iJRASET
International Journal For Research in Applied Science and Engineering Technology

INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY

Volume: 9 **Issue:** X **Month of publication:** October 2021

DOI: https://doi.org/10.22214/ijraset.2021.38512

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International Journal for Research in Applied Science & Engineering Technology (IJRASET)
ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.429
Volume 9 Issue X Oct 2021- Available at www.ijraset.com

A note on Variance-Sum Third Order Slope Rotatable Designs

R. Md. Mastan Shareef[1], B. Guravaiah[2], G. V. S. R. Anjaneyulu[3]
[1]*Department of Statistics, Acharya Nagarjuna University. Guntur-522510(A.P).*

Abstract: ***Response Surface Methodology (RSM) is a collection of mathematical and statistical techniques useful for analyzing experiments where the yield is believed to be influenced by one or more controllable factors. Box and Hunter (1957) introduced rotatable designs in order to explore the response surfaces. The analogue of Box-Hunter rotatability criterion is a requirement that the variance of*** $\partial\hat{y}(x)/\partial x_i$ ***be constant on circles (v=2), spheres (v=3) or hyperspheres (v ≥4) at the design origin. These estimates of the derivatives would then be equally reliable for all points*** $(x_1, x_2, \ldots, x_v)$ ***equidistant from the design origin. This property is called as slope rotatability (Hader and Park (1978)).Anjaneyulu et al (1995 &2000) introduced Third Order Slope Rotatable Designs. Anjaneyulu et al(2004) introduced and established that TOSRD(OAD) has the additional interesting property that the sum of the variance of estimates of slopes in all axial directions at any point is a function of the distance of the point from the design origin. In this paper we made an attempt to construct Variance-Sum Third Order Slope Rotatable in four levels.***

Keywords: Response Surface Methodology. Third Order Slope Rotatable Design; TOSRD (OAD), Variance-Sum Third Order Slope Rotatable Design.

I. INTRODUCTION

Box and Hunter (1957) proved that a necessary and sufficient condition for a design of order d (d=1, 2…) to be rotatable. Gardiner, Grandage and Hader (1959) constructed some third order rotatable designs for two and three factors. Das and Narasimham(1962) constructed TORDs both sequential and non-sequential, uptofifteen factors, using doubly balanced incomplete block designs and complementary BIB designs. Hader and Park (1978) introduced slope rotatability for central composite second order designs analogous to Box and Hunter (1957) central composite second order rotatable designs several authors gave various methods to construct second order slope rotatable designs. Anajaneyulu et al (1993; 1998) have introduced embedded type SOSRDs, Group-Divisible SOSRDs respectively. Anjaneyulu (1995, 2000) introduced Third Order Slope Rotatable Designs over an axial direction analogous to Third Order Rotatable Designs and constructed TOSRDs using Central Composite type Design points and Doubly Balanced Incomplete Block Designs.

Park (1987) studied the necessary and sufficient conditions for Second Order Slope RotatabilityOver All Directions.Anjaneyulu et al (2004) introduced TOSRD (OAD).Slope rotatability in axial directions introduced by Hader and Park (1978) requires that the variance of the estimated slope in every axial direction be constant at points equidistant from the design origin. Sloperotatability over all directions requires that the variance of the estimated slope averaged over all directions through a uniforms distribution be constant at points equidistant from the origin.

Anjaneyulu et al (1997) established that SOSRD (OAD) has the additional interesting property that the sum of the variances of estimates of slopes in all axial directions at any point is a function of the distance of the point from the design origin.

In this paper an attempt is made to introduce Variance – Sum Third Order Slope Rotatable Designs.

II. THIRD ORDER SLOPE ROTATABLE DESIGNS

The general Third Order Response surface is

$$Y(X) = b_0 + \sum_{i=1}^{v} b_i x_i + \sum_{i<}^{v}\sum_{j}^{v} b_{ij} x_i x_j + \sum_{i=1}^{v} b_{ii} x_i^2 + \sum_{i=1}^{v} b_{iii} x_i^3 + \sum_{i\neq}\sum_{j} b_{ijj} x_i x_j^2 + \sum_{i<}\sum_{j<}\sum_{k} b_{ijk} x_i x_j x_k + e \qquad \ldots(2.1)$$

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Where's are independent random errors with same mean zero and Variance σ^2.

Let D = $((x_{ij}))$, i= 1, 2, ,. . . ., N ; j = 1, 2, 3, . . .v , be a set of N design points to fit the Third Order Response Surface in (1.2.1) with v factors.

Let us consider the following N design points in v-factors for fitting the above surface:

		FACTORS
	1.	x_1 x_2……..……x_v
R	2.	x_{11} x_{12}……..……x_{1v}
U	3.	x_{21} x_{22}……..……x_{2v}
N	4.	x_{31} x_{32}……..……x_{3v}
S	.	……..
	.	……..
	.	……..
	N	x_{N1} x_{N2}……..……x_{Nv}

The object of the slope rotatability is to estimate the first order partial derivatives of Y(x) with respect to each of the independent variables with certain desirable criteria.

We define the slope rotatability criterion in general third order response surface design as follows:

1) *Definition of TOSRD:* A general third order response surface design D is said to be a Third Order Slope Rotatable Design (TOSRD) if from this design D, the variance of the estimate of first order partial derivative of Y (x) with respect to each of independent variable (x_i) is only a function of the distance $\left(d^2 = \sum_{i=1}^{v} x_i^2\right)$ of the point (x_1, x_2, . . . , x_v) from the origin (centre), i.e. A third order response surface design is a TOSRD if

$$v\left(\partial \hat{Y} / \partial x_i\right) = f\left(d^2\right) \quad \forall \quad i = 1,2,.....$$

A. Conditions For Third Order Slope Rotatability

The following are the conditions which the design points in D should satisfy for third order slope rotatability (cf. Anjaneyulu et al. (1995)).

1) Symmetry Conditions

All sums of products in which at least one of the x's is with an odd power are zero.

(i) $\sum x_i^2 = N\lambda_2$ = constant

(ii) $\sum x_i^4 = a N\lambda_4$ = constant

(iii) $\sum x_i^6 = b N\lambda_6$ = constant

(i) $\sum x_i^2 x_j^2 = N\lambda_2$ = constant,for i≠j

(ii) $\sum x_i^2 x^4_j = c N\lambda_4$ = constant,for i≠j

(iii) $\sum x_i^2 x_j^2 x_k^2 = N\lambda_6$ = constant, for i≠j≠k

2) Slope Rotatability Conditions

(i) c = 3

(ii) $\Delta_1[\lambda_4[\nu(5-a) - (a-3)^2] + \lambda^2_2[\nu(a-5)+4]]$

$- \Delta[2(a-1)\lambda^2_4[9a(\nu+1) - 9(\nu-1) + 3a - b]] = 0$

Where $\Delta = [(a + \nu - 1)\lambda_4 - \nu\lambda^2_2]$

$\Delta_1 = [\lambda_2\lambda_6\{b(\nu+1) - 9(\nu-1)\} - \lambda^4_2\{a^2(\nu+1) - (6a-b)(\nu-1)\}]$

(iii) $[\lambda_2\lambda_6\{\nu(b-27)\} - \lambda_4^2\{a^2\nu - 6a(\nu-2) + b(\nu-2) - 18(\nu-1)\}] = 0$

(iv) $[\lambda_2\lambda_6\{\nu(b-9)\} - \lambda_4^2\{a^2\nu - 6a(\nu-2) + b(\nu-2) - 6a\}] = 0$

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3) Non - Singularity Conditions

(i) $[\lambda_4/\lambda_2^2] > [\nu(a + \nu - 1)]$

(ii) $\left[\lambda_2\lambda_4/\lambda_4^2\right] > \dfrac{\left\{a^2(\nu+1)-(6a-b)(\nu-1)\right\}}{\left\{b(\nu+1)-9(\nu-1)\right\}}$

III. VARIANCE - SUM THIRD ORDER SLOPE ROTATABLE DESIGNS :

1) Definition (3.1): We define a Variance - Sum Third Order Slope Rotatable Design is one in which the sum of the variances of estimates of slopes of a third order response surface in all axial directions at any point is a function of the distance of the point from the design origin. That is, any symmetric Third Order Response surface Design is a Variance Sum TOSRD, if

$$\sum_{i=1}^{\nu} V\left(\frac{\partial \hat{y}}{\partial x_i}\right) = f\left(d^2\right), \text{ Where } d^2 = \sum_{i=1}^{\nu} x_i^2$$

2) Theorem (3.1): The conditions for Variance-Sum Slope Rotatability for the Symmetric Third Order Response Surface Design are the following :

A. Symmetry Conditions

All sums of products in which at least one of the x's is with an odd power are zero.

(i) $\sum x_i^2 = N\lambda_2 =$ constant

(ii) $\sum x_i^4 = a N\lambda_4 =$ constant

(iii) $\sum x_i^6 = b N\lambda_6 =$ constant

(i) $\sum x_i^2 x_j^2 = N\lambda_4 =$ constant , for $i \neq j$

(ii) $\sum x_i^2 x_j^4 = c N\lambda_4 =$ constant , for $i \neq j$

(iii) $\sum x_i^2 x_j^2 x_k^2 = N\lambda_6 =$ constant , for $i \neq j \neq k$

B. Non - Singularity Conditions

(i) $[\lambda_4/\lambda_2^2] > [\nu (a + \nu - 1)]$

(ii) $\left[\lambda_2\lambda_4/\lambda_4^2\right] > \dfrac{\left\{a^2(\nu+1)-(6a-b)(\nu-1)\right\}}{\left\{b(\nu+1)-9(\nu-1)\right\}}$

Proof: Let D = $((x_{ij}))$, i = 1, 2, ..., N ; j = 1, 2, ...,ν be a ν factor symmetric third order response surface design satisfying conditions given in the statement, to fit third order response surface .

Assume the third order response surface as follows

$$y(x) = b_0 + \sum_{i=1}^{\nu} b_i x_i + \sum_{i<j}^{\nu}\sum^{\nu} b_{ij} x_i x_j + \sum_{i=j}^{\nu} b_{ii} x_i^2 + \sum_{i=1}^{\nu} b_{iii} x_i^3 + \sum_{i\neq j}\sum b_{ijj} x_i x_j^2 + \sum\sum_{i<j<k}\sum b_{ijk} x_i x_j x_k + e$$

Where e's are independent random errors with same mean zero and Variance σ^2.

Thus we have,

$$\frac{\partial \hat{y}}{\partial x_i} = \hat{b}_i + 2\hat{b}_{ii} x_i + \sum_{j\neq i} \hat{b}_{ij} x_j + 3\hat{b}_{iii} x_i^2 + \sum\sum_{j\neq i} \hat{b}_{ijj} x_j^2$$

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$$+2\sum_{j\neq i}\sum_{j<k} b_{ijj}x_i x_j + \sum_{i<j<k}\sum b_{ijk}x_j x_k$$

$$V\left(\partial \hat{y}/\partial x_i\right) = V\left(\hat{b}_i\right) + 4x_1^2 V\left(\hat{b}_{ii}\right) + \sum_{j\neq i}^{\nu} x_j^2 V\left(\hat{b}_{ij}\right) + 9x_i^4 V\left(\hat{b}_{iii}\right)$$
$$+ \sum_{\substack{j\neq i\\ j=i}}^{\nu} x_j^4 V\left(\hat{b}_{ijj}\right) + 4\sum_{\substack{j\neq i\\ j=i}}^{\nu} x_i^2 x_j^2 V\left(\hat{b}_{iij}\right) + \sum_{j<k}^{\nu}\sum x_j^2 x_k^2 V\left(\hat{b}_{ijk}\right)$$
$$+ 6x_i^2 Cov\left(\hat{b}_i \hat{b}_{iij}\right) + 2\sum_{\substack{j\neq i\\ j=1}}^{\nu} x_i^2 Cov\left(\hat{b}_i \hat{b}_{ijj}\right)$$
$$+ 6\sum_{\substack{j\neq 1\\ j=1}}^{\nu} x_i^2 x_j^2 Cov\left(\hat{b}_{iii}\hat{b}_{ijj}\right) + 2\sum_{\substack{j\neq k\neq i\\ j<k}}^{\nu}\sum x_j^2 x_k^2 Cov\left(\hat{b}_{ijj}\hat{b}_{ikk}\right)$$

Therefore, we have,

$$\sum_{i=1}^{\nu} V\left(\partial \hat{y}/\partial x_i\right) = \sum_{i=1}^{\nu} V\left(\hat{b}_i\right) + 4\sum_{i=1}^{\nu} x_i^2 V\left(\hat{b}_{ii}\right) + \sum_{i=1}^{\nu}\left(\sum_{\substack{j\neq i\\ j=1}}^{\nu} x_j^2 V\left(\hat{b}_{ij}\right)\right)$$
$$+ 9\sum_{i=1}^{\nu} x_i^4 V\left(\hat{b}_{iii}\right) + \sum_{i=1}^{\nu}\left(\sum x_j^4 V(b_{ijj})\right)$$
$$+ 4\sum_{i=1}^{\nu}\left(\sum_{\substack{j\neq i\\ j=1}}^{\nu} x_i^2 x_j^2 V\left(\hat{b}_{iij}\right)\right) + \sum_{i=1}^{\nu}\left(\sum_{\substack{j\neq k\neq i\\ j<k}}^{\nu}\sum x_j^2 x_k^2 V\left(\hat{b}_{ijk}\right)\right)$$
$$+ 6\sum_{i=1}^{\nu} x_i^2 Cov\left(\hat{b}_i, \hat{b}_{iii}\right) + 2\sum_{i=1}^{\nu}\left(\sum_{i=1}^{\nu} x_j^2 Cov\left(\hat{b}_i, \hat{b}_{ijj}\right)\right)$$
$$+ 6\sum_{i=1}^{\nu}\left(\sum_{\substack{j\neq i\\ j=1}}^{\nu} x_i^2 x_j^2 Cov\left(\hat{b}_{iii}, \hat{b}_{ijj}\right)\right) + 2\sum_{i=1}^{\nu}\left(\sum_{\substack{j\neq k\neq i\\ j<k}}^{\nu}\sum x_j^2 x_k^2 Cov\left(\hat{b}_{ijj}, \hat{b}_{ikk}\right)\right)$$

…(4.3.4)

$$= \nu V\left(\hat{b}_i\right) + \left[4V\left(\hat{b}_i\right) + (\nu-1)V\left(\hat{b}_{ij}\right) + 6Cov\left(\hat{b}_i, \hat{b}_{iii}\right) + 2(\nu-1)Cov\left(\hat{b}_i \hat{b}_{ijj}\right)\right]\sum_{i=1}^{\nu} x_j^2$$
$$+ \left[9V\left(\hat{b}_{iii}\right) + (\nu-1)V\left(\hat{b}_{ijj}\right)\right]\left(\sum_{i=1}^{\nu} x_i^2\right)^2$$

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$$+\left[V\left(\hat{b}_{iij}\right)(4-2(\nu-1))+\frac{(\nu-i)(\nu-(i+1))}{2}V\left(\hat{b}_{ijk}\right)\right.$$

$$\left.+6Cov\left(\hat{b}_{iii},\hat{b}_{ijj}\right)+2\nu(\nu-1)(\nu-2)Cov\left(\hat{b}_{ijj},\hat{b}_{ikk}\right)-18V\left(\hat{b}_{iii}\right)\right]\sum_{\substack{i\neq \\ i,j=1}}^{\nu}\sum_{j}^{\nu}x_i^2x_j^2$$

$$=\nu V\left(\hat{b}_i\right)+\left[4V\left(\hat{b}_{ii}\right)+(\nu-1)V\left(\hat{b}_{ij}\right)+6Cov\left(\hat{b}_i,\hat{b}_{iii}\right)+2(\nu-1)Cov\left(\hat{b}_i,\hat{b}_{ijj}\right)\right]d^2$$

$$+\left[9V\left(\hat{b}_{iii}\right)+(\nu-1)V\left(\hat{b}_{ijj}\right)\right]\left[d^2\right]^2+\left[V\left(\hat{b}_{iij}\right)(4-2(\nu-1))\right.$$

$$+\frac{(\nu-i)(\nu-(i+1))}{2}V\left(\hat{b}_{ijk}\right)+6Cov\left(\hat{b}_{iii},\hat{b}_{ijj}\right)$$

$$\left.+2\nu(\nu-1)(\nu-2)Cov\left(\hat{b}_{ijj},\hat{b}_{ikk}\right)-18V\left(\hat{b}_{iii}\right)\right]d^2$$

$$= f(d^2)$$

Thus, the sum of the variances of the slopes in axial directions at any point is a function of the distance of the point from the design origin in any symmetric Third Order response surface design. Hence we call these designs as Variance – Sum TOSRD on all axial directions. Thus the conditions for Variance – Sum TOSRD are

All sums of products in which at least one of the x's is with an odd power are zero.

(i) $\sum x_i^2$	$= N\lambda_2$	= constant	for all i = 1,2,...,v	
(ii) $\sum x_i^4$	$= a\,N\lambda_4$	= constant	for all i = 1,2,..., v	
(iii) $\sum x_i^6$	$= b\,N\lambda_6$	= constant	for all i = 1,2,...,v	
(i) $\sum x_i^2 x_j^2$	$= N\lambda_4$	= constant, for i≠j	for all i = 1,...,v	j = 1,...,v
(ii) $\sum x_i^2 x^4_j$	$= c\,N\lambda_4$	=constant, for i≠j	for all i = 1,...,v	j = 1,...,v
(iii) $\sum x_i^2 x_j^2 x_k^2$	$= N\lambda_6$	= constant, for i≠j ≠ k	for all i = 1,...,v	j = 1,...,v k = 1,...,v

C. Non - Singularity Conditions

(i) $[\lambda_4/\lambda_2^2] > [\nu\,(a + \nu - 1)]$

(ii) $\left[\lambda_2\lambda_4/\lambda_4^2\right] > \dfrac{\{a^2(\nu+1)-(6a-b)(\nu-1)\}}{\{b(\nu+1)-9(\nu-1)\}}$

IV. CONSTRUCTION OF FOUR LEVEL VARIANCE-SUM THIRD ORDER SLOPE ROTATABLE DESIGNS

The four level third order slope rotatable design is constructed by combining a pair of second order rotatable designs in four levels.

The Considered Design points are

$[S(\pm\alpha,\pm\alpha,\pm\alpha,\pm\alpha,)+S(\pm\beta,\pm\beta,\pm\beta,\pm\beta)+S(\pm\Upsilon,0,0,0)+S(\pm\Upsilon_1,0,0,0)]$

α α α α

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$$
\begin{array}{cccc}
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\beta & \beta & \beta & \beta \\
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-\beta & -\beta & \beta & -\beta \\
-\beta & -\beta & -\beta & \beta \\
-\beta & -\beta & -\beta & -\beta \\
\Upsilon & 0 & 0 & 0 \\
-\Upsilon & 0 & 0 & 0 \\
0 & \Upsilon & 0 & 0 \\
0 & -\Upsilon & 0 & 0 \\
0 & 0 & \Upsilon & 0 \\
0 & 0 & -\Upsilon & 0 \\
0 & 0 & 0 & \Upsilon \\
0 & 0 & 0 & -\Upsilon \\
\Upsilon_1 & 0 & 0 & 0 \\
-\Upsilon_1 & 0 & 0 & 0 \\
0 & \Upsilon_1 & 0 & 0 \\
0 & -\Upsilon_1 & 0 & 0 \\
0 & 0 & \Upsilon_1 & 0 \\
0 & 0 & -\Upsilon_1 & 0 \\
0 & 0 & 0 & \Upsilon_1 \\
0 & 0 & 0 & -\Upsilon_1
\end{array}
\qquad (4.1)
$$

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The considered design points given us

1. $\sum x_i^2 = 16\alpha^2 + 16\beta^2 + 8\gamma^2 + 8\gamma_1^2 = N\lambda_2$.....(4.2)
2. $\sum x_i^4 = 16\alpha^2 + 16\beta^4 + 8\gamma^4 + 8\gamma_1^4 = aN\lambda_4$.....(4.3)
3. $\sum x_i^6 = 16\alpha^6 + 16\beta^6 + 8\gamma^6 + 8\gamma_1^6 = bN\lambda_6$.....(4.4)
4. $\sum x_i^2 x_j^2 = 16\alpha^4 + 16\beta^4 = N\lambda_4$.....(4.5)
5. $\sum x_i^2 x_j^4 = 16\alpha^6 + 16\beta^6 = 3N\lambda_6$.....(4.6)
6. $\sum x_i^2 x_j^2 x_k^2 = 16\alpha^6 = N\lambda_6$.....(4.7)

Where α=1, β=1.99912, γ=1.4142, γ_1=0.7471

These finally gave

$N = 48$

$\lambda_2 = 2.090509$

$\lambda_4 = 5.657286$

$\lambda_6 = 0.33334$

Solving the equation (4.3) and equation(4.4) gives values of 'a' and 'b'

a = 1.1267538

b = 68.912866

$\square = 16.46280$

$\text{var}(\hat{b}_0) = (0.422955)\sigma^2$

$\text{var}(\hat{b}_i) = (0.009965)\sigma^2$

$\text{var}(\hat{b}_{ij}) = (0.003683)\sigma^2$

$\text{var}(\hat{b}_{ii}) = (0.0016973)\sigma^2$

Where 'α' is arbitrary and has a positive value

The considered design points forms a Variance-Sum Third Order Slope Rotatable arrangement of order three for the values of the constants given in (4.7). Substituting (4.7) in non-singularity conditions gives the values of λ_2, λ_4 and λ_6 which finally satisfies the non-singularity conditions. Hence the considereddesign points forms a Variance-SumThird Order Slope Rotatable Design in fourdimensions.

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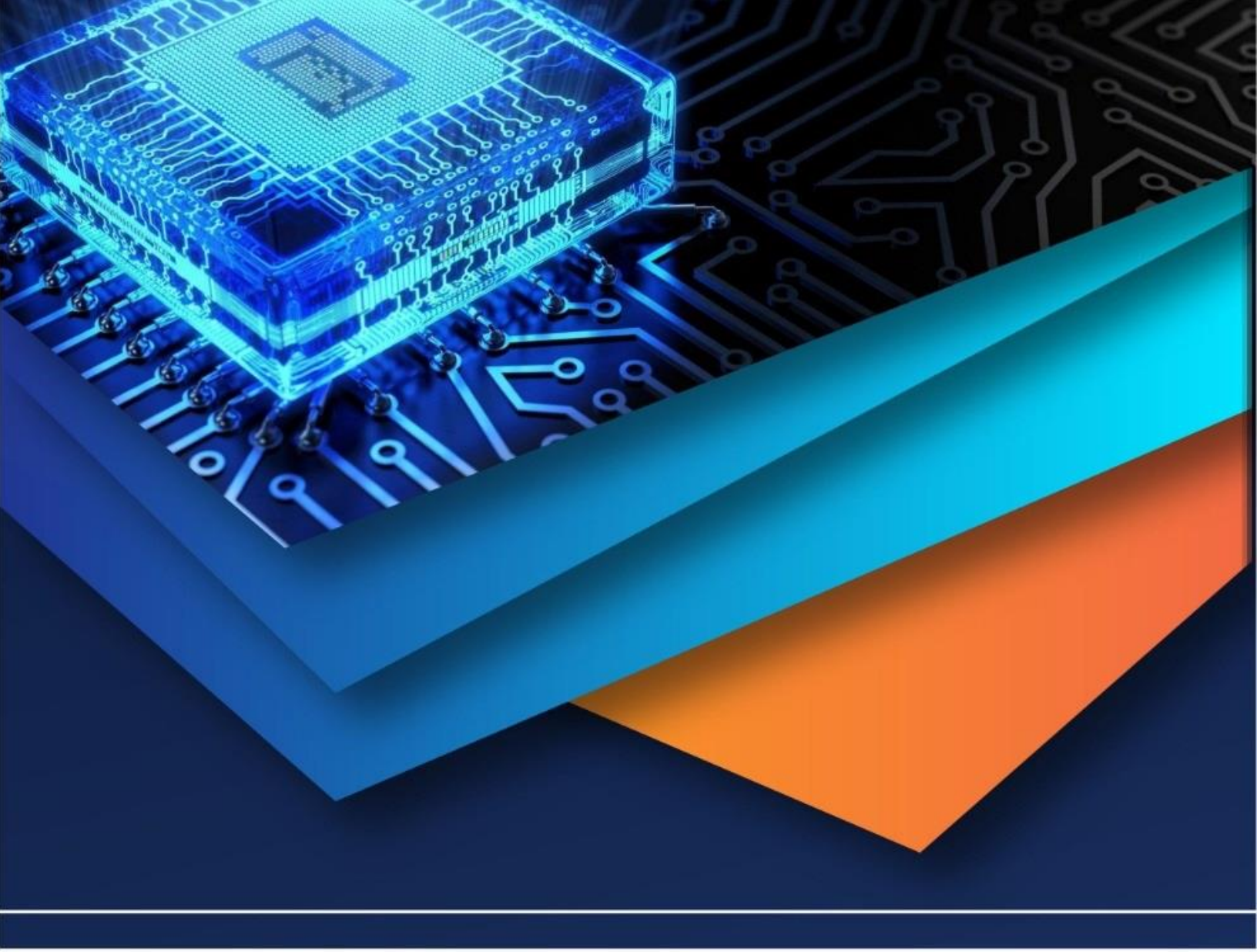

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