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ON COMPARING THE PREDICTION VARIANCES OF SOME CENTRAL COMPOSITE DESIGNS IN SPHERICAL REGIONS: A REVIEW

P.E. Chigbu, E.C. Ukaegbu, J.C. Nwanya

1. INTRODUCTION

Response surface methodology (RSM) is a common framework for many industrial experiments. It is the collection of tools in design of experiments or data analysis that enhances the exploration of a region of design variables in one or more responses, (Myers, Khuri and Carter, 1989). Fitting a second-order model

$$y_{ij} = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_i x_i^2 + \sum_{i<j}^{k} \beta_{ij} x_i x_j + \varepsilon_{ij} \quad (1)$$

is common in response surface methodology, where y_{ij} is a measured response, x_i, $i = 1,...,k$ are the design variables and ε_{ij} is a random error with mean zero and variance, σ^2. There are several second-order model designs in the literature which include Central Composite designs (CCD), Box-Benkhen designs (BBD), Hooke designs, Small Composite designs (SCD), Minimum-run Resolution V designs (MinresV), Hybrid designs, etc (Box and Wilson, 1951; Myers and Montgomery, 2002 and Zarhan, 2002).

A good response surface design possesses the following features: (a) provides a reasonable distribution of data points throughout the region of interest; (b) provides a good profile of the prediction variance in the experimental region; (c) does not require a large number of runs; etc. These attributes were identified by, Myers and Montgomery (2002) and Montgomery (2005) and are typical of the second-order response surface designs, some of whose performances in spherical regions will be investigated in this study.

Several works have been done on response surface designs. Lucas (1976) compared the performances of several types of quadratic response surface designs in symmetric region. He compared the Central Composite designs (CCD), Box-Benkhen designs (BBD), Hooke designs, Pesotchinsky designs, etc, based on *D*- and *G*-optimality criteria. Myers, Vining and Giovanitti-Jensen (1992) presented an extensive study of response variance properties of the following second-order designs: CCD, BBD, and Hybrid designs. These designs were studied using the variance dispersion graph.

Borkowski (1995) studied the analytical properties of the Central Composite designs and Box-Benkhen designs in a spherical region. His studies yielded alternative approach to the computer-based algorithm approach for obtaining the minimum, maximum and average spherical prediction variances for the designs. Zarhan (2002) compared the prediction variances for the CCD, Box-Benkhen Designs, Small Composite designs (SCD) and Hybrid designs for 2, 3, 4, 5 and 6 factors in both spherical and cuboidal regions. These comparisons were made using the Variance Dispersion Graphs (VDG), Fraction of Design Space Criterion and the *G*- and *D*- optimality criteria. Park et al (2005) evaluated the response variance properties of response surface designs on cuboidal region utilizing both the VDG and Fraction of Design Space Graph (FDSG). Borror et al (2006) compared the response variance performance for the variation of the CCD in both the spherical and cuboidal regions. Their interest is to know how these designs perform when axial distance of $\alpha = \sqrt[4]{k}$ is employed. He used a fraction of design space as a criterion for comparison for 6 to 10 factors.

However, in this study, we try to demonstrate that in spherical regions with radius $\alpha = \sqrt{k}$ none of the designs, CCD, SCD and MinResV is uniformly superior when evaluated under the $G-$ and $I-$optimality criteria as well as the VDG. The range of number of factors under consideration is 3 to 7 with 2, 3 and 5 centre points. The $G-$ and $I-$optimality criteria are obviously indispensable since the prediction variances of the designs are the objects of interest and can only be evaluated using these optimality criteria as will also be demonstrated later in section three.

The findings of this research work have wide applications in industrial processes especially in the chemical industry. Response surface designs can be used to solve two types of problems in the chemical industry, as reported by Myers, Khuri and Carter (1989). The first is a procedure in which a region of the best operating conditions is sought. In this case, the method of Evolutionary operation (EVOP) is used. Evolutionary operation was proposed by Box (1957) as a procedure for the continuous monitoring and improvement of a full-scale process with the goal of moving the operating conditions towards the optimum. Here, response surface methodology is applied using the 2^k full factorial designs which form part of the three designs under consideration in this paper. In practice, EVOP can be applied to only two or three variables but in theory, it can be applied to k process variables. However, Montgomery (2005) gives the procedure for two process variables while Box and Draper (1969) discuss in detail the three-variable case and Myers and Montgomery (2002) investigate and discuss the computer implementation of EVOP. The second problem is confirming the exact location of the optimum in the region of interest. In this case, the class of CCD's is used to a large extent to tackle this situation.

2. DEFINITIONS

2.1. *Central composite designs (CCD)*

This class of designs was developed by Box and Wilson (1951) and is the most widely used class of second-order model designs. Assuming there are $k^{3} \geq 2$ design variables, the CCD consists of a 2^k full or 2^{k-1} fractional factorial (of resolution V), $2tk$ axial or star runs and n_0 centre points, where t is the number of replication and for this study, $t = 1$.

Therefore, the CCD uses $n = f + 2tk + n_0$ points to estimate the $(k+1)(k+2)/2$ model parameters (Atkinson and Donev, 1992). According to Montgomery (2005), for a spherical region of interest, the best choice of α from the view point of the prediction variance for the CCD is to set $\alpha = \sqrt{k}$. This gives the spherical CCD in which all the fractorial and axial design points are located on the surface of a sphere. Early recommendation made by Box and Hunter (1957) is to choose the number of centre points, n_0 for which uniform information or precision is achieved. For $k = 2$, the structure of the CCD is

$$
\begin{array}{c|cccc|cccc|c}
 & \multicolumn{4}{c|}{2^k} & \multicolumn{4}{c|}{2k} & n_0 \\
x_0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
x_1 & -1 & -1 & 1 & 1 & -\alpha & \alpha & 0 & 0 & 0 \\
x_2 & -1 & 1 & -1 & 1 & 0 & 0 & -\alpha & \alpha & 0
\end{array}
$$

2.2. *Small composite designs (SCD)*

This class of designs was developed by Hartley in 1959 as small and more economical alternative to the CCD. The basic construction of SCD is similar to that of CCD, except that the factorial component is of resolution III instead of resolution V. That is, no main effects are aliased with any other main effect, but main effects are aliased with two-factor interactions and two-factor interactions may be aliased with each other. The design matrix for $k = 3$ (see Zahran, 2002) is

$$
\mathbf{X} = \begin{bmatrix}
x_1 & -1 & 1 & 1 & -1 & -\alpha & \alpha & 0 & 0 & 0 & 0 \\
x_2 & -1 & 1 & -1 & 1 & 0 & 0 & -\alpha & \alpha & 0 & 0 \\
x_3 & -1 & -1 & 1 & 1 & 0 & 0 & 0 & 0 & -\alpha & \alpha
\end{bmatrix}.
$$

2.3. *Minimum-runs resolution V designs (MinResV)*

The minimum-runs resolution V designs were developed by Ochlert and Whitecomb in 2002 as fractional factorial designs in which the main effects and two-factor interactions are not aliased with the other main effects and two-factor interactions. Rather two-factor interactions are aliased with three-factor interactions. For further study of the resolution V designs, see Montgomery (2005).

2.4. $G-$ *optimality criterion*

The $G-$optimality criterion minimizes the maximum prediction variance over the region of interest. Symbolically, it is given by $min\{max\, v(x)\}$ = $min\{max\, \underline{x}^{/} M^{-1}(\xi)\underline{x}\}$, where $\underline{x}$ is a vector of points in the region of interest and $M^{-1}(\xi)$ is the inverse of the information matrix of the design, ξ.

2.5. $I-$ *optimality criterion*

A design is said to be $I-$optimal if it minimizes the normalized average integrated prediction variance.

$$I = \frac{n}{\sigma^2}\int_R var(x)d\mu(x) \tag{2}$$

where $\text{var}(x) = \underline{x}^{'} M^{-1}(\xi)\underline{x}$ is the prediction variance, R is the region of interest, and μ is uniform measure on R with total measure 1 (Giovannitti-Jensen and Myers, 1989; Atkinson and Donev, 1992 and Hardin and Sloane, 1993).

The values of the $G-$ and $I-$optimality criteria were computed using the MATLAB program for each of the designs compared and the results are presented in Table 1 below.

2.6. *Variance dispersion graphs*

The use of the variance dispersion graphs (VDG) was introduced by Giovannitti-Jesen and Myers (1989) to evaluate the properties of the prediction variance of a design. The VDG displays the minimum, maximum and average prediction variance for a specific spherical design with radius, r, from the centre of the design. Traditionally, the scaled prediction variance (SPV), discussed in section three, is plotted against the radius in the graph (see also Zahran, 2002 and Montgomery, 2005). Comparisons among competing designs can be made easily and the strength and weaknesses of the designs can be assessed using the VDG. This type of information cannot be captured in single number criterion.

2.7. *Prediction variance*

This, according to Montgomery (2005), is the variance of the predicted response at points of interest, x. It is given by

$$v(x) = \sigma^2 X'(X'X)^{-1} X\,. \tag{3}$$

3. ANALYTICAL APPROACH

Fitting a full quadratic response model of equation (1) where there are k variables $x_1, x_2, ..., x_k$; $p = (k+1)(k+2)/2$ unknown coefficients, β, and independent error term, ε, with mean 0 and variance, σ^2, let the design consists of $n \geq p$ points $[x_{j1}, x_{j2}, ..., x_{jk}]$ for $1 \leq j \leq n$, chosen from a spherical region of interest and let X be the n x p expanded design matrix $f(x)$ = $[1, x_1, ..., x_k; x_1^2, ..., x_k^2; x_1x_2, ..., x_{k-1}x_k]$ and let $M_x = \frac{1}{n}X'X$ be the information matrix of the design matrix, then, the prediction variance at an arbitrary point, x, is

$$var(x) = \sigma^2 f'(x)M_x^{-1} f(x) \tag{4}$$

(see Hardin and Sloane, 1993).

The scaled prediction variance (SPV) is obtained by multiplying the above expression by n and dividing by the error variance, σ^2. The resulting expression is given by

$$\frac{nvar(x)}{\sigma^2} = nf'(x)M_x^{-1} f(x) \tag{5}$$

The scaling is used to facilitate comparison among competing designs of various sizes (see Montgomery, 2005). Now the $I-$optimal design has been defined as one which minimizes the normalized average or integrated prediction variance, $I = \frac{n}{\sigma^2}\int_R var(x)d\mu(x)$, R and μ retaining their usual meanings. This integral was simplified by Box and Draper (1963) as

$$I = trace\{S(X'X)^{-1}n\} \tag{6}$$

where

$$S = \int_R f'(x)f(x)d\mu(x) \tag{7}$$

is the moment matrix of region of interest (see also Hardin and Sloane, 1993). For a second-order model with $k = 3$ variables, the moment matrix in a spherical region is given below as

$$S = \begin{bmatrix} x_0 & x_1 & x_2 & x_3 & x_1^2 & x_2^2 & x_3^2 & x_1x_2 & x_1x_3 & x_2x_3 \\ 1 & 0 & 0 & 0 & \sigma_2 & \sigma_2 & \sigma_2 & 0 & 0 & 0 \\ 0 & \sigma_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \sigma_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sigma_2 & 0 & 0 & 0 & 0 & 0 & 0 \\ \sigma_2 & 0 & 0 & 0 & \sigma_4 & \sigma_{22} & \sigma_{22} & 0 & 0 & 0 \\ \sigma_2 & 0 & 0 & 0 & \sigma_{22} & \sigma_4 & \sigma_{22} & 0 & 0 & 0 \\ \sigma_2 & 0 & 0 & 0 & \sigma_{22} & \sigma_{22} & \sigma_4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma_{22} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma_{22} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma_{22} \end{bmatrix}$$

where $\sigma_2 = \int_R x_i^2 dx = \frac{r^2}{k}$ (8)

$$\sigma_4 = \int_R x_i^4 dx = \frac{3r^4}{k(k+2)} \quad (9)$$

$$\sigma_{22} = \int_R x_i^2 x_j^2 dx = \frac{r^4}{k(k+2)} \quad (10)$$

(see Giovannitti-Jensen and Myers, 1989); r is the radius of a ball or sphere and is defined by Onukogu (1997) as

$$r = \left\{ \sum_{i=1}^{k} x_i^2 \right\}^{\frac{1}{2}} = k^{\frac{1}{2}} = \alpha \quad (11)$$

Hence the $G-$optimal design is the one that minimizes the maximum value of equation (5) while $I-$optimal design is one that minimizes equation (6).

The prediction variance function, $V(x) = f'(x)M^{-1} f(x)$ can be expressed in a closed form which will facilitate the calculation of the $V_{\max}$ ($G-$optimal) and average V_p ($I-$optimal) response variances on the surface of a sphere of radius, r. Using the structure of the matrix, X, the information matrix, $X'X$, for a CCD is obtained directly by matrix multiplication and the resulting block matrix, derived by Borkowski (1995), is

$$X'X = \begin{bmatrix} n & J'_k & (f+2t\alpha^2)' & L' \\ J_k & diag(d_i) & \phi'_1 & \phi'_2 \\ (f+2t\alpha^2) & \phi_1 & (f+2t\alpha^4)I_k & L'J_k \\ L & \phi_2 & (L'J_k)' & diag(h_i) \end{bmatrix},$$

where ϕ_1 and ϕ_2 are zero matrices, J_k is a $k\times 1$ unit column vector, L is a $\binom{k}{2}\times 1$ unit column vector, I_k is $k-$dimensional identity matrix while $diag(d_i)$ and $diag(h_i)$ are diagonal matrices such that $d_i = f + 2t\alpha^2$ for $1 \le i \le k$ and $h_i = \binom{k}{2}\times\binom{k}{2}$ for $k > 3$ or $k \times k$ matrix for $k \le 3$. The inverse of the information matrix is given by

$$(X'X)^{-1} = \begin{bmatrix} \alpha_{11} & J'_k & \alpha_{12} & L' \\ \phi_1 & diag(1/d_i) & \phi'_1 & \phi'_2 \\ \alpha_{12} & \phi_1 & \dfrac{1}{2t\alpha^4}[I-\alpha_{22}] & L'J_k \\ L & \phi_2 & (L'J_k)' & diag(1/h_i) \end{bmatrix}$$

where $\alpha_{11} = \dfrac{kf + 2t\alpha^4}{T}$, $\alpha_{12} = -\dfrac{(f+2t\alpha^2)}{T}$, $\alpha_{22} = \dfrac{nf-(f+2t\alpha^2)^2}{T}$ and $T = 2nt\alpha^4 + knf - k(f+2t\alpha^2)^2$.

Borkowski (1995) used this block matrix form to study the scaled response variance through a theorem he proposed. From this theorem, the following are obtained:

$$V_p = n\left\{a + br^2 + \left[c + \left(\frac{d\Gamma(k/2)}{2(\sqrt{\pi})^k}\right)h*(p)\right]r^4\right\}$$

where $h^*(p) = h(p)/r^{k+3}$ and the values are tabulated in Borkowski (1995).

We can derive also the maximum value of variance:

$$V_{max} = n\left[a + br^2 + \left(c + \frac{d}{k}\right)r^4\right] \text{ for } d \le 0$$

or $V_{max} = n[a + br^2 + (c+d)r^4]$ for $d > 0$;

$$a = \alpha_{11}\,,\; b = 2\alpha_{12} + \frac{1}{f + 2t\alpha^2}\,,\; c = \frac{1}{2}\left(\frac{1}{f} - \frac{\alpha_{22}}{t\alpha^4}\right) \text{ and } d = \frac{1}{2}\left(\frac{1}{2\alpha^4} - \frac{1}{f}\right).$$

4. COMPARISON OF THE DESIGNS

4.1. *Comparison using $G-$ optimality*

From Table 1 below, for k = 3, 4 and 5, the order of performance of the designs is SCD $\rightarrow$ CCD $\rightarrow$ MinResV according to the values of their respective variances. For $k > 5$, the order of performance is CCD $\rightarrow$ SCD $\rightarrow$ MinResV. These $G-$optimal values (ie the prediction variances) are consistent for $n_0 = 2$ centre runs and the radius of the sphere is $\alpha = \sqrt{k}$.

4.2. *Comparison using $I-$ optimality*

Under the $I-$optimality criterion, the order of performance is CCD $\rightarrow$ MinResV $\rightarrow$ SCD for $k = 3$, 4, 5 and 6. For $k = 7$, the order is CCD $\rightarrow$ SCD $\rightarrow$ MinResV. These are the results when the radius of the sphere is $\alpha = \sqrt{k}$ but these optimum prediction variances are not consistent for $n_0 = 2$ centre runs.

Particularly, it can be observed that for $k = 5$, SCD and MinResV are optimally equal with respect to the $G-$ and $I-$optimality criteria.

4.3. *Comparison using variance dispersion graphs*

Comparisons done in sections 4.1 and 4.2 are with single number criteria. These criteria do not describe the performance of the designs throughout the region in which responses are to be estimated. This situation, as earlier stated, is captured using the variance dispersion graphs.

For $k = 3$, the VDG of Figure 1 shows that the three designs maintained stable response variance for $r < 1$, but CCD and SCD are optimally good for $r \leq 1.7$. For $k = 4$, the plot in Figure 2 shows that the three designs performed equally when $r = 1.5$, but are optimally best for $r = 2$. For $k \geq 5$, the three designs are unstable for $r < 1.6$, but optimally good for $1.7 \leq r < 2.5$ as shown in figures 3, 4 and 5.

5. CONCLUSION

From the foregoing, none of the designs is judged as superior in the entire three bases for comparison, that is the $I-$ and $G-$optimality criteria as well as the VDG. However, the CCD is found to be at its best (gives minimum prediction variance) under the $I-$optimality for 5 centre points and for $k = 3$ factors.

For the $G-$optimality, the prediction variance of the CCD increases with increasing number of centre points. The SCD behaves in a similar way under the $I-$optimality criterion but achieves its minimum variance under the $G-$optimality using two centre points. The variance deteriorates with increasing number of centre points. Under the $I-$optimality, the MinResV is at its best with 5 centre points and experiences the same deterioration with CCD and SCD under the $G-$optimality.

Finally, using the VDG, the three designs performed well towards the centre of the sphere for $1 \leq r \leq 2$.

Department of Statistics
University of Nigeria, Nsukka

POLYCARP E. CHIGBU
EUGENE C. UKAEGBU
JULIUS C. NWANYA

APPENDIX

TABLE 1

Designs Examined Under the Optimality Criteria in Spherical Region for $\alpha = \sqrt{k}$

Design	k	p	α	f	n_0	n	$G-opt$	$I-opt$
CCD	3	10	$\sqrt{3}$	8	2	16	**10.5715**	10.3048
					3	17	11.2322	7.0031
					5	19	13.4287	**6.6652**
SCD	3	10	$\sqrt{3}$	4	2	12	**10.2000**	16.2576
					3	13	11.0500	10.5623
					5	15	12.7500	**9.8338**
MinResV	3	10	$\sqrt{3}$	7	2	15	**12.2932**	11.8065
					3	16	**12.2932**	10.0456
					5	18	15.4286	**8.3964**
CCD	4	15	2	16	2	26	**15.5689**	**15.5519**
					3	27	16.1677	16.1388
					5	29	16.3521	19.2239
SCD	4	15	2	8	2	18	**15.5250**	**25.5881**
					3	19	16.3875	27.0018
					5	21	16.3333	31.0270
MinResV	4	15	2	11	2	21	**15.5806**	**20.8421**
					3	22	16.3226	21.8254
					5	24	16.3603	23.0992
CCD	5	21	$\sqrt{5}$	16	2	28	**23.9543**	**22.6246**
					3	29	24.8098	23.4519
					5	31	26.0488	24.4189
SCD	5	21	$\sqrt{5}$	11	2	23	**20.9640**	**80.0536**
					3	24	22.2456	83.5501
					5	26	23.9342	85.3241
MinResV	5	21	$\sqrt{5}$	11	2	23	**20.9640**	**80.0536**
					3	24	22.2456	83.5501
					5	26	23.9342	85.3241
CCD	6	28	$\sqrt{6}$	32	2	46	**28.8800**	**28.2810**
					3	47	29.5078	28.8958
					5	49	30.7634	30.1252
SCD	6	28	$\sqrt{6}$	16	2	60	30.4886	**49.2659**
					3	31	**30.0411**	50.9081
					5	33	32.4374	54.5549
MinResV	6	28	$\sqrt{6}$	22	2	36	**33.1145**	39.6809
					3	37	34.0343	40.7831
					5	39	34.9479	**31.5549**
CCD	7	36	$\sqrt{7}$	64	2	80	**42.4640**	**36.1917**
					3	81	43.6534	39.2222
					5	83	44.1743	43.1010
SCD	7	36	$\sqrt{7}$	22	2	38	**44.6424**	**41.1830**
					3	39	45.2399	53.6754
					5	41	46.0097	57.3843
MinResV	7	36	$\sqrt{7}$	30	2	46	**42.4810**	42.7013
					3	47	44.2081	43.1111
					5	49	45.1143	**41.5231**

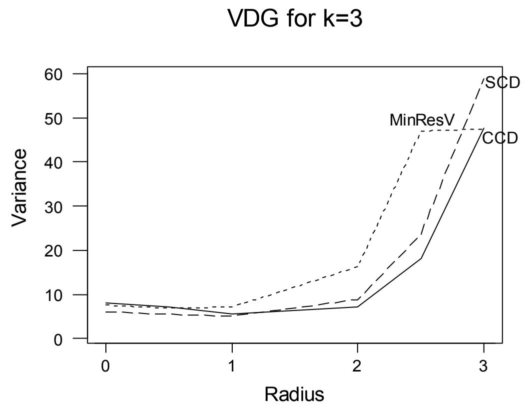

Figure 1

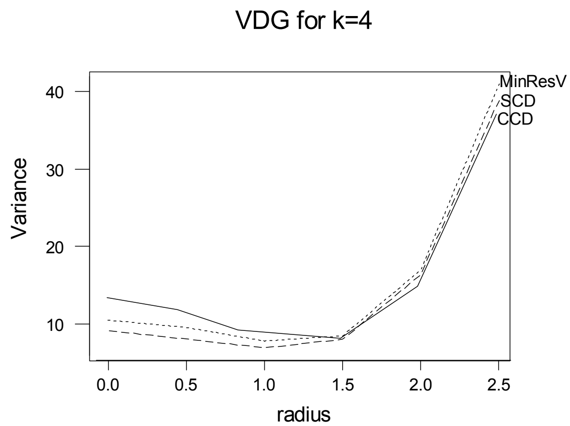

Figure 2

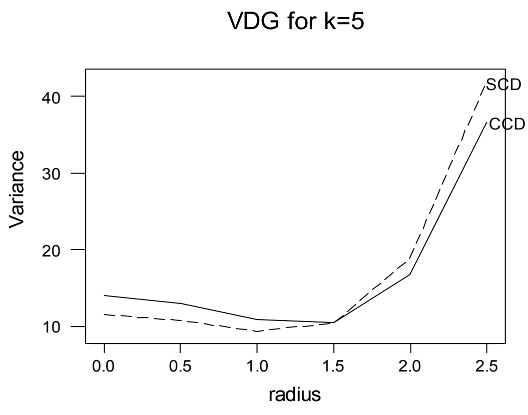

Figure 3

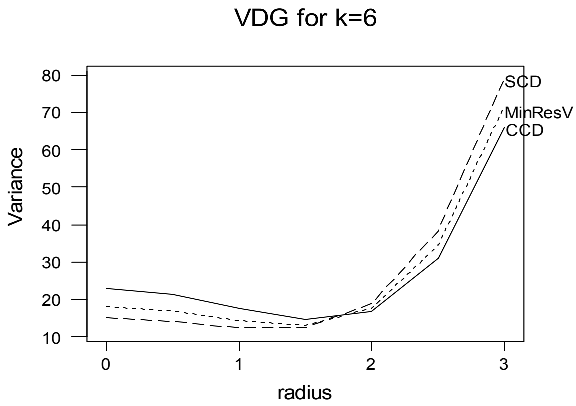

Figure 4

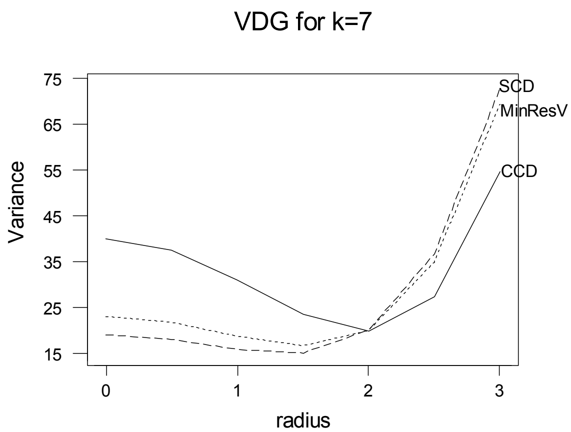

Figure 5

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SUMMARY

On comparing the prediction variances of some central composite designs in spherical regions: a review

Three second-order response surface designs, namely: central composite design, small composite design and minimum-run resolution V design are compared for 3 to 7 factors in spherical regions using the $G-$ and $I-$optimality criteria. The structures of the response variances of the designs are displayed graphically using the variance dispersion graphs. The maximum and average response variances are determined analytically as func-

tions of the radii of the design region. Results for the $G-$ and $I-$optimality criteria are obtained for a spherical region of radius, $\alpha = \sqrt{k}$ where k is the number of factors under consideration. The results suggest that none of the designs is uniformly better than the others with respect to the optimality criteria and the variance dispersion graphs for the factors considered.