

COMPARISON OF MIXTURE EXPERIMENTS MODELS (A BOOTSTRAP SIMULATION APPROACH)

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Abstract

The study investigates the various mixture experiment model and proposed a new polynomial model which is a modified special cubic model. The models were examined via a bootstrap resampling scheme and select model based on bias, AIC, BIC and standard error criteria. The study observed that the modified special cubic model was the second best most using AIC criterion.

Introduction

The task of optimizing mixtures commonly occurs in food processing, refining, or the manufacturing of chemicals industries. The mixtures of components must be sum to a constant for instance to optimize the taste of a fruit-punch consisting the juices of 5 fruits then the sum of the proportions of all fruits in each mixture must be 100%. A number of designs have been developed to address specifically the analysis and modeling of mixtures experiments Cornell (1990a, 1990b), Cornell and Khuri (1987), Deming and Morgan (1993), Montgomery (1991).

When the mixture components are subject to the constraint that the proportion must sum to constant, you can have simplex lattice designs and or simplex-centroid designs can be adopted. When mixture components are subjected to additional constraints like a maximum and/or minimum value for each component thus have constrained mixture design or extreme-vertices designs is adopted.

In a mixture designs where there are constraints on the component proportion, these are often upper and/or lower bound constraints of the form $L_i \leq x_i \leq U_i$, for $i = 1, 2, \dots, q$ where L_i is the lower bound for the i -th component and U_i the upper bound for the i th component. The general form of the constrained mixture problem is $x_1 + x_2 + \dots + x_q = 1$, $L_i \leq x_i \leq U_i$ for $i = 1, 2, \dots, q$ with $L_i \geq 0$ and $U_i \leq 1$ e.g three components mixture with only lower bounds $0.3 \leq x_1$, $0.4 \leq x_2$, $0.1 \leq x_3$ subject to $x_1 + x_2 + \dots + x_q = 1$, $L_i \leq x_i \leq 1$ for $i = 1, 2, \dots, q$. Pseudo components designs: this can be employed to fit the mixture model. This is due to the fact that the constrained design space well usually has relatively high levels of multicollinearity among the predictors. The components x_i^* - pseudo component is defined as $x_i^* = \frac{x_i - L_i}{1 - L}$ with $L = \sum_{i=1}^q L_i < 1$ denoting the sum of all the lower bounds.

Aggarwal and Sarin(1996) were of the opinion that very many products like chemical, oils, juice and perfume which undergo the prediction process are mixture of two or more components or ingredient. In an attempt to meet the right quality or standard, there is always the need to allow the products to pass through series of formulation or blend of components. This is subject to constraint that the sum of the proportion (not quantity) of the components must be equal to a constant. Assume the components are $X_1, X_2, \dots, X_n$, then the sum is $\sum_{i=1}^n X_i = 1$ or constant. Scheffe (1958,1963) happened to be the proponent of the simplex lattice and simplex centroid which are widely adopted as mixture experiment design especially when extreme constraint of upper and lower bound are of components proportion do not require. He proposed the designs in an attempt to fit the canonical polynomial models.

Brown et al (2014) proposed a new class of statistical model for mixture experiment which provide a power for unification and extension of mixture experiment model but require extensive computation effort. They opined that generalized blending mixture model can accurately describe response surface in a situation where standard model would lead to misleading approximation. But their model requires more data compared to standard model. Scheffe (1958) came out with the use of (q, ∞) symmetric canonical polynomial models of design m for q components or proportion subject to the constraint of constancy of components. Piepel, Szychowski and Loepky(2002) proposed partial quadratic mixture model, for detail reader should see Aggarwal and Sain (1996). In their literatures, Cornell(1991,2002), Johnson and Zabik (1981), Becker(1968) and Snee (1973) had demonstrated the application of mixture experiment

designs in their works. The focus of this paper is to compare both linear, quadratic and polynomial models of mixture experiments via bootstrap techniques. And equally extend special cubic model and consider it with existing models.

Mixture Experiments Modelling

The mixture experiment is constructed based on the combination of proportion of ingredients there by excluding intercept and squares of the components in any of its model. The Scheffe polynomials for mixture experiments are described as follows:

$$y_k = \sum_{i=1}^p \beta_i x_i + \epsilon_k \text{ Linear}$$

$$y_k = \sum_{i=1}^p \beta_i x_i + \sum_{i < j} \beta_{ij} x_i x_j + \epsilon_k \text{ Quadratic}$$

$$y_k = \sum_{i=1}^p \beta_i x_i + \sum_{i < j} \beta_{ij} x_i x_j + \sum_{i < j < k} \beta_{ijk} x_i x_j x_k + \epsilon_k \text{ Special Cubic}$$

$$y_k = \sum_{i=1}^p \beta_i x_i + \sum_{i < j} \beta_{ij} x_i x_j + \sum_{i < j} \gamma_{ij} x_i x_j (x_i - x_j) + \sum_{i < j < k} \beta_{ijk} x_i x_j x_k + \epsilon_k \text{ Full cubic}$$

$$y_k = \sum_{i=1}^p \beta_i x_i + \sum_{i < j} \beta_{ij} x_i x_j + \sum_{i < j} \gamma_{ij} x_i x_j (x_i - x_j) + \sum_{i < j} \gamma_{ij} x_i x_j (x_i + x_j) + \sum_{i < j < k} \beta_{ijk} x_i x_j x_k + \epsilon_k \text{ modified}$$

Where $\beta_i, \beta_{ij}, \gamma_{ij}$ are the parameters that are to be estimated for the data.

Data Analysis and Discussion

TABLE 1:

DATA extracted from Guller et al 2008

x1	x2	x3	y
0.05	0.06	0.89	49
0.05	0.22	0.73	47.5
0.05	0.86	0.09	39
0.05	0.7	0.25	40.5
0.05	0.38	0.57	45.5
0.05	0.54	0.41	45.5
0.12	0.06	0.82	59
0.12	0.22	0.66	65
0.12	0.86	0.02	58
0.12	0.7	0.18	59.5
0.12	0.38	0.5	71
0.12	0.54	0.34	59.5
0.19	0.06	0.75	66.5
0.19	0.22	0.59	70
0.19	0.38	0.43	81
0.19	0.54	0.27	75
0.19	0.7	0.11	79
0.26	0.06	0.68	82.5
0.26	0.7	0.04	81.5
0.26	0.54	0.2	85
0.26	0.38	0.36	82
0.26	0.22	0.52	85
0.33	0.06	0.61	82
0.33	0.22	0.45	93
0.33	0.38	0.29	94
0.33	0.54	0.13	91
0.4	0.06	0.54	89.5
0.4	0.22	0.38	102.5
0.4	0.38	0.22	96.5
0.4	0.54	0.06	88.5

Source: Data from Table 4 in Guller, Prickett, Casares, and Bruck(2008)

Table 2:

Showing linear model of mixture experiment

Linear	original	bootBias	bootSE	bootMed	2.5%	97.5%
x1	185.804	-0.0914	9.0132	185.480	168.7070	203.4675
x2	41.955	0.6838	4.1104	42.371	34.6313	49.7881
x3	43.148	-0.1165	2.7639	42.912	38.6330	51.1541

In this model, x1 has the highest value of coefficient i.e 185.804 which means that x1 contributed more to the production of y than other components, followed by x3 with coefficient of 43.148, whereby x2 (41.955) contributed less to the production of y. The absolute bias of the components after simulation of 1000 are:- x1 is $0.0914 < x3$ (0.1165) $< x2$ which is (0.6838). Based on the standard error, the one with the least value is the best, therefore x3 (2.7639) is better compare to the remaining components followed by x2 (4.1104) and followed by x1 (9.0132). At 2.7% confidence interval x1 is (185.480) $> x3$ (38.6330) $> x2$ (34.6313), and at 97.5% x1 is (203.4675) $> x3$ is (51.1541) $> x2$ (49.7881).

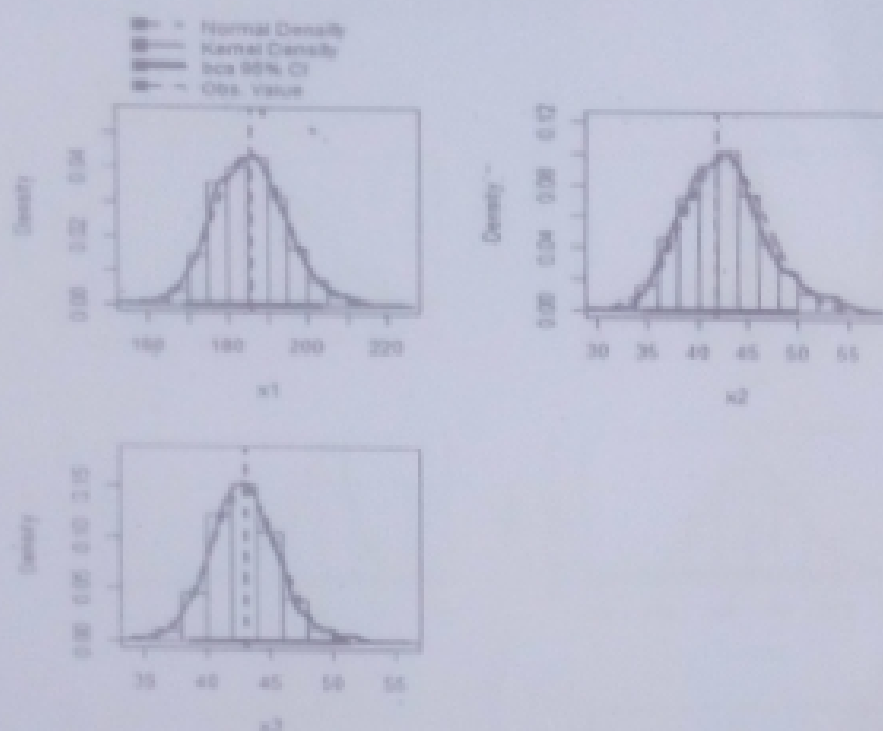


Figure 1 showing Normal, Kernel and histogram of linear model

Histogram:- for x1, x2 and x3, the histogram is fairly skewed to the right and we can see that it has the highest value at the middle point. Kernel density:- is the line with blue color. For x1, it shows that at 4.4% gave rise to a kernel density with a mode at 186 and a pronounce shoulder at 178. X2 has 0.10 which gave rise to a kernel density with a mode at 43 and a pronounce shoulder at 40. And x3 has 15% which gave rise to a kernel density with a mode at 47. Normal density:- x1, x2 and x3 has perfect normal graph, it is neither skewed to left nor to the right with their respective observed value almost at the middle.

Table 3:

Showing Quadratic model of mixture experiment

Quadratic	original	bootBias	bootSE	bootMed	2.5%	97.5%
x1	-11.373	2.2208	48.5561	-10.301	-109.23	83.96
x2	19.533	-0.5551	5.0117	19.197	9.86	30.19
x3	30.141	-1.0035	6.1702	30.441	13.89	37.80
x1.x2	364.314	-0.6402	75.9247	361.123	207.68	518.52
x1.x3	311.289	-2.4892	82.4090	311.456	150.49	477.27
x2.x3	39.591	3.2006	17.5285	41.715	8.99	75.07

In blending of individual components x_3 has the highest coefficient of (30.141) which shows that it contributed more to the production, followed by x_2 (19.533) and followed by x_1 (-11.373) which is negative and it shows that x_1 has no positive effect in the production. Based on absolute bias after simulation of 1000 are: x_1 (2.2208) > x_3 (1.0035) > x_2 (0.5551). The standard error of x_2 (5.0117) is the one with the least value and is the best followed by x_3 (6.1702) and followed by x_1 (48.5561). At 2.5% confidence interval, the confidence interval of x_1 is (-109.23) < x_2 (9.86) < x_3 (13.89). But at 97.5%, the confidence interval of x_1 is (83.96) > x_3 (37.80) > x_2 (30.19). For blending of two components, x_1 and x_2 has the highest coefficient (i.e. 364.314) and it shows that it contributed more to the production of y , followed by x_1 and x_3 (i.e. 311.591) and followed by x_2 and x_3 with the lowest value of (39.591) which has the lowest impact in the production. The coefficients of blending of two components together are positive which shows that they behave synergistically and also complementary. The absolute bias after simulation of 1000 is: x_2 and x_3 is (3.2006), x_1 and x_3 is (2.4892) and x_1 and x_2 is (0.6402). Based on the standard error the one with the least value is the best, then standard error of x_2 and x_3 (17.5285) is the one with the least value and is the best followed by blending of x_1 and x_2 (75.9247), then followed by blending x_1 and x_3 (82.4090). At 2.5% confidence interval, the coefficient of blending of x_2 and x_3 is (8.99) < blending of x_1 and x_3 is (150.49) < blending of x_1 and x_2 (207.68). But at 97.5% confidence interval of blending of x_1 and x_2 is (518.52), x_1 and x_3 is (477.27) and x_2 and x_3 is (75.07).

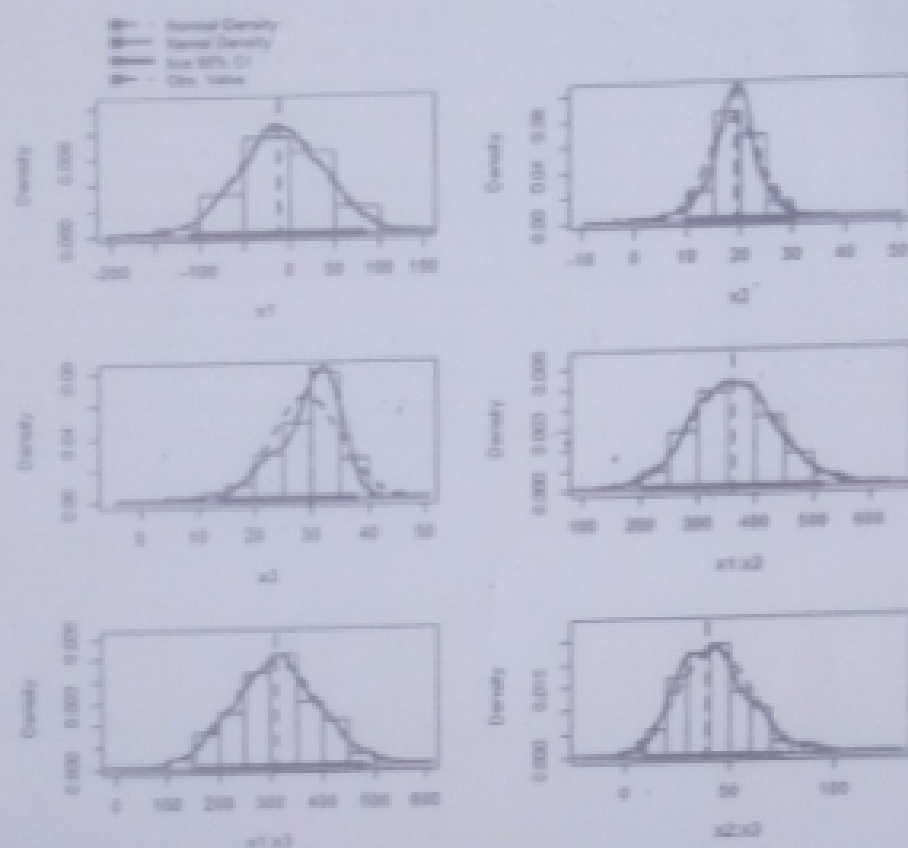


Figure 2 showing Normal, Kernel and histogram of Quadratic model

Histogram:- for x_1 , the histogram was high at about 0.7% and for x_2 with the highest value of 8% which is neither skewed to the right nor to the left while x_3 has the highest value of 7% and skewed to the left. For x_1x_2 with highest value at about 0.5%, x_1x_3 at 0.5% and x_2x_3 at about 0.22%. Kernel density:- For x_1 , it shows that at 0.7% gave rise to a kernel density with a mode at -15, x_2 has 9% which gave rise to a kernel density with a mode at 19. And x_3 has 8% which gave rise to a kernel density with a mode at 32 with a slight shoulder of 23 and it is skewed to the right. For x_1x_2 , it shows 0.5% gave rise to kernel density with mode at 360, x_1x_3 is 0.5% that gave rise to a kernel density with a mode of 0.25%. Normal density:- the normal shape is perfect for all the component, it is neither skewed to left nor to the right with their respective observed value almost at the middle except x_3 which skewed to the right.

Table 4:
Special cubic model of mixture experiment

Special Cubic	original	bootBias	bootSE	bootMed	2.5%	97.5%
x1	17.614	3.8782	47.9412	23.833	-83.89	102.67
x2	28.364	0.4984	8.2505	27.394	19.06	57.94
x3	38.088	-0.3376	5.5051	38.431	23.37	45.72
x1:x2	268.902	-4.2743	95.8354	264.018	67.35	454.73
x1:x3	222.004	-5.3373	86.6768	215.222	65.29	397.22
x2:x3	-12.626	2.2201	29.1336	-10.005	-79.43	39.14
x1:x2:x3	367.318	-20.4859	169.6318	352.766	48.98	718.12

In blending of a components singly, x3 has the highest coefficient of (38.088), so it contributed more to the production, followed by x2 (28.364) and followed by x1 (17.614) which is the least which shows that it has small contribution in the production. Based on absolute bias after simulation of 1000 are: x1 is (3.8782) > x2 is (0.4984) > x3 (0.3376). The standard error of x3 (5.5051) is the best because of its least value, followed by x2 (8.2505) and followed by x1 (47.9412). At 2.5% confidence interval, x1 is (-83.89) < x2 (19.06) < x3 (23.37). But at 97.5% confidence interval x1 is (102.67) > x3 (57.94) > x2 (45.72). For blending of two components, x1 and x2 has the highest coefficient (i.e 268.902), followed by x1 and x3 (i.e 222.004), the two mixtures are positive which means they behave synergistically and complementary in the mixture. But the blending of x2 and x3 (-12.626) is negative and it indicates that the mixture components behave antagonistically i.e the components are against each other and also they are not complementary. The absolute bias after simulation of 1000 is: x1 and x2 is (4.2743), x1 and x3 is (5.3373) and the last one x2 and x3 is (2.2201). The standard error of x2 and x3 (29.1336) is the one with the least value and is the best in the mixture, followed by x1 and x3 (86.6768), then followed by x1 and x2 (95.8354). At 2.5% confidence interval, x2 and x3 is (-79.43) < x1 and x3 is (65.29) < x1 and x2 (67.35). But at 97.5% confidence interval of x1 and x2 is (454.73), x1 and x3 is (397.22) and x2 and x3 is (39.14). and for blending of three components (x1, x2 and x3), the coefficients is 367.318 and it is positive which shows that the components behave synergistically and complementary. The absolute bias is 20.4859, standard error is 169.6318, the confidence interval at 2.5% is 48.98 while at 97.5 is 718.12.

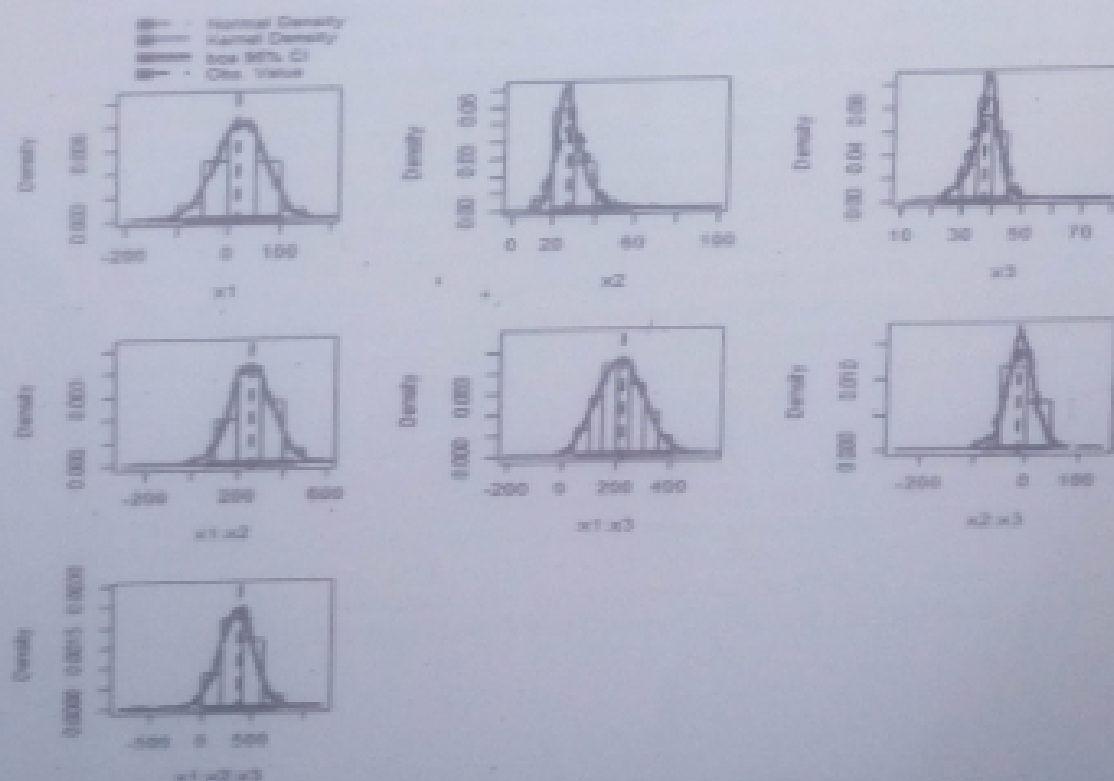


Figure 3 showing Normal, Kernel and histogram of special cubic model

Histogram:- The histogram of x_1 was high at about 0.8% and x_2 with the highest value of 6%, while x_3 has the highest value of 7% which is neither skewed to the right nor to the left except x_2 that slightly skewed to the left. x_1x_2 with highest value at about 0.4%, x_1x_3 at about 0.5% and x_2x_3 at about 0.12% while $x_1x_2x_3$ was 0.022%. Kernel density:- For x_1 , it shows that at 0.7% gave rise to a kernel density with a mode at 25. x_2 has 7% which gave rise to a kernel density with a mode at 28. And x_3 has 8% gave rise to a kernel density with a mode at 38. For x_1x_2 , it shows 0.4% gave rise to kernel density with mode at 280, x_2x_3 is 0.25 which gave rise to a kernel density with a mode at 300. Normal density:- the normal shape was ok for all the components, it is neither skewed to left nor to the right respect to their observed value almost at the middle except x_2 which slightly skewed to the left.

Table 5
Showing fullcubic model of mixture experiment

Full Cubic	original	bootBias	bootSE	bootMed	2.5%	97.5%
x_1	257.18	81.40	333.22	318.83	-399.80	905.29
x_2	19.31	-0.56	15.38	18.90	-9.60	55.96
x_3	39.74	-2.20	16.54	38.81	16.20	71.58
x_1x_2	-199.75	-142.92	605.76	-305.60	-1312.92	1036.40
x_1x_3	-190.72	-139.62	605.77	-290.07	-1402.71	938.00
x_2x_3	-8.66	6.07	43.38	-2.71	-128.40	48.92
$x_1x_2x_3$	889.40	110.83	711.54	965.28	-471.76	2382.11
$x_1x_2^*(x_1-x_2)$	-402.19	-83.78	380.40	-459.56	-1179.55	304.71
$x_1x_3^*(x_1-x_3)$	-132.26	-79.65	374.86	-185.94	-848.21	536.82
$x_2x_3^*(x_2-x_3)$	-27.71	-6.91	43.27	-31.21	-112.38	82.14

Between individual components x_1 has the highest coefficient of (257.18) which shows that it contributed more to the production of y than other components, followed by x_3 (39.74) and then followed by x_2 with (19.31) which is the least and it shows that it has small contribution in the production. Based on absolute bias after simulation of 1000 are: x_1 is (81.40) > x_3 is (2.20) > x_2 (0.56). The standard error of x_2 (15.38) has the least value and is the best followed by x_3 (16.54) and followed by x_1 (333.22) which has the highest value of standard error and it is not that efficient compare to others. At 2.5% confidence interval is x_1 (-399.80) < x_2 (-9.60) < x_3 (16.20). But at 97.5% confidence interval x_1 is (905.29) > x_3 is (71.58) > x_2 is (55.96). For blending of two components, x_1 and x_2 has the coefficient of (-199.75), but x_1 and x_3 has the coefficient of (-190.72) while x_2 and x_3 has the coefficient of (-8.66), the blending of two mixtures are negative which shows that the mixture behave antagonistically that means the components are against each other and also they are not complementary. The absolute bias after simulation of 1000 is: x_1 and x_2 is (-142.92), x_1 and x_3 is (-139.62) and x_2 and x_3 which is the last is (6.07). The standard error of x_2 and x_3 is (43.38) is the one with the least value of standard error and it is the best in the mixture, followed by x_1 and x_2 which is (605.76), then followed by x_1 and x_3 is (605.77) which is approximately to that of the blending of x_1 and x_2 . At 2.5% confidence interval, x_2 and x_3 is (-128.40) > x_1 and x_2 which is (-1312.92) > x_1 and x_3 which is also (-1402.71). But at 97.5% confidence interval of x_1 and x_2 is (1036.40), x_1 and x_3 is (938.00) and x_2 and x_3 is (48.92). And for blending of three components (x_1 , x_2 and x_3), the coefficients is 889.40 and it is positive which shows that the components behave synergistically and complementary. The absolute bias is 110.83, standard error is 711.54, the confidence interval at 2.5% is -471.76 while at 97.5% is 2382.11. In blending of two components in combination with their differences, their coefficients are: for $x_1x_2^*(x_1-x_2)$ is -402.19, $x_1x_3^*(x_1-x_3)$ is -132.26 and $x_2x_3^*(x_2-x_3)$ is -27.71. These coefficients are positive and show that the components react antagonistically. The absolute bias of $x_1x_2^*(x_1-x_2)$ is -83.78 and $x_1x_3^*(x_1-x_3)$ is -79.65 while the absolute bias of $x_2x_3^*(x_2-x_3)$ is -6.91. Based on the standard error, the blending of $x_2x_3^*(x_2-x_3)$ with the least value of (43.27) is the best followed by $x_1x_3^*(x_1-x_3)$ with standard error of (374.86) and the last one with the highest standard error of (380.40). At 2.5% confidence interval, the interval of $x_1x_2^*(x_1-x_2)$ is -1179.55, $x_1x_3^*(x_1-x_3)$ is -848.21 and $x_2x_3^*(x_2-x_3)$ is -112.38. But at 97.5% confidence interval, the confidence interval of $x_1x_2^*(x_1-x_2)$ is 304.71 and $x_1x_3^*(x_1-x_3)$ is 536.82 while the confidence interval of $x_2x_3^*(x_2-x_3)$ is 82.14 which is the least.

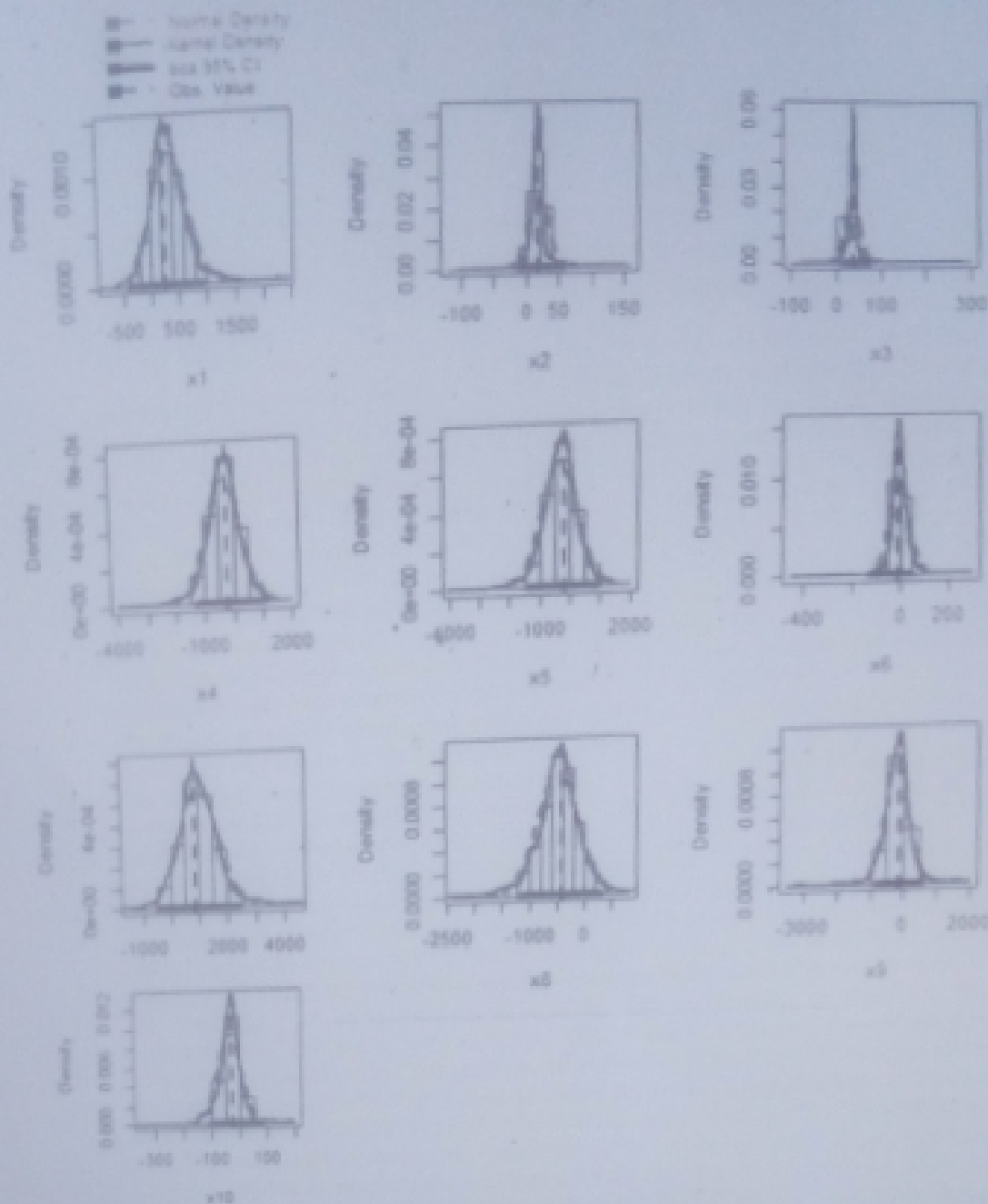


Figure 4 showing Normal, Kernel and histogram of full cubic model

Histogram:- The plots have their highest value almost at the middle, but x_1 and x_7 was a bit skewed to the left and x_4 , x_5 , x_8 and x_{10} are slightly skewed to the right. Kernel density:- For x_1 , it shows that at 0.15% gave rise to a kernel density with a mode at 250, x_2 has 5% which gave rise to a kernel density with a mode at 20. And x_3 has 6% gave rise to a kernel density with a mode at 30. For x_4 and x_5 , it shows at nearly zero (0) gave rise to kernel density with mode at -100, x_6 is 1.5% that gave rise to a kernel density with a mode of 10, x_7 at nearly zero gave rise to kernel density with mode at 990, x_8 is 0.012% with -400, x_9 is 0.012% with -100 and lastly x_{10} is 0.14 which gave rise to a kernel density with a mode at -30. Normal density:- the shape of the plot is normal for some components but for some components it either skewed to left or to the right with their respective observed value almost at the middle which is almost the same with the mode of kernel density.

Table 6
Specialquartic model of mixture experiment

Special Quartic	original	bootBias	bootSE	bootMed	2.5%	97.5%
x1	3.74	29.72	121.80	20.3	-208.10	226.88
x2	28.04	1.18	9.87	27.34	17.97	64.43
x3	36.92	0.09	8.17	37.95	10.89	46.66
x1*x2	296.29	-35.92	181.10	282.17	-56.29	632.71
x1*x3	240.07	-45.26	196.46	216.06	-141.46	596.93
x2*x3	-5.74	-3.87	48.10	-8.93	-93.20	101.71
x1*x2*x3	389.49	149.17	763.17	514.38	-1240.51	1791.78
x1*x1*x2*x3	139.20	-478.32	1960.47	-150.14	-3467.53	3829.37
x1*x2*x2*x3	-245.99	-88.77	569.96	-286.52	-1267.89	853.91
x1*x2*x3*x3						

Among individual components x3 has the highest coefficient of (36.92) which shows that it contributed more to the production of y than other components, followed by x2 (28.04) and then followed by x1 with (3.74) which is the least and it shows that it has the least contribution in the production. Based on absolute bias after simulation of 1000 are: x1 is (29.72) > x2 is (1.10) > x3 (0.09). The standard error of x3 (8.17) is the least value and is the best followed by x2 (9.87) and followed by x1 (121.80) which has the highest value of standard error and it's less efficient compare to others. At 2.5% confidence interval, the confidence interval of x2 is (17.97) which is the highest followed by x3 (10.89) and then x3 (-208.10) which is the least. But at 97.5% confidence interval x1 is (226.88) followed by x2 (64.43) and the x3 (46.66). For blending of two components, the blending of x1 and x2 has the coefficient of (296.29) which is the highest and x1 and x3 has the coefficient of (240.07) which shows that the two components has positive value and they are synergistic and complementary. While x2 and x3 has the coefficient of (-5.74), it's negative which shows that the components behave antagonistically and also they are not complementary. The absolute bias after simulation of 1000 is: for the blending of x1 and x2 is (35.92), x1 and x3 is (45.26) and x2 and x3 is (3.87). The standard error of blending of x2 and x3 is (48.10) is the best because it has the least value of standard error, followed by x1 and x2 which is (181.10), then followed by x1 and x3 is (196.46). At 2.5% confidence interval, the confidence interval of x1 and x2 is (-56.29) > x2 and x3 which is (-93.20) > x1 and x3 which is also (-141.46). But at 97.5% confidence interval, x1 and x2 is (632.71), x1 and x3 is (596.93) and x2 and x3 is (101.71). And for blending of three components (x1, x2 and x3), the coefficients is 389.49 and it is positive which shows that the components behave synergistically and complementary. The absolute bias is 149.17, standard error is 763.17, the confidence interval at 2.5% is -1240.51 while at 97.5 is 1791.78. In blending of three components in combination with a component already appeared in the three components, the coefficient of x1*x1*x2*x3 is 139.20. The coefficient is positive, the components behave synergistically. But for x1*x2*x2*x3 is -245.99 and is negative, the components are antagonistic and x1*x2*x3*x3 has no value. The absolute bias of x1*x1*x2*x3 is -478.32 and x1*x2*x2*x3 is -88.77 while the absolute bias of x1*x2*x3*x3 has no value. Based on the standard error, the blending of x1*x2*x2*x3 with the least value of (569.96) and is the best followed by x1*x1*x2*x3 with standard error of (1960.47). At 2.5% confidence interval, the interval of x1*x1*x2*x3 is -3467.53, x1*x2*x2*x3 is -1267.89. But at 97.5% confidence interval, the confidence interval of x1*x1*x2*x3 is 3829.37 and x1*x2*x2*x3 is 853.91. Looking at this model, the last column (x1*x2*x3*x3) has no contribution in the production based on everything.

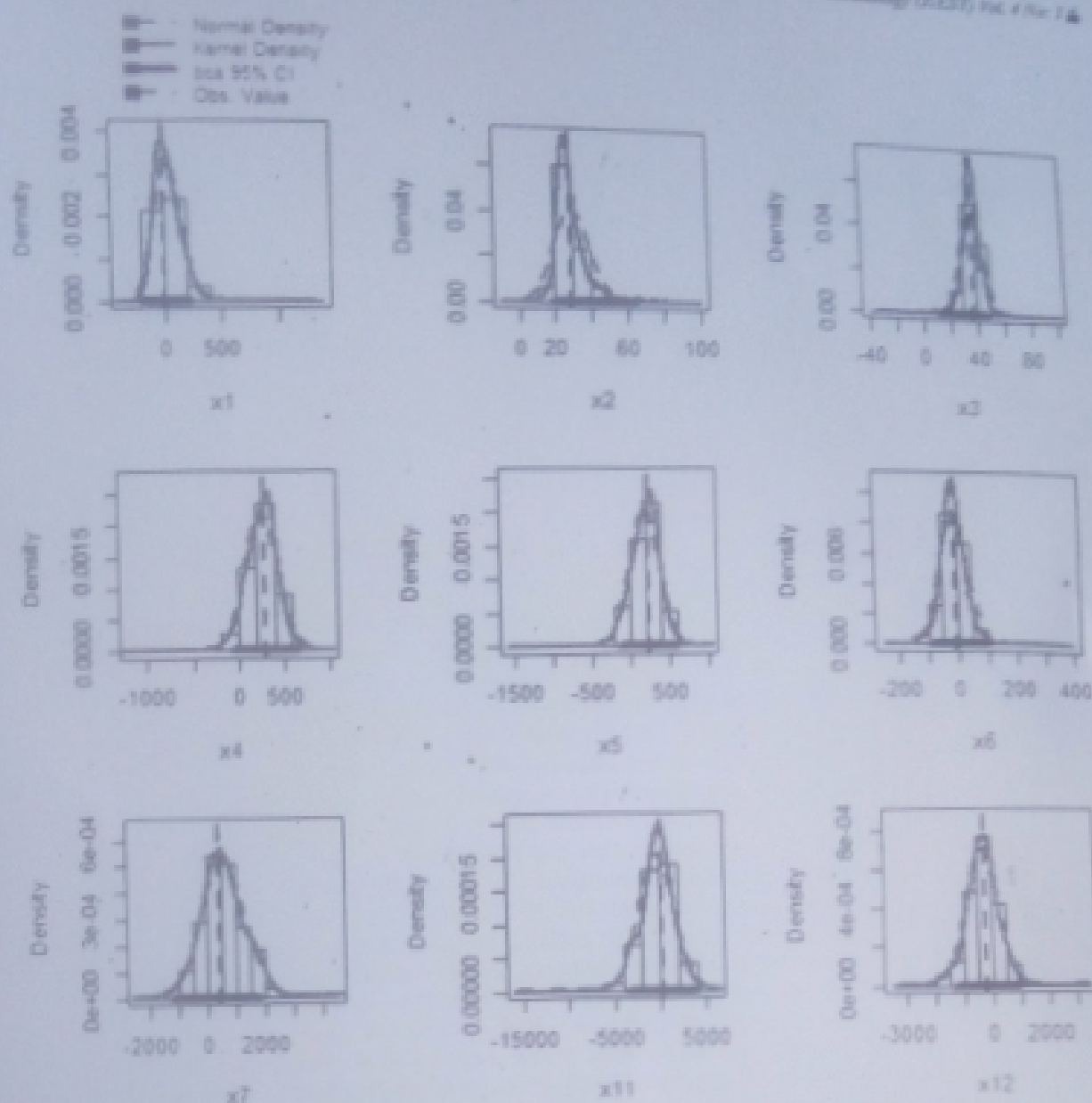


Figure 5 showing Normal, Kernel and histogram of special quartic model

Histogram:- The plots have their highest value almost at the middle of the plot except that x1, x2 and x7 are slightly skewed to the left. **Kernel density:-** For x1, it shows that at 0.35% it gave rise to a kernel density with a mode at 0, x2 has 0.8% which gave rise to a kernel density with a mode at 30. And x3 has 0.55% gave rise to a kernel density with a mode at 35, x4 is at 0.025% with 300, x5 is at 0.025% with 250, x6 is at 0.10% with 10, x7 shows at nearly zero (0) gave rise to kernel density with mode at 400, x11 is 0.015% that gave rise to a kernel density with a mode of 0, x12 at nearly zero gave rise to kernel density with mode at 990, x8 is 0.012% with -400, x9 is 0.012% with -100 and lastly x10 is 0.14 which gave rise to a kernel density with a mode at -30. **Normal density:-** the shape of the plot is normal for some components but for some components it is either skewed to left or to the right with their respective observed value almost at the middle which is almost the same with the mode of kernel density.

Table 7.
Showing full quartic model of mixture experiment

Full Quartic	Original	bootBias	bootSE	bootMed	2.5%	97.5%
x1	-171.03	144.65	16182.29	-890.41	-9320.36	37702.71
x2	10.75	4.54	118.67	16.86	-372.98	135.89
x3	36.63	-17.89	151.52	36.02	-147.08	155.62
x1*x2	641.89	-258.05	31899.98	1969.73	-73168.43	18585.41
x1*x3	640.05	-139.49	31316.06	2082.44	-76591.37	17893.12
x2*x3	20.00	19.59	370.33	20.52	-556.37	679.30
x1*x2*x3	453.69	121.98	20143.19	-314.19	-10969.65	46554.18
x1*x2*(x1-x2)	217.83	-141.88	27146.80	1283.58	-54133.04	15025.31
x1*x3*(x1-x3)	556.57	19.4950	24112.21	1918.99	-49355.64	14618.40
x2*x3*(x2-x3)	1.17	-78.0960	428.27	-17.80	-596.63	905.74
x1*x1*x2*x3	-1616.12	-887.54	77101.77	-5313.89	-48267.92	139859.37
x1*x2*x2*x3	-462.63	316.0042	9138.36	-221.33	-17222.05	6867.25
x1*x2*(x1-x2)^2	337.17	45.87	12488.16	-835.47	-21809.61	8200.65
x1*x3*(x1-x3)^2	382.50	188.72	10051.43	1161.61	-33834.87	5869.3
x2*x3*(x2-x3)^2	-6.6511	-70.4981	454.65	-41.921	-578.3249	894.58

Between the individual components x3 has the highest coefficient of (36.63), it contributed more to the production of y than other components, followed by x2 (10.75) and then followed by x1 with (-171.03). Based on absolute bias when 1000 sample was simulated are: x1 is (144.65) > x2 is (4.54) > x3 (-17.89). The standard error of x2 (118.67) is the least which is the best followed by x3 (151.52), followed by x1 (16182.29) which has the highest value of standard error and it's less efficient compare to others. At 2.5% confidence interval, the confidence interval of x3 is (-147.08) the highest, followed by x2 (-372.98) and then x1 (-9320.36) the least. But at 97.5% confidence interval x1 is (37702.71) followed by x3 (155.62) and x2 (135.89). For blending of two components, the blending of x1 and x2 has the coefficient of (641.89) which is the highest and x1 and x3 has the coefficient of (640.05) While x2 and x3 has the coefficient of (20.00) which shows that the blending of two components are positive, they behave synergistically and complementarily. The absolute bias after simulation of 1000 is: for the blending of x1 and x2 is (258.05), x1 and x3 is (139.49) and x2 and x3 is (19.59). The standard error of blending of x2 and x3 is (370.33) is the best because it has the least value of standard error, for x1 and x2 is (31899.98), then for x1 and x3 is (31316.06). At 2.5% confidence interval, the confidence interval of x1 and x2 is (-73168.43), x2 and x3 is (-556.37) > x1 and x3 is also (-76591.37). But at 97.5% confidence interval, x1 and x2 is (18585.41), x1 and x3 is (17893.12) and x2 and x3 is (679.30). And for blending of three components (x1, x2 and x3), the coefficients is 453.69, it is positive which shows that the components behave synergistically and complementary. The absolute bias is 121.98, standard error is 20143.19, the confidence interval at 2.5% is -10969.65 while at 97.5 is 46554.18. In blending of two components in combination with their differences, their coefficients are: for x1*x2*(x1-x2) is 217.83, x1*x3*(x1-x3) is 556.57 and x2*x3*(x2-x3) is 1.17. These coefficients are positive and show that the components react synergistically. The absolute bias of x1*x2*(x1-x2) is -141.88 and x1*x3*(x1-x3) is 19.4950 while the absolute bias of x2*x3*(x2-x3) is -78.0960. Based on the standard error, the blending of x2*x3*(x2-x3) is (428.27) is the best followed by x1*x3*(x1-x3) with standard error of (24112.21) and the last one x1*x2*(x1-x2) with the highest standard error of (27146.80). At 2.5% confidence interval, the interval of x1*x2*(x1-x2) is -54133.04, x1*x3*(x1-x3) is -49355.64 and x2*x3*(x2-x3) is -596.63. But at 97.5% confidence interval, the confidence interval of x1*x2*(x1-x2) is 15025.31 and x1*x3*(x1-x3) is 14618.40 while the confidence interval of x2*x3*(x2-x3) is 905.74. In blending of three components in combination with a component already appeared in the three components, the coefficient of x1*x1*x2*x3 is -1616.12, but for x1*x2*x2*x3 is -462.63, the coefficients are negative, so the components are antagonistic and x1*x2*x3*x3 has no value. The absolute bias of x1*x1*x2*x3 is -887.54 and x1*x2*x2*x3 is 316.0042 while the absolute bias of x1*x2*x3*x3 is unknown. Based on the standard error, the blending of x1*x2*x2*x3 with the value of (9138.36) is the better compared to x1*x1*x2*x3 with standard error of (77101.77). At 2.5% confidence interval, the confidence interval of x1*x1*x2*x3 is -48267.92 and x1*x2*x2*x3 is -17222.02. But at 97.5% confidence interval, the confidence interval of x1*x1*x2*x3 is 139859.37 and x1*x2*x2*x3 is 6867.25, but x1*x2*x3*x3 is unknown. In blending of two components in combination with square of their differences, the coefficient of x1*x2*(x1-x2)^2 is 337.17, x1*x3*(x1-x3)^2 is 382.50, these coefficients are

positive and show that the components react synergistically but the coefficient of $x_2^2 x_3^2 (x_2 - x_3)^2$ is - 5.8531. The absolute bias after simulation of 1000 is: for $x_1^2 x_2^2 (x_1 - x_2)^2$ is 45.87 and $x_1^2 x_3^2 (x_1 - x_3)^2$ is 188.72 while the absolute bias of $x_2^2 x_3^2 (x_2 - x_3)^2$ is - 70.4981. Based on the standard error, the blending of $x_2^2 x_3^2 (x_2 - x_3)^2$ is (454.63) is the best followed by $x_1^2 x_3^2 (x_1 - x_3)^2$ with standard error of (10051.43) and the last one $x_1^2 x_2^2 (x_1 - x_2)^2$ with the highest standard error of (12488.16). At 2.5% confidence interval, the confidence interval of $x_1^2 x_2^2 (x_1 - x_2)^2$ is -21809.61, $x_1^2 x_3^2 (x_1 - x_3)^2$ is -33834.87 and $x_2^2 x_3^2 (x_2 - x_3)^2$ is -578.3249. But at 97.5% confidence interval, the confidence interval of $x_1^2 x_2^2 (x_1 - x_2)^2$ is 8200.65 and $x_1^2 x_3^2 (x_1 - x_3)^2$ is 5389.3 while the confidence interval of $x_2^2 x_3^2 (x_2 - x_3)^2$ is 894.58.

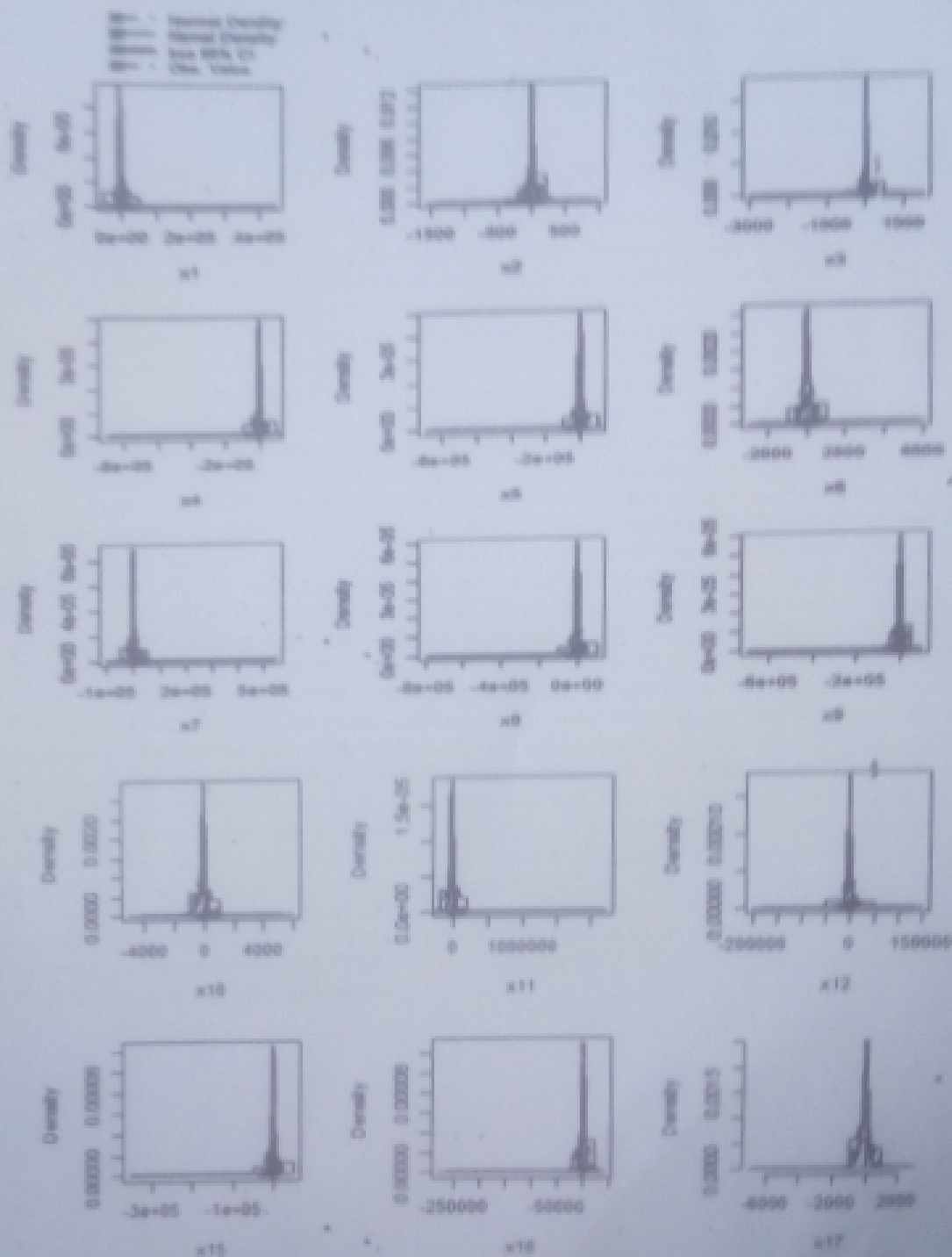


Figure 6: showing Normal, Kernel and histogram of full quartic model

Table 8:
Specialcubic model of mixture experiment

Modified Special Cubic	original	bootBias	bootSE	bootMed	2.5%	97.5%
x1	330.08	110.92	404.43	409.99	-566.67	1031.04
x2	14.07	-3.71	21.91	13.022	-29.18	52.18
x3	35.72	-6.02	31.17	35.139	-12.49	67.87
x1*x2	-348.37	-190.89	758.18	-492.97	-1634.71	1493.81
x1*x3	-339.47	-185.72	757.295	-471.79	-1644.06	1278.22
x2*x3	19.72	20.14	94.916	26.80	-151.35	181.42
x1*x2*x3	1322.63	149.13	1456.972	1427.98	-1691.14	3830.75
x1*x2*(x1-x2)	-553.98	-134.75	583.804	-644.20	-1524.96	851.94
x1*x3*(x1-x3)	-277.04	-125.28	601.747	-338.52	-1363.82	772.13
x2*x3*(x2-x3)	-24.50	-10.96	51.327	-31.40	-112.06	92.07
x1*x2*x3*(abs(x1-x2-x3))	-568.30	-27.46	1474.287	-603.74	-3018.42	2846.34

Among the individual components x1 has the highest value of coefficient of (330.08), it means that x1 contributed more to the production of y than other components, followed by x3 (35.72) and then followed by x2 with (14.07). The absolute bias when 1000 sample was simulated are: x1 is (110.92) > x2 is (-3.71) > x3 (-6.02). The standard error of x2 (21.91) is the least followed by x3 (31.17), followed by x1 (404.43). At 2.5% confidence interval, the confidence interval of x3 is (-12.49), the highest followed by x2 (-29.18) and then x1 (-566.67). But at 97.5% confidence interval x1 is (1031.04) followed by x3 (67.87) and x2 (52.18). For blending of two components, the blending of x1 and x2 has the coefficient of (-348.37) and x1 and x3 has the coefficient of (-339.47) While x2 and x3 has the coefficient of (19.72) which is the highest and also positive then it behave synergistically and complementarily. The absolute bias after simulation of 1000 is: for blending of x1 and x2 is (-190.89), x1 and x3 is (-185.72) and x2 and x3 is (20.14). The standard error of blending of x2 and x3 is (94.916) and it is the best because it has the least value of standard error, for x1 and x2 is (758.18), then for x1 and x3 is (757.295). At 2.5% confidence interval, the confidence interval of x1 and x2 is (-1634.71), x2 and x3 is (-151.35) and x1 and x3 is (-1644.06). But at 97.5% confidence interval, x1 and x2 is (1493.81), x1 and x3 is (1278.22) and for x2 and x3 is (181.42). For blending of three components (x1, x2 and x3), its coefficients is 1322.63, which positive and shows that the components react synergistically and complementary. The absolute bias is 149.13, standard error is 1456.972, the confidence interval at 2.5% is -1691.14 while at 97.5 is 3830.75. In blending of two components in combination with their differences, their coefficients are: for x1*x2*(x1-x2) is -553.98, x1*x3*(x1-x3) is -277.04 and x2*x3*(x2-x3) is -24.50. These coefficients are negative and show that the components react antagonistically. The absolute bias of x1*x2*(x1-x2) is -134.75 and x1*x3*(x1-x3) is -125.28 while the absolute bias of x2*x3*(x2-x3) is -10.96. Based on the standard error, the blending of x2*x3*(x2-x3) is (51.327) is the best followed by x1*x2*(x1-x2) with standard error of (583.804) and the last one is x1*x3*(x1-x3) with the highest standard error of (601.747). At 2.5% confidence interval, the confidence interval of x1*x2*(x1-x2) is -1524.96, x1*x3*(x1-x3) is -1363.82 and x2*x3*(x2-x3) is -112.06. But at 97.5% confidence interval, the confidence interval of x1*x2*(x1-x2) is 851.94 and x1*x3*(x1-x3) is 772.13 while the confidence interval of x2*x3*(x2-x3) is 92.07. for blending of x1*x2*x3*(abs(x1-x2-x3)), its coefficient is -568.30, it is negative and it means the components is antagonistic. The absolute bias is -27.46, with the standard error of 1474.287, but at 2.5% it has -3018.42 of confidence interval and while at 97.5% it has 2846.34 of confidence interval.

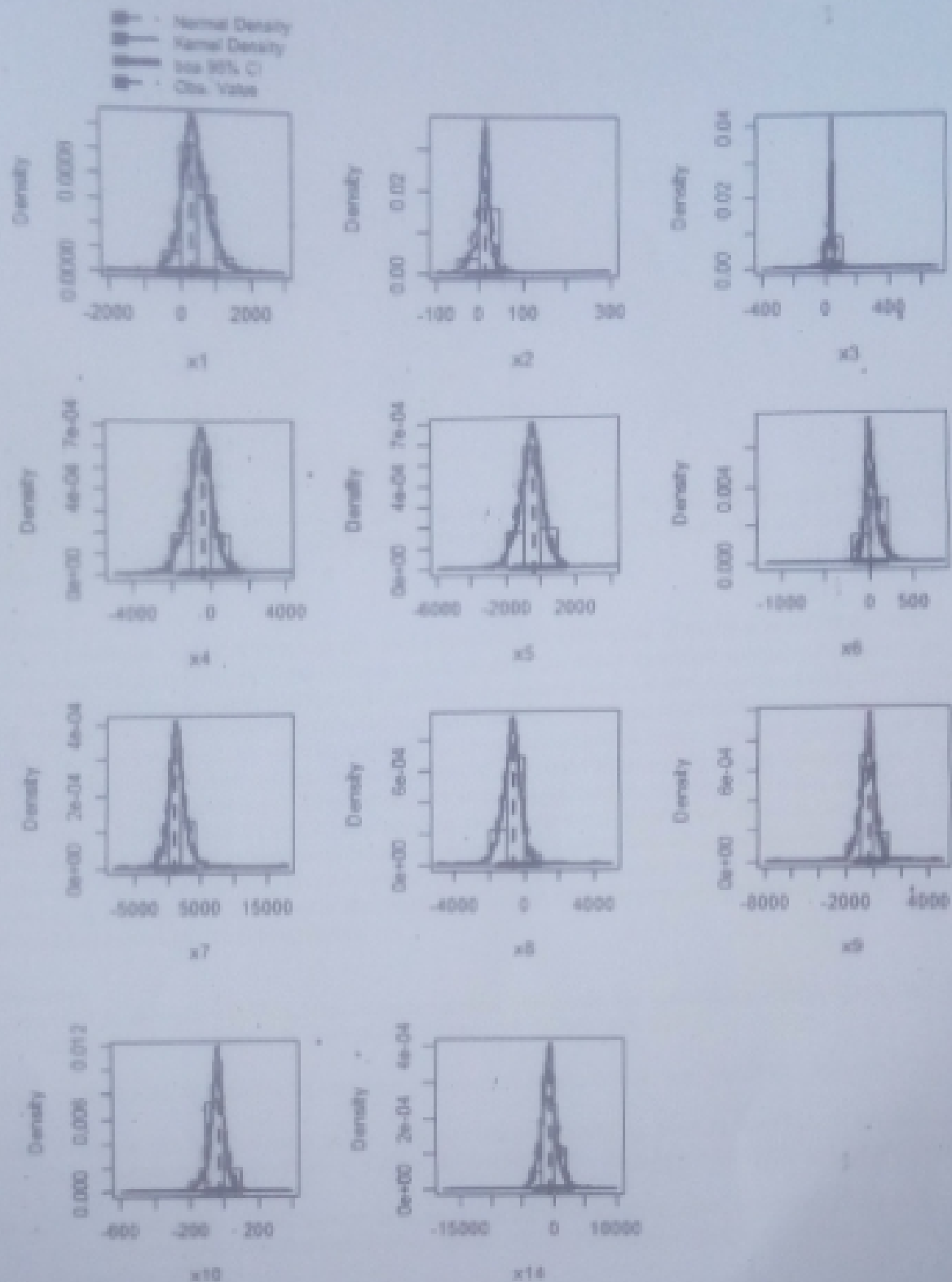


Figure 1: comparing normal, kernel and 95% confidence interval with observed values for various variables

Histogram:- The plots have their highest value almost at the middle of the plot except that x1, x2 and x7 are slightly skewed to the left. Kernel density:- For x1, it shows that at 0.35% it gave rise to a kernel density with a mode at 0, x2 has 0.8% which gave rise to a kernel density with a mode at 30. And x3 has 0.55% gave rise to a kernel density with a mode at 35, x4 is at 0.025% with 300, x5 is at 0.025% with 250, x6 is at 0.10% with 10, x4, x5, x7, x8, x9, and x14 shows at nearly zero (0) gave rise to kernel density with mode at 0, -

200, 1000, -500, -400, and -500 respectively. x_{11} is 0.015% that gave rise to a kernel density with a mode of 0, x_{12} at nearly zero gave rise to kernel density with mode at 990, x_8 is 0.012% with -400, x_9 is 0.012% with -100 and lastly x_{10} is 0.14 which gave rise to a kernel density with a mode at -30. Normal density- the shape of the plot is normal for some components but for some components it either skewed to left or to the right with their respective observed value almost at the middle which is almost the same with the mode of kernel density.

Table 9:
Model comparison with AIC and BIC

Model	AIC	BIC
Linear	200.0636	205.6684
Quadratic	177.7602	187.5686
Special Cubic	172.41	183.62
Full Cubic	168.79	184.2059
Special Quartic	175.9575	189.9695
Full quartic	177.07	199.49
Modified SC	166.56	186.38

Selection of Best Model

Base on AIC, the one with the least value of AIC is the best model. Then the best model is full cubic model because it has the least value of AIC. But based on the BIC the one with the least value is also the best. So, the best model is special cubic model

Conclusion

Mixture experiment was performed on the data extracted from the work of Gallant et al (2008), various models were compared ranging from linear to cubic models, the study modified special cubic model and from the AIC criterion the modified special cubic was the second best out of the seven models compared. The proportion of X_1 component contributed high in linear, full cubic and modified special cubic models whereas the proportion of X_3 contributed high in Quadratic, Special cubic, Special Quartic and Full Quartic. It was further observed that the proportion of X_1 contributed negatively in Quadratic and full Quartic models. The proportion of X_2 contributed low to the production in linear, full cubic and modified special cubic. In blending of X_1 and X_2 components, the Quadratic, Special cubic, Special Quartic and full Quartic designate synergistic and complimentary; whereas full cubic and modified special cubic showed antagonistic. For blending of X_1 and X_3 ditto as the blending of X_1 and X_2 but the blending of X_2 and X_3 , Quadratic, special quartic, full quartic and modified Special cubic expressed synergistic while special cubic and full cubic indicated antagonistic.

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