# A-D -T optimal four factor central composite design with application in a germination of Melia Vonkesii experiment

Okango A.A\*, Koske J, Kasina M.M and Kabue T University of Eldoret, Department of Mathematics and Computer Science, P.O. Box 1125-30100, Eldoret Kenya \*Corresponding author: anapapaa@yahoo.com;

#### Abstract

This paper discusses a four factor central composite design. The efficiency of the general rotatable design is compared to the A-D-T optimal ones. As an application of the theory a detailed illustration is made on the germination of Melia Volkensii experiment.

**Keywords:** Central composite design, Rotatability, A-D-T optimality, Weights.

### Introduction

The central composite design (CCD) was introduced by (Box and Wilson, 1951). It is commonly used to study second order designs. These designs are mixtures of three building blocks: cubes, stars and center points. Consider the case where an experiment consists of m factors  $x_1, x_2, ..., x_m$ . The cube portion is a  $2^{m-h}$  fractional factorial design. If it is replicated n<sub>c</sub> times, then it is a design for sample size  $2^{m-h}n_c$ . The star portion takes one observation at each of the vectors

29 \_\_\_\_\_

 $\pm \alpha e_i$  for i \le m, for some beingstarthei- th radius  $e_i$ Euclidean unit vector. For  $n_s$  replications, the star portion is a design for sample size  $2mn_s$ . The center point portion is the one point design in 0 being replicated  $n_o$  times (Pukelsheim, 2006). Therefore the central composite design is for sample size  $n = 2^{m-h}n_c + 2mn_s + n_o$ .

CCDs have been widely studied. (Box and Hunter, 1957) developed the notion of design rotatability. A design is said to be rotatable when the variance is a function only of the distance from the center of the design and not a function of the direction. (Box and Draper, 1963) proposed several criteria which can be used in design selection. (Myers, 1976) suggested optimal CCDs under several criteria. The concept of slope-rotatable CCDs was discussed by (Hader and Park, 1978). (Myers and Montgomery, 2002) discussed the efficiency of experimental designs and compared the CCD with other designs under D-, A- and E- optimality criterion.

This paper focuses on a four factor rotatable CCD. In Section 2 we discuss the concept of rotatability and the criteria for obtaining the A-, D-, T- designs from a general CCD. In Section 3 results on Optimal CCDs under the A-, D-, T- criteria are presented together with their respective efficiencies. An application of a four factor CCD in the germination of *Melia Volkensii* experiment is given in section 4. Finally in Section 5 some conclusions and recommendations are made on the use of a four factor CCD.

### The Central Composite Design

The central composite design is commonly used to fit the second order response surface model of the form:

$$y_{u} = \beta_{0} + \sum_{i=1}^{m} \beta_{i} x_{iu} + \sum_{i=1}^{m} \beta_{ii} x_{iu}^{2} + \sum_{i
(1)$$

where  $x_{iu}$  is the value of the variable  $x_i$  at the *u*th experimental point and  $\varepsilon_u's$  are uncorrelated random errors with mean zero and variance  $\sigma^2$ 

For a central composite design, the  $x_{iu}$ 's satisfy the following conditions

(A) 
$$\sum_{u=1}^{N} \left\{ \prod_{u=1}^{m} x_{iu}^{\pi_i} \right\} = 0$$
 if any  $\pi_i$  is odd, for  $\pi_i = 0, 1, 2, 3$  and  $\sum \pi_i < 4$   
(B)  $\sum_{u=1}^{N} x_{iu}^2 = n_c 2^{m-h} + 2n_s \alpha^2$   
(C)  $\sum_{u=1}^{N} x_{iu}^4 = n_c 2^{m-h} + 2n_s \alpha^4$   
(D)  $\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 = n_c 2^{m-h}$ 
(2)

(Box and Hunter, 1957) gave the condition that a CCD must satisfy to be rotatable as

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

This gives

$$\alpha^4 = \frac{2^{m-h}n_c}{n_s}$$

(4)

For N regression vectors  $x_1, x_2, ..., x_N$  the detailed contents of the second order design matrix is given by the matrix X below made up with  $x_1, x_2, ..., x_N$  as the rows.

$$X = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & \dots & x_{m1} & x_{11}^2 & x_{11}x_{21} & \dots & x_{m-1,1}x_{m1} \\ 1 & x_{12} & \dots & x_{m2} & x_{12}^2 & x_{12}x_{22} & \dots & x_{m-1,2}x_{m2} \\ \vdots & \vdots & \dots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{1N} & \dots & x_{mN} & x_{1N}^2 & x_{1N}x_{2N} & \dots & x_{m-1,N}x_{mn} \end{bmatrix}$$
(5)

A central composite design can be made better by varying the proportion that a particular regression vector is run. In the simplest case all the regression vectors have uniform weights implying they are run an equal number of times.

Given an s\*s matrix *C*, the matrix means are defined by:

$$\phi_{p}(C) = \begin{cases} \lambda_{max}(C) & \text{for } p = \infty \\ \left(\frac{1}{s} \operatorname{trace} C^{p}\right)^{1/p} & \text{for } p \neq 0, \pm \infty \\ (\det C)^{1/s} & \text{for } p = 0 \\ \lambda_{min}(C) & \text{for } p = -\infty \end{cases}$$
(6)

The matrix means constitute the D-, A-, E- and T- criterion for design optimality with the value of p being respectively 0, -1,  $-\infty$  and 1.

(Pukelsheim, 2006) gives a method for finding optimal weights as follows;

For the matrix means  $\phi_p$ , with parameter  $p \in (-\infty; 1]$  the optimal weights satisfy

$$w_i = \frac{\sqrt{b_{ii}}}{\sum_{j \le N} \sqrt{b_{jj}}} \text{ for all } i = 1, ..., N$$
(7)

Where  $\mathbf{b_{11}}, \dots, \mathbf{b_{NN}}$  are the diagonal elements of the matrix  $B = UC^{p+1}U'$ ,  $U = (XX')^{-1}XK$ , C is the information matrix, K is the coefficient matrix and the N regression vectors  $x_1, x_2, \dots, x_N$  form the rows of the matrix X.

The optimal value is given by:

$$v(\phi_p) = \left(\frac{1}{s} \operatorname{trace} C^p\right)^{1/p} = \left(\frac{1}{s} \left(\sum_{j \le N} \sqrt{b_{jj}}\right)^2\right)^{1/p} \text{ if } p \neq 0$$
(8)

# Application to the Four Factor Rotatable Central Composite Design

Consider the case where m = 4, h = 0,  $n_c = n_s = n_o =$ 

1. The second order response surface is given by:  $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \beta_{44} x_4^2 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{14} x_1 x_4 + \beta_{23} x_2 x_3 + \beta_{24} x_2 x_4 + \beta_{34} x_3 x_4 + \varepsilon$ 

For the CCD to be rotatable the value of  $\alpha$  is computed using (4). This gives  $\alpha = 2$ .

The four factor CCD design matrix X for the second order model is shown in table 1.

# Table 1: Design Matrix for a Four Factor Rotatable CentralComposite Design

Vector	xo	<i>x</i> <sub>1</sub>	<b>x</b> <sub>2</sub>	<i>x</i> <sub>3</sub>	<i>x</i> 4	$x_1^2$	$x_1 x_2$	x1 x3	x1 x4	22	x2 x3	x2 x4	x23	x3 x4	x
1	1	-1	-1	-1	-1	1	1	1	1	1	1	1	1	1	1
2	1	1	-1	-1	-1	1	-1	-1	-1	1	1	1	1	1	1
3	1	-1	1	-1	-1	1	-1	1	1	1	-1	-1	1	1	1
4	1	1	1	-1	-1	1	1	-1	-1	1	-1	-1	1	1	1
5	1	-1	-1	1	-1	1	1	-1	1	1	-1	1	1	-1	1
6	1	1	-1	1	-1	1	-1	1	-1	1	-1	1	1	-1	1
7	1	-1	1	1	-1	1	-1	-1	1	1	1	-1	1	-1	1
8	1	1	1	1	-1	1	1	1	-1	1	1	-1	1	-1	1
9	1	-1	-1	-1	1	1	1	1	-1	1	1	-1	1	-1	1
10	1	1	-1	-1	1	1	-1	-1	1	1	1	-1	1	-1	1
11	1	-1	1	-1	1	1	-1	1	-1	1	-1	1	1	-1	1
12	1	1	1	-1	1	1	1	-1	1	1	-1	1	1	-1	1
13	1	-1	-1	1	1	1	1	-1	-1	1	-1	-1	1	1	1
14	1	1	-1	1	1	1	-1	1	1	1	-1	-1	1	1	1
15	1	-1	1	1	1	1	-1	-1	-1	1	1	1	1	1	1
16	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
17	1	-2	0	0	0	4	0	0	0	0	0	0	0	0	0
18	1	2	0	0	0	4	0	0	0	0	0	0	0	0	0
19	1	0	-2	0	0	0	0	0	0	4	0	0	0	0	0
20	1	0	2	0	0	0	0	0	0	4	0	0	0	0	0
21	1	0	0	-2	0	0	0	0	0	0	0	0	4	0	0
22	1	0	0	2	0	0	0	0	0	0	0	0	4	0	0
23	1	0	0	0	-2	0	0	0	0	0	0	0	0	0	4
24	1	0	0	0	2	0	0	0	0	0	0	0	0	0	4
25	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0

The moment matrix for the general design depicted in table 1 above  $M_G = \frac{X/X}{N}$  is given below.

10<sup>th</sup> AIC Symposium 1: Peer Reviewed Papers

	[25	0	0	0	0	24	0	0	0	24	0	0	24	0	24
	0	24	0	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	24	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	24	0	0	0	0	0	0	0	0	0	0	0
$M_G = \frac{1}{2r}$	0	0	0	0	24	0	0	0	0	0	0	0	0	0	0
	24	0	0	0	0	48	0	0	0	16	0	0	16	0	16
	0	0	0	0	0	0	16	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	16	0	0	0	0	0	0	0
<sup>4</sup> <sup>G</sup> 25	0	0	0	0	0	0	0	0	16	0	0	0	0	0	0
	24	0	0	0	0	16	0	0	0	48	0	0	16	0	16
	0	0	0	0	0	0	0	0	0	0	16	0	0	0	0
	0	0	0	0	0	0	0	0	0	0	0	16	0	0	0
	24	0	0	0	0	16	0	0	0	16	0	0	48	0	16
	0	0	0	0	0	0	0	0	0	0	0	0	0	16	0
	124	0	0	0	0	16	0	0	0	16	0	0	16	0	48-

The optimal values with respect to the D-, A-, E- and T- criterion are computed using (8) with  $C = M_G$  and are given in table 2 below.

# Table 2: D-, A-, E- and T- Optimal Values for the General FourFactor CCD

D	Α	Е	Т
0.7672656	0.3164835	0.0319464	1.090667

The general four factor rotatable CCD can be modified by varying the  $n_0$ , the number of times that the center point is replicated. The effect of this variation on the D-, A-, E- and T- optimal values is shown in table 3.

The table indicates the changes in the D-, A-, E- and T- optimal values as the number of times the center point,  $n_0$  is replicated. For D-Optimality, the optimal value peaks at  $n_0=2$ . For A-Optimality, the optimal values increases from  $n_0=1$  achieving a maximum value at  $n_0=7$  before starting to decrease. For E-Optimality, the optimal value increases steadily achieving a maximum at  $n_0=21$ . For T-

Optimality the optimal value continuously decreases as  $n_0$  increases. Thus the maximum is where  $n_0=0$ .

no	D	Α	Е	Т
0	-	-	-	1.1333330
1	0.7672656	0.3164835	0.0319464	1.0906670
2	0.7726469	0.4539723	0.0613313	1.0512820
3	0.7644165	0.5228758	0.0884377	1.0148150
4	0.7513894	0.5590062	0.1135084	0.9809524
5	0.7363525	0.5773857	0.1367525	0.9494253
6	0.7205120	0.5853659	0.1583512	0.9200000
7	0.7044723	0.5869337	0.1784625	0.8924731
8	0.6885599	0.5844156	0.1972244	0.8666667
9	0.6729580	0.5792438	0.2147583	0.8424242
10	0.6577691	0.5723370	0.2311712	0.8196078
11	0.6430487	0.5643035	0.2465581	0.7980952
12	0.6288233	0.5555556	0.2610031	0.7777778
13	0.6151017	0.5463779	0.2745815	0.7585586
14	0.6018811	0.5369700	0.2873605	0.7403509
15	0.5891518	0.5274725	0.2994005	0.7230769
16	0.5768998	0.5179856	0.3107556	0.7066667
17	0.5651085	0.5085802	0.3214750	0.6910569
18	0.5537596	0.4993065	0.3316029	0.6761905
19	0.5428346	0.4901996	0.3411795	0.6620155
20	0.5323146	0.4812834	0.3502414	0.6484848
21	0.5221811	0.4725738	0.3555556	0.6355556
22	0.5124161	0.4640806	0.3478261	0.6231884
23	0.5030020	0.4558091	0.3404255	0.6113475

Table 3: Effect of n<sub>0</sub> on D-, A-, E- and T- Optimal Values

24	0.4939222	0.4477612	0.3333333	0.6000000
25	0.4851607	0.4399365	0.3265306	0.5891156
26	0.4767023	0.4323326	0.3200000	0.5786667

10<sup>th</sup> AIC Symposium 1: Peer Reviewed Papers

Figure 1 illustrates the effect of the number of times the center point is replicated on the D-, A-, E- and T- optimal values. It shows that the optimal value is a decreasing function of  $n_0$  for T- optimality. For the other criterion the highest optimal value can be directly read from the figure. This value can then be used by an experimenter to achieve an optimal design with respect to the selected criterion.

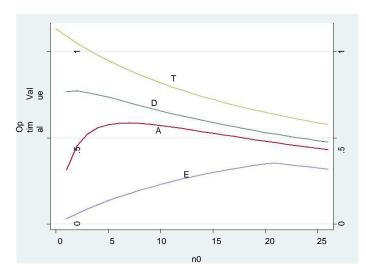


Figure 1: Effect of no on D-, A-, E- and T- Optimal Values

#### **A-Optimal Design**

In this case p = -1. The A-Optimal weights are computed using equation (7) with

B = UU',  $U = (XX')^{-1}X_{and} K = I$ . The optimal weights are 0.03488366, 0.02746118 and 0.22217191 for the cubic, star and center point parts respectively of the general central composite design. In practice these weights can be approximately achieved by setting  $n_c = 4$ ,

 $n_s=3$  and  $n_o=22$ . The A-Optimal design will therefore be of sample size 110. The associated A-Optimal moment matrix is defined by  $M_{Abelow}$ .

	r110	0	0	0	0	88	0	0	0	88	0	0	88	0	88 ]
	0	88	0	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	88	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	88	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	88	0	0	0	0	0	0	0	0	0	0
	88	0	0	0	0	160	0	0	0	64	0	0	64	0	64
1	0	0	0	0	0	0	64	0	0	0	0	0	0	0	0
$M_A = \frac{1}{110}$	0	0	0	0	0	0	0	64	0	0	0	0	0	0	0
110	0	0	0	0	0	0	0	0	64	0	0	0	0	0	0
	88	0	0	0	0	64	0	0	0	160	0	0	64	0	64
	0	0	0	0	0	0	0	0	0	0	64	0	0	0	0
	0	0	0	0	0	0	0	0	0	0	0	64	0	0	0
	88	0	0	0	0	64	0	0	0	64	0	0	160	0	64
	0	0	0	0	0	0	0	0	0	0	0	0	0	64	0
	L 88	0	0	0	0	64	0	0	0	64	0	0	64	0	160

The A-Optimal value is 0.5925926. The A-Optimal value for the general design was found to be 0.3164835. This represents an efficiency of 53.41% of the general design compared to the A-Optimal one.

# **D-Optimal Design**

In this case p = 0. The D-Optimal weights are computed using equation (7) with

B = UCU',  $U = (XX')^{-1}X_{and} K = I$ . The optimal weights are 0.03951116, 0.03951116 and 0.05173225 for the cubic, star and center point parts respectively of the general central composite design. In practice these weights can be approximately achieved by setting  $n_c = 2$ ,  $n_s=2$  and  $n_o=3$ . The D-Optimal design will therefore be of sample size 51. The associated D-Optimal moment matrix is defined by  $M_D$  below.

	۲ <b>5</b> 1	0	0	0	0	48	0	0	0	48	0	0	48	0	481
	0	48	0	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	48	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	48	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	48	0	0	0	0	0	0	0	0	0	0
	48	0	0	0	0	96	0	0	0	32	0	0	32	0	32
1	0	0	0	0	0	0	32	0	0	0	0	0	0	0	0
$M_D = \frac{1}{1}$	0	0	0	0	0	0	0	32	0	0	0	0	0	0	0
<i>b</i> 51	0	0	0	0	0	0	0	0	32	0	0	0	0	0	0
	48	0	0	0	0	32	0	0	0	96	0	0	32	0	32
	0	0	0	0	0	0	0	0	0	0	32	0	0	0	0
	0	0	0	0	0	0	0	0	0	0	0	32	0	0	0
	48	0	0	0	0	32	0	0	0	32	0	0	96	0	32
	0	0	0	0	0	0	0	0	0	0	0	0	0	32	0
	L48	0	0	0	0	32	0	0	0	32	0	0	32	0	96-

The D-optimal value is 0.7728318. The D-Optimal value for the general design was found to be 0.7672656. This represents an efficiency of 99.28% of the general design compared to the D-Optimal one.

## **T-Optimal Design**

In this case p = 1. The T-Optimal weights are computed using equation (7) with

 $B = UC^2U'$ ,  $U = (XX')^{-1}X$  and K = I. The optimal weights are 0.03887431, 0.04599671 and 0.0100373 for the cubic, star and center point parts respectively of the general central composite design. In practice these weights can be approximately achieved by setting  $n_c = 4$ ,

 $n_s=5$  and  $n_o=1$ . The T-Optimal design will therefore be of sample size 105. The associated T-Optimal moment matrix is defined by  $M_T$  below.

MT															
	r105	0	0	0	0	104	0	0	0	104	0	0	104	0	1047
	0	104	0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	104	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	104	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	104	0	0	0	0	0	0	0	0	0	0
	104	0	0	0	0	224	0	0	0	64	0	0	64	0	64
	0	0	0	0	0	0	64	0	0	0	0	0	0	0	0
= 105	0	0	0	0	0	0	0	64	0	0	0	0	0	0	0
105	0	0	0	0	0	0	0	0	64	0	0	0	0	0	0
	104	0	0	0	0	64	0	0	0	224	0	0	64	0	64
	0	0	0	0	0	0	0	0	0	0	64	0	0	0	0
	0	0	0	0	0	0	0	0	0	0	0	64	0	0	0
	104	0	0	0	0	64	0	0	0	64	0	0	224	0	64
	0	0	0	0	0	0	0	0	0	0	0	0	0	64	0
	L104	0	0	0	0	64	0	0	0	64	0	0	64	0	224

The T-Optimal Value is 1.143492. The T-Optimal value for the general design was found to be 1.090667. This represents an efficiency of 95.38% of the general design compared to the T-Optimal one.

#### Application to the Germination of Melia Volkensii Experiment

A four factor rotatable central composite design is used in this experiment. The factors under investigation are temperature, soil PH, chemical concentration and length of time of seed pre-treatment. Four different chemicals are be used. This are; Sulphuric Acid (H<sub>2</sub>SO<sub>4</sub>), Gibberellic Acid (GA<sub>3</sub>), Hydrogen Peroxide (H<sub>2</sub>O<sub>2</sub>), Potassium Nitrate (KNO<sub>3</sub>). The chemical concentrations will be unique to each chemical but will be set as per the requirements of the design. However temperature, soil PH and length of seed pre-treatment will be uniform among all the chemicals. The coded values in conformity to the design and the corresponding raw actual value setting are summarized in table 4.

Table 4. Coded	Variable Setting	and Corres	ponding Actual
Values			

Coded	Temperature	Soil	Pre-treatment	Chemical Concentration (%)						
Value		PH	Time (Hours)	H.SO.	GA;	H:0:	KNO;			
-2	20.0	3.0	4.0	20.0	0.01	1.0	0.1			
-1	35.0	5.0	6.0	35.0	0.02	2.0	0.2			
0	50.0	7.0	8.0	50.0	0.03	3.0	0.3			
1	65.0	9.0	10.0	65.0	0.04	4.0	0.4			
2	80.0	11.0	12.0	80.0	0.05	5.0	0.5			

The experiment is performed by placing 20 seeds in a petri-dish and subjected to each of the condition specified in table 2 for the four

factors  $x_1, x_2, x_3$  and  $x_4$  with the associated raw values transformation illustrated in table 4 above. The outcome is the number of seeds that germinate in a particular petri-dish.

To satisfy the conditions for A-D-T optimality, for each of the four chemicals the cubic part of the design is replicated 5 times, the star portion is replicated 5 times and the center point is replicated 25 times. The entire experiment therefore consists of 580 runs.

## Conclusion

A rotatable factor four central composite design has been presented. Suggestions have been made on improvements of this design with respect to A-D-T optimality. It was found that the improved designs had better efficiency with respect to the respective optimality criteria. An application to a germination of Melia Volkensii Experiment has been given. The application can be extended to any four factor experiment provided appropriate coded value and raw value transformations are made.

#### References

- Box, G.E.P. and Draper, N.R. (1963), The *Choice of a Second* Order Rotatable Design, Biometrika, 50, 335-352.
- Box, G.E.P. and Hunter, J.S. (1957), *Multifactor Experimental* Design for Exploring Response Surfaces, Annals Mathematical Statistics, 28,195-241.
- Box, G. E. P., and Wilson, K. B. (1951), On the Experimental Attainment of Optimum Conditions, Journal of the Royal Statistical Society, Series B, 13, 1–45.
- Hader, R.J. and Park, S.H. (1978), *Slope-Rotatable Central Composite Designs*, Technometrics, 20, 413-417.
- Myers, R.H. (1976), *Response Surface Methodology*, Blacksburg : VA.
- Myers, R.H. and Montgomery, D.C. (2002), *Response Surface Methodology: Process and Product Optimization Using Designed Experiments (2nd ed.)*, John Wiley & Sons, Inc.
- Pukelsheim, F. (2006), *Optimal Design of Experiments*, Society for Industrial and Applied Mathematics