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Replication of Axial Points in Two-Factor Doehlert and Central Composite Designs with a Single Centre Point

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Abstract
This study investigated the effect of replicating axial points in two-factor second-order experimental designs with a single centre point. The designs considered include the Doehlert design (DD), Inscribed Central Composite Design (ICCD), and Face-Centred Central Composite Design (FCCCD), all configured with a common radial distance of 1.0. Among these, the DD and ICCD exhibit spherical geometry, while the FCCCD does not. The objective was to evaluate how replication of axial points influences the statistical properties of these designs compared to their un-replicated counterparts. To assess the impact, various design evaluation metrics were employed, including D-optimality, T-optimality, prediction variance, and G-efficiency. The results showed that the un-replicated FCCCD exhibited both D- and T-optimality. The un-replicated Doehlert and ICCD designs were only D-optimal, whereas their replicated versions were T-optimal. This indicates a consistent shift from D-optimality to T-optimality upon replication of the axial points across all designs. Additionally, the findings suggested that the Doehlert design shares more structural and statistical similarities with the ICCD than with the FCCCD. Based on these results, the study recommended replicating axial distance of Doehlert and Central Composite designs in order to obtain T-optimal designs.

Keywords: Replication, Doehlert, Central Composite Designs, Second-Order Designs, G-Optimality

Introduction

Doehlert design is a second-order design that begins with an equilateral triangle of lengths 1 as seen in Verdooren, (2017). To construct a regular hexagon (six-sided shape) with 1 centre point (0,0), with one center point, we will have a design size such as $N = n + 1$ where n is the radial point obtain from the shape of the design, hence, n=6, making the size of the design N=7-sized design. The design points of a doehlert design are; (1,0), (0.5,0.866), (0,0), (-0.5,0.866), (-1,0), (-0.5,-0.866) and (0.5,-0.866). The points on the hexagon, which is to say the 6 outer points lie on a circle of radius 1. It is a spherical design. Obviously, the designs that are most popular for modeling the second-order (quadratic) models are the central composite designs. Central Composite Design is a second-order design developed by Box & Wilson in1951 which can also be called Box-Wilson design. This design is seen as an alternative to the complete 3^kdesign. It was developed by the combinations of the 2^kfactorial or fractional factorial design points having factor level of -1, 1 with axial points of $\{(\pm 1, 0, \ . \ . \ . \ , 0), \ (0, \pm 1, \ . \ . \ . \ ,0), \ . \ . \ . \ , (0, 0, \ . \ . \ . \ , \pm 1)\}$ and then the centre point(s) c given as (0, 0, ... , 0). This process is called the augmentation of first-order design. The factorial portion as stated above contains the 2^kfactorial points or the fractions of it, while the axial portion contains the $2k$ design points properly arranged such that two points are selected on each axis of the explanatory variables with axial distance of α taken from the design centre. Replication of axial points in experimental design refers to the repetition of experimental runs conducted at the central points and extreme (axial) points of the design space. The importance of replicating axial points are as follows;

a) It increases the reliability and repeatability of results
b) It detects potential outliers or variability
c) It improves estimation of curvature in the response surface
d) It minimizes potential errors.

The A-optimality criterion minimizes the trace of the inverse of the normalized information matrix, this is equivalent to the T-optimality which seeks to maximize the trace of the normalized information matrix.
The D-optimality criterion minimizes the determinant of M^{-1}which is equivalent to maximizing the determinant of M.
Experimental design based on Doehlert and Central Composite (Inscribed and Face centered) designs are widely used in optimization and modelling of processes. However, replicating the axial points of these designs for a single centre point is not commonly practiced. There is a lack of research on the benefits and limitations of replicating axial points for both Designs. Therefore, understanding the implications of replicating axial points for Doehlert and Central Composite designs is essential for optimizing processes effectively and efficiently. Hence, this research was initiated to bridge this gap.
The aim of the study is to compare the effect of Axial point Replication in two-factor Doehlert and Central Composite Designs with a single centre Point, while the objectives include to;

1. compare the efficiency of three two-factor experimental designs (FCCCD, ICCD, and DD) with and without axial point replication using a single center point.
2. evaluate the impact of axial point replication on design properties such as: Prediction variance, D-optimality, A-optimality, T=optimality, G-efficiency, Maximum and minimum prediction variance
3. determine which design provides better estimation capability and model stability when replication at axial points is introduced.

The study examines the impact of replicating axial points for two-factor Doehlert and Central Composite designs with a centre point. This may include investigating how replication affects the accuracy of model prediction, variance component estimation and overall efficiency of the experimental design. The study may also explore different techniques for incorporating axial point replications and trade-offs involved in terms of added resources versus increased reliability. The practical applications of this research could extend to various fields, including, but not limited to, chemistry, engineering, pharmaceuticals and food science, where experiments need to be conducted to determine the optimal setting for different independent variables. Conclusively, replicating axial points for two-factor Doehlert and Central Composite designs is an important aspect of experimental design research, contributing to the advancement of efficient and reliable processes in various industries.

The Central Composite design was proposed by Box and Wilson (1951), it is an easily constructed design which is the reason why the design is widely used, this design comprises of three portions which includes, the full or fractions of 2^kfactorial points, with the $2k$ axial points with the i^{th} pair given as $(0,0\ ...,0,\alpha,0,\ ...\ ,0)$ and $(0,0\ ...,0,-\alpha,0,\ ...\ ,0)$ where α and –α occur in the i^{th} spot and in the k-vector and the centre point c of the form $(0,0,\ ...,0)$. This process is also known as argumentation of first order design. It was constructed as an alternative to the 3^kdesign. (Wardrop, 1985 and Khuri & Cornell, 1996). The fractions of the factorial points are chosen such that no main effect is aliased with main effect or no two factor interaction effects are aliased with two factor effects. Doehlert established an equation in such a way that, when a simplex optimization having two variables come to the point where it encircles the optimum, a hexagon is formed. These designs allow for the calculation of a response surface through a minimum of experimentation. An additional attractive feature of this design is that a neighboring domain can be easily used by the means of addition of a few experiments (Suliman, 2017).

Recently, Alhaddad et al. (2020) applied Doehlert experimental plan in determining the optimal conditions which are the Time, PH, and Temperature for removing Barium ion from aqueous solutions.
Second-Order Model is commonly used in response surface methodology for many reasons which include, the quadratic model that is very flexible because it will often work efficiently as an estimation of the true response surface. Secondly, the method of least squares can be used in order to estimate the model parameters ($\boldsymbol{\beta}'s$) in the second-degree model. lastly, there is significant practical experience showing that quadratic models work well in explaining real response surface problems. (Suliman, 2017).

The Response Surface Methodology is very crucial in developing, formulating, designing and analyzing original scientific studies and products. It proves so efficient in the enhancement of existing studies. RSM are mostly and commonly applied in the industry, Social Science, Biological and Clinical Sciences, Physical and Engineering Sciences and Food Science. Because RMS has an extensive application in the real-life, it becomes paramount to trace the history of Response Surface Methodology which was introduced by Box & Wilson in 1951 (Wikipedia 2006). In their study, it was suggested to use a first-degree polynomial model to approximate the response variable. They acknowledged that this model is only an approximation, not accurate, but such a model is easy to estimate and apply, even when little is known about the process (Wikipedia 2006). Moreover, the origin of RMS started in 1930s. The orthogonal design was motivated by Box and Wilson (1951), in the case of the first-order model. For the second-order models, many subject-matter scientists and engineers have working knowledge of the central composite designs (CCDs) and three-level designs.

Onuet al. (2021) proposed A-optimality criterion as the best criterion among other alphabetic criteria studied for reduced quadratic model.
Iwundu and Oko, (2021) found out that designs may be better in D-optimality criterion, but may not be better in A-optimality criterion. This was observed while studying Design efficiency and optimality values of replicated central composite designs with full factorial portions.

Materials and Methods
The second-order quadratic model used in this study is given as seen in

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_{12} + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \varepsilon \quad (2.1)$$

The Design Matrix X is obtained from the Quadratic Model in (2.1) as seen in Richard-Igweh, et al. (2023), Onu, et al. (2022), Iwundu (2016a &b), Oyejola and Nwanya (2015) and Iwundu & Onu (2017).
The D-optimality is given as seen in Onukogu & Iwundu, (2007) as

$$\emptyset(M(\xi)) = Max(det\{M(\xi)\}) = Min(det\{M^{-1}(\xi)\}) \quad (2.2)$$

The T-optimality is given as

$$\emptyset(M(\xi)) = Max(tr\{M(\xi)\}) \quad (2.3)$$

The G-optimality is given as seen in Iwundu and Oko, (2021), and Iwundu and Onu, (2017) as

$$\emptyset(M(\xi)) = Min\left(Max_{\underline{x}\in R} Var(\underline{x})\right) \quad (2.4)$$

This criterion seeks to minimize the maximum scaled variance of prediction.
The G-efficiency is given as seen in Iwundu and Oko, (2021), Iwundu and Onu, (2017) as

$$G - eff = \frac{p}{MaxV(x)} \times 100 \quad (2.5)$$

Results
The results are as seen summarized in tables 3.1 and 3.2 below.
Table 1 shows the prediction variance along with the D- and A-optimality of the Designs

Un-Replicated					Replicated					
Designs	c	Det(m)	Tr(m)	PV	Designs	C	Det(m)	Tr(m)	PV1	PV2
FCCCD	1	0.0082	4.4286	6.8833	FCCCD1	1	0.0063	4.2500	7.8462	7.8462
				5.9500					6.6154	6.6154
				6.8833	FCCCD2		0.0063	4.2500	7.8462	7.8462
				6.8833					7.8462	6.1538
				5.1333					3.3846	7.8467
				5.1333					3.3846	5.5385
									5.5385	3.3846
DD	1	2.58e-4	2.6070	5.8333	DD1	1	2.12e-4	2.6327	6.5455	6.5455
				5.8333					3.6364	6.5455
				5.8333	DD2		2.12e-4	2.6327	6.5455	6.5455
				5.8333					3.6364	3.6364
				5.8333					6.5455	6.5455
				5.8333					6.5455	3.6364
				7.000					6.5455	6.5455
									8.000	8.000

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ICCD	1	1.38e-4	2.5858	6.6037	ICCD1	1	1.21e-4	2.6376	7.5339	7.4588
				6.1912					7.0487	6.8955
				4.6625	ICCD2		1.04e-4	2.6376	5.2507	4.8080
				6.6037					3.8835	7.4588
				4.7171					3.8835	7.4588
				6.2232					5.3150	3.2207
				6.9987					7.9985	3.2207
										7.9982

Table 2 G-efficiency, D-optimality, maximum and minimum variance of predictions

Un-replicated				Replicated			
FCCCD				FCCCD			
G-eff(m) %	Det(m)	Max var	Min var	G-eff(m) %	Det(m)	Max var	Min var
87.17	0.0082	6.8833	5.1333	76.5	0.0062	7.8462	3.3846
DD				DD			
G-eff(m) %	Det(m)	Max var	Min var	G-eff(m) %	Det(m)	Max var	Min var
85.7	2.58e-4	7.000	5.8333	75	2.12e-4	8.000	3.6364
ICCD				ICCD			
G-eff(m) %	Det(m)	Max var		G-eff(m) %	Det(m)	Max var	Min var
85.7	1.38e-4	6.9987	4.6625	75	1.21e-4	7.9985	3.8835

Table 3 summary

Design	Replication	G-eff (%)	Det(m)	Max Var	Min Var
FCCCD	No	**87.17**	0.0082	6.88	5.13
FCCCD	Yes	76.5	0.0062	7.85	3.38
DD	No	85.7	2.58e-4	7.00	5.83
DD	Yes	75.0	2.12e-4	8.00	3.63
ICCD	No	85.7	1.38e-4	6.99	4.66
ICCD	Yes	75.0	1.21e-4	7.99	3.88

FCCCD-Face centered central composite design
DD-Doehlert design

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ICCD-Inscribed central composite design

Discussion

Comparative Design Efficiency (with and without replication)

FCCCD (Face Centered Central Composite Design):

The Face Centered Central Composite Design without replication of axial distance was found to have High G-efficiency (87.17%) and lower max prediction variance (6.8833) and with D-optimality Det(m) of 0.0082, while without replication distance was found to have G-efficiency dropped to 76.5% with D-optimality Det(m) decreased slightly to 0.0062, but maximum variance increased to 7.8462, inferentially, the above results imply that Replication reduced G-efficiency and increased prediction variance which means that FCCCD performs better without replication.

DD (Doehlert Design):

The Doehlert Design without replication of axial distance was found to have Moderate G-efficiency (85.7%) with a Very low determinant (2.58e-4), indicating less information content, while with replication, it was found to have G-efficiency dropped to 75% and Prediction variance increased (max var from 7.000 to 8.000). the results mean that Replication worsens the prediction performance of DD. It performs better without axial point replication.

ICCD (Inscribed Central Composite Design):

The Inscribed Central Composite Design without replication of axial distance was found to have G-efficiency of 85.7% with the Prediction variance range: 4.6625 to 6.9987 and determinant Det(m) of 1.38e-4, while with replication, it was found that G-efficiency dropped to 75% with Maximum variance increased to 7.9985 and minimum variance dropped to 3.8835. These imply that ICCD follows the same trend, that is to say, replication causes a drop in G-efficiency and increases the range of prediction variance.

Impacts of axial point replication on the Design properties

Axial point replication increased prediction variance across all designs. This implies that Replicating axial points without increasing design diversity adds repeated information rather than new directional information, worsening prediction precision in unexplored regions of the design space.

D-optimality decreased with axial point replication. That is to say, the determinant of the information matrix reflects the volume of the confidence region for parameter estimates. Lower determinants imply less precise estimates.

A-optimality, measured via Tr(m), generally increased slightly or showed mixed behaviour. This implies that A-optimality reflects the average variance of the parameter estimates. An increased trace implies higher overall estimation error.

G-efficiency decreased significantly for all three designs after replication. Which means, G-efficiency measures how uniformly precise the predictions are across the design space (inverse of the worst-case prediction variance). A drop in G-efficiency implies the design is less balanced and has more extreme prediction errors at some points.

Conclusion

Replication of axial points does not improve the statistical properties of two-factor designs with a single center point. FCCCD performs best overall in terms of G-efficiency and D-optimality when not replicated. G-efficiency and determinant of the information matrix consistently decline when replication is applied, and prediction variance increases, indicating reduced model reliability. All three designs are more efficient and stable without axial point replication, especially when the number of experimental runs must be minimized.

Recommendations

The study recommended the following:

1. Avoid axial point replication in two-factor experimental designs when using a single center point, unless absolutely necessary due to process variability concerns.
2. Prefer FCCCD without replication when seeking an optimal balance between efficiency and prediction accuracy in small-scale RSM studies.
3. Future studies should explore higher-order designs or multi-center-point configurations for robustness rather than relying on replication alone.
4. Researchers should consider design-specific trade-offs based on their practical objectives (e.g., variance control vs. number of runs).

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