American Journal of Theoretical and Applied Statistics
2017; 6(6): 303-310
http://www.sciencepublishinggroup.com/j/ajtas
doi: 10.11648/j.ajtas.20170606.17
ISSN: 2326-8999 (Print); ISSN: 2326-9006 (Online)

Construction of Weighted Second Order Rotatable Simplex Designs (Wrsd)

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To cite this article:

Otieno-Roche Emily, Koske Joseph, Mutiso John. Construction of Weighted Second Order Rotatable Simplex Designs (Wrsd). *American Journal of Theoretical and Applied Statistics*. Vol. 6, No. 6, 2017, pp. 303-310. doi: 10.11648/j.ajtas.20170606.17

Received: June 2, 2017; **Accepted**: June 16, 2017; **Published**: December 7, 2017

Abstract: Response surface methodology is widely used for developing, improving, and optimizing processes in various fields. A rotatable simplex design is one of the new designs that have been suggested for fitting second-order response surface models. In this article, we present a method for constructing weighted second order rotatable simplex designs (WRSD) which are more efficient than the ordinary rotatable simplex designs (RSD). Using moment matrices based on the Simplex and Factorial Designs, and the General Equivalence Theorem (GET) for D- and A- optimality, weighted rotatable simplex designs (WRSDs) were obtained. A- and D- optimality criterion was then used to establish the efficiency of the designs.

Keywords: D – Optimal, A – Optimal, Response Surface Designs, Second-Order Designs, Information Surface, Moment Matrices, Weighted Rotatable Simplex Designs

1. Introduction

A rotatable simplex design is one of the newly introduced designs in response surface experiment. Rotatable Simplex Designs have been suggested to have a very wide usage e.g in Food science, Business performance, Health sciences, Bio-processing, Engineering, Construction Industry and so on as its performance was illustrated in Response Surface Analysis (RSA) of percentage crude oil removed by three factors. Rotatable Simplex Designs (RSDs) are constructed using the properties of a Simplex – lattice design (SLD), through Full Factorial Designs (FFDs)

Design points from SLD are used to generate the original design points for the RSD. The levels of the SLD were increased by taking all the combination levels of the original points from the SLD such that the sum of all odd moments is zero. These points were then augmented with all the combination levels of the distance from the centre point (a). Equation (1) was then solved to attain rotatability.

$$\sum t_{iu}^4 = 3 \sum t_{iu}^2 t_{ju}^2 \; for \; all \; i \neq j \tag{1}$$

where the summation in the above relations is over the design points $u = 1, 2, \ldots, N$.

The introduction of weights to RSD in this paper is for the purpose of improving the design by making it more efficient

2. Optimality Criteria and Efficiencies

Optimal designs are experimental designs that are generated based on a particular optimality criterion and are generally optimal only for a specific statistical model. The ultimate purpose of any optimality criterion is to measure the largeness of a non-negative definite $s \times s$ information matrix C.

The optimality criterion used in this study were from the family of matrix means $\emptyset_p \; for \; p = -1, 0$, introduced by Kiefer (1964) and is discussed in detail by Pukelsheim (1993).

Efficiency tests the goodness of a design.

3. Weighted Rotatable Simplex Designs

A WRSD is modified from the general RSD by separating it into Simplex and "Radius" Factorial blocks having weights α_1 and α_2 assigned to the Simplex block (τ_1) and 'Radius' factorial block (τ_2).

In this study, the rotatable WRSD will be expressed as:

$$M(\mathrm{T}) = \alpha_1 M(\tau_1) + \alpha_2 M(\tau_2) \quad (2)$$

An outline of the procedure to be used in obtaining the WRSDs is as follows:

3.1. Construction of $\{2,2\}$ *Wrsd*

The elementary RSD τ_1 and τ_2 are used to generate the WRSD T with points as given from [Table 1]

Table 1. *Design points for* $\{2,2\}$*RSD.*

t_{1u}	1	−1	0	0	½	−½	−½	½	a	$-a$	a	$-a$
t_{2u}	0	0	1	−1	½	−½	½	−½	a	a	$-a$	$-a$

Where $a = \left[\frac{3}{16}\right]^{\frac{1}{4}}$

$$\text{Thu } \tau_1 = \begin{array}{c} \begin{array}{ccc} t_{0u} & t_{1u} & t_{2u} \end{array} \\ \begin{bmatrix} 1 & 1 & 0 \\ 1 & -1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & -1 \\ 1 & \frac{1}{2} & \frac{1}{2} \\ 1 & -\frac{1}{2} & -\frac{1}{2} \\ 1 & -\frac{1}{2} & \frac{1}{2} \\ 1 & \frac{1}{2} & -\frac{1}{2} \end{bmatrix} \end{array} \text{ and } \tau_2 = \begin{array}{c} \begin{array}{ccc} t_{0u} & t_{1u} & t_{2u} \end{array} \\ \begin{bmatrix} 1 & a & a \\ 1 & -a & a \\ 1 & a & -a \\ 1 & -a & -a \end{bmatrix} \end{array} \quad (3)$$

such that, for weights $\alpha_1, \alpha_2 \geq 0$ with $\alpha_1 + \alpha_2 = 1$, the design $\mathrm{T} = \alpha_1\tau_1 + \alpha_2\tau_2$ has

$$M(\tau_1) = \frac{1}{8}\begin{bmatrix} 8 & 31_2' & 0 & 0 \\ 31_2 & \frac{9}{4}\mathrm{I}_2 + \frac{1}{4}(e_1e_2' + e_2e_1') & 0 & 0 \\ 0 & 0 & 3\mathrm{I}_2 & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{bmatrix} \quad (4)$$

and

$$M(\tau_2) = \frac{1}{4}\begin{bmatrix} 4 & (4a^2)1_2' & 0 & 0 \\ (4a^2)1_2 & (4a^4)\mathrm{J}_2 & 0 & 0 \\ 0 & 0 & (4a^2)\mathrm{I}_2 & 0 \\ 0 & 0 & 0 & 4a^4 \end{bmatrix} \quad (5)$$

So that using (4) and (5) in (2) becomes

$$M(\mathrm{T}) = \begin{bmatrix} 1 & b1_2' & 0 & 0 \\ b1_2 & c\mathrm{I}_2 + d(e_1e_2' + e_2e_1') & 0 & 0 \\ 0 & 0 & b\mathrm{I}_2 & 0 \\ 0 & 0 & 0 & d \end{bmatrix} \quad (6)$$

With its corresponding inverse as:

$$\left(M(\mathrm{T})\right)^{-1} = \begin{bmatrix} \frac{(c^2-d^2)}{|M_1|} & -\frac{b(c-d)}{|M_1|} & -\frac{b(c-d)}{|M_1|} & 0 & 0 & 0 \\ -\frac{b(c-d)}{|M_1|} & \frac{ec-b^2}{|M_1|} & \frac{b^2-ed}{|M_1|} & 0 & 0 & 0 \\ -\frac{b(c-d)}{|M_1|} & \frac{b^2-ed}{|M_1|} & \frac{ec-b^2}{|M_1|} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{b} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{b} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{d} \end{bmatrix} \quad (7)$$

where

$$b = \frac{3\alpha_1}{8} + a^2\alpha_2, \quad c = \frac{9\alpha_1}{32} + a^4\alpha_2, \quad d = \frac{\alpha_1}{32} + a^4\alpha_2 \text{ and } \quad |\boldsymbol{M_1}| = (c-d)[a(c+d) - 2b^2]$$

3.2. $\{2,2\}$ ***Optimal Designs***

Optimal designs are experimental designs that are generated based on a particular optimality criterion and are generally optimal only for a specific statistical model. Here we have used the general equivalence theorem to compute the values of the masses assigned to the design points of the RSD to obtain D-optimal and A-optimal WRSDs. Optimality measures the largeness of a non-negative definite $s \times s$ matrix C where C is the subset of M. In this study, the matrix C will be the information matrix based on the full parameter system of the model.

3.2.1. D – Optimal Wrsd

A weighted design $\eta(\alpha)$ is D-optimal for $K'(\theta)$ if and only if

$$\mathrm{trace}\left(\mathrm{C_j C}(\alpha)^{-1}\right)\begin{cases} = trace\ (C(\alpha)^0)\ for\ j \in \{1,2\} \\ < trace\ (C(\alpha)^0)\ otherwise \end{cases} \quad (8)$$

D – optimal WRSD design therefore is:

$$\mathrm{T}\left(\alpha^{(D)}\right) = \alpha_1\tau_1 + \alpha_2\tau_2 \quad (9)$$

Where the GET in (7) is used to obtain the values of α_1 and α_2 which would give a D-optimal design. i.e α_1 and α_2 are solved to satisfy

$$trace\left(M(\tau_i)\left(M(\mathrm{T})\right)^{-1}\right) = trace(M(\mathrm{T}))^0, \text{for } i = 1,2 \quad (10)$$

Thus from (4) and (7), $M(\tau_1)\left(M(\mathrm{T})\right)^{-1}$ becomes

$$\begin{bmatrix} \frac{(c-d)(-4(c+d)+3b)}{4|M_1|} & \left(\frac{(c-d)(-3+8b)}{8|M_1|}\right)1'_2 & 0 & 0 \\ \left(\frac{(c-d)[-6(c+d)+5b]}{16|M_1|}\right)1_2 & \left(\frac{-2b^2+c+d}{4|M_1|}\right)\mathrm{I}_2 + \left(-\frac{-8b^2-c+12b(c-d)+9d}{32|M_1|}\right)\mathrm{J}_2 & 0 & 0 \\ 0 & 0 & \left(\frac{3}{8b}\right)\mathrm{I}_2 & 0 \\ 0 & 0 & 0 & \frac{1}{32d} \end{bmatrix} \tag{11}$$

With its trace being

$$\frac{1}{8}\left[8\left(\frac{(c^2-d^2)}{|\boldsymbol{M_1}|}\right) + 12\left(-\frac{b(c-d)}{|\boldsymbol{M_1}|}\right) + \frac{9}{2}\left(\frac{ec-b^2}{|\boldsymbol{M_1}|}\right) + \frac{1}{2}\left(\frac{b^2-ed}{|\boldsymbol{M_1}|}\right) + \frac{6}{b} + \frac{1}{4d}\right] \tag{12}$$

and

$$trace(M(\mathrm{T}))^0 = trace\,\mathbf{I}_6 = 6 \tag{13}$$

now using (12) and (13) in (9), with $\alpha_1 + \alpha_2 = 1$, we obtain

$$\alpha_1^5 - 11.6781\alpha_1^4 - 40.7289\alpha_1^3 - 46.8974\alpha_1^2 + 16.84662\alpha_1 = 0 \tag{14}$$

This gives $\alpha_1 = 0.283748894$ for $\alpha_1 \in [0,1]$
and $\alpha_2 = 1 - 0.283748894 = 0.716251105$

Thus using (3) in (9) together with values of α_1 and α_2 from (14), the unique D – optimal moment matrix for $\{2,2\}$ WRSD is

$$\begin{pmatrix} 1 & 0.41661_2' & 0 & 0 \\ 0.41661_2 & 0.2141\mathrm{I}_2 + 0.1432(e_1e_2' + e_2e_1') & 0 & 0 \\ 0 & 0 & 0.4166\mathrm{I}_2 & 0 \\ 0 & 0 & 0 & 0.1432 \end{pmatrix} \tag{15}$$

3.2.2. A – Optimal Wrsd

A convex combination

$$\eta(\alpha) = \sum_{j=1}^{m} \alpha_j \eta_j, \tag{16}$$

with

$$\alpha = (\alpha_1, \alpha_2, \dots\dots\dots, \alpha_m)' \in \mathrm{T} \tag{17}$$

is a weighted design with weight vector α_i where

$$\sum_{i=1}^{m} \alpha_i = 1 \tag{18}$$

From the Kiefer-Wolfowitz equivalence theorem in Pukelsheim (1993), if $\eta(\alpha)$ satisfies the side condition $C_k\left(M(\eta(\alpha))\right) \in PD(s)$ and C_i written as $C_i = C_k(M(\eta_i))$ for $i = 1, \dots\dots, m,$ then, $\eta(\alpha)$ Solves the design problem i.e the θ_ρ optimal design problem if for $\rho = -1$

$$\text{Trace } C_i C_k(M(\eta(\alpha)))^{-2} = \text{trace } C_k(M(\eta(\alpha)))^{-1}\ i = 1, \dots\dots, m \tag{19}$$

Therefore, a WRSD $\eta(\alpha)$ is A-optimal if and only if (19) is satisfied

From (6), let $(M(\mathrm{T}))^{-1} = \begin{pmatrix} V^{-1} & 0 \\ 0 & W^{-1} \end{pmatrix}$ so that

$$(M(\mathrm{T}))^{-2} = \begin{pmatrix} V^{-2} & 0 \\ 0 & W^{-2} \end{pmatrix} \tag{20}$$

Where $V = \begin{pmatrix} 1 & b1_2' \\ b1_2 & c\mathrm{I}_2 + d(e_1e_2' + e_2e_1') \end{pmatrix}$ and $W = \begin{pmatrix} b\mathrm{I}_2 & 0 \\ 0 & d \end{pmatrix}$

This gives

$$V^{-1} = \begin{pmatrix} e & f1_2' \\ f1_2 & g\mathrm{I}_2 + h(e_1e_2' + e_2e_1') \end{pmatrix} \text{ and } W^{-1} = \begin{pmatrix} \frac{1}{b}\mathrm{I}_2 & 0 \\ 0 & \frac{1}{d} \end{pmatrix} \tag{21}$$

Similarly, $(V^{-1})^2 = \begin{pmatrix} 2f^2 + e^2 & f(h+g+e)1_2' \\ f(h+g+e)1_2 & (h^2 + g^2 + f^2)\mathrm{I}_2 + (2gh + f^2)(e_1e_2' + e_2e_1') \end{pmatrix}$

and

$$(W^{-1})^2 = \begin{pmatrix} \frac{1}{b^2}\mathrm{I}_2 & 0 \\ 0 & \frac{1}{d^2} \end{pmatrix} \tag{22}$$

from (21), $M(\mathrm{T})^{-2}$ then becomes

$$\begin{pmatrix} p & q1_2' & 0 & 0 \\ q1_2 & rI_2 + s(e_1e_2' + e_2e_1') & 0 & 0 \\ 0 & 0 & \frac{1}{b^2}I_2 & 0 \\ 0 & 0 & 0 & \frac{1}{d^2} \end{pmatrix} \tag{23}$$

Where

$$p = 2f^2 + e^2, \quad q = f(h+g+e), \quad r = h^2 + g^2 + f^2 \text{ and } \quad s = 2gh + f^2$$

In which;

$$e = \frac{c^2 - d^2}{|\boldsymbol{V}|}, \quad f = \frac{-b(c-d)}{|\boldsymbol{V}|}, \quad g = \frac{ac - b^2}{|\boldsymbol{V}|} \text{ and } \quad h = \frac{b^2 - ad}{|\boldsymbol{V}|}$$

Thus $M(\tau_1)(M(\mathrm{T})^{-2})$ becomes

$$\frac{1}{8}\begin{pmatrix} 8p + 6q & (8q + 3r + 3s)1_2' & 0 & 0 \\ \left(3p + \frac{10}{4}q\right)1_2 & \left(3q + \frac{9}{4}r + \frac{1}{4}s\right)I_2 + \left(3q + \frac{9}{4}s + \frac{1}{4}r\right)(e_1e_2' + e_2e_1') & 0 & 0 \\ 0 & 0 & \frac{3}{b^2}I_2 & 0 \\ 0 & 0 & 0 & \frac{1}{4d^2} \end{pmatrix} \tag{24}$$

and

$$trace\left(M(\tau_1)(M(\mathrm{T})^{-2})\right) = \frac{1}{8}\left(8p + 12q + \frac{9}{2}r + \frac{1}{2}s + \frac{6}{b^2} + \frac{1}{4d^2}\right) \tag{25}$$

$p = \frac{\alpha_1^2}{(64|V|)^2}[(6\alpha_1 + 6.9282\alpha_2)^2 + (5\alpha_1 + 6\alpha_2)^2]$

$q = \frac{\alpha_1^2}{(64|V|)^2}[(6\alpha_1 + 6.9282\alpha_2)^2[(7\alpha_1 + 6.7846\alpha_2) + (9\alpha_1 + 9.2154\alpha_2) + (5\alpha_1 + 6\alpha_2)^2]]$

with $r = \frac{\alpha_1^2}{(64|V|)^2}[(7\alpha_1 + 6.7846\alpha_2)^2 + (9\alpha_1 + 9.2154\alpha_2)^2 + (6\alpha_1 + 6.9282\alpha_2)^2]$

$s = \frac{\alpha_1^2}{(64|V|)^2}[(9\alpha_1 + 9.2154\alpha_2)(7\alpha_1 + 6.7846\alpha_2) + (6\alpha_1 + 6.9282\alpha_2)^2]$

$|V| = \frac{1}{4}\alpha_1\left[\frac{2\alpha_1^2 + 2.4308\alpha_1\alpha_2}{64}\right]$

Now from [20],

$$trace(M(\mathrm{T})^{-1}) = e + 2g + \frac{2}{b} + \frac{1}{d} \tag{26}$$

Using (25) and (26) in (19) results in

$$1 + 11.0408\alpha_1 + 18.1390\alpha_1^2 - 55.7918\alpha_1^3 - 214.6311\alpha_1^4 - 1189.2271\alpha_1^5 - 2567.6833\alpha_1^6 + 2528.7509\alpha_1^7 - 1273.3248\alpha_1^8 - 254.5424\alpha_1^9 = 0 \tag{27}$$

Which when solved within $[0, 1]$ we get $\alpha_1 = 0.279637843$
and $\alpha_2 = 1 - \alpha_1 = 0.720362156$
Hence the unique A-optimal design is

$$\eta(\alpha^{A}) = 0.279637843\tau_1 + 0.720362156\tau_2 \tag{28}$$

using (4) and (5) together with α_1 and α_2 values from (27) in (9), we have

$$\begin{pmatrix} 1 & 0.4168 1_2' & 0 & 0 \\ 0.4168 1_2 & 0.2137I_2 + 0.1438(e_1e_2' + e_2e_1') & 0 & 0 \\ 0 & 0 & 0.4168I_2 & 0 \\ 0 & 0 & 0 & 0.1438 \end{pmatrix} \tag{29}$$

the required A-optimal design.

3.3. Construction of $\{3, 2\}$ Wrsd

Similar to 3.1 above, the elementary RSD τ_1 and τ_2 are used to generate the WRSD T such that:
For weights $\alpha_1, \alpha_2 \geq 0$ with $\alpha_1 + \alpha_2 = 1$, the design $\mathrm{T} = \alpha_1\tau_1 + \alpha_2\tau_2$
Has the moment matrix (2) i.e. $M(\mathrm{T}) = \alpha_1 M(\tau_1) + \alpha_2 M(\tau_2)$
Where

$$\tau_1 = \begin{array}{c} \begin{array}{cccc} t_{0u} & t_{1u} & t_{2u} & t_{3u} \end{array} \\ \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & -1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 1 & \frac{1}{2} & \frac{1}{2} & 0 \\ 1 & -\frac{1}{2} & \frac{1}{2} & 0 \\ 1 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 1 & -\frac{1}{2} & -\frac{1}{2} & 0 \\ 1 & \frac{1}{2} & 0 & \frac{1}{2} \\ 1 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 1 & \frac{1}{2} & 0 & -\frac{1}{2} \\ 1 & -\frac{1}{2} & 0 & -\frac{1}{2} \\ 1 & 0 & \frac{1}{2} & \frac{1}{2} \\ 1 & 0 & -\frac{1}{2} & \frac{1}{2} \\ 1 & 0 & \frac{1}{2} & -\frac{1}{2} \\ 1 & 0 & -\frac{1}{2} & -\frac{1}{2} \end{bmatrix} \end{array} \text{ and } \tau_2 = \begin{array}{c} \begin{array}{cccc} t_{0u} & t_{1u} & t_{2u} & t_{3u} \end{array} \\ \begin{bmatrix} 1 & -a & -a & -a \\ 1 & -a & -a & a \\ 1 & -a & a & -a \\ 1 & -a & a & a \\ 1 & a & -a & -a \\ 1 & a & -a & a \\ 1 & a & a & -a \\ 1 & a & a & a \end{bmatrix} \end{array} \tag{30}$$

From (30) we have:

$$M(\tau_1) = \frac{1}{18}\begin{pmatrix} 18 & 4 1_3' & 0 & 0 \\ 4 1_3 & \frac{9}{4}\mathrm{I}_3 + \frac{1}{4}\mathrm{J}_3 & 0 & 0 \\ 0 & 0 & 4\mathrm{I}_3 & 0 \\ 0 & 0 & 0 & \frac{1}{4}\mathrm{I}_3 \end{pmatrix} \tag{31}$$

and

$$M(\tau_2) = \frac{1}{8}\begin{pmatrix} 8 & (8a^2)1_3' & 0 & 0 \\ (8a^2)1_3 & (8a^4)\mathrm{J}_3 & 0 & 0 \\ 0 & 0 & (8a^2)\mathrm{I}_3 & 0 \\ 0 & 0 & 0 & (8a^4)\mathrm{I}_3 \end{pmatrix} \tag{32}$$

So that (2) becomes

$$\begin{pmatrix} 1 & \left(\frac{2\alpha_1}{9} + a^2\alpha_2\right)1_3' & 0 & 0 \\ \left(\frac{2\alpha_1}{9} + a^2\alpha_2\right)1_3 & \frac{1}{8}\mathrm{I}_3 + \left(\frac{\alpha_1}{72} + a^4\alpha_2\right)\mathrm{J}_3 & 0 & 0 \\ 0 & 0 & \left(\frac{2\alpha_1}{9} + a^2\alpha_2\right)\mathrm{I}_3 & 0 \\ 0 & 0 & 0 & \left(\frac{\alpha_1}{72} + a^4\alpha_2\right)\mathrm{I}_3 \end{pmatrix} \tag{33}$$

Where $a = \left[\frac{7}{64}\right]^{\frac{1}{4}}$

3.4. $\{3,2\}$ *Optimal Designs*

Similarly, the general equivalence theorem is used to compute the values of the masses assigned to the design points of the RSD to obtain D-optimal and A-optimal WRSDs

3.4.1. D – Optimal Wrsd

D – optimal WRSD design is:

$$\eta\left(\alpha^{(D)}\right) = \alpha_1\tau_1 + \alpha_2\tau_2$$

such that:

$$M(\mathrm{T}) = \alpha_1 M(\tau_1) + \alpha_2 M(\tau_2) \tag{34}$$

Using the GET to obtain values of α_1 and α_2 which would give a D-optimal design. i.e solving α_1 and α_2 to satisfy

$$trace\left(M(\tau_i)\left(M(\mathrm{T})\right)^{-1}\right) = trace(M(\mathrm{T}))^0 \; for\; i = 1, 2 \tag{35}$$

$M(\tau_1)\left(M(\mathrm{T})\right)^{-1}$ is as in APENDIX I

$$\therefore\; trace\left(M(\tau_1)\left(M(\mathrm{T})\right)^{-1}\right)$$

$$= \frac{1}{18}\left[\frac{18(c-d)^2(c+2d)-12b(c-d)^2}{|V|} + \frac{3}{|V|}\left[\frac{5(c-d)\left[a(c+d)-2b^2\right]}{2} + \frac{(b^2-ad)(c-d)}{2} - 4b(c-d)^2\right] + \frac{12}{b} + \frac{3}{4d}\right] \tag{36}$$

and

$$trace(M(\mathrm{T}))^0 = trace\; \mathrm{I}_{10} = 10 \tag{37}$$

now using (36) and (37) in (34) with $\alpha_1 + \alpha_2 = 1$, we obtain

$$1 - 3.564144\alpha_1 + 5.924622\alpha_1^2 - 5.2839\alpha_1^3 + 3.4871\alpha_1^4 - 4.36076\alpha_1^5 + 0.5915\alpha_1^6 = 0 \tag{38}$$

This gives $\alpha_1 = 0.596127182$ for $\alpha_1 \in [0, 1]$, and $\alpha_2 = 1 - 0.596127182 = 0.403872817$

Therefore using (30) with α_1 and α_2 values from (38) in (34), the unique D – optimal moment matrix for $\{3, 2\}$ WRSD is

$$\begin{pmatrix} 1 & 0.26601_3' & 0 & 0 \\ 0.26601_3 & 0.0745\mathrm{I}_3 + 0.0525\mathrm{J}_3 & 0 & 0 \\ 0 & 0 & 0.2660\mathrm{I}_3 & 0 \\ 0 & 0 & 0 & 0.0525\mathrm{I}_3 \end{pmatrix} \tag{39}$$

3.4.2. A – Optimal Wrsd

Similarly, a WRSD $\eta(\alpha)$ is A-optimal if and only if (18) is satisfied

From (32), let $M(\mathrm{T}) = \begin{pmatrix} V & 0 \\ 0 & W \end{pmatrix}$ where;

$$V = \begin{pmatrix} 1 & \left(\frac{2\alpha_1}{9} + a^2\alpha_2\right)1_3' \\ \left(\frac{2\alpha_1}{9} + a^2\alpha_2\right)1_3 & \frac{1}{8}\mathrm{I}_3 + \left(\frac{\alpha_1}{72} + a^4\alpha_2\right)\mathrm{J}_3 \end{pmatrix} \text{ and } W = \begin{pmatrix} \left(\frac{2\alpha_1}{9} + a^2\alpha_2\right)\mathrm{I}_3 & 0 \\ 0 & \left(\frac{\alpha_1}{72} + a^4\alpha_2\right)\mathrm{I}_3 \end{pmatrix}$$

Such that

$$(M(\mathrm{T}))^{-1} = \begin{pmatrix} V^{-1} & 0 \\ 0 & W^{-1} \end{pmatrix} \text{ then } (M(\mathrm{T}))^{-2} = \begin{pmatrix} V^{-2} & 0 \\ 0 & W^{-2} \end{pmatrix} \tag{40}$$

With $V^{-1} = \begin{pmatrix} e & f1_3' \\ f1_3 & (h-g)\mathrm{I}_3 + g\mathrm{J}_3 \end{pmatrix}$ and $W^{-1} = \begin{pmatrix} \frac{1}{b}\mathrm{I}_3 & 0 \\ 0 & \frac{1}{d}\mathrm{I}_3 \end{pmatrix}$

Then

$$(V^{-1})^2 = \begin{pmatrix} 3f^2+e^2 & \big(f(2h+g+e)\big)1_3' \\ \big(f(2h+g+e)\big)1_3 & (h-g)^2\mathrm{I}_3 + (h^2+2gh+f^2)\mathrm{I}_3 \end{pmatrix} \text{ and}$$
$$(W^{-1})^2 = \begin{pmatrix} \frac{1}{b^2}\mathrm{I}_3 & 0 \\ 0 & \frac{1}{d^2}\mathrm{I}_3 \end{pmatrix} \tag{41}$$

Thus $trace\left(M(\tau_1)\left(M(\mathrm{T})\right)^{-2}\right)$ is

$$\frac{1}{18}\left[\frac{1}{|V|^2}\left\{24ef+24fg+48fh+18e^2+63f^2+3gh+\frac{15}{2}g^2+\frac{33}{2h^2}\right\}+\frac{12}{b^2}+\frac{3}{4d^2}\right] \tag{42}$$

Where

$$e=(c-d)^2(c+2d),\qquad f=-b(c-d)^2,\qquad g=(c-d)[(c+d)-2b^2],$$
$$h=(c-d)(b^2-d) \text{ and } |V|=(c-d)^2[(c+d)-2b^2]$$

With

$$b=\frac{2}{9}\alpha_1+\left(\frac{7}{64}\right)^{\frac{1}{2}}\alpha_2,\quad c=\frac{5}{36}\alpha_1+\frac{7}{64}\alpha_2 \text{ and } d=\frac{\alpha_1}{72}+\frac{7}{64}\alpha_2$$

$$\text{Now from (A2), } trace\left(M(\mathrm{T})^{-1}\right)=\frac{e}{|V|}+\frac{3g}{|V|}+\frac{3}{b}+\frac{3}{d} \tag{43}$$

Using (42) and (43) in (19) results in

$$\alpha_1^{11}-21.8288\alpha_1^{10}+44.0225\alpha_1^{9}-494.7780\alpha_1^{8}+283.3541\alpha_1^{7}-236.8855\alpha_1^{6}+233.7964\alpha_1^{5}-55.2344\alpha_1^{4}-166.1101\alpha_1^{3}+35.0103\alpha_1^{2}+0.4652\alpha_1=0 \tag{44}$$

Which when solved within $[0,1]$ we get $\alpha_1=0.219614833$
and

$$\alpha_2=1-\alpha_1=0.780385166$$

Hence the unique A-optimal design is

$$\eta(\alpha^{A})=0.219614833\eta_1+0.780385166\eta_2 \tag{45}$$

Using values of α_1 and α_2 from (44) in (30) we have;

$$\begin{pmatrix} 1 & 0.30691_3' & 0 & 0 \\ 0.30691_3 & 0.0275\mathrm{I}_3+0.0884\mathrm{J}_3 & 0 & 0 \\ 0 & 0 & 0.3069\mathrm{I}_3 & 0 \\ 0 & 0 & 0 & 0.0886\mathrm{I}_3 \end{pmatrix} \tag{46}$$

the required A-optimal design.

4. Efficiencies of the Designs

The performance of the RSD and WRSD was measured using the D- and A- criterion.

Table 2. *Optimal values.*

	Rotatable Simplex Design (RSD)		Weighted Rotatable Simplex Design (WRSD)	
Factors (k)	$D-$	$A-$	$D-$	$A-$
2	0.1908	2.5295	0.1618	0.0372
3	0.1075	4.3744	0.0258	0.0409

4.1. D - Efficiency

The performance of the WRSD in comparison to the RSD is measured by the D-efficiency which is defined by $(\tau)=\left\{\frac{|M(\tau)|}{|M(\tau^0)|}\right\}^{\frac{1}{s}}$. Using the D- optimal $\emptyset_0(C_k(M))$ values for the two designs from Table 1, the D – Efficiency values are:

Table 3. *D – Efficiency values.*

Design Factors	Rotatable Simplex Design (RSD)	Weighted Rotatable Simplex Design (WRSD)	D - efficiency $D_{eff}(\eta^*)$
2	0.1908	0.1618	0.8480
3	0.1075	0.0258	0.24

From the efficiencies, it is noted that the WRSD is 15.2% more D - efficient for two factors and 76% more D - efficient for three factors.

4.2. A - Efficiency

Similarly the A – optimal $\emptyset_{-1}(C_k(M))$ values for the two designs from Table 1 are used to obtain the A – Efficiency values as $\frac{\emptyset_{-1}(C_1)}{\emptyset_{-1}(C_2)} = \frac{\left(\frac{1}{s}\,traceC_1{}^{-1}\right)^{-1}}{\left(\frac{1}{s}\,traceC_2{}^{-1}\right)^{-1}}$:

Table 4. *A – Efficiency values.*

Design Factors	Rotatable Simplex Design (RSD)	Weighted Rotatable Simplex Design (WRSD)	A – efficiency $A_{eff}(\eta^*)$
2	2.5295	0.0372	0.0147
3	4.3744	0.0409	0.0093

From the efficiencies, it is also noted that the WRSD is 98.53% more A - efficient for two factors and 99.07% more A - efficient for three factors.

5. Conclusion

In this study, we have presented a method for constructing a WRSD. The constructed design has achieved estimation efficiency as shown by the results in relation to their moment matrices. These designs have also proved to be D- and A-optimal.

Appendix

I. Matrices for $\{3, 2\}$ RSD A - Optimality

$M(\tau_1)\left(M(\mathrm{T})\right)^{-1}$ for $\{3, 2\}$ RSD

$$M(\tau_1)\left(M(\mathrm{T})\right)^{-1} = \frac{1}{18}\begin{bmatrix} 18 & 41_2' & 0 & 0 \\ 41_2 & \frac{9}{4}\mathrm{I}_3 + \frac{1}{4}\mathrm{J}_3 & 0 & 0 \\ 0 & 0 & 4\mathrm{I}_3 & 0 \\ 0 & 0 & 0 & \frac{1}{4}\mathrm{I}_3 \end{bmatrix}\begin{bmatrix} V^{-1} & 0 \\ 0 & W^{-1} \end{bmatrix} \tag{A1}$$

Where

$$V^{-1} = \begin{pmatrix} (c-d)^2(c+2d) & (-b(c-d)^2)1_3' \\ (-b(c-d)^2)1_3 & |V|\mathrm{I}_3 + (c-d)(b^2-ad)\mathrm{J}_3 \end{pmatrix}$$

With

$$|V| = (c-d)^2[a(c+2d) - 3b^2] \text{ and } \quad W^{-1} = \begin{pmatrix} \frac{1}{b}\mathrm{I}_3 & 0 \\ 0 & \frac{1}{d}\mathrm{I}_3 \end{pmatrix} \tag{A2}$$

References

[1] Box, G. E. P., & Draper, N. R. (1959). A basis for the selection of a response surface design. *Journal of American Statistical Association, 54*, 622-654.

[2] Das, M. N., & Narasimham, V. L. (1962). Construction of rotatable designs through balanced incomplete block designs. *Annals of Mathematical Statistics*, *33*(4), 1421-1439.

[3] Das, R. N. (1997). Robust second order rotatable designs: Part I RSORD. *Calcutta Statistical Association Bulletin*, *47*, 199-214.

[4] Das, R. N. (1999). Robust Second Order Rotatable Designs: Part - II RSORD. *Calcutta Statistical Association Bulletin*, *49*, 65-76.

[5] Otieno-Roche E., Koske J. & Mutiso J. (2017). Construction of Second Order Rotatable Simplex Designs. *Manuscript submitted for publication.*

[6] Panda, R. N., & Das, R. N. (1994). First order rotatable designs with correlated errors. *Calcutta Statistical Association Bulletin*, *44*, 83-101.

[7] Rajyalakshmi, K., & Victorbabu B. R. (2014). Construction of second order rotatable designs under tri-diagonal correlation structure of errors using central composite designs. *Journal of Statistics: Advances in Theory and Applications*, *11*(2), 71-90.

[8] Rajyalakshmi, K., & Victorbabu, B. R. (2011). Robust Second Order Rotatable Central Composite Designs. *JP Journal of Fundamental and Applied Statistics*, *1*(2), 85-102.

[9] Tyagi, B. N. (1964). Construction of second order and third order rotatable designs through pairwise balanced designs and doubly balanced designs. *Calcutta Statistical Association Bulletin*, *13*, 150-162.

[10] Victorbabu, B. R., & Rajyalakshmi, K. (2012). A new method of construction of robust second order rotatable designs using balanced incomplete block designs. *Open Journal of Statistics*, *2*(2), 88-96.

[11] Victorbabu, B. R., & Rajyalakshmi, K. (2012). Robust second order slope rotatable designs using balanced incomplete block designs. *Open Journal of Statistics, 2*(2), 65-77.