hypercube region. However, most research on robust missing observations in Box-Behnken design recently focused on third-order designs, called *ABBD*.

This paper conducts a comparative analysis of the classical *BBD* and the *SBBD* focusing on the robustness of these designs when a single observation is missing. The *SBBD* [24] is noted for its advantage of requiring fewer runs than the *BBD*. The paper evaluates these designs using relative *A*-, *D*-, and *G*-efficiency to assess parameter estimation accuracy and explores a fraction of the design space plot in terms of scaled prediction variance. The paper is structured as follows: Section 2 Outlines the methodology used in the study. Section 3.1: Presents the results and discussions on scaled prediction variance and relative efficiencies. Section 3.2: Provides an analysis and discussion using the Fraction of Design Space graph of both *BBD* and *SBBD*. Section 4: Summarizes the findings and conclusions of the study.

II. Methodology

I. Description of Second Order Model

In numerous instances involving response surface methodology, we may not understand the relationship between the predictor variables and the response. A first-order model might not be sufficient to capture the curvature of the response function. Therefore, we often use higher-degree polynomials, such as a second-order model, to better evaluate curvature in optimization experiments. For k quantitative factors denoted by $x_1, x_2, \dots, x_k$, a second-order model is

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

where $\beta_0, \beta_i, \beta_{ii}$, and β_{ij} are the intercept, linear, quadratic, and bilinear terms, respectively, and ϵ_i is a random error with mean zero, variance σ^2 and independent between any pair of runs. The number of unknown parameters to be estimated is denoted as $p = k + k + \binom{k}{2} + 1$, and to have sufficient degrees of freedom to estimate the model coefficients, the number of runs or observations n must be greater than or equal to p.

II. Small Box-Behnken Design

Box and Behnken [6] combined balanced incomplete block design and factorial design to create a three-level factorial design called Box-Behnken design. Box-Behnken Designs are three-level, second-order spherical designs with all points on a sphere. They are typically used for fitting second-order response surface models and are available for 3–12 and 16 factors. This design is widely used for second-order models in analytical chemistry and industrial applications. Small Box-Behnken Design is specially constructed by using a Balanced incomplete block design (*BIBD*) and Partially Balanced incomplete block design (*PBIBD*) and replaces treatments partly by 2_{III}^{3-1} designs and partly by full factorial designs. A unique feature of *SBBD* is that it has minimum runs compared to classical *BBD*. *SBBD* consists of two design point categories: Full Factorial design 2^2 or 2^3 denoted as (*F*), and 2_{III}^{3-1} Fractional Factorial design denoted as (*FF*), which has runs in the form $\begin{pmatrix} 1 & 1 & 1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix}$.

Appendix A of the article outlines the detailed structures of the design point types or called as design matrix X for the Small Box-Behnken Design. Using the design matrix X of *BBD* and *SBBD*, we can calculate further computational analysis. To know about the further construction methods of *SBBD*, refer to article [24].

III. Scaled Prediction Variance

Borkowski [5] gives an analytical form for calculating scaled prediction variance values of central composite design and Box-Behnken design. Scaled prediction variance criteria is an essential tool for selecting response surface designs. It allows for good prediction of response variables at various points of interest throughout the experimental region. This scaling is widely used to facilitate comparisons among designs of various sizes. The prediction variance at a point $\mathbf{x}$ is given by

$$v(x) = \frac{n \cdot var[\hat{y}_{(x)}]}{\sigma^2} = n \cdot X^{(m)'} (X'X)^{-1} X^{(m)} \quad (2)$$

$x^{(m)}$ is the design point vector in the design space expanded to model form, n is the design size or runs, and σ^2 is the observation error. Desirable designs are those which have the smallest value of scaled prediction variance.

IV. Fraction of Design Space

The *FDS* plot is a useful tool to compare two or more designs, as it shows the *SPV* distributions of designs with a single curve and their *G*-efficiency and *V*-average values. *FDS* plot is [15] constructed by sampling many values, say n, from throughout the design space and obtaining the corresponding *SPV* values. The *FDS* plot informs the experimenter how the *SPV* varies throughout the design space, including the minimum and maximum *SPV*s. The idea is that the design is better if a larger fraction of the design space is close to the minimum *SPV* value. Moreover, the design is more stable if the line is flatter. The *FDS* plot helps summarize the range and the proportions of *SPV* values in the design space and easily compares designs with a single curve. In addition, [23] it provides the researcher with a single plot to compare designs or study the properties of a specific design. Accordingly, the *FDS* technique could be applied to regular and non-regular design regions.

V. Relative G-, D-, and A-, Efficiency

G-optimality is defined as minimizing the maximum variance of any predicted value over the experimental space. Iwundu[10] investigates how single or multiple missing observations affect cuboidal designs' Relative *A-*, *D-*, and *G*-efficiency. It is defined as the ratio of the determinant of the information matrix of the design to the determinant of the information matrix of an optimal design.

$$G_{\text{eff}} = \frac{p}{n \cdot MAX_{X \in R} v(x)} \tag{3}$$

Here p is the number of parameters of estimated model, n is the number of observations in the respective design and $MAX_{X\in R} v_{(x)}$ is the maximum value of the variance of predicted response. Thus, relative G-efficiency denoted by RE_G is given as the ratio of G_{eff} of reduced design and of complete design.

$$RE_G = \frac{G_{\text{eff (reduced)}}}{G_{\text{eff}}} = \frac{n \cdot MAX_{X\in R} v(x)}{n_r \cdot MAX_{X\in R} v(x)_{\text{reduced}}} \tag{4}$$

where n is the size of the runs of the complete design, and n_{r} is the size of the runs of the reduced design. According to this definition of RE_G, a design with a higher value of RE_G will be preferred. By utilizing equations (3) and (4), we can compute the relative G-efficiency value. These values are then presented in tables 3 and 4.

D- efficiency is defined as maximizing the determinant of the information matrix or minimizing the determinant of the inverse of the information matrix. Thus, relative D-efficiency is given as

$$RE_D = \left(\frac{|X'X|_{\text{reduced}}}{|X'X|}\right)^{\frac{1}{p}} \tag{5}$$

Where, p is the number of parameters of the model to be estimated, $|X'X|_{\text{reduced}}$ is the determinant of the information matrix of reduced design and $|X'X|$ is the determinant of the complete design matrix. A value approaching one will represent a minor loss, whereas a value below one will represent a more significant loss in model estimation. Through the application of equation (5), we are able to determine the relative *D*-efficiency value. These computed values are then listed in tables 3 and 4.

The A-Criterion considers the individual variances of the regression coefficients rather than the covariances among coefficients. Thus, relative A-efficiency is given as

$$RE_A = \frac{\text{trace}(X'X)^{-1}}{(\text{trace}(X'X)^{-1})_{\text{reduced}}} \tag{6}$$

where the trace is the sum of the main diagonal values of $(X'X)^{-1}$, where (trace $(X'X)^{-1})_{\text{reduced}}$ is the trace of $(X'X)^{-1}$ of the reduced design, and a design with a higher value of RE_A will be preferable. By utilizing equation (6), we can ascertain the relative *D*-efficiency value. The calculated values are subsequently enumerated in tables 3 and 4.

III. Result and Discussion

I. Scaled Prediction Variance of One Missing Box-Behnken Design

The insignificant difference in the Average Scaled Prediction Variance (*ASPV*) between instances of missing and non-missing observations is evident from the values in Table 1. The smallest prediction value is preferred for optimal prediction performance among each factor's design points. Regarding missing factorial design points, factor k = 8 has the lowest SPV value of 24.08 compared to all other factors k = 3,4,5,6,7 and 9, all of which have *SPV* values ranging from 34 to 45.

Table 1: *SPV values of one missing observation of BBD k = 3 to 9 factors.*

Number of Factors	Missing Design Points	Runs	SPV		
			Min	Avg	Max
k = 3	None		3.2521	7.3627	16.6260
	F	12	3.0656	8.9792	42.2400
	Centre	5	3.6256	7.0704	15.7584
k = 4	None		4.6440	10.4340	17.4960
	F	24	4.4892	10.9765	39.4400
	Centre	6	5.1591	10.1732	16.9157
k = 5	None		6.6424	14.9776	24.9964
	F	40	6.5025	15.3540	40.3875
	Centre	6	7.3260	14.8095	24.5565
k = 6	None		7.7598	13.1220	21.8160
	F	48	7.7009	13.3666	33.7663
	Centre	6	8.5807	13.3030	21.1735
k = 7	None		9.3248	15.3698	20.0942
	F	56	9.1744	15.6709	40.1258
	Centre	6	10.5530	15.5733	19.9958
k = 8	None		12.1800	16.7040	21.0480
	F	112	12.0309	16.7076	24.0856
	Centre	8	12.7449	17.3621	21.5985
k = 9	None		11.8170	24.9730	34.4110
	F	120	11.7648	24.8325	34.8945
	Centre	10	12.7839	25.0647	34.4301

II. Scaled Prediction Variance of One Missing Small Box-Behnken Design

In the case of the Small Box-Behnken Design, there is an upward trend in the Scaled Prediction Variance for most factors when there are non-missing design points and a center. However, factor k = 7 deviates from this increasing trend. When comparing the difference between full factorial and 2_{III}^{3-1} fractional factorial design points based on average and Max SPV, there is a moderate difference in the average SPV of all the factors. Interestingly, factors k = 8 and 9 have similar differences. In contrast, Max SPV for factors k = 4,7 and 9 shows significant differences between *F* and *FF* design points, while other factors such as k = 5,6 and 8 exhibit moderate differences. Therefore, we can infer that full factorial observations perform better in terms of prediction when a factorial type of observation is missing, compared to fractional factorial observations.

Table 2: *SPV values of one missing observation of SBBD k = 4 to 9 factors.*

Number of Factors	Missing Design Points	Runs	SPV		
			Min	Avg	Max
k = 4	None		3.1856	14.1042	44.0000
	F	12	3.0954	18.6249	113.4000
	FF	4	2.8371	27.5100	307.2300
	Centre	6	3.3411	13.5639	43.2600
k = 5	None		4.8030	18.8430	60.6000
	F	8	4.7096	19.9404	65.2500
	FF	16	4.7908	21.9820	123.8300
	Centre	6	5.1881	18.2294	58.2900
k = 6	None		6.0458	21.2116	74.1000
	F	16	5.8793	21.7375	74.0000
	FF	16	5.9385	24.1092	109.1500
	Centre	6	6.6304	21.0974	75.8500
k = 7	None		6.0000	23.5152	67.2000
	F	24	5.8750	25.9534	94.4700
	FF	16	5.7528	29.6429	248.6300
	Centre	8	6.4719	23.0723	70.5000
k = 8	None		7.7760	30.6688	85.1200
	F	28	7.6608	32.4198	102.0600
	FF	28	7.6734	32.8734	121.5900
	Centre	8	8.7129	30.4668	85.0500
k = 9	None		7.0000	40.4110	108.5000
	F	24	6.9000	46.1817	180.7800
	FF	36	6.9000	46.1196	325.6800
	Centre	10	7.6659	40.1373	100.0500

III. Relative G, A, and D efficiency values of Box-Behnken Design

Regarding the impact on relative efficiencies, let's first consider the relative A-efficiency. Table 3 presents the variations in relative A-efficiencies resulting from the absence of a factorial point, a center point, and a non-missing point for all factors from k = 3 to 9. The numerical data indicates that A-efficiency is marginally influenced by the absence of a factorial point for only factor k=3. On the other hand, the absence of a factorial point has a statistically significant effect on all other factors. When a center point is missing, the relative A efficiency is similar to that when no design points are missing. Therefore, estimating the precision of individual variances of regression coefficients of the second-order model performs quite well when either factorial or center run points are missing.

The relative *D*-efficiencies closely mirror the *A*-efficiencies. When a factorial or center run observation is missing, the relative D-efficiencies are similar to the efficiencies of a complete design for factors *k* = 3 to 9. Furthermore, the relative *D*-efficiency value significantly estimates the covariances among coefficients when some observations are absent.

The relative *G*-efficiencies exhibit notable similarities with the relative *A*- and *D*-efficiencies. The absence of a factorial point significantly impacts the relative G-efficiencies for factors *k* = 3,4 and 7, moderately affects factors *k* = 5,6, and is less concerning for factors *k* = 8,9. Regarding the missing center point, the relative G-efficiency exceeds one compared to when no observations are missing.

Table 3: *Relative G, A, and D efficiency values one missing observation of BBD k = 3 to 9 factors*

Number of Factors	Missing Design Points	G Efficiency	Relative G efficiency	Relative A efficiency	Relative D efficiency
$k = 3$	None	60.1400	1.0000	1.0000	1.0000
	F	23.6900	0.3939	0.7846	0.8706
	Centre	63.4600	1.0552	0.9577	0.9779
	None	85.7300	1.0000	1.0000	1.0000
$k = 4$	*F*	37.9100	0.4422	0.9181	0.9433
	Centre	88.6700	1.0343	0.9736	0.9879
	None	85.5100	1.0000	1.0000	1.0000
$k = 5$	*F*	52.0000	0.6081	0.9569	0.9675
	Centre	13.7400	0.1607	0.9780	0.9914
	None	64.17	1.0000	1.0000	1.0000
$k = 6$	*F*	82.9200	0.6461	0.9607	0.9709
	Centre	66	1.0303	0.9818	0.9935
	None	89.5	1.0000	1.0000	1.0000
$k = 7$	*F*	89.7100	0.5007	0.9574	0.9731
	Centre	90.025	1.0049	0.9836	0.9949
	None	71.28	1.0000	1.0000	1.0000
$k = 8$	*F*	93.405	0.8736	0.9853	0.9890
	Centre	69.45	0.9744	0.9853	0.9970
$k = 9$	None	79.84	1.0000	1.0000	1.0000
	F	78.81	0.9871	0.9957	0.9932
	Centre	79.88	1.0004	0.9957	0.9981

IV. Relative G, A, and D efficiency values of SBBD K = 4 to 9 factors.

Relative A and D efficiencies exhibit similar effects for all factors from k = 5 to 9, except for factor k = 4. For factor k = 4, the relative A efficiency for 2_{III}^{3-1} fractional factorial points is 0.3906, while the relative D efficiency is 0.7179. Both full factorial and 2_{III}^{3-1} fractional factorial points demonstrate good accuracy for individual coefficients and covariances among coefficients when observations are missing for factors k = 5 to 9 in terms of relative A and D efficiency. The numerical data indicates that the absence of a center point does not impact all factors' relative A and D efficiency.

Relative G efficiencies are significantly influenced by factor k = 4. However, factors k = 7 and 9 exhibit superior prediction performance compared to factor k = 4. Moreover, factors k = 5,6 and 8 excel in minimizing the maximum prediction variance compared to all other factors when the full factorial observation is missing. When it comes to missing 2_{III}^{3-1} fractional factorial observations, only factors k= 6 and 8 have a marginally better effect than all other factors of SBBD. The absence of a center point does not impact the relative G efficiency for any factor.

Table 4: *Relative G, A, and D efficiency values one missing observation of SBBD K = 4 to 9 factors.*

Number of Factors	Missing Design Points	G Efficiency	Relative G efficiency	Relative A efficiency	Relative D efficiency
	None	34.07	1.0000	1.0000	1.0000
$k = 4$	*F*	13.2300	0.3883	0.7360	0.8874
	FF	4.5600	0.1338	0.3906	0.7179
	Centre	34.6900	1.0182	0.9855	0.9879

$k = 5$	None	34.6200	1.0000	1.0000	1.0000
	F	32.2000	0.9301	0.9101	0.9399
	FF	16.9700	0.4902	0.8006	0.9127
	Centre	35.9900	1.0396	0.9883	0.9914
$k = 6$	None	37.8100	1.0000	1.0000	1.0000
	F	37.8200	1.0003	0.9553	0.9582
	FF	25.6800	0.6792	0.8147	0.9285
	Centre	36.8300	0.9741	0.9904	0.9935
	None	53.6200	1.0000	1.0000	1.0000
$k = 7$	*F*	38.0800	0.7102	0.9097	0.9573
	FF	14.0700	0.2624	0.7087	0.8710
	Centre	51.0700	0.9524	0.9959	0.9963
	None	53.0100	1.0000	1.0000	
$k = 8$	*F*	44.0600	0.8312	0.9426	0.9700
	FF	37.0600	0.6991	0.9013	0.9613
	Centre	52.7300	0.9947	0.9956	0.9971
$k = 9$	None	50.7400	1.0000	1.0000	1.0000
	F	30.4500	0.6001	0.8923	0.9661
	FF	16.8800	0.3327	0.8130	0.9519
	Centre	54.8300	1.0023	0.9864	0.9981

V. Discussion on Box-Behnken Design by FDS plot

If we interpret Figure 1 (a) intending to identify the most effective design point types based on *G*-efficiency and maximum *SPV*, it appears that the center and non-missing design points outperform factorial. They achieve a maximum *SPV* value of 15.98, which equates to a *G*-efficiency of 60.6%; this is considerably better than the factorial design points, which reach a high *SPV* value of 42.44 and a *G*-efficiency of 23.69%.

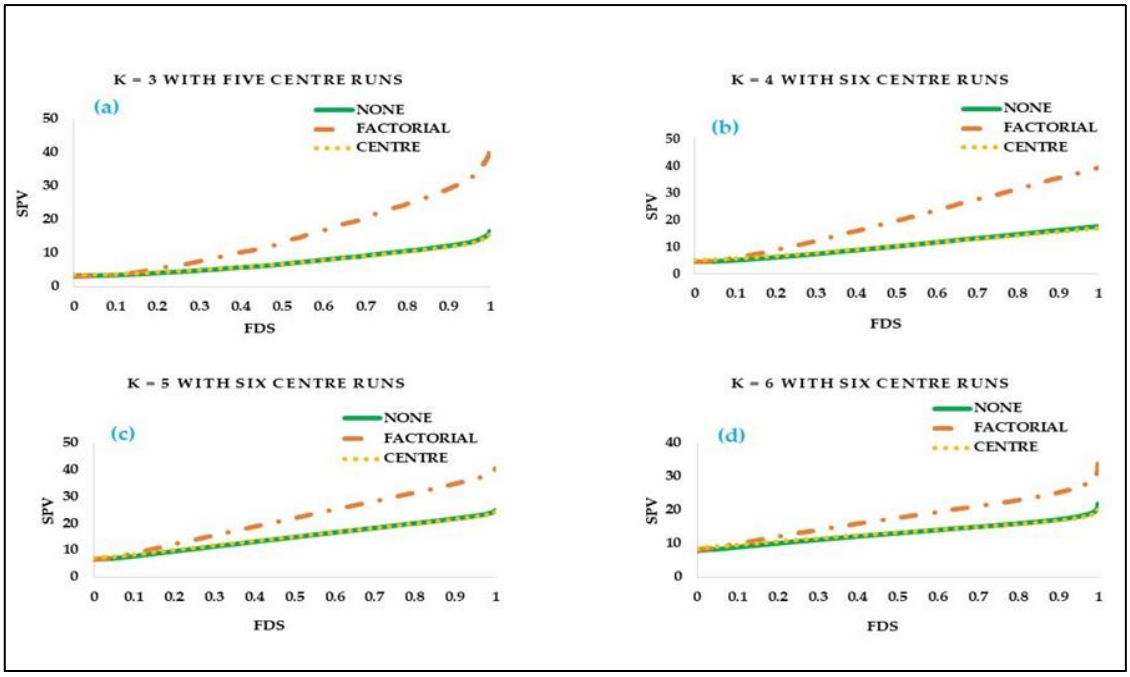

Figure 1: *(a) FDS for BBD K = 3. (b) FDS for BBD K = 4. (c) FDS for BBD K = 5. (d) FDS for BBD K = 6*

When evaluating *BBD k*=4 in Figure 1 (b), we can see a clear difference between the 50th and 75th percentiles of the design points. For the factorial points, the *SPV* at the 50% *FDS* is 19.80, and at the 75% *FDS*, it is 29.92, resulting in a difference of 10.12. On the other hand, for the center and non-missing points, the *SPV* at the 50% *FDS* is 10.29, and at the 75% *FDS*, it is 13.68, yielding a smaller difference of only 3. This percentile-based assessment leads us to conclude that the center and non-missing points demonstrate more consistent and superior performance across the design space than the factorial points.

The *FDS* plot depicted in Figure 1 (c) for *BBD k*=5 suggests that the absence of both the center and factorial design points significantly reduces the likelihood of obtaining a horizontal flat line. The median *FDS* value for the center and non-missing points is 15.21 *SPV*, with a mean or average *SPV* value of 14.8, indicating a lack of symmetry in the *SPV* and FDS distributions [11]. When a factorial point is missing, the maximum *SPV* reaches 40.38, and the average *SPV* is 15.34, suggesting that 50% of the design space exhibits moderate prediction performance.

The *FDS* plots in Figures 1 (d) and (e) reveal that the curves for the center and non-missing design points exhibit similar prediction performance. Both reach a maximum *SPV* value of approximately 20 at *FDS*=1 for factors six and seven. A slight flat line is noticeable in the horizontal curve of the center and non-missing design points for both factors. This increase begins from the median of the *FDS* and extends to roughly 90% of the design space region, suggesting a certain level of stability in the *SPV* distribution of the design points. When a factorial point is missing, factor six achieves a maximum *SPV* value of 33.76, indicating better prediction performance than factor seven, which has an *SPV* value of 40.13.

Based on comparing factors eight and nine from the *FDS* plot in Figures 1 (f) and (g), BBD k=8 exhibits a very similar curve across the entire design space region, with a slightly increasing horizontal line. The *SPV* values range from a minimum of 12 to a maximum of 21. For *BBD* k=9, the curves for the center, factorial, and non-missing design points have similar prediction performance and are very close to each other, with *SPV* values ranging from 12 (*min*) to 34 (*max*) across the entire design space region. Interestingly, each factor's prediction performance is comparable when both design points are missing in factors k = 8 and 9.

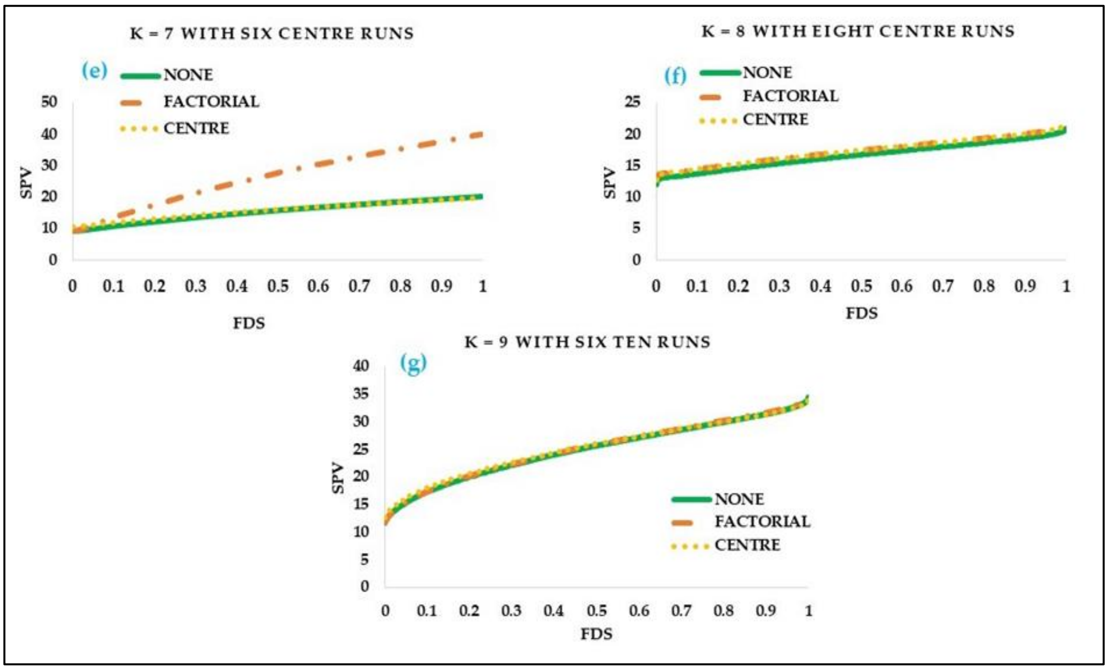

Figure 1: *(e) FDS for BBD K = 7. (f) FDS for BBD K = 8. (g) FDS for BBD K = 9.*

VI. Discussion on Small Box-Behnken Design by FDS plot

Indeed, Figure 2 (a) presents four types of design points: full factorial, 2_{III}^{3-1} fractional factorial, and center and non-missing design points. The point at approximately (0.50,12.15) represents that 50% of the total design space has an SPV value at or below 12 for the design point of one missing center run and non-missing run, where these design points exhibit a flat horizontal curve for the maximum design space region up to 1. A flatter curve implies that the maximum and minimum SPV values are closer together, indicating a more stable distribution of the SPV [11]. The full factorial design points of $SBBD$ k = 4 consist of 12 runs. When 2^2 full factorial points are missing, the maximum SPV value is 113 for the maximum (FDS = 1) design space region, and 80% of the design region has an SPV value of 47 or below. This is similar to missing a center run for the max SPV value. From this, we can infer that 80% of the 2^2 full factorial design space region has moderate SPV compared to 100% of FDS. The 2_{III}^{3-1} fractional factorial design point in $SBBD$ has four runs. When an FF point is missing, it results in a large SPV value of 307 for the maximum (FDS = 1) design space region. However, 50% of the total design space has an SPV value at or below 76.6, and 75% of the total design space region has an SPV value at or below 111.78. This suggests that FF has moderate SPV for 75% of the design space region compared to the large SPV value for the maximum (FDS = 1) region.

The FDS plot of the 2^3 full factorial, center, and non-missing design points is depicted in Figure 2 (b). These design points exhibit similar performance, as indicated by their comparable curves and G-efficiencies of 32.20, 35.99, and 34.62, respectively. Upon closer inspection, the center and non-missing design points are strikingly similar across the entire design space region, from the minimum (FDS=0) to the maximum (FDS=1), with SPV values of 60.60 and 58.29, respectively. However, the 2^3 full factorial design point deviates slightly from the other two similarity curves in the FDS region of 75%. The average SPV values for the center, full factorial, and non-missing points are also similar at 18.84, 19.94, and 18.22, respectively, suggesting that the absence of these design points during experimentation does not significantly impact the prediction performance of SPV on average.

Despite having a high SPV value of 123.83 at maximum (FDS=1), 2_{III}^{3-1} fractional factorial design points maintain a median SPV value of 31.82 in the design space curve and an SPV value of 60.42 for 88% of the total design space. This roughly equates to the maximum SPV value (FDS =1) of the center, factorial, and non-missing runs. Therefore, we can conclude that 2_{III}^{3-1} fractional factorial design points generally provide good prediction performance for most of the design space (90%), except for the maximum region (100%), where their performance is subpar.

As depicted in Figure 2 (c), the design points for the factor k = 6, including centre, 2^3 full factorial, and non-missing, exhibit a similar horizontal curve across the entire design space region, from the minimum (FDS = 0) to the maximum (FDS = 1). These design points have a G-efficiency of 37% and a maximum SPV value of 74. The SPV value fluctuates between 21 and 30, covering 55% to 80% of the design space region. It's interesting to note that while both full factorial and fractional factorial design points consist of the same sixteen runs, the absence of a run from the 2_{III}^{3-1} fractional factorial alone results in a significant SPV value of 109.45 in the maximum (FDS =1) region. The curves for 2_{III}^{3-1} fractional factorial are closely aligned with other design points from the minimum (FDS =0) region to 80% of the design space, with an SPV of 40.47 or less. All design points demonstrate moderate or average prediction performance up to 80% of the total design space region, indicating satisfactory prediction performance within this FDS region.

As shown in Figure 2 (d), 2_{III}^{3-1} fractional factorial design points are the only ones that do not exhibit a flat horizontal curve among all design points. The center and non-missing design points share the same horizontal curve, with an average SPV of 22.79 and similar G-efficiencies of 51 and 53.62, respectively. The 2^3 full factorial design points of $SBBD$ k = 7 consist of 24 runs. If a run is missing from the experiment, the prediction performance of the design remains relatively consistent over approximately 80% of the total design space region, with an SPV value of 42.76. The 2_{III}^{3-1} fractional factorial design points have a substantial SPV value of 248.63 in the maximum (FDS=1) design space region. However, the median of the FDS curve has an average SPV of 70, where the maximum SPV is more than twice the average SPV value. Therefore, we can conclude that the prediction performance of 2_{III}^{3-1} fractional factorial is moderate for only 50% of the total design space region.

As per the *FDS* plot in Figure 2 (e), it's observed that the prediction performance across all shrinkage levels is quite similar for all types of design points, ranging from the lowest to the highest *SPV* value. Approximately half of the *FDS* curves for all design points closely follow the average *SPV* values, while the remaining curves diverge towards the maximum of (*FDS*=1). The global *FDS* curve suggests that less than 25% of the design space has an *SPV* value of 29.61 or lower, and 50% has an *SPV* value of 39.62 or lower for all types of points, including those without missing values. For up to 75% of the design space, the prediction performance of non-missing and center points is significantly better than that of 2^2 or 2^3 full factorial points, and 2^2 or 2^3 full factorial missing points outperform 2_{III}^{3-1}fractional factorial points.

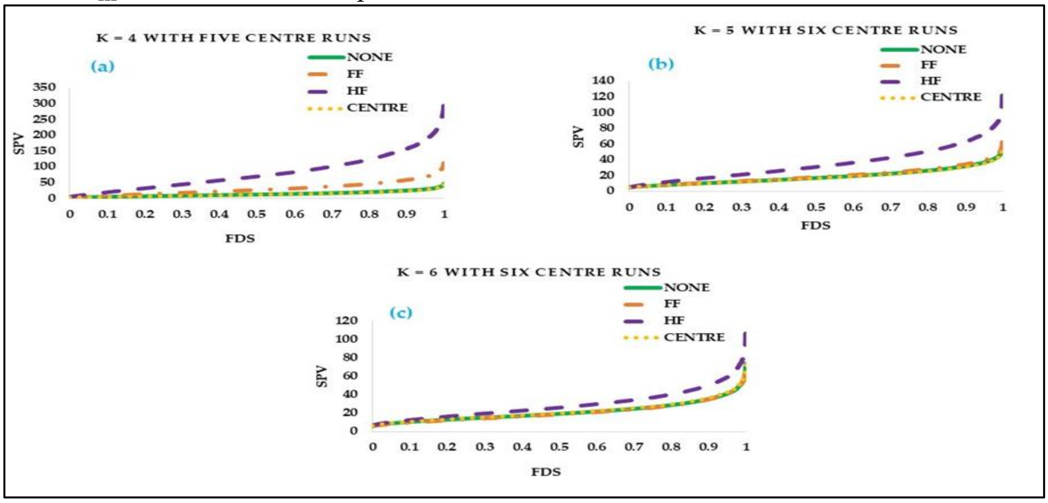

Figure 2: *(a) FDS for SBBD K = 4. (b) FDS for SBBD K = 5. (c) FDS for SBBD K = 6*

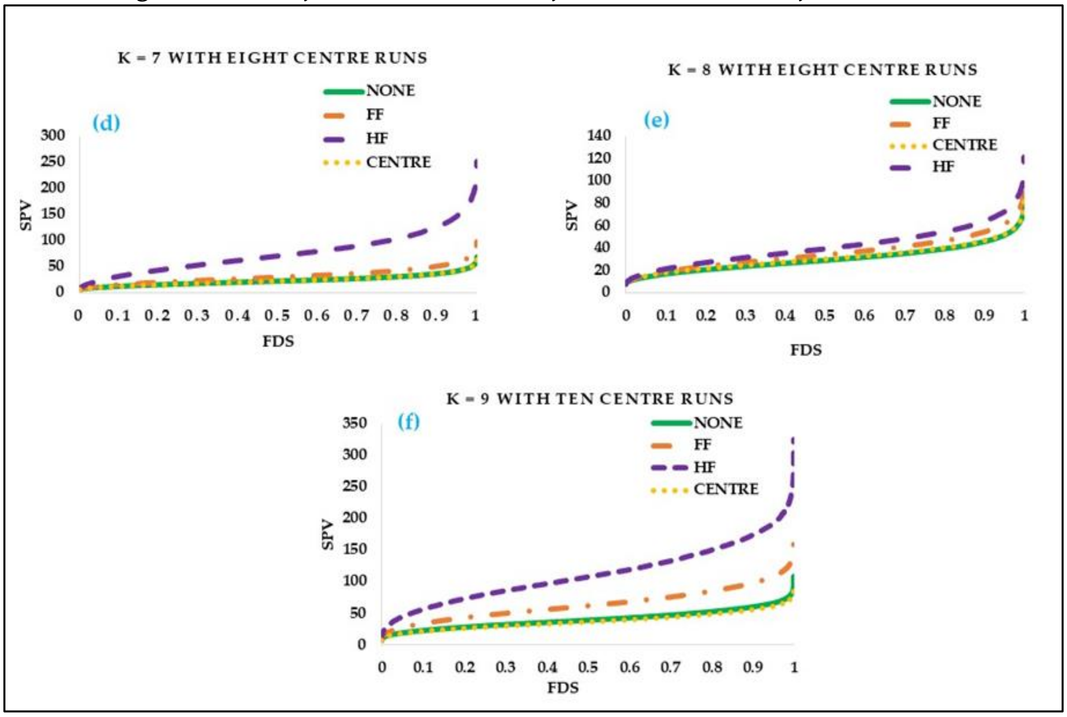

Figure 2: *(a) FDS for SBBD K = 7. (e) FDS for SBBD K = 8. (f) FDS for SBBD K = 9*

IV. Conclusion

The robustness of a single missing observation in *BBD* and *SBBD* is examined to determine which design points offer the best design efficiency and model parameter estimation using an information-based criterion. *BBD* and *SBBD* show good accuracy in estimating individual coefficients and covariances among coefficients when a design point is missing for all factors, except for factor k = 3 in *BBD* and k = 4 in *SBBD*, which show poor accuracy. The relative *G*- efficiency of *BBD* indicates that factors with increasing numbers have lower maximum variance across the experimental space, except for factor k = 7. In *SBBD*, full factorial and center design points have lower maximum variance across the experimental space than fractional factorial design points. The *FDS* plot reveals that missing a center and non-missing run have similar *SPV* values for all factors across the entire design space region for both *BBD* and SBBD. In comparison, the factorial design point type in *SBBD* has higher *SPV* values than BBD despite the fewer runs in *SBBD*. For *BBD*, all factors have similar performance for factorial design points. However, in *SBBD*, full factorial design points outperform 2_{III}^{3-1} fractional factorial design points have a high *SPV* value at the maximum region (FDS =1). If a design point is missing in the 2_{III}^{3-1} fractional factorial design points of *SBBD*, it results in subpar prediction performance.

This research work indeed holds significant potential in identifying robust missing design point types when observations are missing in an experimental situation for both Box-Behnken Design and Small Box-Behnken Design for certain factors. The findings can be beneficial when data may be lost or corrupted during the experimental process. Moreover, the scope for further research is vast. Future studies could extend this work to include more factors and more than one missing observation with multiple combinations. This would allow for a more comprehensive understanding of the robustness of these designs under various conditions.

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