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Evaluation of Second-Order Response Designs with Errors in Factor Levels in the Cuboidal Region

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Abstract. Errors in factor levels often occur in response surface modeling. A design in which these errors have minimal effect is the desired design. This study evaluates the prediction capability of second-order Orthogonal Array Composite Design (OACD) and Orthogonal Uniform Composite Design (OUCD) with and without errors in factor levels for $3 \leq k \leq 5$ factors using 2, 3, and 5 center points in the cuboidal region. Design optimality criteria (in terms of G- and IV-optimality values) and quantile dispersion plots are used to examine the prediction capability of these designs. The results show that OUCD is the preferred design in terms of G-optimality, while IV-optimality and quantile plots indicate that OACD is the preferred design in both the presence and absence of errors in factor levels.

Keywords. Response surface designs, Errors in factor levels, Predictive variance, Design optimality criteria, Quantile dispersion plot.

MSC: 62-XX, 62Rxx, 62R10.

1 Introduction

The assumption in response surface modeling is that the experimental factors (independent variables) are measured without errors. However, in practice, it is often difficult to use a good experimental design due to challenges in setting the values of the factors

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specified by the design or controlling inherently random noise variables during the experimentation phase (Donev, 2000; Winker and Lin, 2011; Ardakani, 2016). According to Ardakani (2016), there are two types of errors that might occur in experimental settings: undiscovered noise factors that are not being assessed and noise factors that cannot be precisely set at the appropriate level. Errors in factor levels occur when factor levels can only be set to target values in the same way as in the experiment or when the error in determining factor levels differs from the error in the experiment (Donev, 2004; Winker and Lin, 2011; Myers et al., 2016). Draper and Beggs (1971) noted that errors can occur in one or more of the following ways: the true function η may be observed with error, the function $f(x_{1u}, x_{2u}, \ldots, x_{ku})$ may not be the correct model, and the observations on the independent variables may contain errors. The presence of errors in factor levels results in poor estimates of regression coefficients, increased variance of model coefficients, loss of efficiency and reduced prediction accuracy in designs, increased uncertainty in parameter estimates, and difficulty in discovering new phenomena. In some cases, the design's efficiency remains high even in the presence of these errors (Donev, 2004; He and Fang, 2011; Myers et al., 2016; Loken and Gelman, 2017; Fang et al., 2019; Wu et al., 2021).

The effects of errors in factor levels have been considered by several authors (Box, 1963; Draper and Beggs, 1971; Fedorov, 1974). These studies highlighted how such errors increase variance and bias in parameter estimates, which motivates the need for robust design strategies. Vuchkov and Boyadjieva (1983) introduced robustness criteria, while Donev (2000, 2004) proposed statistical frameworks to analyze the behavior of designs in the presence of factor uncertainty. Winker and Lin (2011); Ardakani et al. (2011) extended these ideas by exploring the robustness of uniform and second-order designs in various error structures. Fang et al. (2015, 2019); Wu et al. (2021); Didiugwu et al. (2025) compared various response surface designs in the presence of errors. These errors can often be ignored because their effects on important results are believed to be negligible or relatively small, but there is no clear guide for how small errors should be for this to be justified (Donev, 2000; Fang et al., 2019). Wu et al. (2021) stated that since these errors are not ignoreable in model fitting and optimization, it is important to assess the effects of these errors on design performance.

Orthogonal Array Composite Designs (OACDs) and Orthogonal Uniform Composite Designs (OUCDs) are efficient second-order response surface designs (RSDs) for fitting second-order models. These designs have appealing properties such as high efficiencies, good prediction variance capabilities, small run sizes, and uniformity (Zhang et al., 2020). Also, these designs allow users to perform multiple analyses with various parts of the data for cross-validation (Zhou and Xu, 2016). However, errors in factor levels can affect these properties. In response surface modeling, the primary interest lies more in predicting the response variable than in estimating parameters. Prediction variance criteria are important techniques for selecting RSDs because they provide crucial information about the worst-case prediction variance. Thus, examining the prediction capability of different designs when errors in factor levels occur can offer valuable insights for choosing suitable designs for practical use.

This work, therefore, seeks to evaluate the prediction capability (in terms of design optimality and graphical criteria) of OACDs and OUCDs in the cuboidal region, both with and without errors in factor levels. Here, the variability due to errors in factor levels is assumed to be known. The remaining part of this work is organized as follows. In Section 2, the second-order model with and without error, second-order RSDs, design optimality criteria (in terms of G- and IV-optimality), and graphical criterion (quantile dispersion plot (QDP)) are discussed. Prediction capability based on the G- and IV-optimality values and quantile dispersion plot are discussed in Sections 3 and 4, respectively. Section 5 presents the conclusion.

2 Methodology

2.1 Second-order Model with and without Error

The general linear model for fitting the relationship between the response variable Y and the independent variables $X = \{x_1, x_2, \ldots, x_k\}$ is expressed in matrix form as

$$Y = X\beta + \varepsilon, \tag{2.1}$$

where Y is an $(N \times 1)$ matrix of observations of the response, X is an $(N \times p)$ design matrix, β is a $(p \times 1)$ vector of p unknown parameters to be estimated, and ε is an $(N \times 1)$ vector of random response disturbances assumed to be normally distributed with mean 0 and constant variance $\sigma^2 I$, where I is the identity matrix. The number of parameters (p) to be estimated are $p = 2^{-1}(k+1)(k+2)$, where N and k are the number of design points and factors, respectively.

The predicted (fitted) response at any arbitrary point X is given by

$$\hat{Y}(X) = f(X)'\hat{\beta}, \tag{2.2}$$

where $f(X)$ is the appropriate expansion of X to accommodate the assumed model and $\hat{\beta} = (X'X)^{-1}X'Y$ is the ordinary least squares estimate of β.

The full standard second-order model without errors in factor levels is written in quadratic form as

$$Y(X) = \beta_0 + X'\beta + X'BX + \varepsilon, \tag{2.3}$$

where X is a point in the region of interest spanned by the design, β_0 is the intercept, and B is a $p \times p$ symmetric matrix whose diagonal elements are the unknown coefficients of the pure quadratic terms while the off-diagonal elements are the interaction (mixed quadratic) terms.

The predicted response surface model is given by

$$\hat{Y}(X) = \hat{\beta}_0 + X'\hat{\beta} + X'\hat{B}X. \tag{2.4}$$

The variance of the predicted response at any point X is

$$Var[\hat{Y}(X)] = \sigma^2 f(X)'(X'X)^{-1}f(X). \tag{2.5}$$

The scaled prediction variance $SPV(X)$ is defined as

$$SPV(X) = \ nf(X)'(X'X)f(X). \tag{2.6}$$

The general linear model with errors in its factor levels is given by

$$Y = Z\beta + \varepsilon_Y, \tag{2.7}$$

where Y and ε are as defined in (2.1), Z is an $(N \times p)$ true design matrix of those factors that are measured with error, and ε_Y is an $(N \times 1)$ vector of the factor errors on Y, assumed to be independently and normally distributed with mean zero and variance $\sigma_Y^2 I$.

The least squares estimate of β in (2.7) is

$$\hat{\beta} = (Z'Z)^{-1}Z'Y, \tag{2.8}$$

and the predicted response at any point X_0 is

$$\hat{Y}_Z(X_0) = X_0'\hat{\beta}_Z. \tag{2.9}$$

The standard second-order model with errors in factor levels is given by

$$Y(Z,X) = \beta_0 + X'\beta + X'BX + Z'\gamma + X'\Gamma Z + Z'\Delta Z + \varepsilon, \tag{2.10}$$

where Y is the $(N \times 1)$ response matrix, X is the $(p \times 1)$ vector for those factors measured without error, z is the $(m \times 1)$ vector for those factors measured with errors, β_0, β, and B are as defined in (2.3), γ is a vector of coefficients for the linear effects of the factors measured with errors, Γ is a $(p \times m)$ matrix containing the coefficients for the interaction effects between the factors measured with and without errors, Δ is an $(m \times m)$ symmetric matrix whose diagonal elements are the unknown coefficients of the pure quadratic terms while the off-diagonal elements are the interaction (mixed quadratic) terms for factors measured with errors, and ε is the $(N \times 1)$ random error vector assumed to be independent and normally distributed with mean 0 and variance σ_ε^2.

2.2 Second-order Response Surface Designs

The Orthogonal Array Composite Designs (OACDs) introduced by Xu et al. (2014) are types of second-order response surface design (RSD). They consist of three components: a 2-level factorial design with factor levels of $[-1, 1]$; a 3-level orthogonal array $\mathrm{OA}(n, s^k)$ with n runs, k factors, and s levels as the axial portion with levels of $x_i = -\alpha, 0,$ or α $(\alpha > 0)$; and center points where $x_i = 0$.

The Orthogonal Uniform Composite Designs (OUCDs) developed by Zhang et al. (2020) are another type of second-order RSD. OUCDs are noted for being nearly orthogonal, optimal, and space-filling. These designs also consist of three parts: a factorial portion with factor levels of $[-1, 1]$; a 3-level uniform design $\mathrm{UD}(n, s^k)$ as the axial portion with levels of $x_i = -\alpha, 0,$ or α $(\alpha > 0)$; and center points, where $x_i = 0$.

The factorial, axial, and center portions of the OACDs and OUCDs are denoted by n_f, n_α, and n_c, respectively. For a cuboidal region of interest, the axial portion has $\alpha = 1$.

Remark: The OACDs and OUCDs used in this work, as presented in Table 1, were obtained from (Xu et al., 2014; Zhang et al., 2020). The 2-level factorial designs shown in Table 1 were used for the factorial portion (either full or fractional), while the 3-level orthogonal arrays $\text{OA}(9, 3^4)$ and $\text{OA}(18, 3^5)$ formed the axial portion of the OACDs, and the 3-level uniform designs $\text{UD}(9, 3^4)$ and $\text{UD}(18, 3^5)$ comprised the axial portion of the OUCDs.

The total design points N in the OACDs and OUCDs is given by:

$$N = n_f + n_\alpha + n_c, \tag{2.11}$$

where n_f, n_α, and n_c denote the numbers of factorial, axial, and center points, respectively. For the purpose of this work, n_c, the number of center points, was set to 2, 3, and 5.

For example, a 19-run OACD and OUCD for $k = 3$ were obtained by using $n_f = 2^3$ (i.e., an 8-run factorial design) for the factorial portion, an axial portion, n_α, based on $\text{OA}(9, 3^3)$ with columns (1–3) or $\text{UD}(9, 3^3)$ for the 3-level designs when $\alpha = 1$, and $n_c = 2$ center points.

Table 1: 2- and 3-level portions used for OACDs and OUCDs

k	2-level factorial design	n_f	n_α	Generator	3-level OA / Column	3-level UD
3	2^3	8	9	–	$\text{OA}(9, 3^3)$ / (1–3)	$\text{UD}(9, 3^3)$
4	2^4	16	9	–	$\text{OA}(9, 3^4)$ / (1–4)	$\text{UD}(9, 3^4)$
5	$2_v^{(5-1)}$	16	18	E = ABCD	$\text{OA}(18, 3^5)$ / (2–6)	$\text{UD}(18, 3^5)$

2.3 Design Optimality Criteria

Design optimality criteria are used to evaluate and choose a response surface design (RSD) among competing RSDs on the basis of a single-valued criterion often referred to as alphabetic optimality criteria. The four most commonly used design optimality criteria are D-, A-, G-, and IV-optimality. These criteria are based on the information matrix $(X'X)$ of the RSD under consideration. D-optimality minimizes the determinant of the variance–covariance matrix of the parameter estimates, and A-optimality minimizes the trace of the inverse information matrix. The D- and A-optimality criteria are widely used for parameter estimation. G-optimality minimizes the worst-case prediction variance, while IV-optimality addresses the average prediction variance across the design region—both directly relevant to evaluating design robustness in prediction. The smaller the value of a single-valued optimality criterion, the better the design based on that criterion. Here, the G- and IV-optimality criteria that address the prediction variance performance of RSDs are considered.

G-optimality criterion: The G-optimality or global optimality criterion minimizes the maximum variance of any predicted value over the design region R (i.e., a design in which the maximum $SPV(X)$ in the region of interest is minimized). Minimizing the maximum variance ensures that predictions are uniformly reliable across the entire experimental region, avoiding areas with highly uncertain estimates. A G-optimal design ξ is defined as:

$$G_{\text{opt}} = \min_{\xi} \left(\max_{\mathbf{x} \in R} SPV(\mathbf{x}) \right) \tag{2.12}$$

IV-optimality criterion: The IV-optimality criterion minimizes the integrated or average prediction variance of the model over the design region R. The IV-optimal design criterion of a design ξ is given as:

$$IV_{\text{opt}} = \min_{\xi} \frac{1}{A} \int_{R} \text{Var}\left(\hat{Y}(\mathbf{x})\right) d\mathbf{x} \tag{2.13}$$

where A is the area (in general, the volume) of the design space.

2.4 Quantile Dispersion Plot (QDP)

Khuri et al. (1996) proposed the use of quantile dispersion plots due to the inability of the variance dispersion graph (VDG) to provide detailed information about the distribution of prediction variance. The quantile dispersion plot overcomes this challenge and enables information extraction regarding predictive capability throughout the region of interest.

Quantile dispersion plots are obtained from $q-1$ independent coordinates (δ_1, δ_2, …, δ_{q-1}) organized from a uniform distribution, where a large number of points are randomly selected on a sphere of radius r from a sample of 10,000. The scale prediction variances (SPV) are then evaluated for a given r at each selected point. The SPV values obtained at each point denoted by $R(r)$ are then plotted against q for $0 \leq q \leq 1$ at each selected point. The combined quantile dispersion plot is used for evaluating the prediction capability of two designs by superimposing the plots corresponding to each design for several values of r inside the R region. This provides a comprehensive visualization of the distribution of SPV values within R. Designs with flat and small SPV values are more desirable over $0 \leq q \leq 1$.

3 Prediction Capability Based on Design Optimality Criteria

The G- and IV-optimality values of OACD and OUCD with and without errors in the cuboidal region for $3 \leq k \leq 5$ factors using 2, 3, and 5 center points are presented in Table 2. The values of errors in factor levels are obtained by simulating 500 designs from an independent and normally distributed term error (ε), with mean zero and standard deviation $0.1 \leq \sigma_{\varepsilon} \leq 0.3$. The simulated values of the errors in factor levels are used to compute and obtain the G- and IV-optimality values of OACDs and OUCDs with errors.

In Table 2, the OACDs had the highest and least G-optimality values with and without errors at $k = 3$ and $k = 5$ factors respectively. The G-optimality values of OACDs with and without errors increased with an increase in number of factors. The

Table 2: G- and IV-optimality values of OACD and OUCD

Design	k	p	n_c	N	Gopt	Gεopt(0.1)	Gεopt(0.2)	Gεopt(0.3)	IVopt	IVεopt(0.1)	IVεopt(0.2)	IVεopt(0.3)
OACD	3	10	2	19	15.32	15.62	15.65	15.57	6.27	6.08	6.08	5.89
			3	20	16.05	16.43	16.44	14.85	6.20	6.00	6.00	5.80
			5	22	14.77	14.98	14.98	14.99	6.82	6.16	6.60	6.60
OUCD	3	10	2	19	13.25	13.57	13.60	13.59	8.17	8.17	8.36	8.17
			3	20	13.80	14.23	14.24	14.24	8.00	8.20	8.40	8.20
			5	22	13.29	15.58	15.59	15.59	7.92	9.02	9.24	9.02
OACD	4	15	2	27	23.36	25.16	23.47	25.17	10.58	9.89	9.98	9.90
			3	28	23.90	24.50	24.67	24.54	10.14	9.72	9.77	9.77
			5	30	19.32	19.91	19.92	19.92	9.87	9.73	9.75	9.73
OUCD	4	15	2	27	20.22	27.00	26.99	27.00	16.38	31.86	32.40	30.78
			3	28	20.77	28.00	28.00	28.00	16.26	31.36	31.92	30.24
			5	30	24.48	30.00	30.00	30.00	16.55	31.80	32.10	30.60
OACD	5	21	2	36	21.22	36.78	37.39	37.62	11.19	10.76	10.81	10.81
			3	37	29.99	35.51	35.85	38.69	10.82	10.59	10.63	10.63
			5	39	21.97	22.04	22.05	22.06	10.57	10.54	10.56	10.56
OUCD	5	21	2	36	28.31	28.38	28.36	28.33	11.19	10.73	10.77	10.84
			3	37	29.08	29.11	29.13	29.11	10.82	10.59	10.60	10.64
			5	39	30.63	30.67	30.67	30.67	10.57	10.54	10.55	10.57

G-optimality values of OUCDs with and without errors increased with an increase in the number of factors and center points respectively. The design had the least G-optimality values at $k = 3$ factors and the highest values at $k = 5$ factors for with and without errors. The OUCDs showed greater predictive capability than OACDs design in terms of G-optimality for with and without errors.

Also, the IV-optimality values for OACDs without errors and in the presence of errors had the least IV-optimality values at $k = 3$ factors and the highest values at $k = 5$ factors respectively. In the presence of errors, the IV-optimality values of OACDs decreased with an increase in center points and increased with the number of factors except for few fluctuations. The IV-optimality values of OUCDs had the highest values at $k = 4$ factors and the least values at $k = 3$ factors for with and without errors. The predictive capability of OACDs is higher under IV-optimality criterion for with and without error than OUCDs.

4 Prediction Capability Based on Graphical Evaluation

The combined quantile dispersion plots for OACDs and OUCDs at $3 \leq k \leq 5$ factors using 2, 3, and 5 center points respectively were plotted with radius $r = 0.1, 0.3, 0.5, 0.7, \ldots, \sqrt{k}$. Lines A1, A2, A3, and A4 represent OACDs with no error, 0.1 error, 0.2 error, and 0.3 error, respectively, while lines B1, B2, B3, and B4 represent OUCDs with no error, 0.1 error, 0.2 error, and 0.3 error, respectively.

Three Factors

From Figure 1, it was observed that OACD with 0.1 error had the smallest SPV values, followed closely by its 0.2 and 0.3 errors, exhibiting slight dispersion in SPV values as indicated by the flatness of the quantile dispersion plots across q at $r = 0.1$. As the

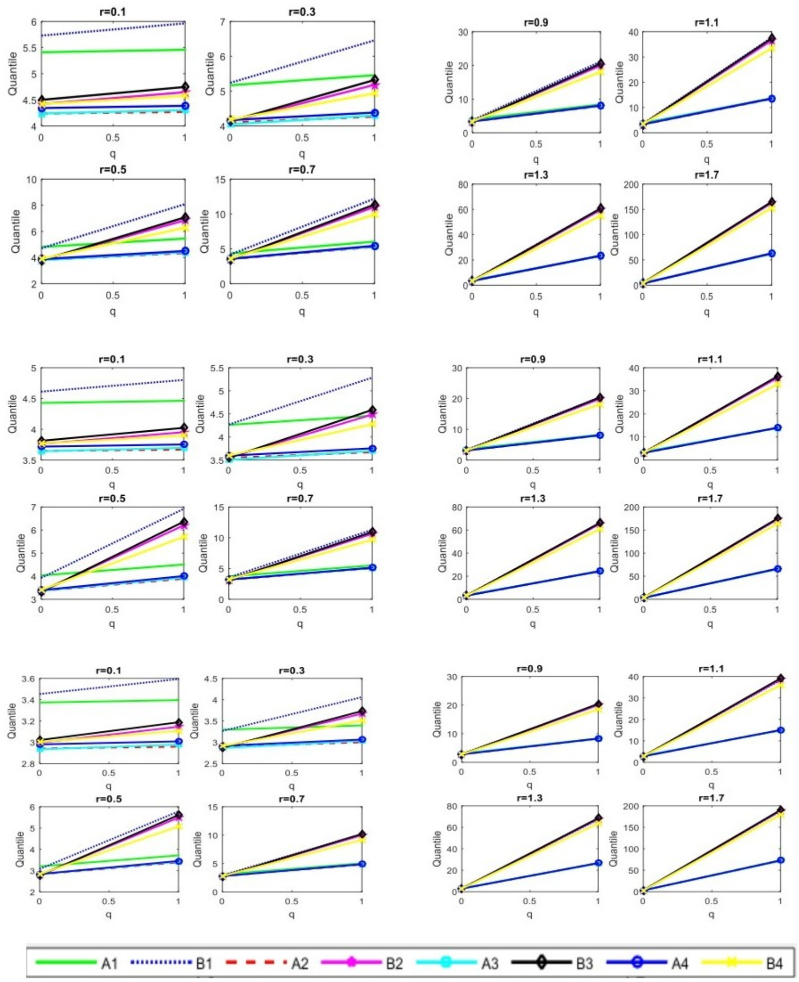

Figure 1: Combined quantile plots for $k = 3$ factors with 2, 3 and 5 center points respectively

radius increased from 0.5 to 0.9, the SPV values of OACD with no error reduced to levels comparable with its 0.1, 0.2, and 0.3 errors, while those of OUCD with no error reduced to match its 0.1 and 0.2 errors. At $r = 1.7$, the plot showed that OACD (with and without error) performed best, with smaller SPV values compared to OUCDs. With an increase in center points, a similar trend was observed, but the designs exhibited smaller SPV values and collapsed together at a faster rate. OACDs, both with and without errors, demonstrated superior predictive capability compared to OUCDs across 2, 3, and 5 center points.

Four Factors

The combined quantile dispersion plots in Figure 2, show that at $r = 0.1$, OACD with 0.1 and 0.3 errors exhibited the smallest SPV values, while OACD with no error had

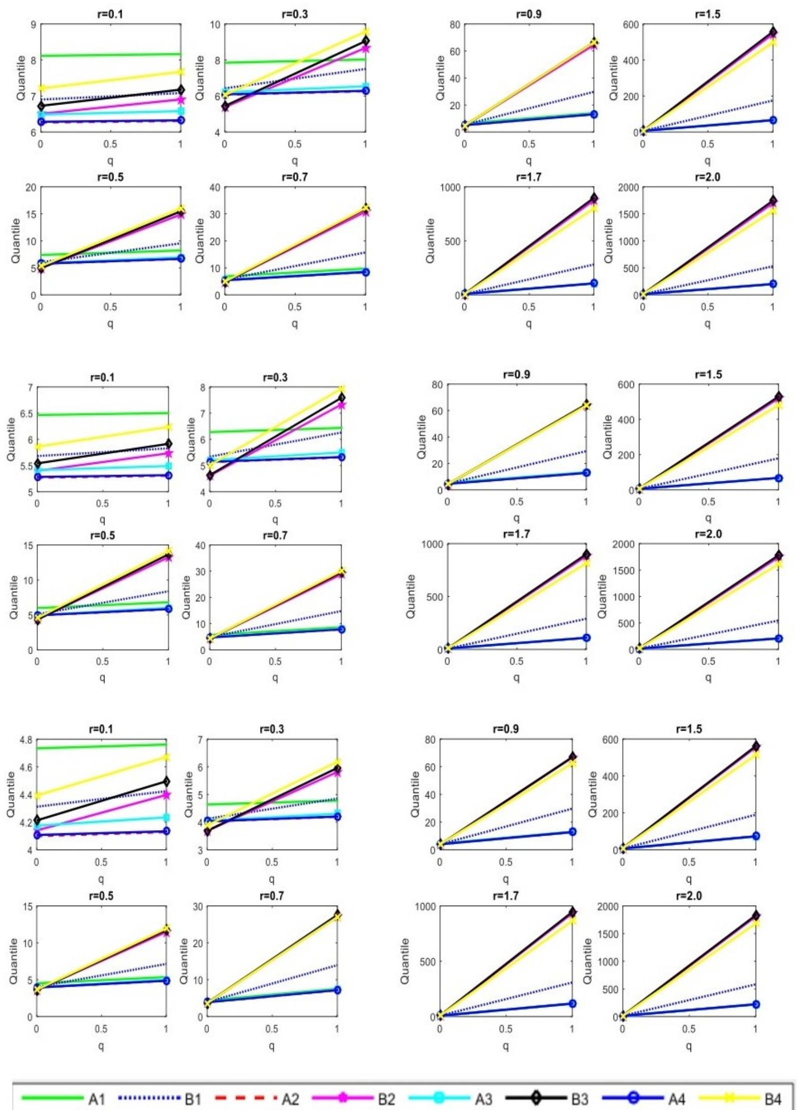

Figure 2: Combined quantile plots for $k = 4$ factors with 2, 3 and 5 center points respectively

the highest SPV value. Additionally, OUCD with 0.1 and 0.2 errors showed the smallest SPV values for $q < 0.2$ at $r = 0.3$. As the radius increased to 0.7 and 0.9, the SPV values of OACD with no error decreased to match those with errors, followed by OUCD with no error, and then OUCD with errors, respectively. At $r = 1.1, 1.3$, and 1.5, OACD (with and without error) collapsed together with the smallest SPV values, followed by OUCD with no error, and then OUCD with 0.3 error, with OUCD with 0.1 and 0.2 errors collapsing together. Similarly, at $r = 1.7$ to 2.0, OACD (with and without error) showed the smallest SPV values with slight dispersion, followed by OUCD with no error

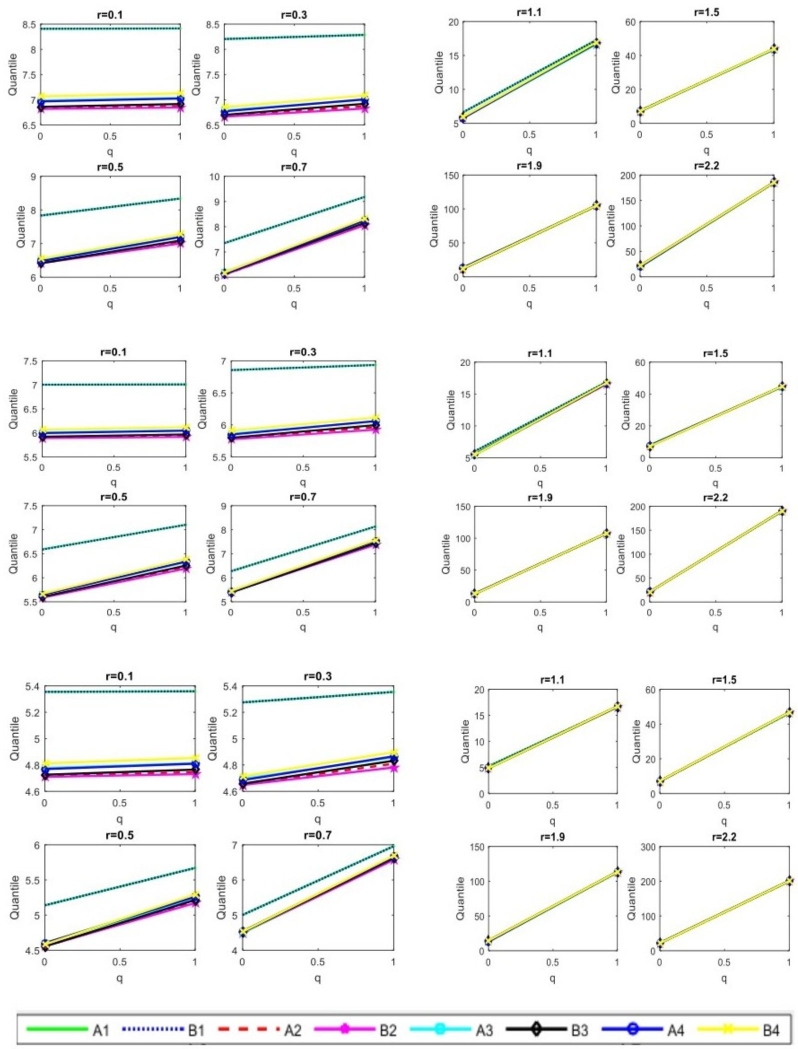

Figure 3: Combined quantile plots for $k = 5$ factors with 2, 3 and 5 center points respectively

with minor dispersion, and then OUCD with errors with higher dispersions. The same trends were observed with 3 and 5 center points, but with smaller SPV values as the number of center points increased. Generally, OACDs, both with and without errors, demonstrated better predictive capability compared to OUCDs with varying error levels (0.3, 0.1, and 0.2) respectively.

Five Factors

From Figure 3, at $r = 0.1$, OUCD with 0.1 error exhibited the smallest SPV values, followed by OACD with 0.1 error, OUCD with 0.2 error, OACD with 0.3 error, OACD with 0.2 error, and OUCD with 0.3 error, while both OACD and OUCD with no error collapsed together with high SPV values. All designs showed slight dispersion in their SPV values across varying q. As the radius increased from 0.3 - 0.9, the SPV values for each design reduced and began to converge. However, at larger radii ($r = 1.1$ to 2.2), all designs collapsed together with high dispersion, evident from the slope shape of the plot across varying q. Similar observations were made with 3 and 5 center points, where the designs exhibited smaller SPV values compared to those with 2 center points. Both OACDs and OUCDs showed comparable predictive capabilities.

5 Conclusion

In this work, the prediction capability of OACDs and OUCDs for $3 \leq k \leq 5$ factors using 2, 3, and 5 center points was examined with and without errors in factor levels. The G- and IV-optimality values, along with quantile dispersion plots, were obtained in the cuboidal region. It was observed that the presence of errors in the factor levels increases the G-optimality values and decreases the IV-optimality values for both designs. The G-optimality values for OACDs increased as the number of factors increased, while those for OUCDs increased with both the number of factors and the number of center points. In contrast, the IV-optimality values for both designs increased as the number of factors increased and decreased as the number of center points increased. The quantile dispersion plots showed that OACDs performed better than OUCDs at each center point. In general, the OUCDs achieved better G-optimality, indicating lower maximum prediction variance, while OACDs were preferred based on IV-optimality and quantile dispersion plots, reflecting better average prediction performance.

These findings offer practical guidance for selecting robust designs in applications where controlling factor levels is difficult, such as industrial experiments and process optimization. However, this work focuses on factor dimensions up to $k = 5$. As the number of factors increases, maintaining orthogonality and space-filling properties may become more difficult, and the efficiency of OACDs and OUCDs may decline. This dimensional limitation suggests that further investigation is needed for high-dimensional experimental spaces. Future research could extend this work by exploring higher-dimensional designs with more factors, assessing the impact of other types of error distributions, and comparing additional optimality criteria, such as D- and A-optimality, to better balance prediction accuracy and estimation precision.

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