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Prediction Variance Assessment of Variations of Two Second-Order Response Surface Designs

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Abstract
Two second-order response surface designs have been evaluated. The designs are the small composite designs and the minimum-run resolution V designs. The cube and star portions of these second-order designs are replicated with different amounts and the variations of the designs generated by replication are compared independently to assess the performance of the prediction variances for each of the second-order design under consideration. Two optimality criteria, *G*- and *I*-optimality, that are prediction variance-oriented are used to evaluate the maximum and average prediction variance of the designs while fraction of designs space plots are constructed to track the prediction variance performance of these designs throughout the design space. For the two second-order designs, the results indicate that it is advantageous to replicate the star than replicating the cube.
Keywords: Optimality criteria, fraction of design space plot, small composite design, minimum-run resolution V design, design replication, cube, star.

1. Introduction
Response surface methodology (RSM) is a collection of mathematical and statistical techniques that are very useful when modeling and analyzing experimental situations. The objective is, by careful design of experiments, a response variable (output variable) that is being influenced by several independent variables (input variables) is optimized (see Montgomery, 2005). Designs used to describe these experimental situations are called response surface designs. A second-order response surface design is often chosen based on many considerations such as those identified by Box and Draper (1959), Montgomery (2005), Myers et al (2009) and Anderson-Cook et al (2009a).

As the number of factors in a second-order model increases, the number of terms also increases. Therefore, economic second-order designs with reasonable prediction variance are highly desirable. Two second-order response surface designs with similar components (cube, star and centre point) and used as smaller alternatives to the central composite designs are considered. They are the small composite designs (SCD) and minimum-run resolution V (MinResV) designs. Hartley (1959) and Oehlert and Whitcomb (2002) are useful references for detailed discussion on the two designs. Several other second-order response surface designs have been evaluated and compared using various criteria: see, for example, Zahran et al (2003) ad Ozol-Godfrey (2004).

Replication of experimental observations is considered indispensible for efficient and optimal performance of the second-order designs. Traditionally, the centre point of the design is replicated to ensure proper estimation of the experimental error with $n_0 - 1$ degrees of freedom as it is assumed that the optimum response is at the centre of the design. However, recent researches have shown that replicating at the centre alone may lead to estimating error that may be too small for correct evaluation of the model. Since there is no assurance that variability will remain constant throughout the design region, Dykstra (1960) posits that it is sound experimental strategy to replicate at other locations in the design region. See also, Giovannitti-Jensen and Myers (1989) for further contributions on replication at other design locations apart from the centre point.

Several works on replicating at other design locations have been focused on the central composite designs (CCD). Such works include Dykstra (1960), Draper (1982), Borkowski (1995), Borkowski and Valeroso (2001) and recently, Chigbu and Ohaegbulem (2011). In this study, we extend this idea to the SCD and MinResV designs since these designs share similar components (cube, star and centre point) with the CCD. We adopt the replication procedure introduced by Draper (1982).

The distance of the star points (axial distance), α, from the centre of the design plays significant role in the distribution of the prediction variance in the design region of interest. Several axial distances have been proposed in the literature and each axial distance affects the structure and performance of the design. Some of the available values of α can be found in Box and Hunter (1957), Montgomery (2005), Myers et al (2009) and

Li et al (2009).

We consider the practical α value in evaluating the replicated versions of the SCD and MinResV designs in this study. The practical α value is proposed by Myers et al (2009) as compromise between the spherical α value when $\alpha = \sqrt{k}$, k being the number of design factors, and the rotatable α value when $\alpha = \sqrt[4]{f}$, f being the size of the cube. The practical α is given by $\alpha = \sqrt[4]{k}$. It has been observed by Li et al (2009) that placing the axial runs at practical α levels results in the stability of the estimated parameters and this yields gain in prediction precision. The practical α is very useful especially when the number of factors is large ($k > 5$) as it provides design point that is less extreme.

2. Model Development

The relationship between the response variable, y , and the design variables, $x_1, x_2, \ldots, x_k$, is described by the model

$$\boldsymbol{Y} = \boldsymbol{X\beta} + \boldsymbol{\varepsilon}, \tag{1}$$

where $\boldsymbol{Y}$ is an N? vector of the responses, $\boldsymbol{X}$ is an N譸 expanded design matrix obtained from the N譳 design matrix, ξ , p being the number of model parameters, $\boldsymbol{\beta}$ is the vector of unknown coefficients while $\boldsymbol{\varepsilon}$ is the random error that is normally and independently distributed with mean zero and variance, σ^2 . However, some experimental situations can best be described with the second-order response surface model

$$\boldsymbol{y} = \boldsymbol{\beta_0} + \mathbf{x}'\boldsymbol{\beta} + \mathbf{x}'\boldsymbol{B}\mathbf{x} + \boldsymbol{\varepsilon}, \tag{2}$$

where $\mathbf{x}$ is a point in the design space spanned by the design and $\boldsymbol{B}$ is a k譳 matrix whose diagonal elements are the coefficients of the pure quadratic terms while the off-diagonal elements are one-half coefficients of the mixed quadratic (interaction) terms.

At a point, $\mathbf{x}$, in the design space, the prediction variance is given by

$$Var\left[\hat{y}(\mathbf{x})\right] = \sigma^2 x'\left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1} x, \tag{3}$$

where $x = \left[1; x_1, x_2, \ldots, x_k; x_1^2, x_2^2, \ldots, x_k^2; x_1x_2, \ldots, x_{k-1}x_k\right]$ is the vector of design point in the design matrix expanded to model form. Equation (3) is scaled by multiplying by N , the total number of runs, and dividing by σ^2 , the process variance. The resulting expression,

$$\frac{NVar\left[\hat{y}(\mathbf{x})\right]}{\sigma^2} = Nx'\left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1} x, \tag{4}$$

is the scaled prediction variance (SPV). The benefits of SPV in model assessment has been widely acknowledged: see, for example, Giovannitti-Jensen and Myers (1989), Borkowski (1995), Montgomery (2005), Anderson-Cook et al (2009a) and Li et al (2009).

Often, the standardized or unscaled prediction variance (UPV), given by

\ $$\frac{Var\left[\hat{y}(\mathbf{x})\right]}{\sigma^2} = x'\left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1} x \tag{5}$$

is preferred by some experimenters in design assessment. See Piepel (2009), Goos (2009), Li et al (2009) and Anderson-Cook et al (2009b) for the benefits of using UPV in design evaluation. The benefits of both the scaled and unscaled prediction variances will be explored in evaluating the performances of the variations of the second-order response surface designs.

3. Optimality Criteria

Two optimality criteria that are prediction variance-oriented are employed in the assessment of the replicated second-order designs. They are the *G*- and *I*-optimality criteria. The *G*-optimality criterion minimizes the maximum SPV. That is

$$G - \text{opt} = \min\left\{\max Nx'\left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1} x\right\}. \tag{6}$$

The *I*-optimality criterion minimizes the average SPV. That is

$$I - opt = min \frac{1}{k} \int_R V\left[\hat{y}(x)\right] dx. \tag{7}$$

4. Partial Replication of Design

Let the cube be replicated n_c times, the star replicated n_s and the centre point replicated n_0 times, then the SCD and MinResV designs use a total of $N = n_c f + 2n_s k + n_0$ number of observations or runs for model parameter estimation. For each replication of the cube portion, the star portion is not replicated and for each replication of the star portion, the cube portion is not replicated. In this study, the number of centre points used is $n_0 = 1$.

Six versions of the designs are generated by replicating the cube and star portions by different amount. The first design is where the cube is replicated twice and the star is not replicated. This design is denoted by C_2S_1. The second is C_1S_2, where the star is replicated twice and the cube is not replicated. Other designs are C_3S_1, C_1S_3, C_4S_1 and C_1S_4. These designs are generated for each of the second-order response surface designs for 6 to 10 factors. The spread of the prediction variance of the replicated designs over the entire design region is evaluated using the fraction of design space (FDS) plots.

5. Comparison of Designs

In this section, variations of the SCD and MinResV designs are created and compared using the two optimality criteria and the graphical technique. The FDS plots are constructed for both the scaled (SPV) and unscaled (UPV) prediction variances. The optimality values are displayed in Table 1 for SCD and Table 2 for MinResV designs.

5.1. Small Composite Designs

We first study the prediction variances of the six variations of the SCD using the criteria already stated above.

Comparison Using *G*-Optimality Criterion

The results of the *G*-optimality criterion for the SCD are presented in Table 1. From the results, replicating the star reduces the *G*-optimality for six-factor design while it increases the *G*-optimality for seven, eight and nine-factor designs. Replicating the cube increases the *G*-optimality for all the factors. However, the *G*-optimality values for the replicated star designs, C_1S_2, C_1S_3 and C_1S_4, are far smaller than those of the replicated cube designs, C_2S_1, C_3S_1 and C_4S_1, for all the factors under consideration. Again, the number of runs for the replicated cube designs far exceeds those of the replicated star designs. Therefore, it is more beneficial to replicate the star than replicating the cube.

Comparison Using *I*-Optimality Criterion

The *I*-optimality values are presented in Table 1. The replicated designs display similar behaviour as in the case of *G*-optimality. The *I*-optimality values decrease by replicating the star for the six-factor designs and increases for the other factors. Also, for all the factors, replicating the cube increases the *I*-optimality. Again, the *I*-optimality values of the replicated cube designs are higher than those of the replicated star designs, making replication of the cube designs undesirable.

Comparison Using Fraction of Design Space Plots

The FDS plots for six, seven, eight and nine factors displayed in Figures 1, 2, 3 and 4. For the UPV and SPV, the replicated star designs have graphs that are flatter and maintain minimum prediction variances distributed throughout the design space. For the UPV, the three replicated cube designs are the same for six and eight factors and show dispersion for the replicated star designs. For seven and nine factors, the FDS plots for UPV show that the replicated designs compete favourably with the replicated star designs having lower prediction variance than the replicated cube designs. In all, for the UPV, the higher replicated star design, C_1S_4, seem to be more stable with low prediction variance.

On the other hand, the FDS plots of the replicated star designs show that the designs have equal and minimum scaled prediction variance spread throughout the entire design space for all the factors under consideration. Slight deviation from this general result for the SPV is in factor six where C_1S_2 competes favourably with C_1S_3 and C_1S_4 for about 30% of the entire design space and then slightly deviate with moderately higher SPV.

5.2. Minimum-run Resolution V Designs

In this section, we take a look at the prediction variance properties of the six variations of the replicated MinResV designs.

Comparison Using *G*-Optimality Criterion

The G-optimality values are presented in Table 2. The results indicate that replicating the star portion of the MinResV designs reduces the *G*-optimality for the six-factor designs and increases the *G*-optimality for the remaining factors with very slight margin among the three variations of the replicated star designs. The replicated cube designs increase the *G*-optimality for all the factors under consideration and the values increase significantly as the cube replication increases.

Comparison Using *I*-Optimality Criterion

The *I*-optimality values for all the factors are displayed in Table 2. The values show that the three star designs compete favourably in terms of the *I*-optimality values with very slight differences among the values for the factors under consideration. However, for the replicated cube designs, the *I*-optimality values increase rapidly as the size of replication increases for all the factors under consideration.

Comparison Using Fraction of Design Space Plots

The FDS plots for the scaled and unscaled prediction variances are displayed in Figures 5, 6, 7 and 8. The plots show that for both UPV and SPV, the replicated star designs display minimum prediction variance spread throughout the design space than the replicate designs. Among the star designs, C_1S_4 show stronger prediction capability than the other designs, displaying the most minimum of the prediction variances with the graphs flatter incase of the SPV.

6. Conclusion

Six variations of two second-order response surface designs generated by replication of the cube and star portions have been independently evaluated using three design criteria. The following conclusions are obvious from the results.

1. For the two response surface designs, the replicated star designs have smaller number of runs than the cube designs replicated with the same amount.
2. The replicated star designs have smaller *G*- and *I*-optimality values than the cube designs replicated with the same amount.
3. The FDS plots of the replicated cube and star designs show that the replicated star designs maintained minimum prediction variance throughout the entire design space unlike those of the cube designs.
4. The FDS plots for UPV show that the higher replicated star design, C_1S_4, display stronger prediction capability than the other replicated designs and competes favourably with the other replicated star designs in terms of SPV.

Since the replicated star designs excellently perform better than the replicated cube designs for the three criteria used to evaluate the designs, we recommend that it will be more beneficial to replicate the star. The cube portion should not be replicated for obvious reasons. When it is economically feasible, the higher replicated star design, C_1S_4, should be the best choice for experiments involving any of the two second-order response surface designs.

References

Anderson-Cook, C.M., Borror, C.M. and Montgomery, D.C. (2009a), Response Surface Design Evaluation and Comparison, *Journal of Statistical Planning and Inference*, vol.139, pp. 629-641. Doi: 10.1016/j.jspi2008.04.004.

_____(2009b), Rejionder for "Response Surface Design Evaluation and Comparison", *Journal of Statistical Planning and Inference*, vol.139, pp. 671-674. Doi: 10.1016/jspi.2008.04.009.

Borkowski, J.J (1995), Spherical Prediction Properties of Central Composite and Box-Behnken Designs, *Technometrics*, vol. 37 (4), pp. 399-410.

Borkowski, J.J and Valeroso, E.S. (2001), Comparison of Design Optimality Criteria of Reduced Models for Response Surface Designs in the Hypercube, *Technometrics*, 43 (4), pp. 468 – 477.

Box, G.E.P. and Draper, N.R. (1959), Basis for the Selection of a Response Surface Design, *Journal of the American Statistical Association,* vol.54 (287), pp. 622-654.

Box, G.E.P. and Hunter, J.S. (1957), Multi-Factor Expeerimental Designs for Exploring response Surfaces, *Annals of Mathematical Statistics,* vol. 28, pp. 195-241.

Chigbu, P.E. and Ohaegbulem, U.O. (2011), On the Preference of Replicating Factorial Runs to Axial Runs in Restricted Second-Order Designs, *Journal of Applied Sciences*, 11 (22), pp. 3732-3737.

Draper, N.R. (1982), Centre Points in Second-Order Response Surface Designs, *Technometrics*, vol. 24 (2), pp. 127-133.

Dykstra, O. Jr. (1960), *Partial* Duplication of Response Surface Designs, *Technometrics*, vol. 2 (2), pp. 185-195.

Giovannitti-Jensen, A. and Myers, R.H. (1989), Graphical Assessment of the Prediction Capability of Response Surface Designs, *Technometrics*, vol. 31 (2), pp. 159-171.

Goos, P. (2009), Discussion of "Response Surface Design Evaluation and Comparison", *Journal of Statistical Planning and Inference*, vol.139, pp. 657-659. Doi: 10.1016/j.jspi.2008.04.012.

Hartley, H.O. (1959), Small Composite Designs for Quadratic Response Surfaces, *Biometrics*, 15 (4), pp. 611-

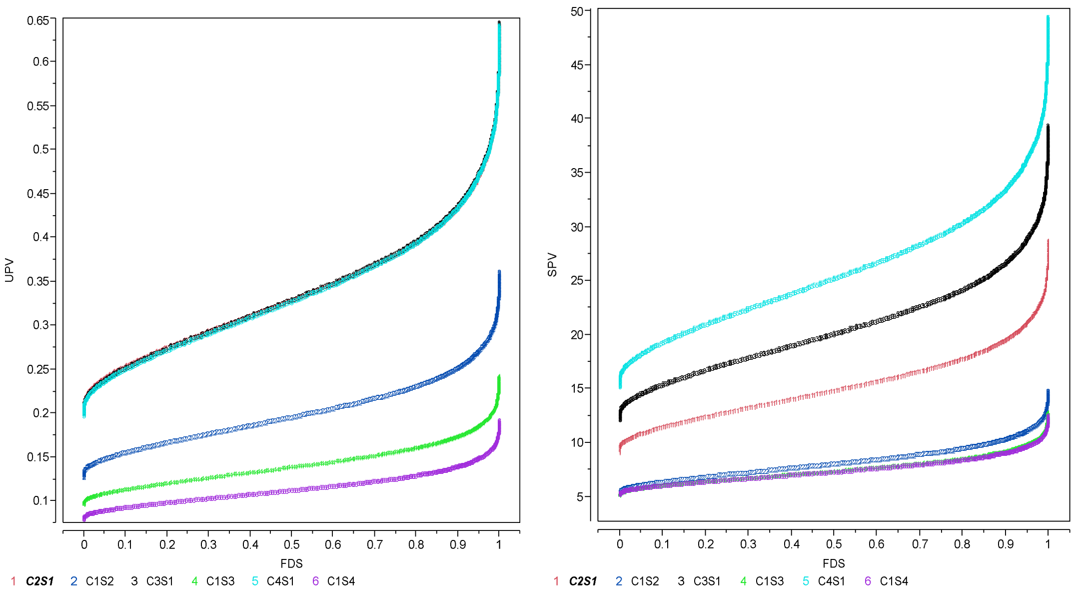
624.
Li, J., Liang, L., Borror, C.M., Anderson-Cook, C.M. and Montgomery, D.C. (2009), Graphical Summaries to Compare Prediction Variance Performance for Variations of the Central Composite Design for 6 to 10 Factors, *Quality Technology and Quantitative Management,* vol. 6(4), pp. 433-449.
Montgomery, D.C. (2005), *Design and Analysis of Experiments, 6th Edition*, John Wiley and Sons, Inc. N.J.
Myers, R.H., Montgomery, D.C. and Anderson-Cook, C.M. (2009), *Response Surface Methodology: Process and Product Optimization Using Designed Experiments*, 3rd Edition, Wiley and Sons Inc. New York, N.Y.
Oehlert, G. W. and Whitcomb, P. (2002), Small, Efficient, Equireplicated Resolution V Fractions of 2^k Designs and Their Application to the central Composite Designs. 46th Annual Fall Technical Conference of the ASQ and ASA.
Ozol-Godfrey, A. (2004), *Understanding Scaled Prediction Variance Using Graphical Methods for Model Robustness, Measurement Error and Generalized Linear Models for Response Surface designs*, Unpublished PhD Dissertation, Virginia Polytechnic Institute and State University
Piepel, G.F. (2009), Discussion of "Response Surface Design Evaluation and Comparison" by C.M. Anderson-Cook, C.M. Borror and D.C. Montgomery, *Journal of Statistical Planning and Inference*, vol. 139, pp. 653-656. Doi: 10.1016/j.jspi.2008.04.008.
Zahran, A., Anderson-Cook, C.M. and Myers, R.H. (2003), Fraction of Design Space to Access Prediction Capability of Response Surface Designs, *Journal of Quality Technology*, vol. 35 (4), pp. 377-386.

Table 1: Summary Statistics for Small Composite Designs with Practical α

k	Design	N	G-Optimal	I-Optimal
6	C_2S_1	45	28.6075	18.8447
	C_1S_2	41	14.7612	9.9892
	C_3S_1	61	39.2833	25.7005
	C_1S_3	53	12.7934	8.9283
	C_4S_1	77	49.3747	32.2665
	C_1S_4	65	**12.4330**	**8.7752**
7	C_2S_1	59	354.5628	182.0658
	C_1S_2	51	**186.3948**	**95.7297**
	C_3S_1	81	407.2287	210.0975
	C_1S_3	65	216.6904	110.7382
	C_4S_1	103	478.1585	247.2061
	C_1S_4	79	249.2863	127.0226
8	C_2S_1	77	73.6989	42.0189
	C_1S_2	63	**38.7620**	**21.8717**
	C_3S_1	107	99.1850	56.7019
	C_1S_3	79	39.3681	21.9527
	C_4S_1	137	129.8632	73.9868
	C_1S_4	95	39.7198	22.0557
9	C_2S_1	95	422.2032	216.5080
	C_1S_2	75	246.6701	125.7679
	C_3S_1	133	497.1299	256.0740
	C_1S_3	93	**243.2588**	**123.7821**
	C_4S_1	171	611.6754	315.4536
	C_1S_4	111	247.0996	125.5580

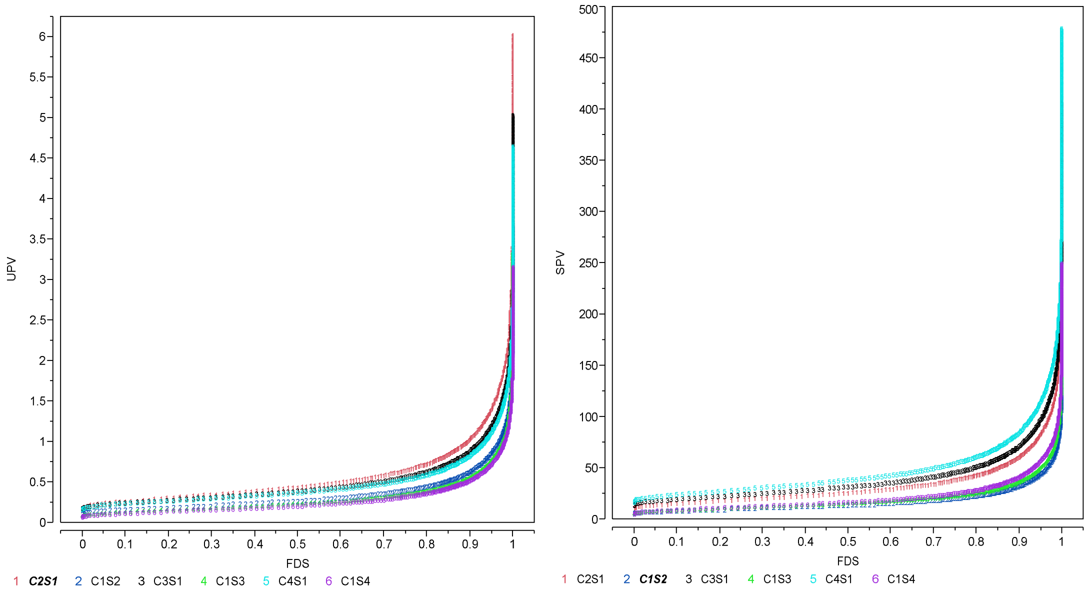
Table 2: Summary Statistics for Minimum-run Resolution V Designs with Practical α

k	Design	N	*G*-Optimal	*I*-Optimal
6	C_2S_1	57	20.9617	14.9600
	C_1S_2	47	14.9999	10.0523
	C_3S_1	79	23.7173	17.7247
	C_1S_3	59	14.1684	9.5852
	C_4S_1	101	27.1577	20.9720
	C_1S_4	71	13.7877	9.4176
7	C_2S_1	75	15.1402	12.7260
	C_1S_2	59	9.9602	7.7673
	C_3S_1	105	20.3037	17.0933
	C_1S_3	73	9.8860	7.5336
	C_4S_1	135	25.1295	21.1935
	C_1S_4	87	10.3508	7.6800
8	C_2S_1	93	16.8595	13.8720
	C_1S_2	71	11.3767	8.4347
	C_3S_1	131	21.5316	18.0880
	C_1S_3	87	11.4421	8.1413
	C_4S_1	169	27.1013	22.8352
	C_1S_4	103	11.3953	7.9834
9	C_2S_1	111	16.9785	14.3133
	C_1S_2	83	11.5176	8.4641
	C_3S_1	157	22.1719	18.9360
	C_1S_3	101	11.8183	8.2617
	C_4S_1	203	28.6613	24.2260
	C_1S_4	119	12.0754	8.2389



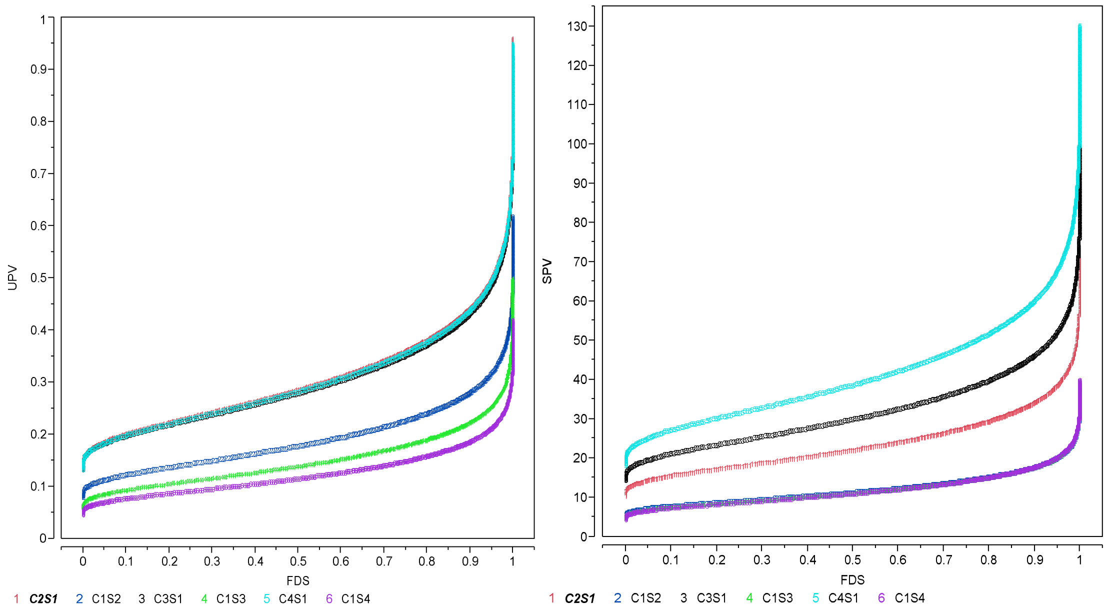
(a) (b)

Figure 1: (a)UPV and (b) SPV for the SCD for $k = 6$ Factors.



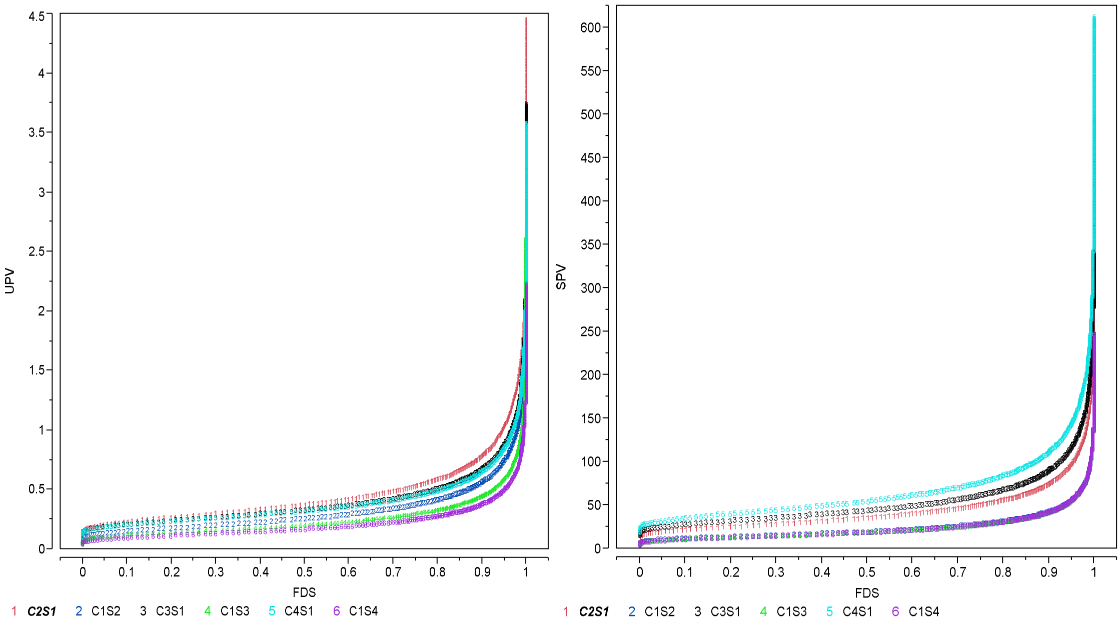
(a) (b)

Figure 2: (a) UPV and (b) SPV for the SCD for $k = 7$ Factors.



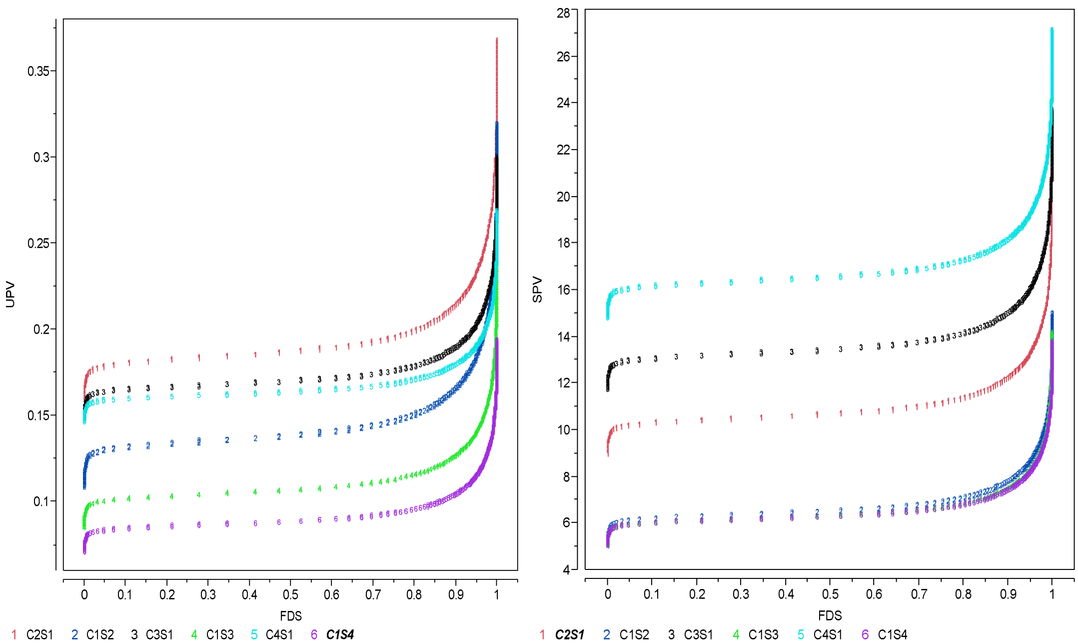
(a) (b)

Figure 3: (a) UPV and (b) SPV for the SCD for $k = 8$ Factors.



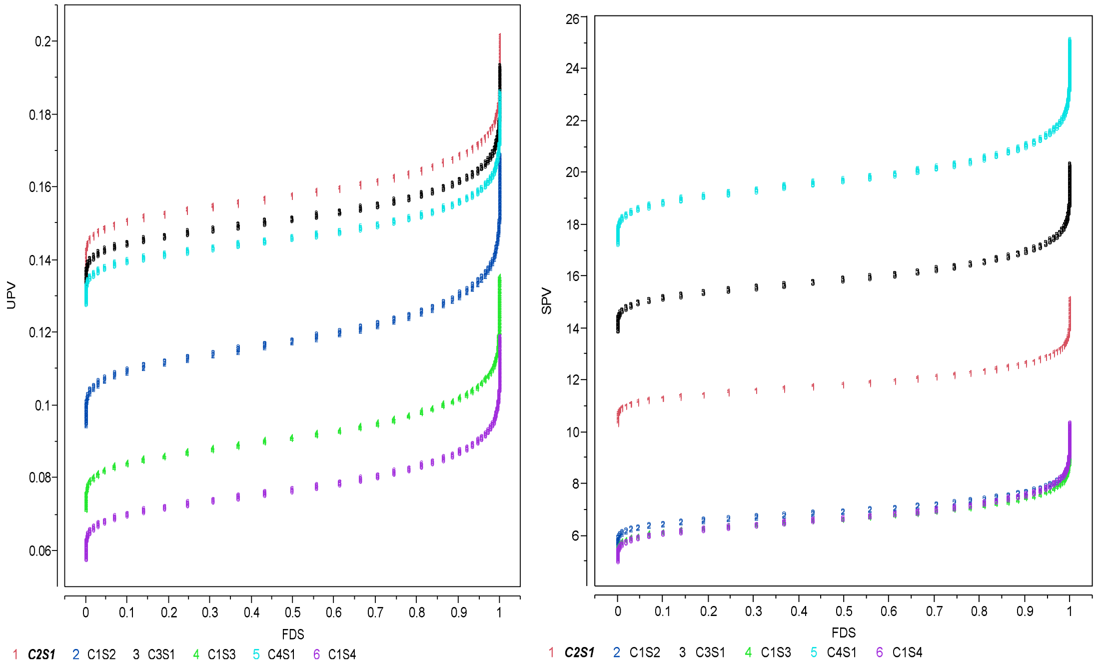
(a) (b)

Figure 4: (a) UPV and (b) SPV for the SCD for $k = 9$ Factors.



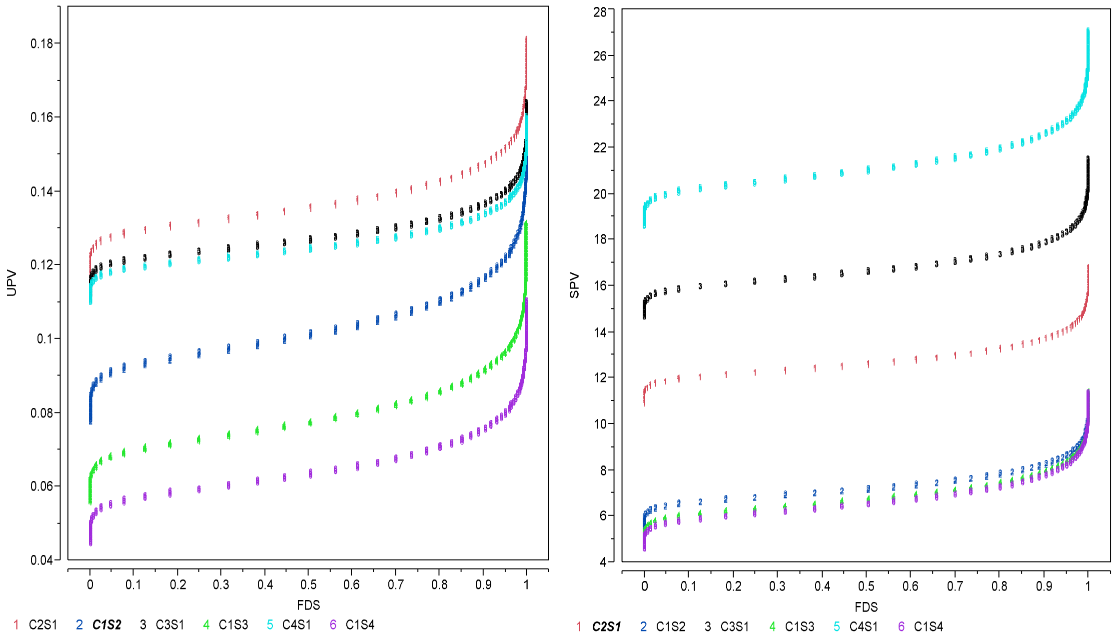
(a) (b)

Figure 5: (a) UPV and (b) SPV for the MinResV Designs for $k = 6$ Factors.



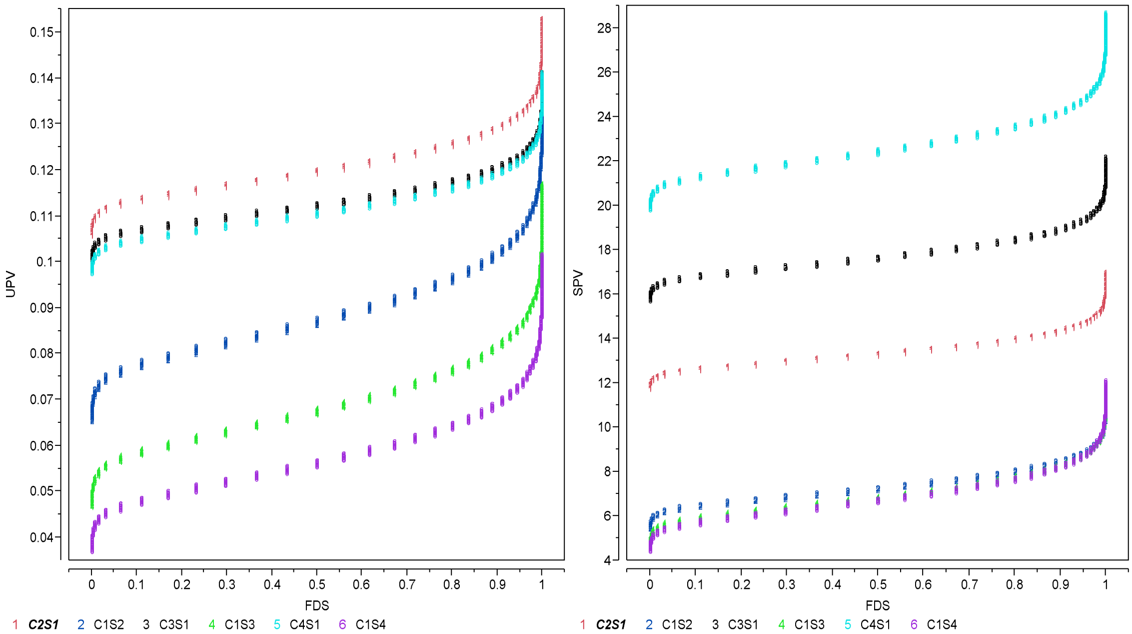
(a) (b)

Figure 6: (a) UPV and (b) SPV for the MinResV Designs for $k = 7$ Factors.



(a) (b)

Figure 7: (a) UPV and (b) SPV for the MinResV Designs for $k = 8$ Factors.



(a) (b)

Figure 8: (a) UPV and (b) SPV for the MinResV Designs for $k = 9$ Factors.