Quantile Dispersion Graphs for Assessing the Prediction Capability of Third-Order Box-Behnken Designs

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The prediction capability of response surface models within a specified experimental region depends on the magnitude and behaviour of the scaled prediction variance (SPV). In this paper, quantile dispersion graphs (QDGs), boxplots and a prediction performance measure were used to assess the distribution, stability, and prediction capability of three third-order Box-Behnken designs: augmented Box-Behnken designs (ABBDs), augmented fractional Box-Behnken designs (AFBBDs), and new augmented Box-Behnken designs (NABBDs). The assessment was conducted for $3 \le k \le 6$ factors using $1 \le n_c \le 3$ centre points. The results show that AFBBDs consistently provide superior predictive capability, particularly at moderate and large radii, while ABBDs demonstrate greater stability near the design centre. NABBDs perform least well across most radii. Overall, AFBBDs are identified as the most efficient of the three designs for providing accurate third-order response surface predictions across the experimental region.

Keywords: Third-order response surface designs**,** Third-order model, Box-Behnken designs, Scaled prediction variance, Quantile dispersion graphs, Boxplots.

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1. Introduction

In response surface methodology (RSM), effective estimation of model parameters is achieved when appropriate experimental designs are used to collect data. These experimental designs are referred to as response surface designs (RSDs) (Montgomery, 2013). A response surface design (RSD) can be expressed as a design matrix D for k factors given in (1) with an $N \times k$ dimension, where N is the number of runs. The columns and rows of D show a factor and the value settings for a collection of factors corresponding to a run, respectively. A design point in a k-dimensional design space indicates each run.

$$D = \begin{bmatrix} x_{11} & x_{12} & \mathbf{K} & x_{1k} \\ x_{21} & x_{22} & \mathbf{K} & x_{2k} \\ x_{31} & x_{32} & \mathbf{K} & x_{3k} \\ \mathbf{M} & \mathbf{M} & \mathbf{L} & \mathbf{M} \\ x_{n1} & x_{n2} & \mathbf{K} & x_{Nk} \end{bmatrix} \tag{1}$$

To estimate the coefficients of the response surface model in (2), the design matrix D in (1) is expanded into the model matrix X, given in (3), where each column corresponds to a model coefficient, including the intercept.

$$\underline{\mathbf{Y}} = \mathbf{X}\underline{\boldsymbol{\beta}} + \underline{\boldsymbol{\varepsilon}} \tag{2}$$

where $\underline{\boldsymbol{Y}}$ is an $N \times 1$ vector, $\boldsymbol{X}$ is the $N \times p$ model matrix, $\underline{\boldsymbol{\beta}}$ is the $p \times 1$ vector of parameters, and $\underline{\boldsymbol{\varepsilon}}$ is the $N \times 1$ vector of random error.

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$$X = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} \\ 1 & x_{31} & x_{32} & \cdots & x_{3k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{Nk} \end{bmatrix} \tag{3}$$

The expansion of D into X depends on the order of the design; moreover, the choice of D is crucial in response surface investigation because the prediction variance depends on it (Khuri, 2017).
The Box-Behnken design (BBD) is considered one of the appropriate second-order RSDs for studying the effects of formulation variables (independent factors) and their interactions on responses (dependent variables) (Karmoker et al., 2019). Developed by Box and Behnken (1960), BBDs are regarded as more efficient than other second-order RSDs such as 3^k factorial designs, central composite designs (CCDs), and Doehlert designs, despite their poorer coverage of the corners of non-linear design spaces (Ferreira et al., 2007; Marasini et al., 2012).

BBDs that are rotatable (or nearly rotatable), require three levels for each factor, and ensure that all design points fall within a safe operating zone. They require fewer runs than 3^k factorial designs and CCDs and allow efficient estimation of first- and second-order coefficients while ensuring no factor is set simultaneously at its high level. However, the second-order representation can become inadequate when third-order terms exist in the true response surface. In such cases, BBDs have limited ability to estimate these third-order terms (Arshad et al., 2018). To address this limitation, augmented Box-Behnken designs (ABBDs) (Arshad et al., 2012), augmented fractional Box-Behnken designs (AFBBDs) (Rashid et al., 2017), and new augmented Box-Behnken designs (NABBDs) (Arshad et al., 2018) were proposed. These designs allow estimation of third-order model parameters and are commonly used to build predictive models, making prediction variance a critical metric for comparing designs.

Myers and Montgomery (2002) noted that a common approach for comparing designs involves alphabetical optimality criteria (D-, A-, G-, or V-optimality), which summarise key optimality characteristics. Additional criteria include pure error estimation, lack-of-fit assessment, design size, and prediction variance behaviour. Park et al. (2005) and Myers et al. (2016) emphasised selecting designs based on the stability of prediction variance (PV) over the experimental region. Stability corresponds to a small difference between the maximum and minimum PV values. PV represents the error associated with predicting a response $\hat{y}(x)$ at a point x using the fitted model and reflects prediction quality especially when design size is not the primary concern (Montgomery, 2013; Myers et al., 2016; Fang et al., 2019). The G-optimality criterion compares designs by minimising the maximum PV. Alternatively, average PV may be computed by summing the variances over the entire design space and dividing by the region's area or volume (Myers et al., 2016). Generally, the maximum and minimum PVs indicate the spread of prediction variances across the design space (Khuri & Mukhopadhyay, 2010).

Several authors, including Myers et al. (1992), Borkowski (2003), Park et al. (2005), Liang et al. (2006), Li et al. (2009), Jang et al. (2012), Ukaegbu and Chigbu (2015), Yankam and Oladugba (2021), and Oladugba et al. (2024) have examined the prediction variance capability of RSDs. They noted that single-valued criteria such as D-, G-, and I-optimality compress high-dimensional information into a single value and thus do not fully represent the distribution of PV across the experimental region.

Therefore, graphical methods such as contour plots, variance dispersion graphs (Giovannitti-Jensen & Myers, 1989), fraction of design space (FDS) plots (Zahran et al., 2003), and three-dimensional VDGs (Goldfarb et al., 2004) have been developed. However, these methods do not describe the full distribution of PV on a hypersphere; they only provide information about the centre and the extremes (Jang et al., 2012). To overcome this limitation, Khuri et al. (1996) introduced quantile dispersion graphs (QDGs), which use PV quantiles at each radius to characterise the distribution of prediction variances within concentric spheres. In addition to QDGs, boxplots are employed as a supplementary graphical tool to provide a simple descriptive summary of the prediction variance distribution at each radius. Despite extensive work on second-order designs, no study in the available literature has examined the prediction capability of third-order Box-Behnken designs using QDGs.

In this paper, the prediction capability of third-order Box-Behnken designs, specifically ABBDs, AFBBDs, and NABBDs, is evaluated to determine how well these designs perform throughout the experimental region. The prediction capability of these designs is evaluated using the QDGs, boxplots, and numerical prediction performance measures for $3 \leq k \leq 6$ factors using $1 \leq n_c \leq 3$ centre points in the spherical region. The assessment is based on scaled prediction variance summaries, variance of prediction, integrated prediction variance, and *D*- and *G*-efficiency values.
The remainder of this paper is organised as follows: Section 2 presents the methodology, including the construction of the designs and computational procedures. Section 3 presents and discusses the results. Section 4 concludes the study.

2. Methodology

This section presents the designs considered for comparison, the third-order response surface model, the scaled prediction variance (*SPV*), and the procedures used to construct QDGs.

2.1 Designs Considered for Comparison

The study evaluates the prediction capability of three third-order Box-Behnken designs: the augmented Box-Behnken designs (ABBDs) of Arshad et al. (2012), the augmented fractional Box-Behnken designs (AFBBDs) of Rashid et al. (2017), and the new augmented Box-Behnken designs (NABBDs) of Arshad et al. (2018). These designs were examined for $3 \leq k \leq 6$ factors, each with $1 \leq n_c \leq 3$ centre points. The number of design points for each case is presented in Table 1. It should be noted that NABBDs do not exist for $k = 3$. A typical design matrix for the three design classes is shown in Figure 1.

Augmented Box-Behnken Designs (ABBDs)

ABBDs (Arshad et al., 2012) are constructed by augmenting a classical second-order BBD with additional factorial, axial, and complementary points to allow estimation of third-order model coefficients. For k factors: Factorial points are generated at levels $\{-a, 0, a\}$, Axial points lie at $(0, \ldots, \pm a, \ldots, 0)$, and Complementary points are added to increase the estimability of cubic terms. Thus, an ABBD consists of: the base BBD core, added factorial points, added axial points, and complementary points.

Augmented Fractional Box-Behnken Designs (AFBBDs)

AFBBDs (Rashid et al., 2017) reduce the number of added factorial points by using fractional factorial designs rather than full factorial designs. This reduction preserves estimability of third-order terms while significantly decreasing the number of additional experimental runs. Consequently, AFBBDs are more cost-efficient and time-efficient than ABBDs while maintaining strong model-fitting capability.

New Augmented Box-Behnken Designs (NABBDs)

NABBDs (Arshad et al., 2018) were proposed to further reduce the number of augmented points required to estimate third-order terms. NABBDs achieve smaller run sizes and better geometric distribution of points compared to ABBDs and AFBBDs, especially for higher-factor designs. Their construction uses a strategic combination of: fractional factorial augmentation, minimal complementary points, and improved axial-point placement.

2.2 Third-Order Response Surface Model

For *k* factors, the third-order response surface model used in this paper is:

$$y = \beta_0 + \sum_{i=1}^{k} \beta_1 x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i=1}^{k} \beta_{iii} x_i^3 + \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} \beta_{ij} x_i x_j + \varepsilon \qquad (4)$$

where *y* is the response variable, x_i's are the explanatory variables, β_i's are model coefficients, *k* represents the number of factors, and ε is a random error. The matrix form of (4) is given in (2). Using (2), the least squares estimator of $\underline{\beta}$ in (2) is given by

$$\hat{\underline{\beta}} = (X^T X)^{-1} X^T Y \qquad (5)$$

and the predicted response denoted by $\hat{\underline{Y}}$ is expressed as

$$\hat{\underline{Y}} = \underline{X}\hat{\underline{\beta}} \qquad (6)$$

2.3 Prediction Variance and Scaled Prediction Variance

The prediction variance (*PV*) of the estimated response $\hat{y}(x)$ at point *x* is:

$$PV(x) = Var(\hat{y}(x)) = \sigma^2 f^T(x)(X^T X)^{-1} f(x) \qquad (7)$$

where $(X^T X)$ and $(X^T X)^{-1}$ denote the information matrix and its inverse, respectively; *f(x)* is the general form of the $1\times p$ model vector at point *x*; and σ^2 is the variance.

The scaled prediction variance (*SPV*) at any point *x* in the region of interest was computed using

$$SPV(x) = Nf^T(x)(X^T X)^{-1} f(x) \qquad (8)$$

SPV was used to eliminate the influence of error variance and permit fair comparison across designs of different sizes. Lower *SPV* values indicate better predictive capability.

2.4 Quantile Dispersion Graphs (QDGs)

Quantile Dispersion Graphs (QDGs), introduced by Khuri et al. (1996), were developed to overcome the limitations of Variance Dispersion Graphs (VDGs) in displaying detailed information on the distribution of prediction variance in response surface designs. QDGs provide a graphical summary of the distribution of the *SPV* throughout the experimental region and facilitate comparisons among competing designs. The prediction performance of the competing designs was examined over concentric hyperspheres of radius *r* centred at the origin. The maximum radius considered varies with the dimensionality of the spherical region. Consequently, radii were selected proportionally to the design-space dimension so that comparable relative locations (near the centre, intermediate region, and near the boundary) could be examined for each value of *k*. This allows a fair comparison of prediction variance behaviour across designs with different numbers of factors.

For a given radius *r*, points were generated uniformly on the surface of the hypersphere. Following Khuri et al. (1996), a vector $\mathbf{z} = (z_1, z_2, ..., z_k)^T$ was generated from a multivariate standard normal distribution. The sampled point was then obtained as $x = r\,(z / ||z||)$, where $||z|| = (z_1^2 + z_2^2 + ... + z_k^2)^{1/2}$.

This procedure ensures that the generated points are uniformly distributed on the surface of the hypersphere of radius r. For each selected radius, *SPV* values were computed at a large number of randomly generated points. Let $F_r(v)$ denote the cumulative distribution function of the *SPV* values computed at a fixed radius r. The corresponding quantile function is defined as $Q_r(p) = \inf\{v : F_r(v) \geq p\}$, $0 < p < 1$, where $Q_r(p)$ represents the p^{th} quantile of the *SPV* distribution at radius r. The QDG is obtained by plotting $Q_r(p)$ against the quantile level p for selected radii. QDGs provide a graphical summary of the distribution and variability of prediction variance throughout the experimental region and facilitate comparisons among competing response surface designs.

Procedure for Constructing QDGs

For each design, QDGs were generated using the following steps:

1. Generate points on a sphere: Randomly generate a large number of points (10,000 in this study) uniformly on the surface of the sphere $P(r)$ using the normalisation procedure described above.
2. Compute *SPV* at each point: For each sampled point, compute the corresponding scaled prediction variance $SPV(x)$.
3. Obtain the distribution of *SPV*: For each radius r, compute the empirical distribution of *SPV* values, denoted by $R(r)$.
4. Compute quantiles: For each r, compute the p^{th} quantile, $Q_r(p)$, for $0 \leq p \leq 1$.
5. Plot QDGs: Plot $Q_r(p)$ against p for each selected value of r. A combined QDG is created by superimposing the quantile curves of the three competing designs, enabling comparison of prediction performance throughout the design region.

Remark 1: A lower quantile curve corresponds to better predictive capability at that region of the experimental space. When the quantile curves of one design lie consistently below those of another, it indicates uniformly superior prediction accuracy across the design region.

In addition to the QDGs, side-by-side boxplots were constructed to provide a descriptive summary of the SPV distributions at the selected radii. The boxplots display the median, interquartile range (IQR), overall range, whiskers, and extreme *SPV* values for each design and radius. The median represents the central tendency of the distribution, while the IQR and overall range provide measures of variability and stability in the *SPV* values. The whiskers indicate the minimum and maximum *SPV* values, and any isolated points represent extreme observations.

Consequently, the boxplots provide information on the centre, spread, skewness, and variability of the *SPV* distributions and facilitate visual comparisons of prediction stability among the competing designs. By complementing the QDGs, the boxplots highlight features such as skewness, variability, and outliers that may not be readily apparent from the quantile curves alone. Collectively, the QDGs and boxplots provide a comprehensive graphical assessment of prediction accuracy and stability throughout the experimental region.

Furthermore, numerical prediction performance measures were computed for each design. These measures include the minimum, maximum, and average scaled prediction variances, selected *SPV* quantiles, variance of prediction (*VP*), integrated prediction variance (*IPV*), D- and G-efficiency values. These measures provide additional information on prediction accuracy, stability, and overall design efficiency.

Remark 2: All computations, including generating hyperspherical points, computing *SPV* values, and constructing QDGs and boxplots, were performed using the MATLAB software.

Table 1: Designs Considered for Comparison

k	Design	n_b	n_f	n_α	α	N
3	ABBD	12	8	6	1.73	$26 + n_c$
	AFBBD	6	8	6	1.73	$20 + n_c$
	NABBD	-	-	-	-	-
4	ABBD	24	16	8	2.00	$48 + n_c$
	AFBBD	18	16	8	2.00	$42 + n_c$
	NABBD	24	32	8	2.00	$64 + n_c$
5	ABBD	40	32	10	2.24	$82 + n_c$
	AFBBD	20	32	10	2.24	$62 + n_c$
	NABBD	40	80	10	2.24	$130 + n_c$
6	ABBD	$48 + n_b$ (48)	64	12	2.45	$172 + n_c$
	AFBBD	$24 + n_b$ (24)	64	12	2.45	$124 + n_c$
	NABBD	48	112	12	2.45	$172 + n_c$

3. Evaluation of Designs' Prediction Capability

This section presents the evaluation of the prediction capabilities of the three third-order Box-Behnken designs: ABBDs, AFBBDs, and NABBDs. The assessment is based on both graphical and numerical measures. The graphical evaluation employs QDGs and boxplots to examine the distribution, variability, and stability of the *SPV* throughout the experimental region. The numerical evaluation is based on *SPV* summary measures, prediction variance statistics, and *D*- and *G*-efficiency values. The analyses were conducted for selected radii within the spherical design region for $3 \leq k \leq 6$ factors and $1 \leq n_c \leq 3$ centre points. Sections 3.1-3.4 present the graphical assessment according to the number of factors, while Section 3.5 provides a numerical comparison of the competing designs.

The graphical summaries obtained from the QDGs and boxplots are presented in Figures 2-17. QDGs provide information about the distribution of *SPV* across quantiles, while boxplots summarise the spread and variability of *SPV* values at each radius. Collectively, these graphical tools provide insight into the stability, variability, and overall predictive capability of the competing designs.

3.1 Three-Factor Designs (k = 3)

Figures 2-4 and 14 show the QDGs and boxplots for $k = 3$. For small radii (e.g., $r = 0.1, 0.5$), both the QDGs and boxplots show that ABBDs tend to exhibit slightly smaller *SPV* quantiles than AFBBDs, indicating better prediction capability near the centre of the design region. The QDG curves for ABBDs are relatively flat, indicating greater stability. As r increases toward the perimeter (e.g., $r = 1.1, 1.7$), AFBBDs begin to outperform ABBDs, with smaller *SPV* quantiles at larger values of p. This pattern becomes more evident as the number of centre points increases. The boxplots confirm that both designs are stable at small radii, but AFBBDs show improved prediction capability at larger radii. Overall, for $k = 3$, ABBDs perform better near the centre, whereas AFBBDs outperform ABBDs at larger radii.

3.2 Four-Factor Designs (k = 4)

Figures 5-7 and 15 display the QDGs and boxplots for $k = 4$. At small radii ($r = 0.1$), QDGs show that ABBD and NABBD have nearly identical *SPV* distributions, and both are slightly more stable than AFBBD. However, as the radius increases ($r = 0.7, 1.3$), AFBBD begins to exhibit smaller *SPV* values, particularly at the lower quantiles of the distribution. The boxplots similarly show that AFBBD becomes more competitive as r increases. At the design boundary ($r = 2.0$), ABBD and AFBBD show closer *SPV* values, and both outperform NABBD. Increasing centre points strengthens the performance of ABBD and AFBBD, but the overall advantage at higher radii still lies with AFBBD. For k = 4, AFBBD generally has superior prediction capability at moderate to large radii, while ABBD and NABBD are more stable at small radii.

3.3 Five-Factor Designs (k = 5)

Figures 8-10 and 16 display QDGs and boxplots for k = 5. The QDGs and boxplots show that all three designs display comparable stability at small radii (r = 0.1). At this radius, AFBBD has slightly smaller *SPV* quantiles, followed by ABBD and then NABBD. As the radius increases (e.g., r = 0.9), ABBD becomes the most stable design, with AFBBD and ABBD overlapping for a large portion of the distribution. At higher radii (r = 1.5, 2.2), AFBBD begins to perform slightly better than ABBD, with both designs outperforming NABBD. The boxplots confirm these observations, showing narrower spreads for AFBBD at larger radii. As centre points increase, the performance of AFBBD improves and becomes consistently better than ABBD and NABBD across most radii. Overall, for k = 5, AFBBD shows the best performance, particularly at moderate and large radii.

3.4 Six-Factor Designs (k = 6)

Figures 11-13 and 17 present QDGs and boxplots for k = 6. The QDGs indicate that at small radii (r = 0.1), ABBD and AFBBD are stable and outperform NABBD. At (r = 0.9), ABBD and AFBBD overlap at small quantiles but separate at larger quantiles. At intermediate radii (r = 1.9), both designs continue to outperform NABBD. At the design boundary (r = 2.4), AFBBD becomes clearly superior to ABBD and NABBD. Increasing the number of centre points reduces the gap between ABBD and AFBBD at small radii, but at higher radii, AFBBD consistently has better performance. Boxplots confirm that AFBBD demonstrates lower median and interquartile *SPV* values at large radii. Overall, for k = 6, AFBBD exhibits the best prediction capability, followed by ABBD, while NABBD performs worst.

3.5 Numerical Comparison of Prediction Performance and Efficiency Measures

Tables 2-5 present a numerical comparison of the competing designs using the maximum, minimum, and average *SPV*, selected *SPV* quantiles, variance of prediction (*VP*), integrated prediction variance (*IPV*), and *D*- and *G*-efficiency values. These numerical measures complement the graphical assessment provided by the QDGs and boxplots and provide a basis for comparing prediction accuracy, stability, and overall design efficiency.

From Tables 2-5, AFBBDs generally exhibit the highest *D*- and *G*-efficiency values together with lower average and maximum *SPV* values, indicating superior prediction performance across the experimental region. ABBDs perform competitively and, in several cases, display greater prediction stability, particularly near the design centre; however, they generally exhibit larger prediction variances than AFBBDs. NABBDs consistently show the poorest performance, characterised by larger SPV values and lower efficiency measures. As the number of factors increases, prediction variance tends to increase, and efficiency decreases for all designs. Nevertheless, AFBBDs experience the least deterioration in performance and maintain superior predictive properties across most radii and centre-point configurations.

Table 2: Prediction Performance Metrics and Efficiency Ratios for Three-Factor Designs (k = 3)

n_c	r	Design	SPV_{max}	SPV_{min}	SPV_{avg}	SPV_{25Q}	SPV_{50Q}	SPV_{75Q}	VP	IPV	D_{Eff}	G_{Eff}
1	0.1	ABBD	6.0505	6.0502	6.0504	6.0503	6.0504	6.0505	0.0003	6.0504	58.0785	59.0672
		AFBBD	15.2062	14.2341	14.7207	14.4800	14.7242	14.9646	0.9722	14.7207	65.0095	79.0751
	0.5	ABBD	6.2725	6.0799	6.1944	6.1581	6.2068	6.2320	0.1926	6.1944	58.0785	59.0672
		AFBBD	15.7509	11.3545	13.4590	12.3111	13.4119	14.5886	4.3964	13.4590	65.0095	79.0751
	1.1	ABBD	7.6036	5.2360	6.5358	6.0929	6.6392	6.9718	2.3675	6.5358	58.0785	59.0672
		AFBBD	13.7752	5.9449	9.3458	7.4400	9.0329	11.0603	7.8304	9.3458	65.0095	79.0751
	1.7	ABBD	22.0083	12.6056	15.6861	13.9102	14.7139	17.2676	9.4027	15.6861	58.0785	59.0672
		AFBBD	16.4571	9.3830	13.0439	11.4519	13.1680	14.6736	7.0741	13.0439	65.0095	79.0751
2	0.1	ABBD	9.4213	9.4210	9.4212	9.4211	9.4212	9.4213	0.0003	9.4212	59.8078	63.1780
		AFBBD	9.3749	8.7763	9.0760	8.9276	9.0783	9.2264	0.5985	9.0760	64.6494	75.4857
	0.5	ABBD	8.9703	8.7905	8.8973	8.8634	8.9090	8.9325	0.1798	8.8973	59.8078	63.1780
		AFBBD	10.2279	7.4282	8.7777	8.0387	8.7448	9.5101	2.7997	8.7777	64.6494	75.4857
	1.1	ABBD	8.2098	6.0002	7.2133	6.8000	7.3098	7.6202	2.2097	7.2133	59.8078	63.1780
		AFBBD	11.2783	4.7816	7.6536	6.2627	7.4407	8.9987	6.4966	7.6536	64.6494	75.4857
	1.7	ABBD	20.5763	11.8005	14.6756	13.0180	13.7682	16.1516	8.7758	14.6756	59.8078	63.1780
		AFBBD	17.2399	9.7741	13.6213	11.9461	13.7665	15.3368	7.4658	13.6213	64.6494	75.4857
3	0.1	ABBD	7.3105	7.3101	7.3103	7.3103	7.3103	7.3104	0.0003	7.3103	59.0508	61.0649
		AFBBD	6.9651	6.5098	6.7318	6.6218	6.7335	6.8433	0.4433	6.7318	63.5047	72.2044
	0.5	ABBD	7.2701	7.0839	7.1946	7.1595	7.2066	7.2310	0.1862	7.1946	59.0508	61.0649
		AFBBD	7.9691	5.8194	6.8645	6.2940	6.8355	7.4337	2.1497	6.8645	63.5047	72.2044
	1.1	ABBD	7.7812	5.4926	6.7491	6.3210	6.8490	7.1705	2.2886	6.7491	59.0508	61.0649
		AFBBD	10.2883	4.3658	7.0730	5.8639	6.8803	8.2762	6.0637	7.0730	63.5047	72.2044
	1.7	ABBD	21.2883	12.1991	15.1769	13.4601	14.2370	16.7056	9.0892	15.1769	59.0508	61.0649
		AFBBD	18.0231	10.1942	14.2215	12.4650	14.3780	16.0154	7.8289	14.2215	63.5047	72.2044

Table 3: Prediction Performance Metrics and Efficiency Ratios for Four-Factor Designs (k = 4)

n_c	r	Design	SPV_{max}	SPV_{min}	SPV_{avg}	SPV_{25Q}	SPV_{50Q}	SPV_{75Q}	VP	IPV	D_{Eff}	G_{Eff}
1	0.1	ABBD	8.4356	8.4354	8.4355	8.4355	8.4355	8.4356	0.0002	8.3455	65.9031	46.1626
		AFBBD	9.6172	9.1957	9.4014	9.3151	9.4012	9.4863	0.4215	9.4014	70.2238	51.4355
		NABBD	14.4925	14.4285	14.4449	14.4449	14.4393	14.4550	0.0640	14.4449	43.5195	21.6705
	0.7	ABBD	8.0808	7.6534	7.9325	7.8829	7.9493	8.0012	0.4274	7.9325	65.9031	46.1626
		AFBBD	10.3485	7.5464	8.7063	8.1210	8.6258	9.2214	2.8021	8.7063	70.2238	51.4355
		NABBD	14.2835	11.4494	12.8152	11.8844	12.6942	13.7529	2.8342	12.8152	43.5195	21.6705
	1.3	ABBD	9.5572	7.2787	8.5342	8.2032	8.5732	8.9193	2.2785	8.5342	65.9031	46.1626
		AFBBD	12.1610	6.6114	8.7828	7.9089	8.4637	9.5975	5.5496	8.7828	70.2238	51.4355
		NABBD	22.9448	7.8783	15.4987	10.2043	15.6056	20.7470	15.0664	15.4987	43.5195	21.6705
	2.0	ABBD	41.1077	22.5105	26.0429	23.3182	24.2515	27.5192	18.5872	26.0429	65.9031	46.1626
		AFBBD	36.8323	20.0866	24.1596	21.5842	23.1886	25.5016	16.7457	24.1596	70.2238	51.4355
		NABBD	87.6214	19.1795	59.5535	41.4362	61.5826	79.8203	68.4418	59.5535	43.5195	21.6705
2	0.1	ABBD	7.3476	7.3474	7.3475	7.3475	7.3475	7.3476	0.0002	7.3475	65.1280	45.2940
		AFBBD	8.0799	7.7259	7.8984	7.8259	7.8983	8.0799	0.3540	7.8984	69.3469	50.3137
		NABBD	12.0521	11.9861	12.0029	11.9887	11.9972	12.0521	0.0660	12.0029	43.3166	21.4487
	0.7	ABBD	7.3233	6.8871	7.1720	7.1214	7.1891	7.2421	0.4361	7.1720	65.1280	45.2940
		AFBBD	9.0574	6.6056	7.6288	7.1246	7.5562	8.0720	2.4518	7.6288	69.3469	50.3137
		NABBD	12.6748	9.7657	11.1634	10.2092	11.0367	12.1221	2.9092	11.1634	43.3166	21.4487
	1.3	ABBD	9.4441	7.1191	8.4002	8.0625	8.4400	8.7932	2.3250	8.4002	65.1280	45.2940
		AFBBD	11.6967	6.4105	8.5214	7.7172	8.2319	9.2830	5.2863	8.5214	69.3469	50.3137
		NABBD	22.8568	7.5202	15.2764	9.8848	15.3986	20.6179	15.3366	15.2764	43.3166	21.4487
	2.0	ABBD	41.8959	22.9192	26.5237	23.7433	24.6957	28.0301	18.9767	26.5237	65.1280	45.2940
		AFBBD	37.6513	20.5056	24.6712	22.0133	23.6981	26.0468	17.1458	24.6712	69.3469	50.3137
		NABBD	88.5256	19.1145	60.0690	41.7072	62.1166	80.6208	69.4110	60.0690	43.3166	21.4487
3	0.1	ABBD	6.5388	6.5386	6.5387	6.5387	6.5387	6.5387	0.0002	6.5387	64.3137	44.4459
		AFBBD	7.0111	6.7041	6.8535	6.7906	6.8533	6.9153	0.3070	6.8535	68.3981	49.2278
		NABBD	10.3648	10.2970	10.3143	10.2997	10.3084	10.3250	0.0678	10.3143	43.0478	21.2017
	0.7	ABBD	6.7701	6.3253	6.6158	6.5642	6.6333	6.6873	0.4449	6.6158	64.3137	44.4459
		AFBBD	8.1739	5.9595	6.8918	6.4439	6.8206	7.2840	2.2144	6.8918	68.3981	49.2278
		NABBD	11.5831	8.6079	10.0344	9.0593	9.9031	11.0122	2.9753	10.0344	43.0478	21.2017
	1.3	ABBD	9.3993	7.0278	8.3345	7.9900	8.3751	8.7354	2.3715	8.3345	64.3137	44.4459
		AFBBD	11.4359	6.3000	8.3839	7.6236	8.1189	9.1135	5.1358	8.3839	68.3981	49.2278
		NABBD	22.8940	7.2975	15.1845	9.7000	15.3037	20.6169	15.5963	15.1845	43.0478	21.2017
	2.0	ABBD	42.6953	23.3391	27.0157	24.1797	25.1512	28.5522	19.3563	27.0157	64.3137	44.4459
		AFBBD	38.4804	20.9373	25.1961	22.4556	24.2087	26.6115	17.5430	25.1961	68.3981	49.2278

		NABBD	89.5552	19.1513	60.6978	42.0818	62.7751	81.5358	70.4039	60.6978	43.0478	21.2017

Table 4: Prediction Performance Metrics and Efficiency Ratios for Five-Factor Designs (*k* = 5)

n_c	r	Design	SPV_{max}	SPV_{min}	SPV_{avg}	SPV_{25Q}	SPV_{50Q}	SPV_{75Q}	VP	IPV	D_{Eff}	G_{Eff}
1	0.1	ABBD	6.1528	6.1527	6.1528	6.1528	6.1528	6.1528	0.0002	6.1528	68.8005	42.0125
		AFBBD	9.6885	8.9766	9.3302	9.2043	9.3298	9.4532	0.7119	9.3302	81.6338	52.6636
		NABBD	8.5143	8.4667	8.4767	8.4682	8.4730	8.4822	0.0476	8.4767	44.4850	15.8838
	0.9	ABBD	6.9845	6.2981	6.7629	6.6928	6.7864	6.8562	0.6864	6.7629	68.8005	42.0125
		AFBBD	11.8635	6.4405	8.8421	7.8302	8.7865	9.7943	5.4231	8.8421	81.6338	52.6636
		NABBD	13.3900	7.4277	10.3553	8.5482	10.0876	12.1536	5.9623	10.3553	44.4850	15.8838
	1.5	ABBD	11.6859	10.2784	10.8903	10.6594	10.8585	11.0906	1.4074	10.8903	68.8005	42.0125
		AFBBD	14.8052	8.0727	10.7780	9.4943	10.6304	11.8987	6.7325	10.7780	81.6338	52.6636
		NABBD	41.9061	9.8060	24.8467	14.4222	23.5309	35.2808	32.1000	24.8467	44.4850	15.8838
	2.2	ABBD	62.7524	30.9097	35.5530	32.0410	33.2601	36.8966	31.8427	35.5530	68.8005	42.0125
		AFBBD	62.7524	24.3486	29.3230	26.5497	28.0987	30.4192	25.3817	29.3230	81.6338	52.6636
		NABBD	163.5211	33.2647	95.6025	53.7909	9.9885	138.4702	130.2564	95.6025	44.4850	15.8838
2	0.1	ABBD	5.7997	5.7995	5.7996	5.7996	5.7996	5.7996	0.0002	5.7996	68.1686	41.5196
		AFBBD	8.5753	7.9453	8.2582	8.1468	8.2578	8.3670	0.6299	8.2582	80.7868	51.8486
		NABBD	7.8946	7.8458	7.8522	7.8473	7.8522	7.8616	0.0488	7.8561	44.1597	15.7307
	0.9	ABBD	6.7898	6.0952	6.5656	6.4946	6.5893	6.6599	0.6946	6.5656	68.1686	41.5196
		AFBBD	10.8483	5.9671	8.1447	7.2356	8.0939	9.0009	4.8812	8.1447	80.7868	51.8486
		NABBD	13.1303	7.0800	10.0479	8.2143	9.7740	11.8710	6.0503	10.0479	44.1597	15.7307
	1.5	ABBD	11.7355	10.3111	10.9303	10.6967	10.8982	11.1331	1.4244	10.9303	68.1686	41.5196
		AFBBD	14.3588	8.0737	10.6179	9.4185	10.4884	11.6647	6.2851	10.6179	80.7868	51.8486
		NABBD	42.2868	9.8141	25.0275	14.4816	23.7036	35.5847	32.4727	25.0275	44.1597	15.7307
	2.2	ABBD	63.4975	31.2711	35.9703	32.4160	33.6498	37.3301	32.2264	35.9703	68.1686	41.5196
		AFBBD	50.5189	24.6936	29.7669	26.9568	28.5282	30.8848	25.8254	29.7669	80.7868	51.8486
		NABBD	165.1168	33.5308	96.5112	54.2739	91.8603	139.8296	131.5860	96.5112	44.1597	15.7307
3	0.1	ABBD	5.4921	5.4920	5.4921	5.4921	5.4921	5.4921	0.0002	5.4921	67.5397	41.0375
		AFBBD	7.7167	7.1501	7.4315	7.33113	7.4312	7.5294	0.5667	7.4315	79.9163	51.0570
		NABBD	7.3706	7.3207	7.3312	7.3223	7.3273	7.3369	0.0499	7.3312	43.8300	15.5784
	0.9	ABBD	6.6249	5.9220	6.3980	6.3262	6.4220	6.4935	0.7029	6.3980	67.5397	41.0375
		AFBBD	10.0750	5.5963	7.6158	6.7815	7.5712	8.3967	4.4787	7.6158	79.9163	51.0570
		NABBD	12.9249	6.7898	9.7969	7.9373	9.5171	11.6431	6.1350	9.7969	43.8300	15.5784
	1.5	ABBD	11.7449	10.3536	10.9801	10.7437	10.9476	11.1853	1.4414	10.9801	67.5397	41.0375
		AFBBD	14.0495	8.1002	10.5243	9.3889	10.4107	11.5204	5.9492	10.5243	79.9163	51.0570
		NABBD	42.6769	9.8352	25.2199	14.5538	23.8791	35.9028	32.8417	25.2199	43.8300	15.5784
	2.2	ABBD	64.2437	31.6337	36.3889	32.7922	34.0407	37.7648	32.6100	36.3889	67.5397	41.0375
		AFBBD	51.3078	25.0469	30.2152	27.3691	28.9612	31.3551	26.2609	30.2152	79.9163	51.0570
		NABBD	166.7351	33.8092	97.4358	54.7699	92.7465	141.1961	132.9259	97.4358	43.8300	15.5784

Table 5: Prediction Performance Metrics and Efficiency Ratios for Six-Factor Designs (*k* = 6)

n_c	r	Design	SPV_{max}	SPV_{min}	SPV_{avg}	SPV_{25Q}	SPV_{50Q}	SPV_{75Q}	VP	IPV	D_{Eff}	G_{Eff}
1	0.1	ABBD	8.9826	8.9825	8.9826	8.9826	8.9826	8.9826	0.0001	8.9826	66.2889	28.2585
		AFBBD	11.9354	11.5616	11.7542	11.6951	11.7551	11.8145	0.3738	11.7542	79.4713	36.7128
		NABBD	16.8473	16.8470	16.8472	16.8472	16.8472	16.8472	0.0003	16.8472	40.5314	27.4288
	0.9	ABBD	8.9023	8.5827	8.7952	8.7627	8.8057	8.8377	0.3196	8.7952	66.2889	28.2585
		AFBBD	12.2040	8.8284	10.7369	10.2335	10.8161	11.2831	3.3755	10.7369	79.4713	36.7128
		NABBD	14.0843	12.5987	13.6807	13.5644	13.7443	13.8528	1.4856	13.6807	40.5314	27.4288
	1.9	ABBD	34.9144	18.6826	20.8694	19.4933	20.0755	21.3385	16.2318	20.8694	66.2889	28.2585
		AFBBD	28.6258	13.9797	18.4348	17.1378	18.2594	19.4284	14.6460	18.4348	79.4713	36.7128
		NABBD	39.8946	32.1483	35.6747	34.4394	35.6854	36.8933	7.7464	35.6747	40.5314	27.4288
	2.4	ABBD	123.3443	39.8386	50.9028	43.2231	46.8351	54.0613	83.5057	50.9028	66.2889	28.2585
		AFBBD	94.6020	30.8476	41.7115	36.1312	38.9355	44.2056	63.7544	41.7115	79.4713	36.7128
		NABBD	125.5340	88.9766	95.0830	93.0120	94.2861	65.7501	36.5574	95.0830	40.5314	27.4288
2	0.1	ABBD	8.5896	8.5895	8.5895	8.5895	8.5896	8.5896	0.0001	8.5895	66.0062	28.0998
		AFBBD	10.9973	10.6530	10.8306	10.7761	10.8314	10.8861	0.3443	10.8306	79.0496	36.4250
		NABBD	15.4392	15.4390	15.4392	15.4391	15.4392	15.4392	0.0003	15.4392	40.4092	27.4337
	0.9	ABBD	8.6440	8.3226	8.5363	8.5036	8.5469	8.5790	0.3214	8.5363	66.0062	28.0998
		AFBBD	11.4646	8.3019	10.0882	9.6148	10.1627	10.6000	3.1627	10.0882	79.0496	36.4250
		NABBD	13.2884	11.7941	12.8824	12.7655	12.9364	13.0555	1.4942	12.8824	40.4092	27.4337
	1.9	ABBD	35.0874	18.7618	20.9612	19.5772	20.1628	21.4330	16.3256	20.9612	66.0062	28.0998
		AFBBD	28.7539	14.0717	18.4734	17.1822	18.2890	19.4437	14.6822	18.4734	79.0496	36.4250
		NABBD	40.1190	32.3278	35.8746	34.6322	35.8854	37.1003	7.7912	35.8746	40.4092	27.4337

	2.4	ABBD	124.0411	40.0527	51.1808	43.4567	47.0896	54.3576	83.9884	51.1808	66.0062	28.0998
		AFBBD	95.3506	31.0211	42.0327	36.4083	39.2256	44.5465	64.3296	42.0327	79.0496	36.4250
		NABBD	125.5208	88.7521	94.8938	92.8108	94.0924	95.5647	36.7687	94.8938	40.4092	27.4337
3	0.1	ABBD	8.2335	8.2334	8.2335	8.2335	8.2335	8.2335	0.0001	8.2335	65.7222	27.9426
		AFBBD	10.2080	9.8885	10.0534	10.0028	10.0542	10.1050	0.3196	10.0534	78.6179	36.1412
		NABBD	14.2615	14.2612	14.2614	14.2614	14.2614	14.2614	0.0003	14.2614	40.2792	27.4136
	0.9	ABBD	8.4115	8.0882	8.3032	8.2703	8.3138	8.3461	0.3233	8.3032	65.7222	27.9426
		AFBBD	10.8484	7.8612	9.5452	9.1009	9.6165	10.0290	2.9872	9.5452	78.6179	36.1412
		NABBD	12.6266	11.1238	12.2183	12.1007	12.2726	12.3925	1.5028	12.2183	40.2792	27.4136
	1.9	ABBD	35.2628	18.8434	21.0554	19.6634	20.2524	21.5300	16.4194	21.0554	65.7222	27.9426
		AFBBD	28.8965	14.1666	18.5278	17.2408	18.3347	19.4811	14.7300	18.5278	78.6179	36.1412
		NABBD	40.3442	32.5083	36.0755	34.8259	36.0863	37.3082	7.8359	36.0755	40.2792	27.4136
	2.4	ABBD	124.7392	40.2681	51.4602	43.6917	47.3455	54.6553	84.4711	51.4602	65.7222	27.9426
		AFBBD	96.1005	31.2051	42.3556	36.6909	39.5256	44.8898	64.8954	42.3556	78.6179	36.1412
		NABBD	125.6207	88.6406	94.8177	92.7227	94.0116	95.4924	36.9800	94.8177	40.2792	27.4136

4. Conclusion

This paper evaluates the prediction capabilities of ABBDs, AFBBDs, and NABBDs using QDGs, boxplots, and numerical prediction performance measures. The evaluation was conducted for $3 \leq k \leq 6$ factors and $1 \leq n_c \leq 3$ centre points in the spherical region.

The graphical and numerical results consistently revealed clear differences in the predictive performance of the competing designs. For smaller radii near the design centre, ABBDs often exhibited competitive performance and, in some cases, greater stability than the other designs. However, as the radius increased, AFBBDs generally demonstrated lower scaled prediction variances and superior prediction performance. The numerical results further showed that AFBBDs consistently achieved higher D- and G-efficiency values and lower average prediction variances than the competing designs across most factor levels and centre-point configurations. NABBDs consistently displayed the weakest prediction performance, characterised by larger prediction variances and lower efficiency values. Although prediction variance increased and efficiency decreased with increasing numbers of factors for all designs, AFBBDs experienced the least deterioration in performance and maintained superior predictive properties throughout most of the experimental region.

Overall, the results indicate that AFBBDs provide the most favourable balance between prediction accuracy, stability, and design efficiency among the three third-order Box-Behnken designs considered. Consequently, AFBBDs are recommended for third-order response surface modelling when reliable and uniform prediction capability over the experimental region is desired, particularly in applications such as pharmaceutical formulation, industrial process optimisation, chemical engineering, and agricultural experimentation.

Future studies may extend the assessment to higher-order response surface designs and investigate the robustness of these designs under model misspecification, missing observations, or the presence of outliers.

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$$\left(\begin{array}{ccc} x_1 & x_2 & x_3 \\ -1 & -1 & 0 \\ -1 & 1 & 0 \\ 1 & -1 & 0 \\ 1 & 1 & 0 \\ -1 & 0 & -1 \\ -1 & 0 & 1 \\ 1 & 0 & -1 \\ 1 & 0 & 1 \\ 0 & -1 & -1 \\ 0 & -1 & 1 \\ 0 & 1 & -1 \\ 0 & 1 & 1 \\ +a & +a & +a \\ +a & +a & -a \\ +a & -a & +a \\ +a & -a & -a \\ -a & +a & +a \\ -a & +a & -a \\ -a & -a & +a \\ -a & -a & -a \\ +\alpha & 0 & 0 \\ -\alpha & 0 & 0 \\ 0 & +\alpha & 0 \\ 0 & -\alpha & 0 \\ 0 & 0 & +\alpha \\ 0 & 0 & -\alpha \\ 0 & 0 & 0 \end{array}\right) \begin{array}{l} \vphantom{x_1} \\ \left.\vphantom{\begin{matrix}0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\end{matrix}}\right\} n_b \\ \left.\vphantom{\begin{matrix}0\\0\\0\\0\\0\\0\\0\\0\end{matrix}}\right\} n_f \\ \left.\vphantom{\begin{matrix}0\\0\\0\\0\\0\\0\end{matrix}}\right\} n_a \\ \left.\vphantom{0}\right\} n_c \end{array}$$

$$\left[\begin{array}{ccc} x_1 & x_2 & x_3 \\ -1 & -1 & 0 \\ 1 & -1 & 0 \\ -1 & 0 & -1 \\ 1 & 0 & -1 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \\ +a & +a & +a \\ +a & +a & -a \\ +a & -a & +a \\ +a & -a & -a \\ -a & +a & +a \\ -a & +a & -a \\ -a & -a & +a \\ -a & -a & -a \\ +\alpha & 0 & 0 \\ -\alpha & 0 & 0 \\ 0 & +\alpha & 0 \\ 0 & -\alpha & 0 \\ 0 & 0 & +\alpha \\ 0 & 0 & -\alpha \\ 0 & 0 & 0 \end{array}\right] \begin{array}{l} \vphantom{x_1} \\ \left.\vphantom{\begin{matrix}0\\0\\0\\0\\0\\0\end{matrix}}\right\} n_b \\ \left.\vphantom{\begin{matrix}0\\0\\0\\0\\0\\0\\0\\0\end{matrix}}\right\} n_f \\ \left.\vphantom{\begin{matrix}0\\0\\0\\0\\0\\0\end{matrix}}\right\} n_a \\ \left.\vphantom{0}\right\} n_c \end{array}$$

$$\left[\begin{array}{cccc} x_1 & x_2 & x_3 & x_4 \\ B_4 & B_4 & B_4 & B_4 \\ +a & +a & 0 & +a \\ +a & +a & 0 & -a \\ +a & -a & 0 & +a \\ +a & -a & 0 & -a \\ -a & +a & 0 & +a \\ -a & +a & 0 & -a \\ -a & -a & 0 & +a \\ -a & -a & 0 & -a \\ +\alpha & 0 & 0 & 0 \\ -\alpha & 0 & 0 & 0 \\ 0 & +\alpha & 0 & 0 \\ 0 & -\alpha & 0 & 0 \\ 0 & 0 & +\alpha & 0 \\ 0 & 0 & -\alpha & 0 \\ 0 & 0 & 0 & +\alpha \\ 0 & 0 & 0 & -\alpha \\ 0 & 0 & 0 & 0 \end{array}\right] \begin{array}{l} \vphantom{x_1} \\ \left.\vphantom{B_4}\right\} n_b \\ \left.\vphantom{\begin{matrix}0\\0\\0\\0\\0\\0\\0\\0\end{matrix}}\right\} n_f \\ \left.\vphantom{\begin{matrix}0\\0\\0\\0\\0\\0\\0\\0\end{matrix}}\right\} n_a \\ \left.\vphantom{0}\right\} n_c \end{array}$$

Figure 1: Design matrıces for ABBD, AFBBD and NABBD respectively

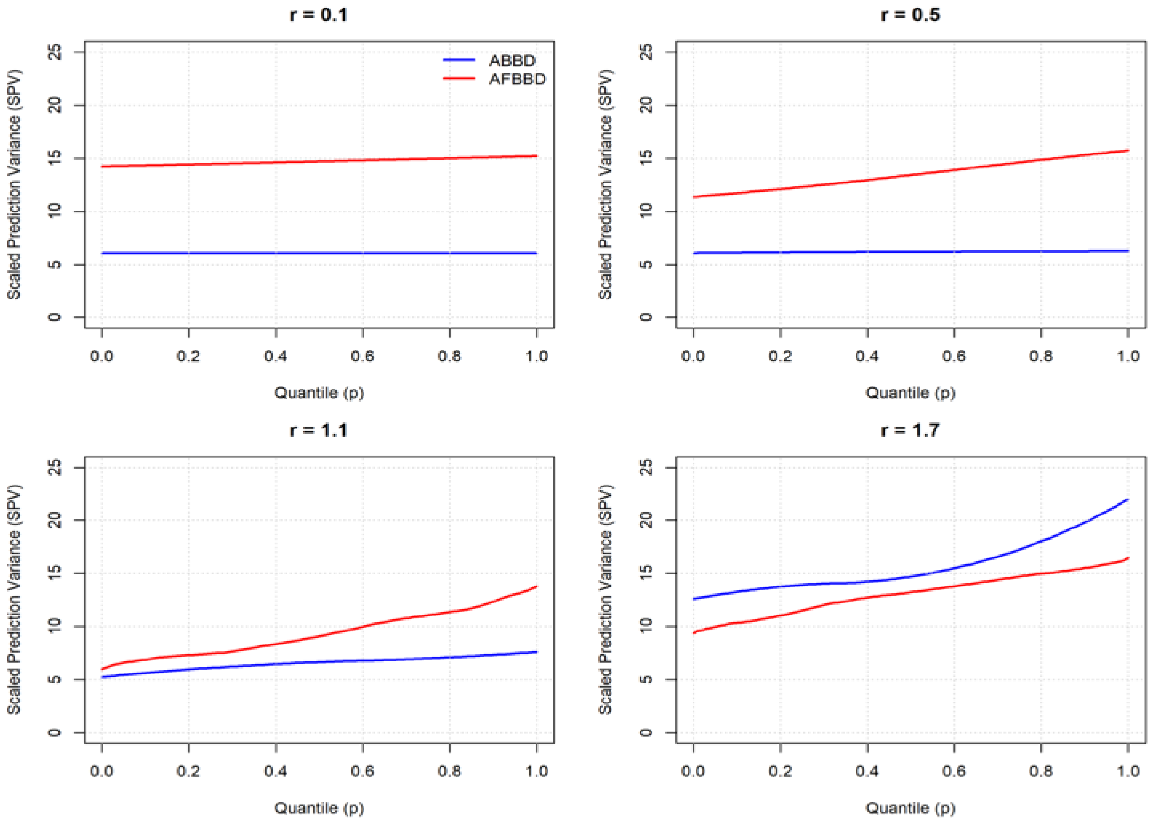


Figure 2: QDG for k = 3 and n_c = 1

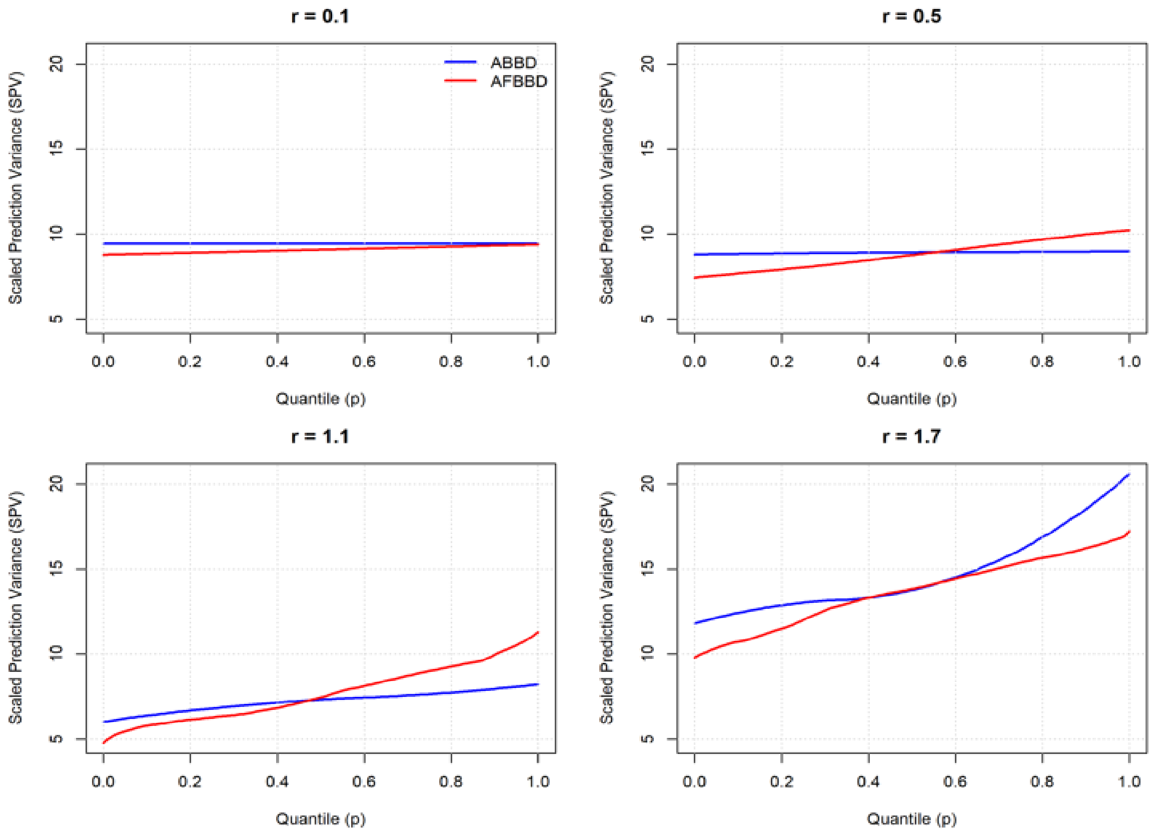


Figure 3: QDG for k = 3 and n_c = 2

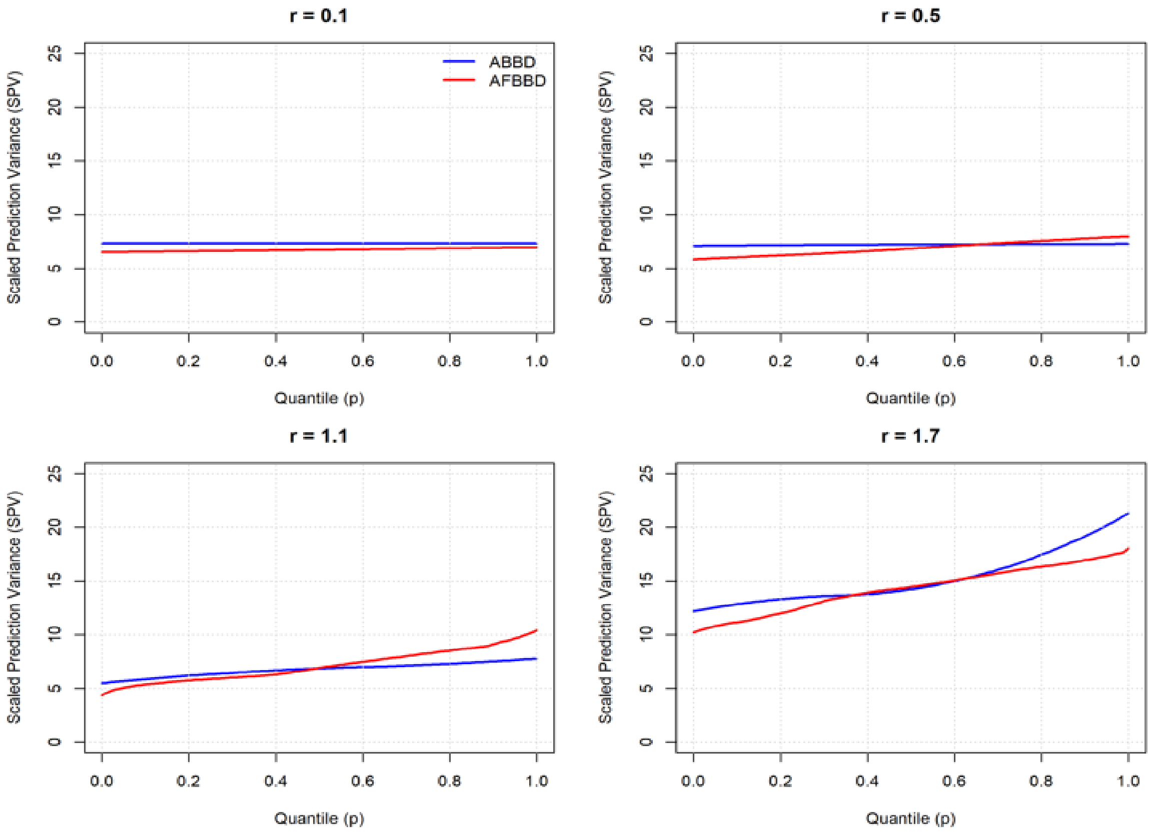


Figure 4: QDG for $k = 3$ and $n_c = 3$

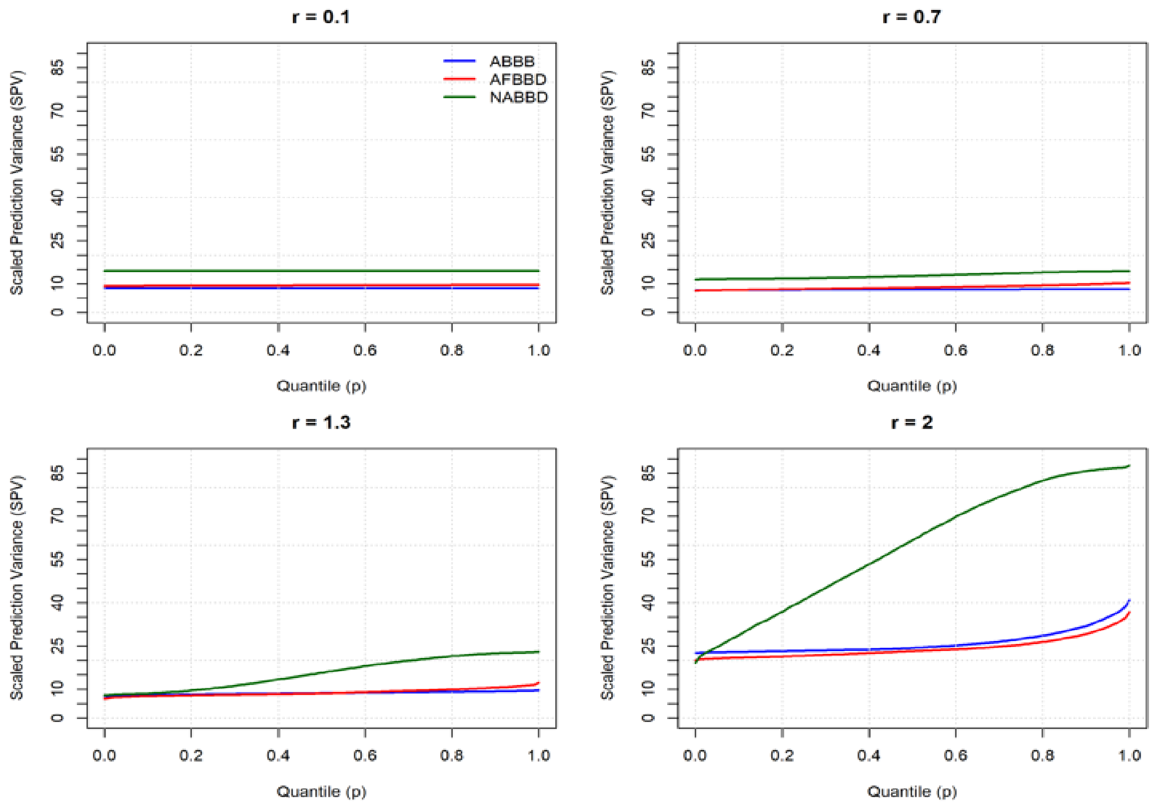


Figure 5: QDG for $k = 4$ and $n_c = 1$

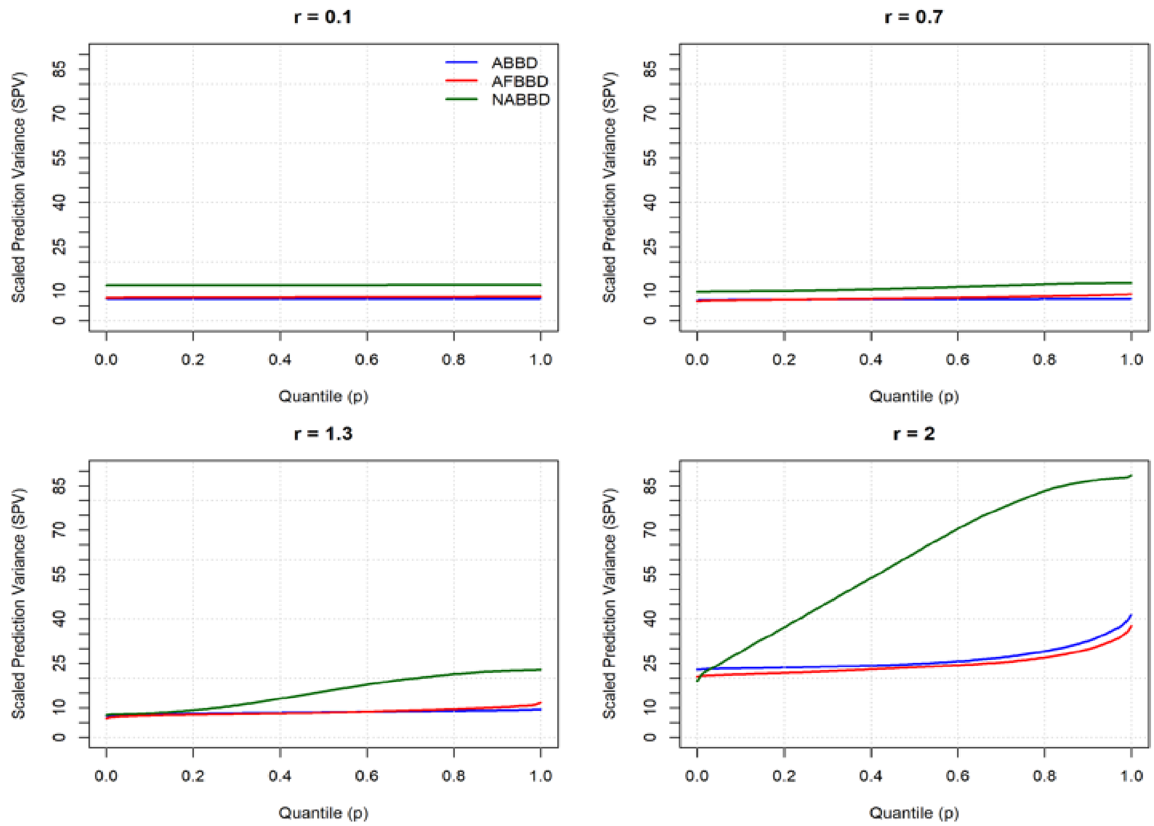


Figure 6: QDG for k = 4 and n_c = 2

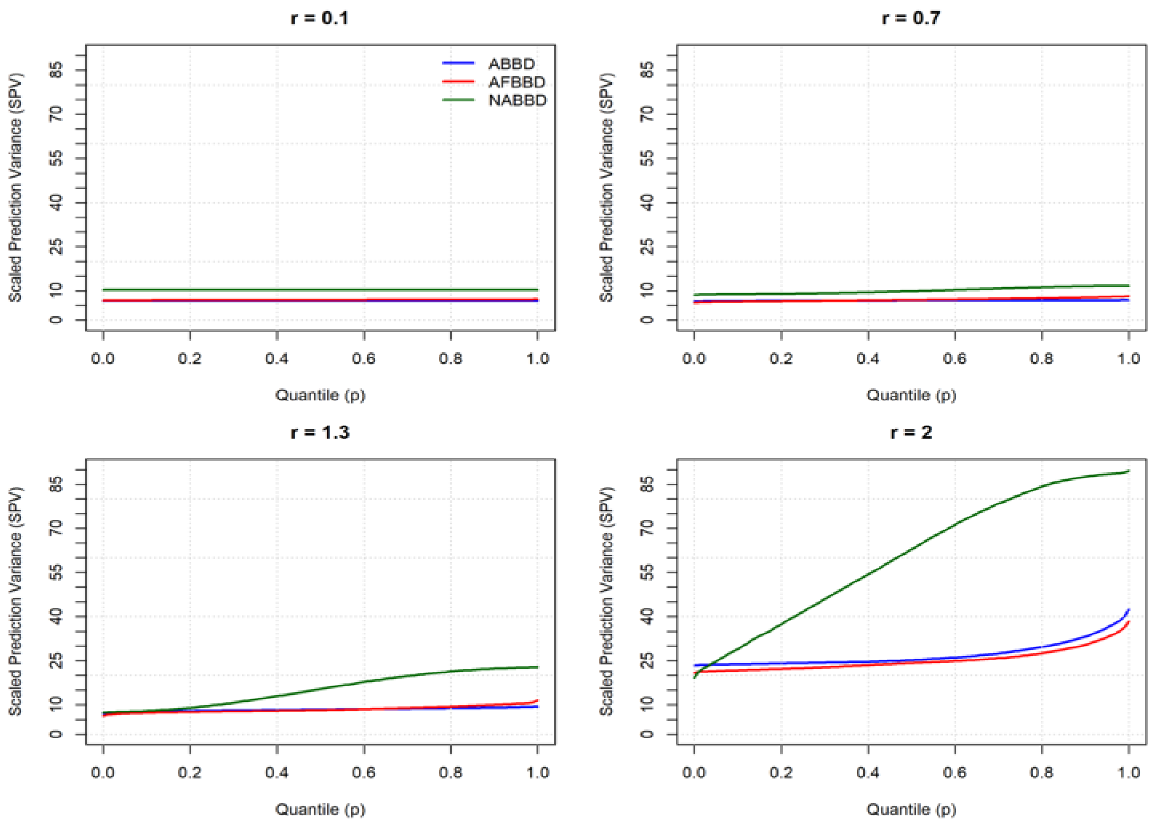


Figure 7: QDG for k = 4 and n_c = 3

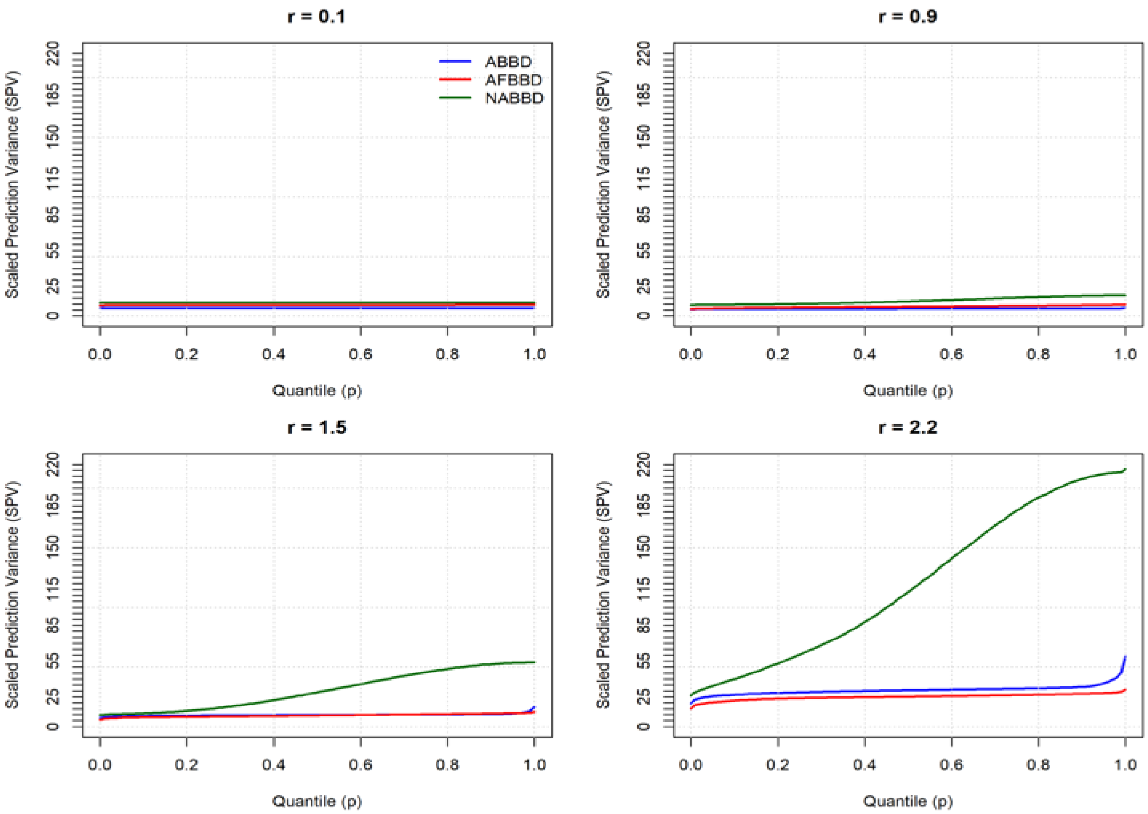


Figure 8: QDG for k = 5 and n_c = 1

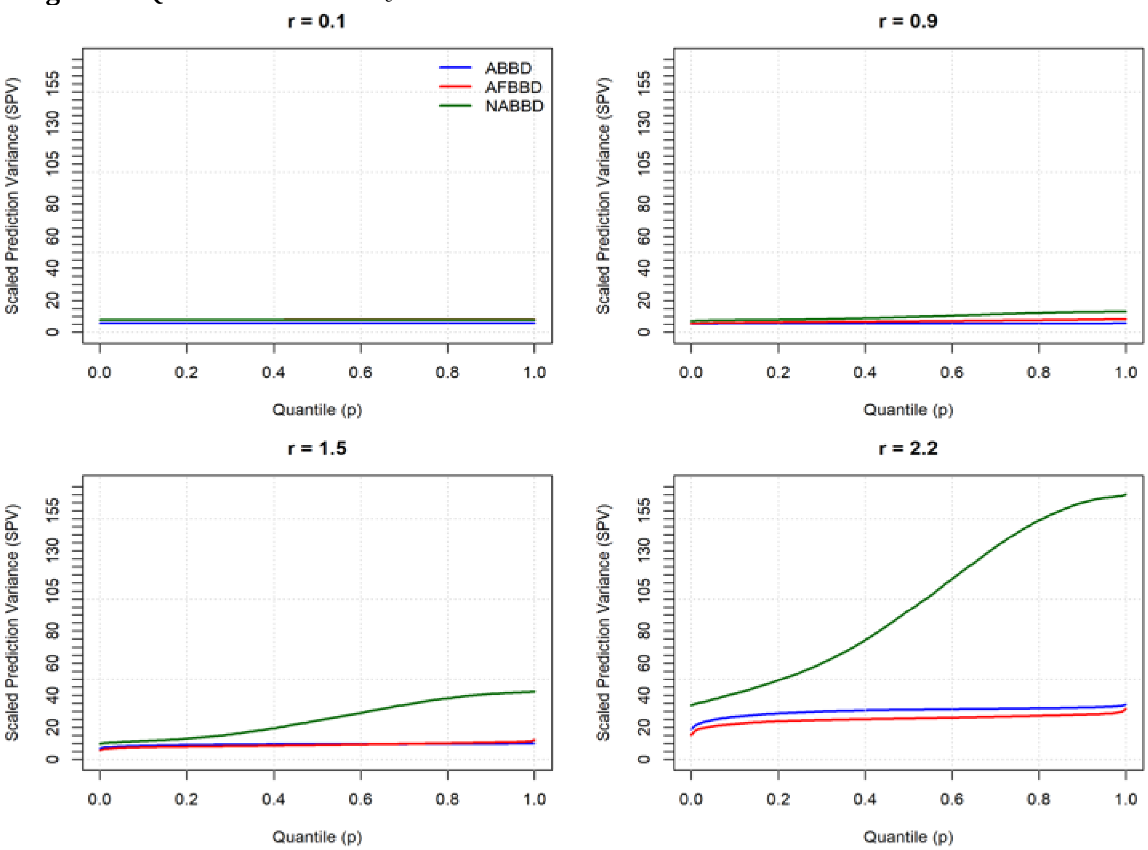


Figure 9: QDG for k = 5 and n_c = 2

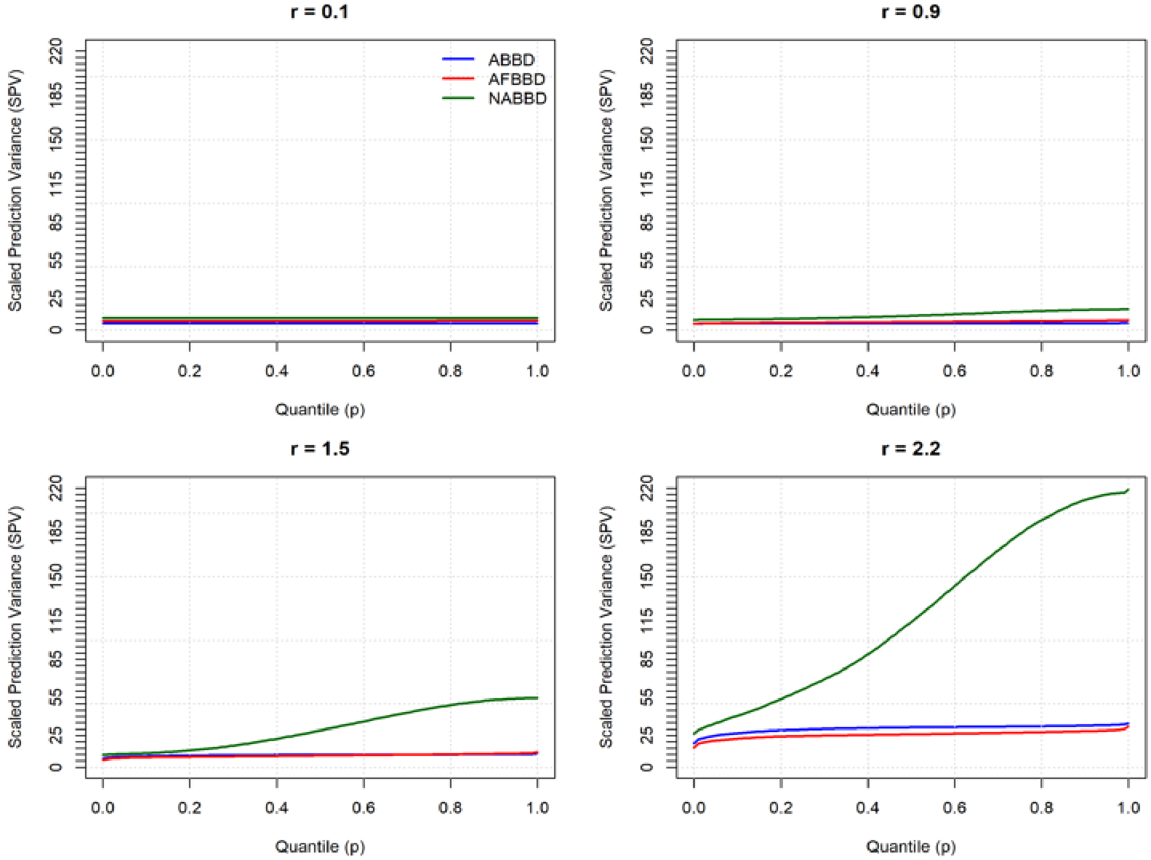


Figure 10: QDG for $k = 5$ and $n_c = 3$

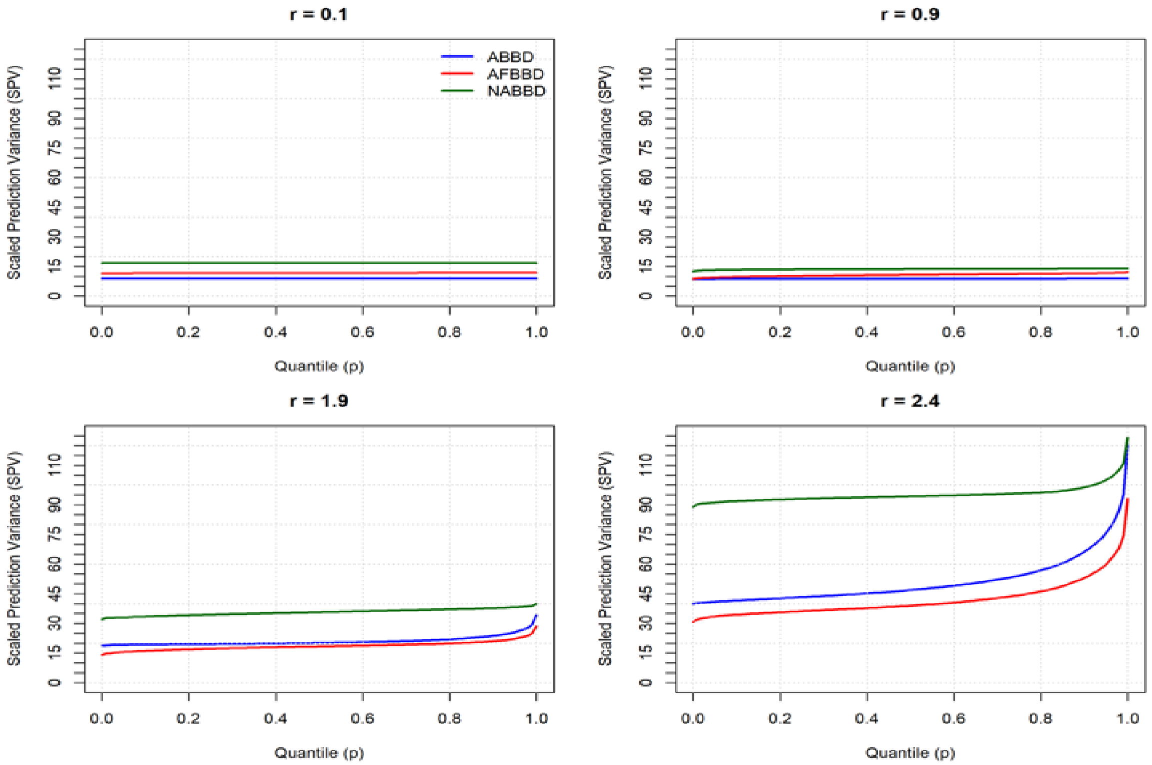


Figure 11: QDG for $k = 6$ and $n_c = 1$

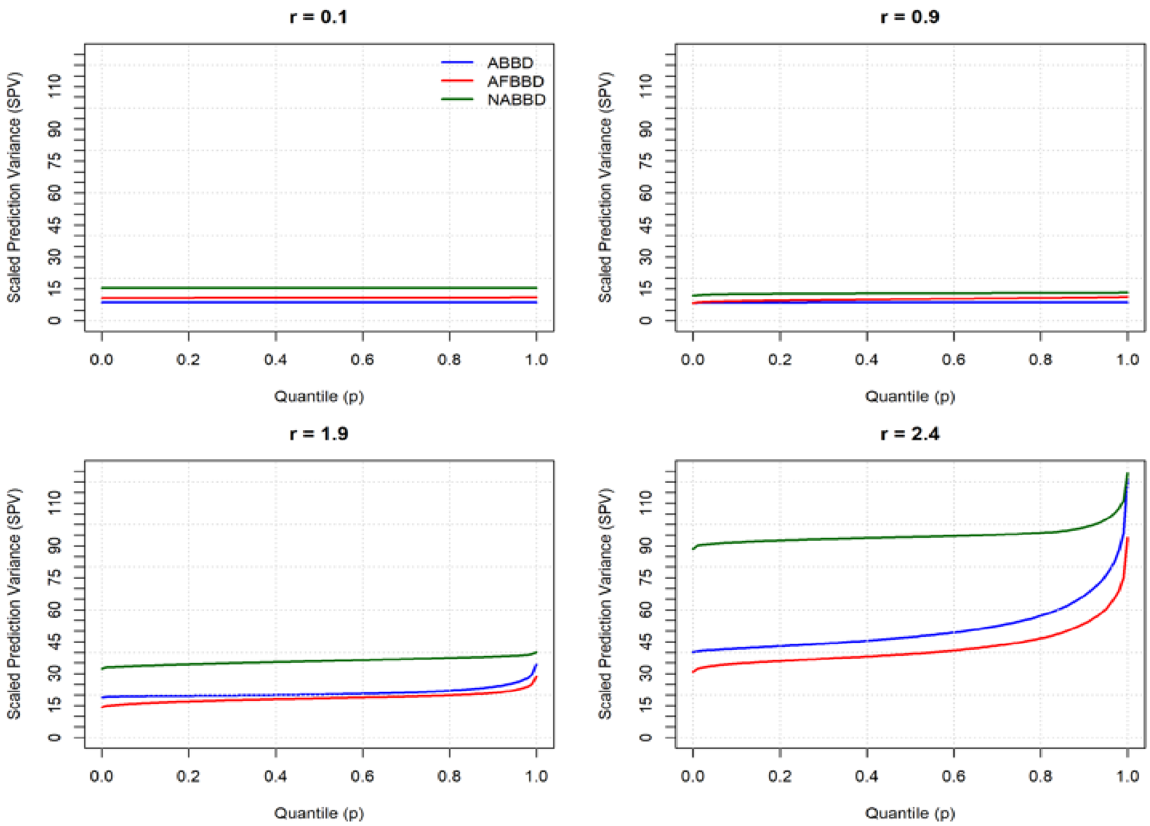


Figure 12: QDG for $k = 6$ and $n_c = 2$

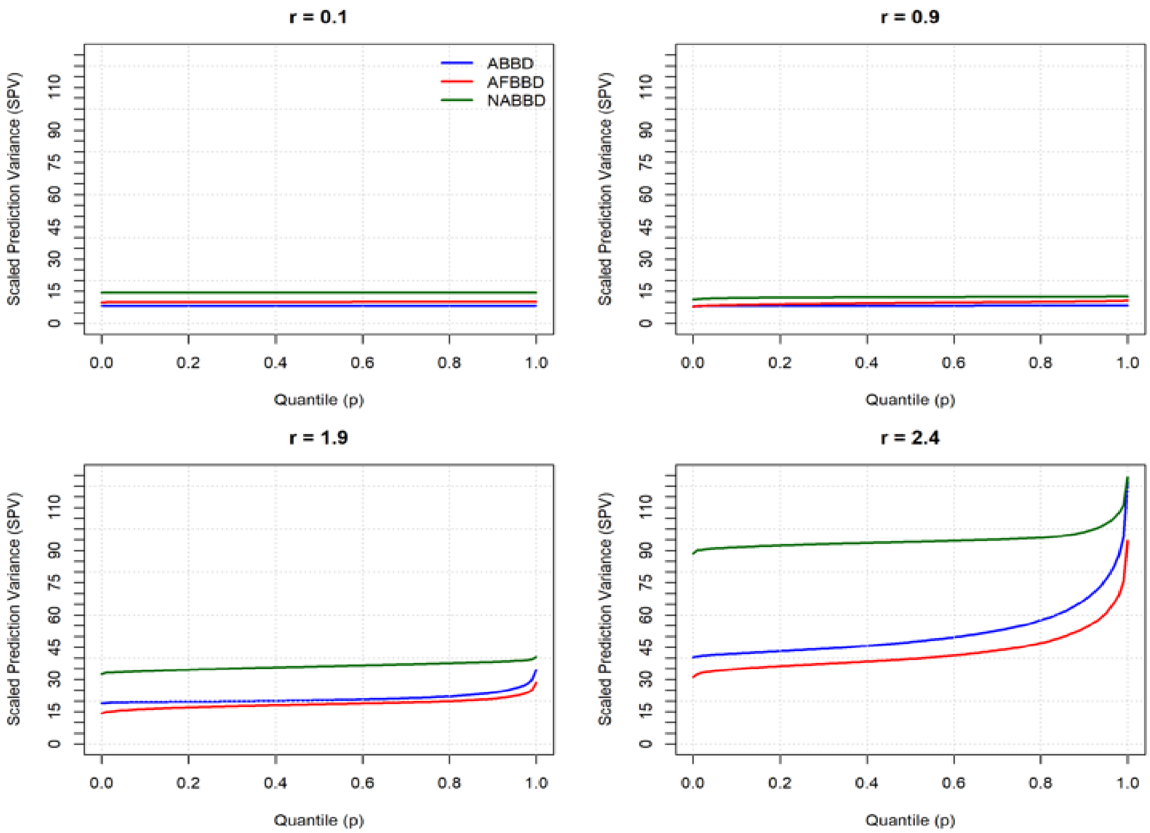


Figure 13: QDG for $k = 6$ and $n_c = 3$

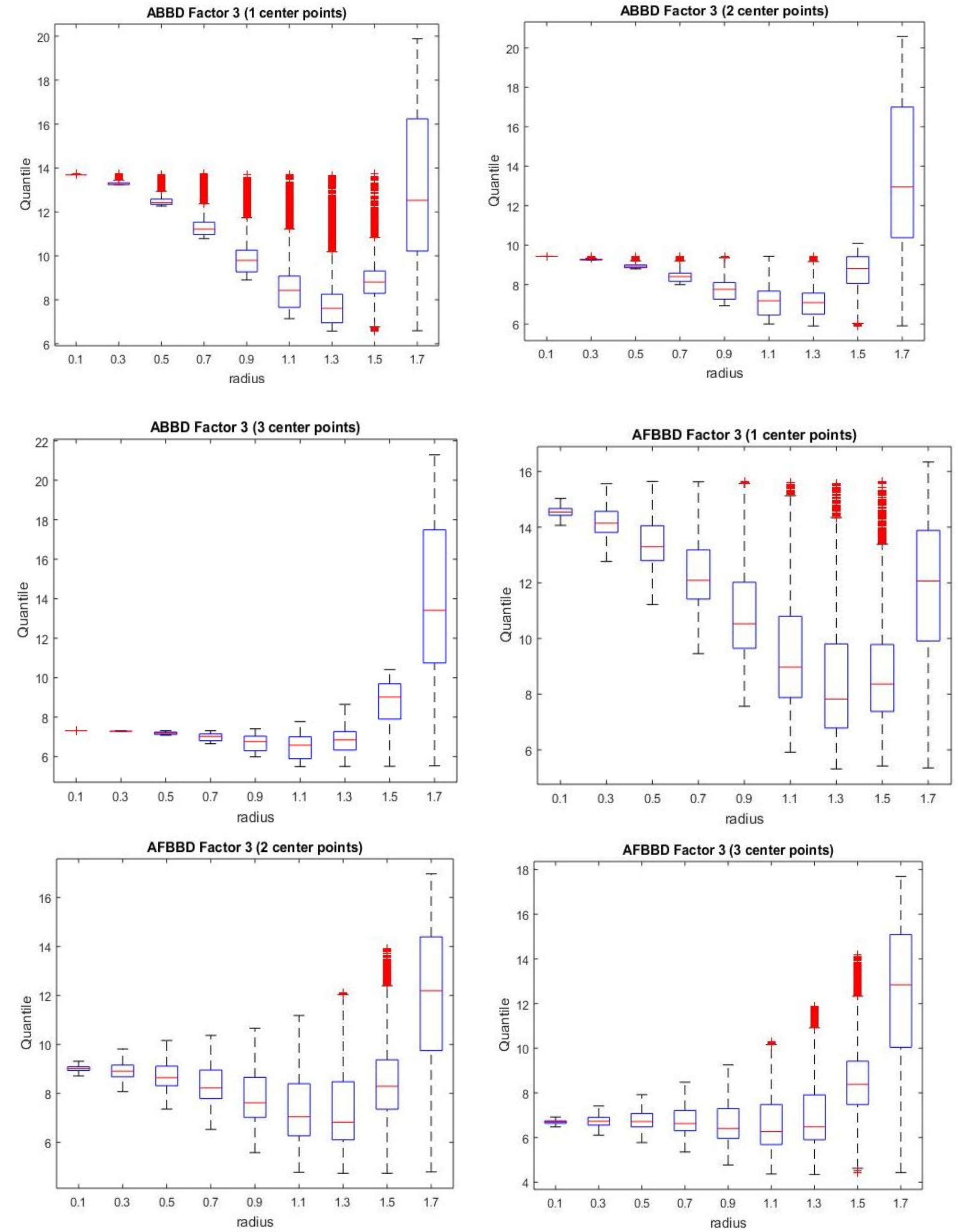
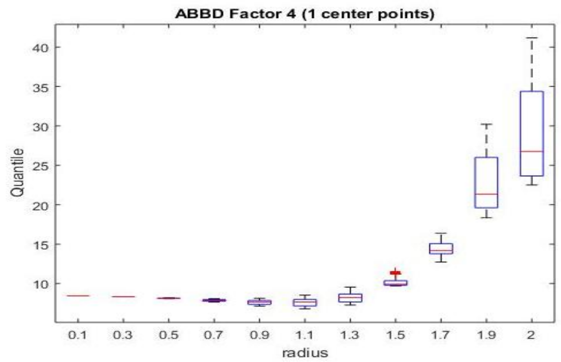
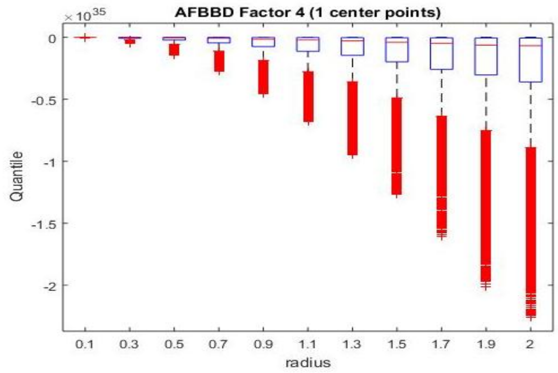
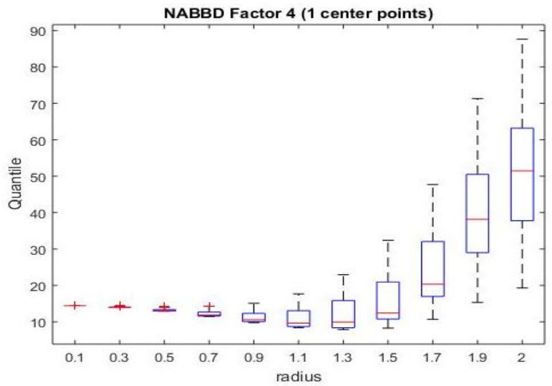
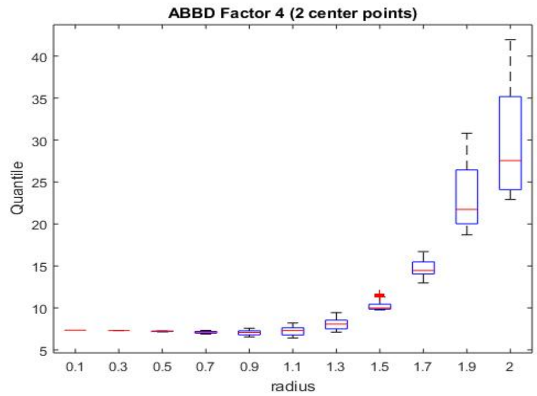


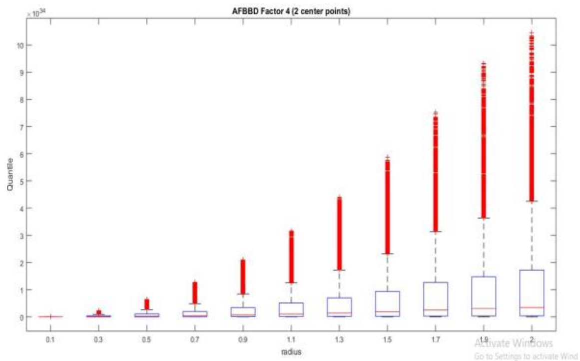
Figure 14: Box plots for k =3 and $1 \leq n_c \leq 3$

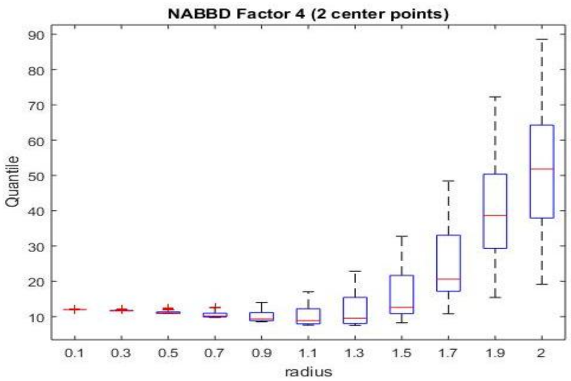

ABBD Factor 4 (1 center points)
Quantile
radius

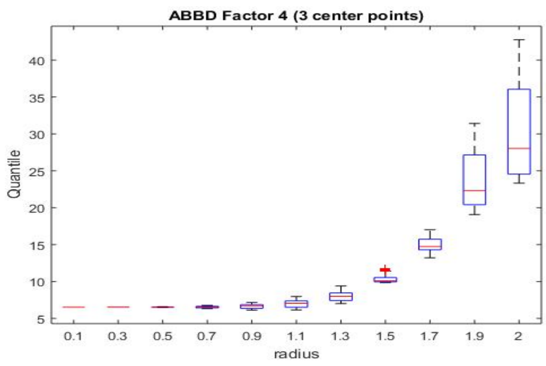

AFBBD Factor 4 (1 center points)
Quantile
radius

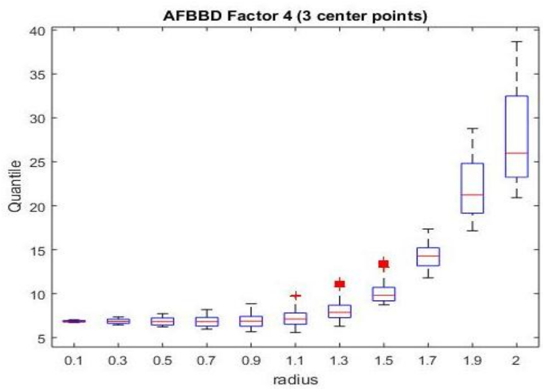

NABBD Factor 4 (1 center points)
Quantile
radius


ABBD Factor 4 (2 center points)
Quantile
radius


AFBBD Factor 4 (2 center points)


NABBD Factor 4 (2 center points)
Quantile
radius


ABBD Factor 4 (3 center points)
Quantile
radius


AFBBD Factor 4 (3 center points)
Quantile
radius

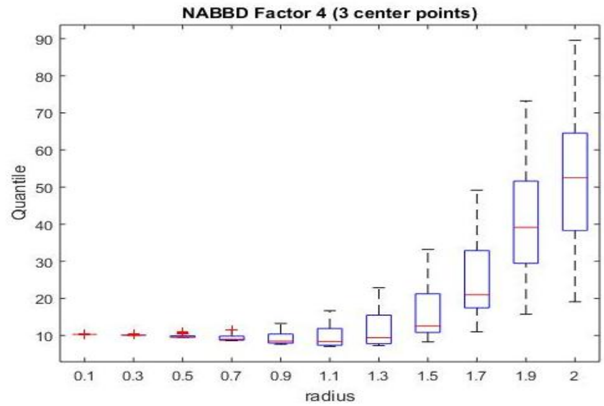
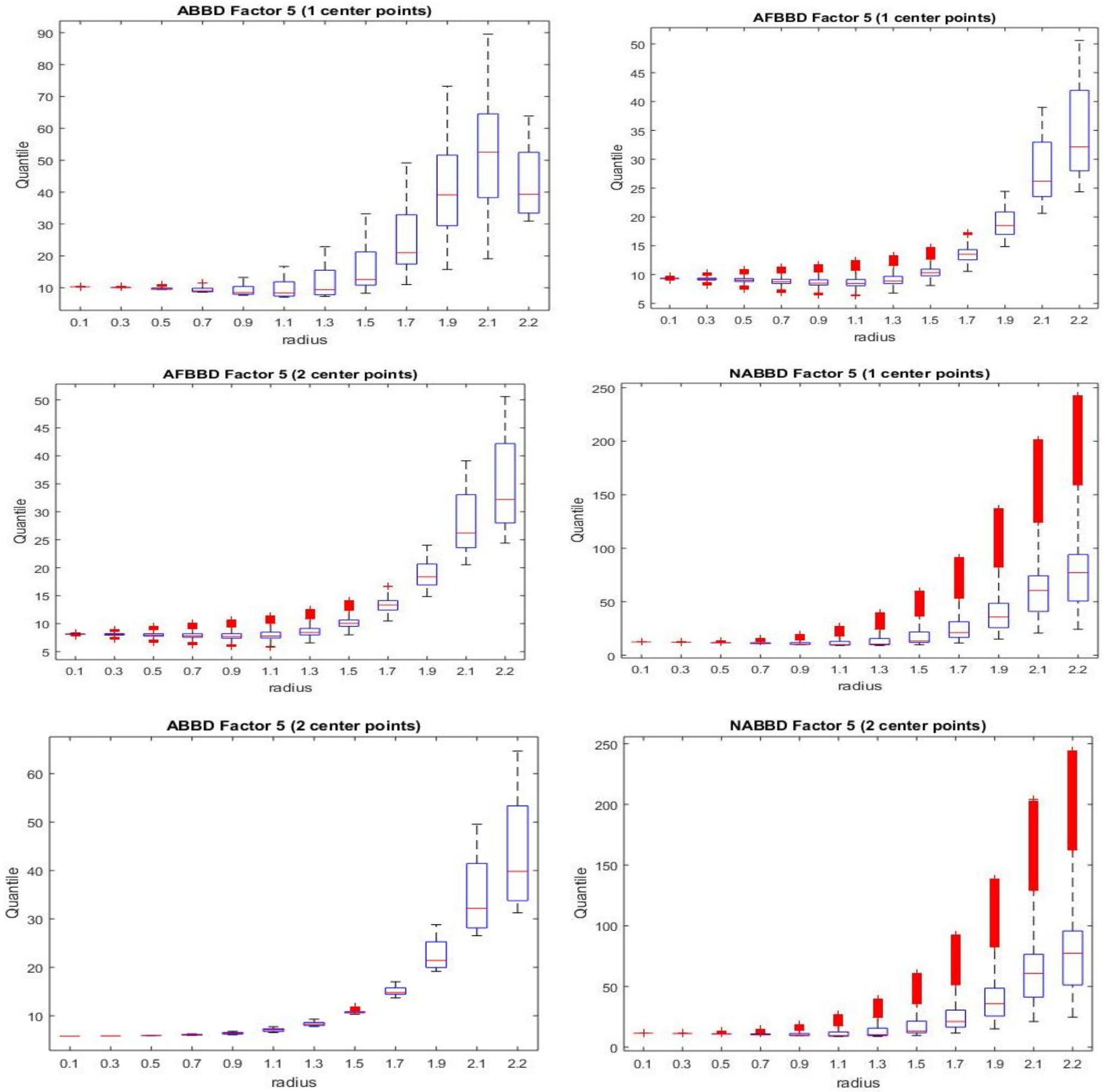


Figure 15: Boxplots for $k = 4$ and $1 \leq n_c \leq 3$



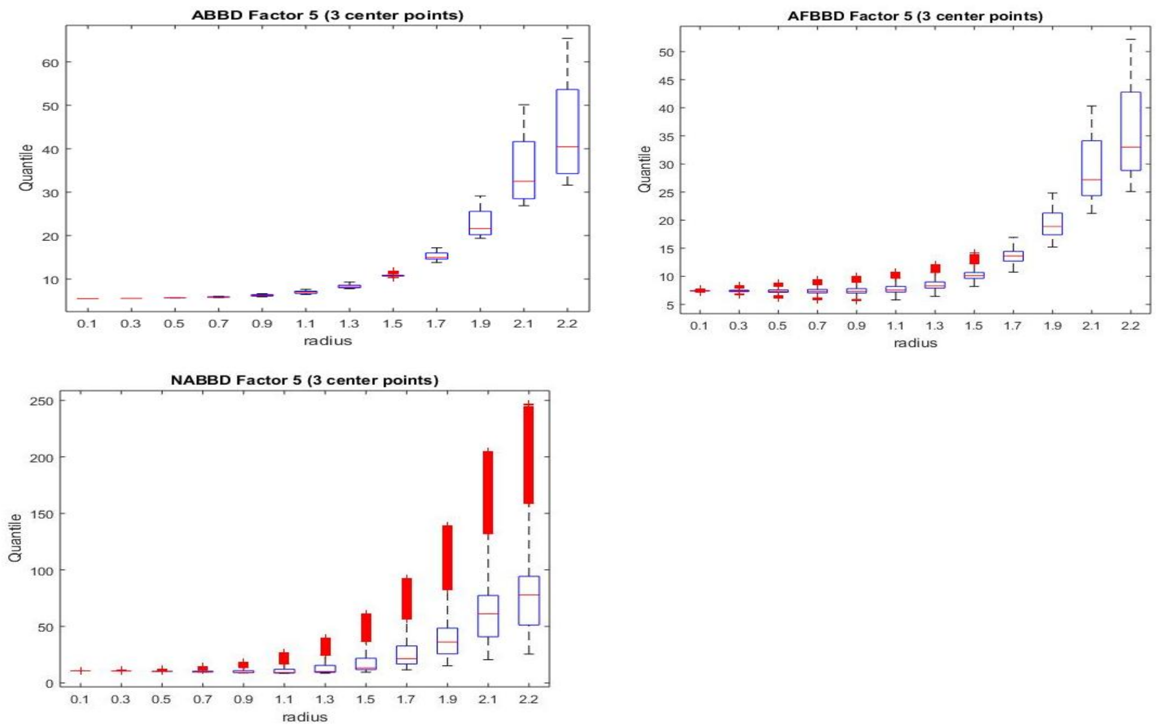
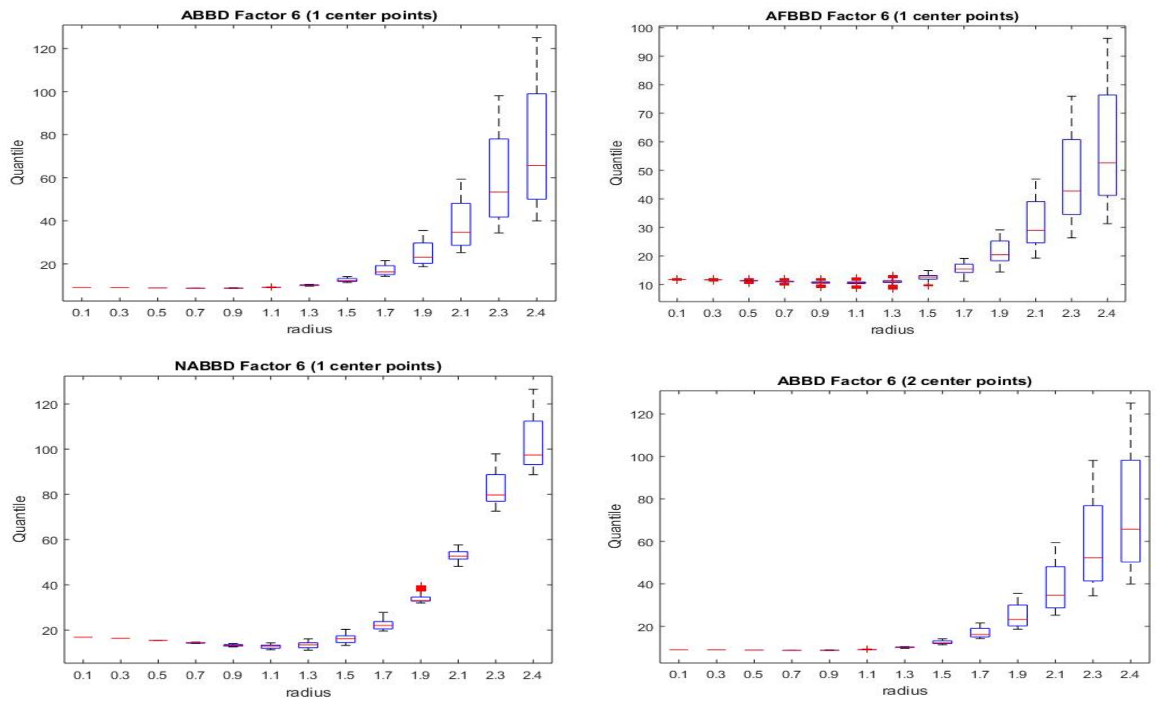


Figure 16: Boxplots for $k = 5$ and $1 \leq n_c \leq 3$



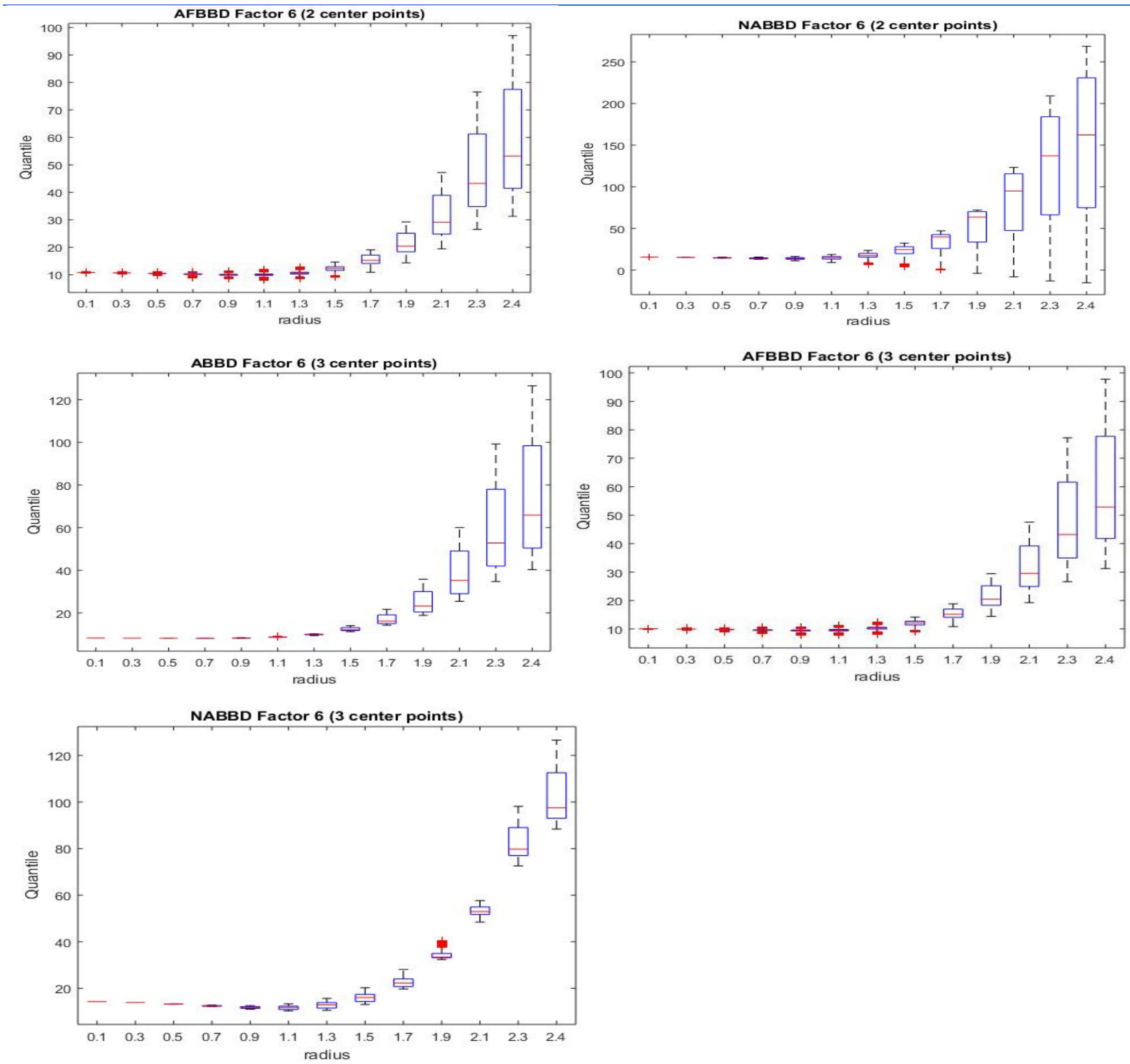


Figure 17: Boxplots for $k = 6$ and $1 \leq n_c \leq 3$