ConstructionofTwenty-fivePointsSecondOrderRotatableDesign in Three Dimensions using Trigonometric functions.

ABSTRACT

This study focuses on the construction of (25SOR) in Three Dimensions (3D) engaging trigonometric functions. Designing experiments in multiple dimensions is crucial for efficiently exploring complex systems and optimizing various processes. The proposed methodology utilizes trigonometric functions to generate a set of experimental points that exhibit desirable properties, such as rotatability, orthogonality, and uniformity, in the three-dimensional space. By employing trigonometric transformations, a design with twenty-five equally spaced points is constructed, ensuring the ability to conduct thorough investigations across the entire experimental region. The advantages of utilizing trigonometric functions in the design construction process include the flexibility to achieve rotational symmetry and the capability to control the distribution of points systematically. The resulting 25SOR design facilitates comprehensive experimentation and enables researchers to efficiently evaluate response surfaces and identify optimal operating conditions in three-dimensional spaces. This approach holds promise for applications in various fields, including agriculture, where the exploration of multidimensional parameter spaces is essential for enhancing performance and efficiency.

Keywords: Trigonometric functions,ResponseSurface,RotatableDesigns, 25SecondOrder.

1. INTRODUCTION

Designing experiments is a fundamental aspect of scientific inquiry across numerous disciplines, ranging from engineering and chemistry to agriculture and pharmaceuticals (Box and Draper, 1957). In many practical scenarios, researchers seek to explore complex systems and optimize processes that involve multiple factors or variables (Box and Hunter, 1957). In such cases, designing experiments in multiple dimensions becomes crucial for obtaining comprehensive insights and achieving optimal outcomes.

Atkinson (1992) presents the Second Order Rotatable Design (SOR) as a frequently employed method for developing experimental designs across multiple dimensions. SOR designs offer several desirable properties, including rotatability, orthogonality, and uniformity, making them particularly valuable for efficiently exploring response surfaces and identifying optimal operating conditions (koske,1987). These designs are especially useful in situations where the relationship between factors and responses is nonlinear or complex (Box and Draper,1963).

In recent times, there has been an increasing interest in broadening the use of SOR designs to encompass three-dimensional (3D) domains. According to Bose and draper (1959)three-dimensional experimental setups are common in various fields, such as engineering, where processes often involve interactions between multiple factors acting in different spatial

dimensions. Additionally, in fields like chemistry and pharmaceuticals, studying reactions and formulations in 3D environments is essential for understanding their behavior and optimizing their performance.
As per kosgei et al (2013) Designing experiments is a fundamental aspect of scientific inquiry across numerous disciplines, ranging from engineering and chemistry to agriculture and pharmaceuticals. In many practice.al scenarios, researchers seek to explore complex systems and optimize processes that involve multiple factors or variables (Box and Draper,1965). In such cases, designing experiments in multiple dimensions becomes crucial for obtaining comprehensive insights and achieving optimal outcomes. One promising avenue for constructing 3D SOR designs is the utilization of trigonometric functions. To Box and Draper (1980)trigonometric functions offer a versatile framework for systematically distributing points in three-dimensional space while ensuring desirable design properties. By leveraging trigonometric transformations, researchers can construct designs with predefined characteristics, such as rotational symmetry and equal spacing, thus facilitating comprehensive experimentation and efficient exploration of response surfaces.
Adekayo et al (2017), in his study highlighted the potential benefits of using second-order rotatable designs where he was able to identify optimal conditions for crop growth, reduce resource use, crop breeding and minimize environmental impacts.Ahmed et al (2017) demonstrated the utility of second-order rotatable designs in investigating the impacts of various fertilizer combinations on wheat yield.Yanis et al (2019), focused on the exploration and exploitation of second order rotatable design where they determined the optimal levels of six ingredients (soybean flour, skimmed milk powder, canola oil, brown sugar, salt, and water).
This study centers on developing a Twenty-five Points Second Order Rotatable Design (25SOR) in three dimensions through the utilization of trigonometric functions. We aim to develop a systematic methodology for generating 3D SOR designs that exhibit desirable properties, such as rotatability, orthogonality, and uniformity. By harnessing the power of trigonometric functions, we seek to provide researchers with a valuable tool for efficiently exploring complex parameter spaces and optimizing processes in three-dimensional environments.

2. MOMENTSANDNON-SINGULARITYCONDITIONS.

As per Box and Hunter (1957), a second-order response surface is attained when the design points fulfill the subsequent conditions:

$$\sum_{u=1}^{N} x_{iu}^2 = N\lambda_2$$

$$\sum_{u=1}^{N} x_{iu}^4 = 3N\lambda_4 \quad (1)$$

$$\sum_{u=1}^{N} x_{iu}^2\, x_{ju}^2 = N\lambda_4$$

$$\sum_{u=1}^{N} x_{iu}^4 = 3\sum_{u=1}^{N} x_{iu}^2\, x_{ju}^2\,, \ (i < j = 1,2, \dots k)$$

Any further computations involving powers and products up to the fourth order result in zero. A set of points is deemed to form a second-order rotatable design if it satisfies the stated conditions and if the matrix X^' X employed in the least squares estimation is non-singular. Box and Hunter (1957) illustrated that the crucial condition for this to happen is:

$$\frac{\lambda_4}{\lambda_2^2} > \frac{k}{k+2} \qquad (2)$$

3. CONSTRUCTIONOF 25 SET POINT DESIGNS

3.1 Construction of 3s – Points

Bose and Draper (1959) pioneered the incorporation of trigonometric functions in the development of second-order rotatable designs. They introduced transformations characterized by the form:

$$T_1=\begin{bmatrix} Cos\alpha, -Sin \propto , & 0 \\ sin \propto , \; cos \propto , 0 \\ 0 \quad 0 & -1 \end{bmatrix} \qquad (3)$$

and

$$T_2=\begin{bmatrix} Cos\frac{\propto}{2}, & Sin\frac{\propto}{2}, & 0 \\ sin\frac{\propto}{2}, & cos\frac{\propto}{2}, & 0 \\ 0 & 0 & -1 \end{bmatrix} \qquad (4)$$

Where $\propto = \frac{2\pi}{s}$

In the present study, these transformations are utilized to create second-order rotatable designs. The transformations outlined in equations (3) and (4) are employed on the point sets structured as G (r, 0, b), representing points on the plane where y = 0, and on all other points derived from successive applications of T_1 and T_2. The permutation group (I, W,W^2) generated by;

$$W=\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}, \qquad (5)$$

Consider a set T(r, o, b). Assuming b= 0, then T(r, o, b) becomes T(r, o, o). Applying (3) and (5) respectively on T(r,o,o) yields the following set of coordinates,

(r cos t$\alpha r sint\alpha$ 0)

(r sin t $\propto$ 0 r cos t $\propto$) (6)

$$(0 \quad r\cos t \propto \quad r\sin t \propto)$$

For t = 0, 1, 2… (s-1) and s≥5, When $S \geq 5$ set $T_0(r,0,0)$ and points (rcostα, rsintα, 0) = $3S$
The sums and products of the set up to power four for the coordinates listed in equation (6) are given by:

$$\sum_{u=1}^{N} x_{iu}^2 = sr^2,$$

$$\sum_{u=1}^{N} x_{iu}^4 = \frac{3}{4} sr^4, \qquad (7)$$

$$\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 = \frac{1}{8} sr^4,$$

The excess function for T(r,o,o) is given by;

$$\sum_{u=1}^{N} x_{iu}^4 - 3\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 = \frac{3}{8} sr^4 \qquad (8)$$

3.2FOUR POINT SET

Similarly, the co-ordinates for the four points set denoted G (a, a, a) are as listed below,

When no of points is 8 given by sets $\frac{1}{3}$ $G(a,a,a)$ and points $(\pm a, \pm a, \pm a)$ but this runs are halved.
G (a, a, a)

G (-a, a, a)

G (a, -a, a) (9)

G (a, a, -a)

The sums and products up to power four for G (a, a, a) is given by,

$$\sum_{u=1}^{N} x_{iu}^2 = 4a^2$$

$$\sum_{u=1}^{N} x_{iu}^4 = 4a^4 \qquad (10)$$

$$\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 = 4a^4$$

The excess for the above set of points is given by

$$\sum_{u=1}^{N} x_{iu}^4 - 3\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 = -8a^4 \quad (11)$$

3.3 THE SIX POINT SET

For the six points set denoted by G(c, o, o), When the number of points is 6 given by set $\frac{1}{4} G(0,0,c)$ and the points $(\pm c, 0,0)$, $(0, \pm c, 0)$, $(0,0,\pm c)$

The co-ordinates for the six points are listed as below,

G(c, o, o)

G (-c, o, o)

G (o, -c, o) (12)

G (o, c, o)

G (o, o, c)

G (o, o, -c)

The sums and products up to power four for G (c, o, o) is given by

$\sum_{u=1}^{N} x_{iu}^{2}$ =2c^2

$\sum_{u=1}^{N} x_{iu}^{4}$ =2c^4 (13)

$\sum_{u=1}^{N} x_{iu}^{2}\ x_{ju}^{2}$ =0

The excess for the above set of points is given by

$$\sum_{u=1}^{N} x_{iu}^{4} - 3\sum_{u=1}^{N} x_{iu}^{2}\ x_{ju}^{2} = 2c^4 \quad (14)$$

By augmenting specific sets of points in equations (6), (9), and (12), second-order rotatable designs in three dimensions can be obtained. The augmentation is given by $3S + \frac{1}{2}\ of$ 8+6 = $3S$+4+6. But S ≥ 5 when S =5, Combining 3s given in (6) with four-point set given in (9) and six-point set given in (12) was obtained as3s+G (a, a, a) + G(c,0,0), by letting s=5,25 points will be obtained.

3.4 Optimality Criteria for 25SOR

3.4.1 Evaluation of D-optimality criterion

The D-optimality criterion design stands as the predominant criterion in optimal designs theory. This criterion aims to minimize $|(X'X)^{-1}|$, or, conversely, maximize the determinant of the information matrix X'X of the design.
The determinant criterion $\phi(C)$ deviates from the determinant $\det(C)$ by considering s^{th} root

$$\phi(C) = \det(C)^{\frac{1}{s}} . \quad (15)$$

3.4.2 Evaluation of T-optimality criterion

This criterion maximizes the trace of the information matrix. A T-optimal design is a plan where optimality is achieved by distinguishing between two or more models, one of which is true, aiming to minimize the optimality criteria for the variance of predictions. T-optimality is achieved by utilizing the following expression: The evaluation of the trace criterion is given by

$$\phi_{-\infty}(\mathrm{C})=\frac{1}{s}trace(C) \qquad (16)$$

3.4.3 Evaluation of A-optimality criterion

The A-optimality criterion aims to reduce the trace of the inverse of the information matrix. This criterion decreases the trace of the precision matrix or maximizes the trace of the information matrix, as illustrated by the equation below.

$$\phi_{-1}(\mathrm{C})=\left(\frac{1}{s}traceC^{-1}\right)^{-1} \text{ if C is positive definite.} \qquad (17)$$

3.4.4 Evaluation of E-optimality criterion

Another design criterion is E-optimality, which focuses on minimizing the largest

eigenvalues of the dispersion matrix. E-optimality is assessed using the equation below:
The smallest eigenvalue criterion

$$\phi_{-\infty}(\mathrm{C})=\lambda_{(\min)}(C) \qquad (18)$$

3.5 Relative efficiencyfor 25SOR

3.5.1 Relative D-efficiency

Burgess (2004) describes the relative D-efficiency of a design as the absolute value of the ratio between the value of a specific D-criterion for a given design, denoted as M(ε), and the numerical value of a D-optimal design, denoted as M(ε*).

$$\left|\frac{M(\varepsilon)}{M(\varepsilon^*)}\right|. \qquad (19)$$

where

3.5.2Relative A-efficiency

A-efficiencyis achieved by using the followingequation

$$\text{Relative A-efficiency}=\frac{tr(M^{-1}(\xi^*))}{tr(M^{-1}(\xi))} \qquad (20)$$

3.5.2Relative E-efficiency

The E-optimality criteria for is given design as;

$$\text{Relative E-efficiency}=\frac{\lambda_{\min}(\xi)}{\lambda_{\min}(\xi^*)} \qquad (21)$$

3.5.3 Relative T-efficiency

The Relative T-efficiency of any design is defined as the ratio of the value of the optimal design, to the value of a specific T-design as;

$$\text{Relative T-efficiency}=\frac{tr(M\ \ (\xi^*))}{tr(M\ \ (\xi))} \qquad (22)$$

4.1Construction of 25-points set design

When $S \geq 5$ set $T_0(r, 0,0)$ and points (rcostα, rsintα, 0) = 3S

When no of points is 8 given by sets $\frac{1}{3}\ G(a, a, a)$ and points $(\pm a, \pm a, \pm a)$

When the number of points is 6 given by set $\frac{1}{4} G(0,0, c)$ and the points $(\pm c, 0,0)$, $(0, \pm c, 0)$, $(0,0, \pm c)$

The combination is given by

3S + $\frac{1}{2}$ of 8+6 = 3s+4+6

But S ≥ 5 when S =5

Then 3S+4+6= 15+4+6= 25points

The moment conditions for second order rotatable arrangement are given by

$$\sum_{u=1}^{N} x_{iu}^2 = N\lambda_2$$

$$\sum_{u=1}^{N} x_{iu}^4 = 3N\lambda_4$$

$$\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 = N\lambda_4$$

$$\sum_{u=1}^{N} x_{iu}^4 = 3\sum_{u=1}^{N} x_{iu}^2\, x_{ju}^2$$

The excess is given by

$$\sum_{u=1}^{N} x_{iu}^4 - 3\sum_{u=1}^{N} x_{iu}^2\, x_{ju}^2 = 0$$

Additionally, all other sums of powers and products up to the fourth order are zero. A set of points is considered to constitute a second-order rotatable design if the aforementioned conditions are met and the matrix used in the least square's estimation is non-singular. The non-singular necessary and sufficient condition is:

$$\frac{\lambda_4}{\lambda_2^2} > \frac{K}{K+2}$$

In this context, K denotes the number of factors. The set of twenty-five points must adhere to specific moment conditions to constitute a rotatable arrangement of second order.

3S+4+6

$$\sum_{u=1}^{25} x_{iu}^2 = \mathrm{S}r^2 + 4a^2 + 2c^2 = N\lambda_2$$

$\sum_{u=1}^{25} x_{iu}^4 = \frac{3}{4}sr^4 + 4a^4 + 2c^4 = 3N\lambda_4$

$$\sum_{u=1}^{25} x_{iu}^2 x_{ju}^2 = \frac{1}{8}sr^4 + 4a^4 = N\lambda_4$$

The excess is;

$\frac{3}{4}sr^4 + 4a^4 + 2c^4 - 3(\frac{1}{8}sr^4 + 4a^4)=0$

When s=5

$\frac{15}{4}r^4 + 4a^4 + 2c^4$ - $\frac{15}{8}r^4 + 12a^4$=0

$$\frac{15}{4}r^4 + 8a^4 + 2c^4 = 0$$

$$\frac{15r^4 - 16a^4 + 16c^4}{8} = 0$$

$$15r^4 + 16c^4 - 64a^4 = 0$$

$$15r^4 + 16c^4 = 64a^4$$

Let

$$r^2 = xa^2$$

$$c^2 = ya^2$$

$$15x^2a^4 + 16y^2a^4 = 64a^4$$

We drop a^4

$$15x^2 + 16y^2 = 64$$

When x=1

$$15 + 16y^2 = 64$$

$$16y^2 = 49$$

$$y^2 = \sqrt{\frac{49}{16}}$$

$$y = \frac{7}{4} = 1.75$$

Thus,

$$r^2 = 1a^2$$

$$c^2 = 1.75a^2$$

But

$$\sum_{u=1}^{25} x_{iu}^2 = Sr^2 + 4a^2 + 2c^2 = N\lambda_2$$

$$5a^2 + 4a^2 + 3.5a^2 = 25\lambda_2$$

$$12.5a^2 = 25\lambda_2$$

$$\lambda_2 = 0.500a^2 \qquad (23)$$

$$\sum_{u=1}^{25} x_{iu}^4 = \frac{3}{4} sr^4 + 4a^4 + 2c^4 = 3\mathrm{N}\lambda_4$$

$$\frac{15}{4} a^4 + 4a^4 + 6.125a^4 = 75\lambda_4$$

$$3.75a^4 + 4a^4 + 6.125a^4 = 75\lambda_4$$

$$13.875a^4 = 75\lambda_4$$

$$\lambda_4 = 0.185a^4 \qquad (24)$$

The condition for non-singularity in the context of second order designs is;

$$\frac{\lambda_4}{\lambda_2{}^2} > \frac{k}{k+2}$$

$$\frac{\lambda_4}{\lambda_2^2} = \frac{0.185}{(0.500)^2} = 0.74$$

$$\frac{k}{k+1} = \frac{3}{5} = 0.6$$

therefore

$$\frac{\lambda_4}{\lambda_2^2} > \frac{k}{k+2}$$

$$0.74 > 0.6$$

which satisfy the non-singularity condition for second order rotatability.

4.2 Optimality Criteria for 25SORD

The provided moment matrix pertains to a second-order rotatable design in three dimensions Substituting the values of λ_2 and λ_4 given in (23) and (24) to (25)

$$Z_2=\begin{bmatrix}1.00 & 0.50 & 0.50 & 0.50 & 0 & 0 & 0 & 0 & 0 & 0\\ 0.50 & 0.57 & 0.19 & 0.19 & 0 & 0 & 0 & 0 & 0 & 0\\ 0.50 & 0.19 & 0.57 & 0.19 & 0 & 0 & 0 & 0 & 0 & 0\\ 0.50 & 0.19 & 0.19 & 0.57 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0.50 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0.50 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0.50 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.19 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.19 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.19\end{bmatrix} \quad (25)$$

4.2.1 D-Criterion

The determinant criterion is derived by assessing the expression $\text{Det}(Z_2)^{\frac{1}{S}}$: where $Z_2$is defined as stated in equation (25), and S represents the count of parameters in the parameter system. Therefore,

$$\text{Det}(Z_2)^{\frac{1}{10}} = 0.3371216702 \quad (26)$$

4.2.2 T-Criterion

The T-criterion is obtained by evaluating $\frac{1}{S}$ trace (Z_2) where Z_2 was given in (25) and S is the number of parameters to be estimated.

Thus,

$$\frac{1}{s}\text{ trace }(Z_2) = \frac{1}{10} \times 4.78 = 0.472 \quad (27)$$

4.2.3 A-Criterion

The T-criterion is obtained by evaluating (17) where Z_2 was given in (25) and s is the number of parameters to be estimated.

Thus,

$$\frac{1}{s}\text{ trace }(Z_2)^{-1})^{-1}=0.25892233045 \quad (28)$$

4.2.4 E-Criterion

The determinant of the matrix $Z_{2(10x10)}$, Gives ten characteristic roots and by taking the smallest value from the list of Eigen values gives the E-Criterion,

Thus $eig(Z_2)$ = 0.175 (29)

4.3 Relative Efficiency for 25SOR

4.3.1 Relative D-efficiency for 25 points

Using the equation provided in (19), the D-efficiency for k=3 is expressed as follows:

$$\text{D-efficiency}=\frac{|M(\xi)|}{|M(\xi^*)|},$$

Given that M(ε^*) = 0.156705 represents the value of the optimal design and M(ε) = 0.3371216702 denotes the value of the specific design. Hence;

$$= \frac{0.3371216702}{0.156705} \times 100 = 215.1314\% . \quad (30)$$

Relative T-efficiency for 25 points

Using the formula provided in (22), the T-efficiency for k=3 is expressed as

$$\frac{\Delta_1(\varepsilon_T^*)}{\Delta_1(\varepsilon)}$$

where $\Delta_1(\varepsilon_T^*)$ = 0.274537 represents the value of the optimal design and $\Delta_1(\varepsilon)$= 0.5440474286 denotes the value of the specific design. Hence;

$$=\frac{0.274537}{0.5440474286} \times 100 = 34.20\% \quad (31)$$

Relative A-efficiency for 25 points

Applying the equation provided in (20), the relative efficiency for the C-criterion for k=3 is expressed as;

$$\text{Relative A-efficiency} = \frac{tr\,(M^{-1}(\varepsilon_A^*))}{tr\,(M^{-1}(\varepsilon))}$$

Here, the numerator value of 36.62092 represents the value of the optimal design, while the denominator holds the same value for the specific design. Hence;

$$\frac{36.62092}{36.62092} \times 100 = 100\ \% (32)$$

Relative E-efficiency for 25 points

Utilizing the equation provided in (21), the relative efficiency for the DT-criterion for k=4 is expressed as;

$$\text{Relative E-efficiency} = \frac{\boldsymbol{\lambda}_{\mathbf{min}(\mathbf{m}(\boldsymbol{\varepsilon}))}}{\boldsymbol{\lambda}_{\mathbf{min}(\mathbf{m}(\boldsymbol{\varepsilon}_{\mathbf{F}}^*))}}$$

Here, the denominator value of 0.535503991 represents the value of the optimal design, and the numerator maintains the same value for the specific design. Hence;

$$\frac{0.5355039691}{0.5355039691} \times 100 = 100\% \quad (33)$$

Conclusions

In conclusion, the construction of Twenty-five Points Second Order Rotatable Designs in Three Dimensions using trigonometric functions represents a promising avenue for enhancing experimental design methodologies. By leveraging the principles of SOR designs, researchers can systematically distribute points in three-dimensional space while ensuring desirable properties such as rotatability and uniformity. The incorporation of trigonometric functions offers a flexible framework for generating designs with predefined characteristics, facilitating comprehensive experimentation and efficient exploration of response surfaces. While current literature may be limited on this specific topic, existing knowledge in experimental design, rotatable designs, and trigonometric functions provides a foundation for further research and innovation. Moving forward, interdisciplinary collaboration and advanced computational techniques could propel the development and application of 3D SOR designs with trigonometric functions, unlocking new possibilities for optimizing processes and understanding complex systems across various domains.

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