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Assessment of prediction capability of response surface designs using graphical methods

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Abstract
The goal of many studies is to choose a design that allows a good estimate of the relationship between explanatory factors and the response of interest. The design of the RESPONSE surfaces allows adjustment of the response surfaces and provides a means of checking their suitability. There are many measure to study the predictive performance of responsive surface designs for comparison of designs, but these are mainly the single-valued efficiency type criteria. The graphical method is a useful tool for assessing the overall predictability of an experimental design over the entire area of interest. Variance dispersion graph (VDG) are useful for comparing competing designs over a fixed design space. However, they do not provide all useful information about the predictability of a design. The fraction of design space (FDS) technique provides more detailed information by quantifying the portion of the design space where the scale prediction variance (SPV) is less than or equal to any predefined value. The FDS technique complements the use of VDGs to better understand the predictability of a design. Here, these two graphical tools have been described. Several standard response surface designs with varying number of elements are discussed with these two methods.

Keywords: Fraction of design space plot, response surface design, scaled prediction variance, variance dispersion graph

1. Introduction

Research has often sought to determine and quantify the relationship between a large number of explanatory variables and one or more measurable responses. Many studies seek to determine and quantify the relationship between a large number of explanatory variables and one or more measurable responses. Response surface methodology (RSM) is used to examine the relationship between the response and the explanatory variables. The process is used for developing, improving, or optimizing a process through various graphical, statistical, and mathematical methods. The least squares method is frequently used to fit first-order regression models by RSM

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_{iu} + \varepsilon \qquad (1)$$

or a second-order model

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_{iu} + \sum_{i=1}^{k} \beta_{ii} x_{iu}^2 + \sum_{i<}\sum_{i'} \beta_{ii'} x_{iu} x_{i'u} + \varepsilon \qquad (2)$$

In this model, $x_1, x_2, \ldots, x_k$ are k independent variables, y is the response variable, and N observations are made. The x_{iu} level represents the level of the i^{th} (i = 1, 2, ..., k) factor in the u^{th} treatment combination (u = 1,2, ..., N). ε is a random error with mean 0 and variance σ^2. β_0 is a constant, β_i is the i^{th} linear regression coefficient, β_{ii} is the i^{th} quadratic regression coefficient and $\beta_{ii'}$ is the $(i, i')^{th}$ interaction coefficient. It is common to use the central composite design introduced by Box and Wilson (1951) [3] for second order polynomial models because its structure enables good estimation of all model parameters. On the other hand, Plackett-Burman designs (1946) [11] or factorial designs are most suitable for first-order models.

In the literature, attempts have been made to compare response surface designs on the basis of single-valued efficiency-type criteria. Mostly alphabetical optimality criteria, like D, A, G, or V, has been used where each attempts to summarize one important characteristic of the design

(Kiefer and Wolfowitz, 1959) [6]. These are single number criteria where each criterion intends to capture a different aspect of the ‘goodness’ of a design.
The intention of the researcher can be to have suitable prediction at a specific vicinity within the design space. To achieve this, Box and Hunter (1957) [2] described a variance function, i.e., the scaled prediction variance (SPV). The SPV gives a degree of the precision of the estimated response at any point within the design space. It is desirable that the distribution of the scaled prediction variance throughout the design space need to be moderately stable. Box and Hunter (1957) [2] additionally described the idea of rotatability that is attained while a design has the identical value of scaled prediction variance for any two point which can be on the identical distance from the centre.

The SPV is defined as

$$v(x_0) = \frac{N var(\widehat{y}(x_0))}{\sigma^2} = N x_0'((X'X)^{-1})x_0 \qquad (3)$$

where x_0 corresponds to the location in the design space which is also a function of the model used, the total sample size, N, is used to penalise larger designs, $var(\widehat{y}(x_0))$ is the variance of the estimated response at x_0, X is the design matrix, and σ^2 is the variance.
The aim of G-optimality is to reduce the max SPV all through the vicinity of the design. i.e., a design which satisfies $\min[\max(v(x))_{x\epsilon R}]$ is a G-optimal design. The lower bound for the maximum SPV is equal to p, the number of parameters in the model (Myers and Montgomery, 2002) [9]. Therefore,

$$\text{G-efficiency} = \frac{p}{\max(v(x))_{x\epsilon R}} \qquad (4)$$

A best design can be more complicated than may be summarized via way of means of single numbers. Consequently, graphical techniques for design evaluation had been advanced to allow researchers to take a look at designs more thoroughly.
Variance Dispersion Graphs (VDGs) have been proposed to evaluate a response surface design with spherical regions (Giovannitti-Jensen and Myers, 1989) [4]. VDGs cannot provide more information about the distribution of SPV on the sphere, as they only display three prediction variance values in concentric spheres. A solution to this is the fraction of design space (FDS) which has been described by Zahran *et al.* (2003) [15] to study how well the design predicts throughout the design space. In FDS, the plot displays the SPV versus the volume of the design region and show the maximum, minimum and quantiles of the SPV distribution. This summary provides insight into the prediction performance of the experimental designs. It additionally has a bonus of requiring only a single line to symbolize every design, bearing in mind a clear evaluation of numerous competing designs in a single plot.
Central composite design (CCD) and Box-Behnken designs are an important class of response surface design. The central composite design introduced by Box and Wilson (1951) [3] is one of the most popular response surface designs. It is designed to fit a second order model. It exists for spherical or cuboidal regions for $k \geq 2$, where k is the number of factors. The CCD has three components: the factorial points, the 2k axial points and the n_c center runs. The axial points are at a distance of α from the design center. They mainly contribute to the estimation of the quadratic terms. The center runs are located in the center of the design space and help to estimate the quadratic terms as well as the pure error. The choice of the number of center runs affects the distribution of the SPV (Myers and Montgomery, 2002) [9]. Box–Behnken designs (Box and Behnken, 1960) [1] are the designs for response surface methodology to achieve the following goals: Each factor, is placed at one of three equally spaced values, usually coded as −1, 0, +1. The design should be sufficient to fit a quadratic model, that is, one containing squared terms, products of two factors, linear terms and an intercept. Box-Behnken design is considered to be more proficient and most powerful than other designs such as the three-level full factorial design, central composite design despite its poor coverage of the corner of nonlinear design space.
In the next section two graphical method have been described. Some standard response surface designs with different number of factors are discussed with both these methods.

2. Methodology and Application
2.1 Variance Dispersion Graph
A variance dispersion graph allows one to visualize the uniformity of the scaled prediction variance of a value in multidimensional space. It consists of three curves: the maximum, the minimum and the average scaled variance of a predicted value on a hypersphere. Each value is plotted against the radius of the hypersphere. The VDG plots the maximum and minimum over spheres of radius r from the center of the design, as well as the spherical average of the SPV against the radius r throughout the region of interest. The degree of rotatability of the SPV at any given radius of spheres is illustrated by comparing the maximum to the minimum of SPV across the range of radii.
Figure 1 shows the VDG of a 3-factor CCD for a second order model in a spherical region. It is rotatable, i.e. $\alpha = \sqrt[4]{8}$. Therefore the minimum, the maximum, and the average SPV curves are identical. The number of center runs considered is one, three, and five. As the number of center runs increases, the SPV improves closer to the center of the design space.

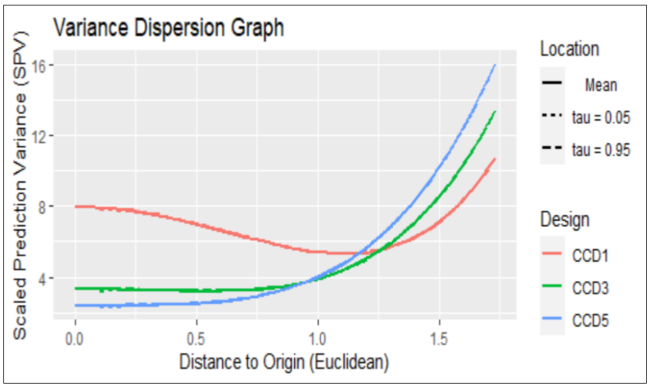


Fig 1: VDG for examining the effect of center runs in CCDs

In Figure 2, CCD and BBD for 3 factors are compared. The designs have all been scaled to the unit sphere. Nearness to rotatability of a design can be evaluated by comparing the spread of the maximum and minimum curves. The VDG also allows the user to see the specific locations where the SPV is maximized and where it is minimized. The CCD performs better than the BBD with almost over the whole region.

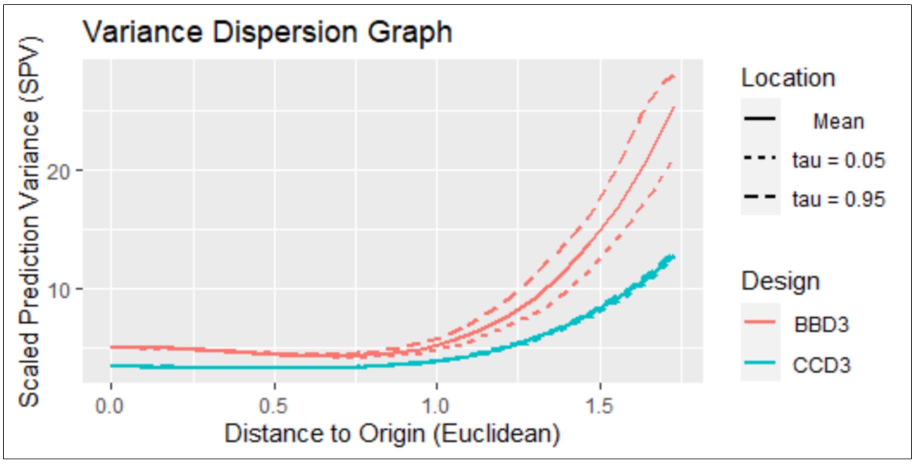


Fig 2: VDG of three-factor designs for a spherical region

2.2 The Fraction of Design Space Plot

Fraction of design space plot examine a design's prediction variance properties through graphs and it is introduced by Zahran *et al.* (2003) [15]. They display the fraction of the design space where the scaled prediction variance (SPV) is less than or equal to a predefined value for all observed values. The SPV distribution of a design can be studied by examining its FDS plot and also compare designs. The FDS plot provides the information about the distribution of the SPV throughout the design space, including the minimum and the maximum SPVs. Similar to the VDG, one can determine the approximate G-efficiencies for a design by looking at an FDS plot. The idea is that the closer the design space of the SPV is to the minimum, the better the design. Also, the flatter the line, the more stable the SPV distribution for that design. Graphs are given so that one can evaluate the predictive performance of a design or compare different design based on the fraction of the plan space contained in multiple cut-off points for some measure of variance. The larger the fraction of design space that is at or below a given value, the better the design.

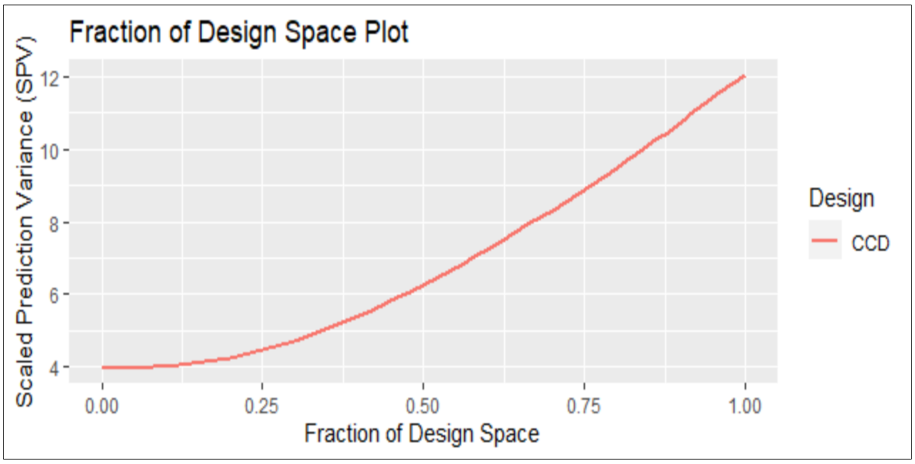


Fig 3: FDS plot for CCD (nc = 2) on a spherical region

In Figure 3, the SPV values for the 3-factor CCD range between 4 and 12. The G-efficiency is approximately 83.33% (10 parameters in the model divided by the maximum SPV value of 12). The corresponding FDS value on the x-axis of the plot indicates about the skewness of distribution.

The FDS graph helps to study the design of any linear model chosen. Consequently, this allows for a comparison of the properties of the prediction variance of the design at the same time on the basis of different models. This information is useful as the envisaged model may change after data collection. To compare the different designs, the size of the cut-off point in relation to the volume of the design area can be considered. For a practitioner who a priori doesn't know where he or she might want to predict in the design space, it is very desirable to have a larger area relatively close to the minimum SPV. To estimate the predictability of the FDS graph, the percentage of the design space values relative to the whole range of cut points is shown in the range of minimum to maximum SPV. This allows the researcher to compare the effectiveness of the design in terms of prediction. By plotting multiple designs on the same graph, researchers can see the global minimum and maximum SPV for each design. The slope of the curve shows how quickly the design reaches the maximum SPV, preferably closer to horizontal.

A variant of the FDS plots is the scaled FDS plot, which focuses on the stability of the forecast variance in area X of the design. Here, the normal FDS plot is adjusted using the scaled SPV. A design with a steeper scaled SPV curve than another has an SPV that is less stable in the design region. This version of the FDS chart also allows the analyst to determine the ratio of the maximum SPV to the minimum.

Variance Ratio FDS (VRFDS) plot is another variant of FDS. This graph is especially useful when comparing a range of candidate design to a reference design. To plot such a plot, the

SPV is calculated for a number of different designs at the same randomly modelled points in the design region X. The VRFDS plot is then plotted by replacing the SPV with the natural logarithm of the ratio of each design's SPV to the reference design's SPV. Supposing that two designs, d_1 and d_2 are of interest, the VRFDS plot is constructed by calculating the log variance ratio Log VR (x^{*}, d_1, d_2) = log v(x^*, d_1)/v(x^*, d_2), for each simulated point x^*. d_2 is the reference design and is represented by a constant log variance ratio of zero in the plot. If the log variance ratio for a design is negative, it has a lower SPV than the reference design and is therefore the preferred design. Similarly, when the log variance ratio is positive it has a larger SPV than the reference design and is therefore not preferred. A design which leads to better predictions over much of the experimental region will have a curve largely below the horizontal line representing the reference design. These VRFDS plots can be useful for eliminating designs which are not admissible in the sense that they perform worse compared to any other candidate design over most of the experimental region.

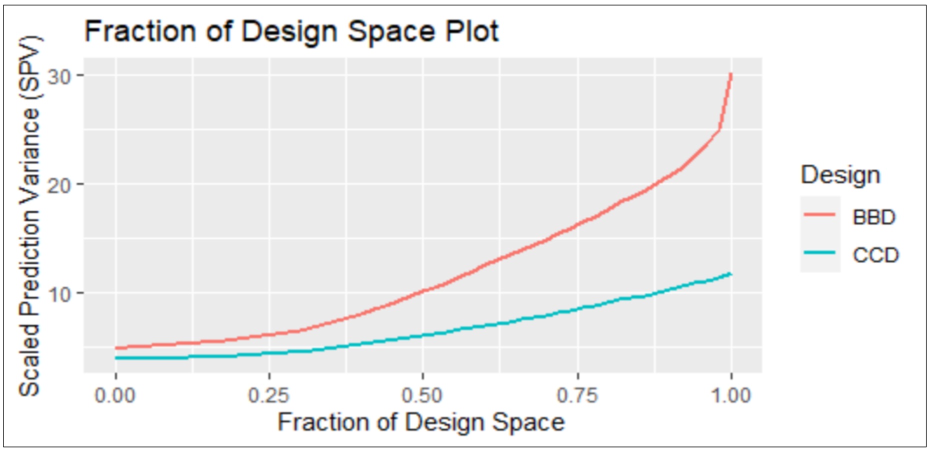


Fig 4(a): FDS plot for 3 factor CCD and BBD

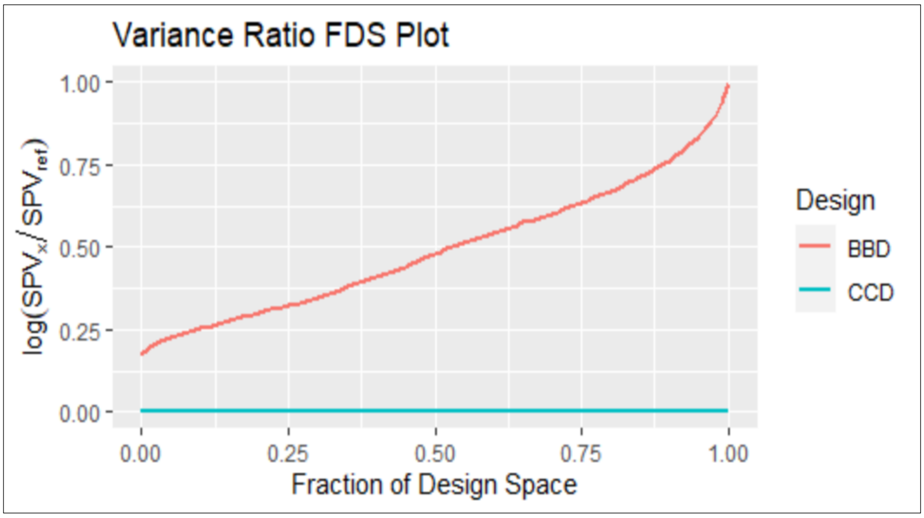


Fig 4(b): Variance Ratio FDS plot for 3 factor CCD and BBD

From Fig 4(a) CCD is preferable to BBD for this model and design space. This is confirmed by the Variance Ratio FDS plot shown in fig. 4(b) which shows that CCD is largely superior over the majority of the design region.

2.3 Comparison between Central Composite, D- and A-optimal Designs

In this example, optimal design is considered alternatives to central composite designs (CCDs) for three design factors. A hyper spherical design region is assumed, and the axial distance for the CCD is assumed to be $\alpha = \sqrt{3}$. This spherical CCD is based on a full factorial design, augmented with four center runs and the usual six axial runs. The CCD hence contains 22 runs. D-optimality seeks to maximize the determinant of the information matrix. A-optimality seeks to minimize the trace of the inverse information matrix, which minimizes the average variance of the regression parameters.

From the figure 5(a), VDG it is clear that the CCD and A-optimal designs have comparable SPV profiles over X, where the SPV is exceptionally low close to the origin however turns out to be progressively more terrible towards the border. The D-optimal design does more regrettable in the inside and yet have better SPV close to the edge of X. The FDS plot shows that the D-optimal design has the most stable SPV. And it gets clearer from the FDS plots shown in figure 5(b), FDS allows global comparisons easier than VDGs and makes comparisons with fixed radii easier. Although the CCD and A- optimal designs accomplish lower SPV values close to the origin, this comes at the expense of an altogether higher SPV close to the border of X. The FDS plot puts more accentuation on the edge since this is in the same place as most of the volume of X found. Consequently the D- optimal designs gives an option in contrast to the CCD which features better forecast over most of the plan area.

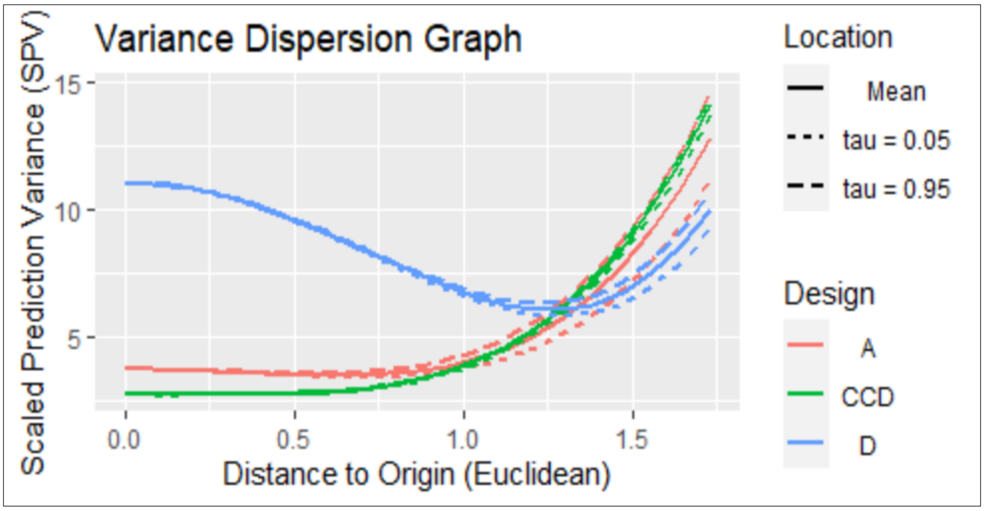


Fig 5(a): VDG plot for 3 factor CCD, A and D optimal design

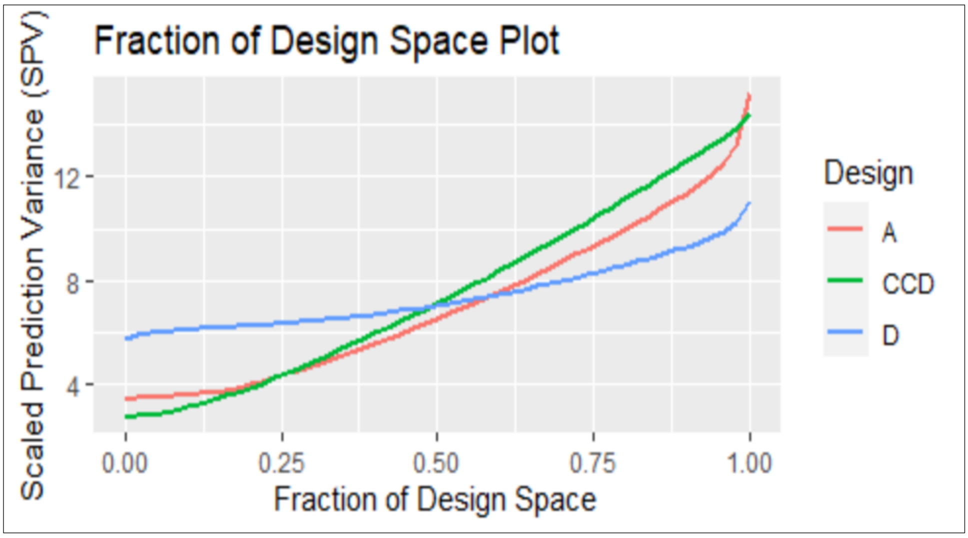


Fig 5(b): FDS plot for 3 factor CCD, A and D optimal design

2.4 Comparisons of CCD with different center runs

Figure 6 illustrates an FDS graph for CCD with three factors and different center runs. G efficiency can be easily read from the graph. More stable designs have FDS graphs with more nearly horizontal lines. Here, a 1-center run CCD is the most stable. The 5 center run CCD has the most variable SPV range, with the smallest predictive variance being about eight times the best predictive variance.

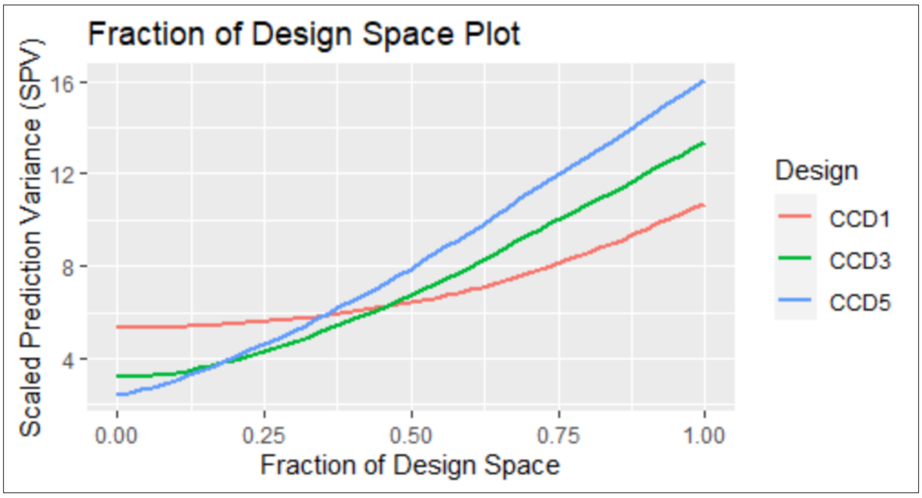


Fig 6: FDS for examining the effect of center runs in CCDs

2.5 Comparison of some Three-Factor Designs
FDS plots for the following designs: The CCD design with center run=2, the small composite design (SCDH) by Hartley (1959) [5], the Box Behnken design (BBD), Hybrid design D416B, D311B by Roquemore (1976. Hartley (1959) [12, 5] introduced the small composite designs (SCD). These designs have the same construction as the CCD except that they employ a resolution III fractional factorial design in the factorial portion, are often near-saturated, and are more economical than the CCD. Another near-saturated class of designs is the hybrid class (Roquemore (1976)) [12]. These designs are available for k = 3, 4, and 6. This class contains some designs that are highly efficient and nearly rotatable.

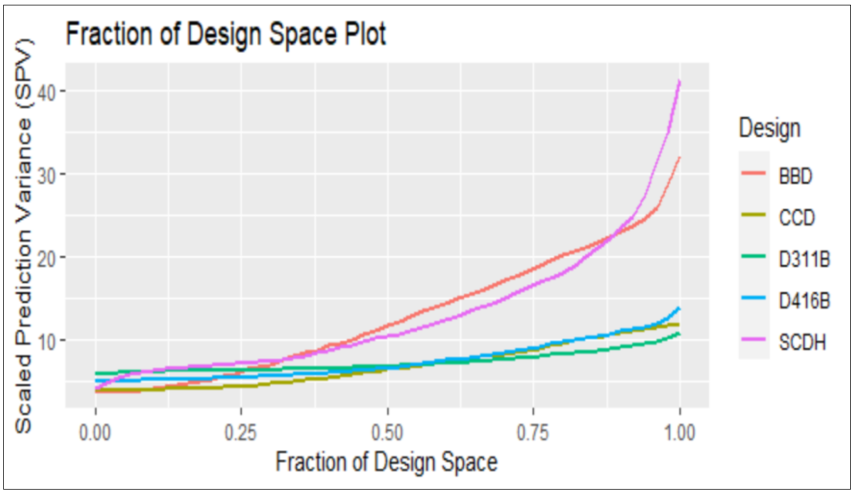


Fig 7: Comparison of some three factors design

The SCDH and BBD designs have substantially higher G-efficiencies (max SPV values). The hybrid D311B has lower SPV values for approx. 97% of the total design space compared with the other designs.

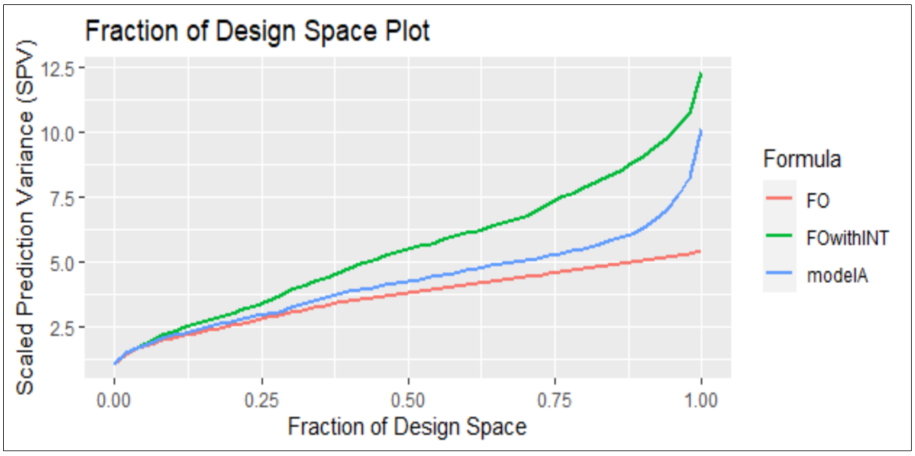
2.6 Testing model adequacy for 3-factor CCD
On account of the 10-term three-factor quadratic model, there are various models that might be nested inside the complete model. The table1 shows a few potential nested designs that might be fascinating while inspecting a three-factor CCD. The comparing FDS curves for these 7 models are displayed in Figure 7.

From the figure we can note the interesting feature of the different designs: FDS curve of the first-order model with interactions has a very different slope from the remaining curves with similar numbers of terms. There is much larger effect of adding interaction term on the stability of the SPV values (as described by FDS curves that are closer to horizontal) than the addition of a similar number of quadratic terms. This happen because in CCD small number of runs are involved in estimation of interaction terms. As the model get reduced, G optimal bound automatically get reduced since is related to the number of parameters in model.

Second, for all fraction of design space, any model that is nested inside another should have a FDS curve that is at or beneath the greater model. This is due to the SPV's design, which means that adding terms to the model will only raise its SPV value. This is connected to the basic bias-variance trade-off in model selection, in which a model that is small may suffer from bias issues due to its inability to correctly explain the underlying relationship, while a model that is too large may suffer from inflated prediction variance. The maximum SPV values for the second-order model and the first-order model with interaction are 12.70 and 11.8, respectively. However, the G-efficiencies associated with them are far different, because of the number of associated parameters. The G-efficiencies of the design for these two models are 78.7% (10/12.70) and 59.3% (7/11.8), respectively.

Table 1: Information for the reduced models in Figure 8 (factor = 3)

Type of model (k=3)	Terms in model	No of parameters p (G optimal bound)	Maximum SPV
First order (FO) model	x_1, x_2, x_3	4	5.80
Model A	x_1, x_2, x_3, x_1x_2	5	7.80
FO model with interactions	$x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3$	7	11.80
Model B	$x_1, x_2, x_3, x_1x_2, x_1^2$	6	8.40
Model C	$x_1, x_2, x_3, x_1x_2, x_1^2, x_3^2$	7	10.29
Model D	$x_1, x_2, x_3, x_1^2, x_3^2$	6	8.29
Second order model	$x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3, x_1^2\, x_2^2, x_3^2$	10	12.70



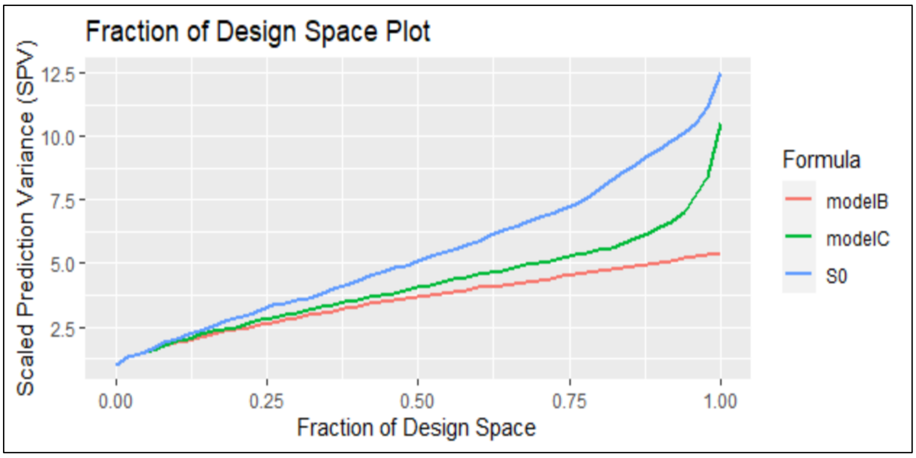


Fig 8: FDS plot for a 3-factor CCD (n_c = 2) for several models

3. Package for Creating VDGs and FDS Plots in R programming

All the graphs shown above was developed in R programming. Lawson (2012) [7] developed a package *Vdgraph* for creating Variance Dispersion Graphs of response surface designs. The package includes functions that make the variance dispersion graph of one design or compare variance dispersion graphs of two designs, which are stored in data frames or matrices. The package also contains several minimum run response surface designs (stored as matrices). Schoonees *et al.* (2016) [13] developed vdg package that provides a customizable interface for generating graphical summaries of the prediction variance associated with specified linear model specifications and experimental designs. These methods include variance dispersion graphs, fraction of design space plots and quantile plots which can assist in choosing between a catalogues of candidate experimental designs. Package rsm (Lenth, 2010) [8] has been used to generate CCD and BBD and Package AlgDesign (Wheeler & Braun, 2019) [14] has been used to generate A and D optimal design.

4. Conclusions

Alphabetic optimality criteria as well as variance dispersion graphs are all useful measures for comparing competing designs. The VDG is a useful tool for visualizing the range of the values possible for the scaled prediction variance for different designs and their location in the design space. The fraction of design space (FDS) technique is a complement to the existing VDG technique. FDS, focuses on how well it predicts for any fraction of the design space. It gives the fraction of the design space that is less than or equal to a pre-specified value of the SPV. The FDS graph represents the cumulative fraction of design at each value of the SPV throughout the design region. It allows comparison of the global minimum and maximum of SPV for different designs. Since the model robustness properties of a design can be an important consideration, adaptations of the FDS plot can assist in choosing a design that will perform well for a broad range of nested models within the maximal model specified. One can see the approximate G-efficiency for that design with the specific model directly from the FDS plot.

5. Acknowledgement

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Appendix 1: CCD and BBD design for 3 factors is given below

x_1	x_2	x_3
-1	-1	1
1	-1	1
0	0	1.6818
-1	1	1
-1	1	-1
0	0	-1.6818
0	-1.6818	0
0	1.6818	0
-1.6818	0	0
-1	-1	-1
1	1	-1
1.6818	0	0
0	0	0
0	0	0
1	-1	-1
1	1	1
	CCD for 3 factors	
x_1	x_2	x_3
1	0	1
1	0	-1
-1	0	-1
0	1	-1
0	-1	1
0	1	1
0	0	0
0	-1	-1
1	1	0
-1	-1	0
-1	0	1
-1	1	0
1	-1	0
	BBD for 3 factors	