DETERMINING THE BEST COVARIANCE STRUCTURE IN 3^3 FACTORIAL DESIGN

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Abstract
This research evaluated the performance of covariance structure in seed rates, row spacing and varieties of bread wheat yield. 3^3 full factorial design method and mixed model methods were used for the analysis. The four covariance structure used were compound symmetry (CS), huynh-feldt (HF), first order auto-regressive (AR(1)) and heterogeneous first order auto-regressive (ARH(1)). The goodness of fit criteria used to evaluate the performance of covariance structures were Akaike Information Criterion (AIC) and Bayesian Information Criterion (BIC). The data used composed of 270 observations for yield and were divided into three factors and three levels. The factors were A, B and C and the levels are 1, 2 and 3 for each factor. Analysis shows that the data satisfied all the assumptions. Based on the results in this study, it was found that First order auto-regressive (AR(1)) was found to be the best covariance structure for the data set.

Keywords: 3^3 Factorial Design, Covariance Structures, First Order Auto-regressive, Compound Symmetry, Huynh-Feldt and Heterogeneous First Order Auto-regressive.

Introduction

Factorial design is an important method or design to determine the effect of multiple variables on a response. Traditionally, experiments are designed to determine the effect of one variable upon one response. Fisher, (1935) Showed that there are advantages of combining the study of multiple variables in the same factorial experiment. Factorial design can reduce the number of experiments to be performed by studying multiple factors simultaneously. Additionally, it can be used to find both main effects (from each independent factor) and interaction effects (when both factors must be used to explain the outcome). Factorial design is a useful method of designing experiments in both laboratory and industrial settings (Drafter, 2007). Design of experiment (DOE) is a standard technique to identify key factors and levels that influence system performance and variability. This technique is especially useful when there is the need to understand the interactions and effects of several variables and absence of concrete information (Richard, 1999). Factorial design works well when interactions between variables are strong and important and where every variable contributes significantly (Trochim, 2006). It is clear that factorial designs can become cumbersome and have too many groups even with only a few factors (Williams, et al., 2006). *Design of experiments is applicable to both physical processes and computer simulation models. Experimental design is an effective tool for maximizing the amount of information gained from a study while minimizing the amount of data to be collected. Factorial designs allow estimation of the sensitivity to each factor and also the combined effects of two or more factors* (Box & Draper, 1987).

As noted by several authors (Algina & Oshima, 1994), each analysis has distinct advantages and disadvantages, and each type of analysis will provide a more powerful result under certain conditions and when certain statistical assumptions are satisfied. Analysis of variance procedures can be used to analyze if assumption about the observation are valid; that is normality, independence and homogeneity of variance.

Analysis of full factorial designs or regular fractional factorial design has long been an uncharted territory of research. It is relatively a systematic target driven research that has emerged significantly. Factorial designs are widely used in experiments involving several factors where it is necessary to study the impact of the factors or factor combinations on a process. Special cases of the general factorial designs are widely used in scientific endeavors and they form the basis for other designs of considerable practical value. Recent advances in the analysis of cigarettes smokers and the maize grain data have galvanized the need for techniques to analyze full factorial design data. Apart from a very few examples, most of the research works have surfaced in the scientific body of literature in the past decade or so. Numerous researchers have addressed the problem and have meaningfully contributed to the development of the design (Gurbuz, et al., 2003).

Recently, Planta, (2006) determined low-temperature tolerance and genetics potential in wheat (Tricitum aestivum) in 2^3 factorial design. Fareha, (2013), determined the effects of process parameters on single fixation of reactive printing and crease resistance finishing of cotton fabric using 2^3 factorial designs.

As pointed out by Garratt, (2001) in the discussion of (Lewis, *et al*., 2001) experimentation that is limited to small number of noise factors often results in only small improvements in product performance in laboratory experiments. These improvements then tend to be masked when products are manufactured in full scale production due to variation in unexplored noise factors.

The purpose of this paper is to determine the best covariance structure among the four in 3^3 factorial design using seed rates, row spacing and varieties of bread wheat yield.

Methodology

Observation/Experimental Design

The data used for this study is secondary data obtained from the Irrigation Scheme Maiduguri. The materials used composed of: V1-Local Variety, V2-R_{23}-BB-PCBWH-98 and V3-TOP'S NARO-CMB-PCBWH-1729. Seed Rate: 50kg/ha, 100kg/ha and 150kg/ha and Row Spacing:

5cm, 25cm and 35cm, the design was replicated 10 times in a 3^3 factorial design. The trial was conducted at Lake Chad Research Institute Experimental Farm Maiduguri during the 2011 planting season. These consist of making plot sizes of 3m x 5m with 1m in-between. The experiment was completed same day to avoid introducing error due to planting same experiment on different days. The NPK and urea fertilizer were applied at split dosage, half at planting and the other half two weeks after germination. Weeding was carried out regularly as it was not part of the design.

Full Factorial Design

The three-level design is written as a 3^k full factorial design. It means that k factors are considered, each at three levels. These are (usually) referred to as low, intermediate and high levels. The levels are numerically expressed as 0, 1 and 2. We used the 0, 1, 2 scheme, because the three-level designs were proposed to model possible curvature in the response function and to handle the case of nominal factors at 3 levels. A third level for a continuous factor facilitates investigation of a quadratic relationship between the response and each of the factors.

The 3^3 Design Model

This is a design that consists of three factors, each at three levels. It can be expressed as 3x3x3=3^3 design. The model for such an experiment is given as follows

$$Y_{ijk} = \mu + A_i + B_j + AB_{ij} + C_k + AC_{ik} + BC_{jk} + ABC_{ijk} + \varepsilon_{ijk} \quad (1)$$

Where each factor is included as a nominal factor rather than as a continuous variable. Main effect have 2 degree of freedom, two-factor interactions have 4 degree of freedom and three-factor interactions have 8 degree of freedom and Y_{ijk} is the yield of i^{th} level of factor A, j^{th} level of factor B and k^{th} level of factor C μ is the general mean independent of treatment effect or intercept (overall mean response of all observations).

A_i Effect of i^{th} level of factor A (variety).

B_j Effect of j^{th} level of factor B (seed rate).
AB_{ij} Interaction effect of i^{th} level of factor A (variety) and j^{th} level of factor B (seed rates).
C_k Effect of k^{th} level of factor C (Row spacing).
AC_{ik}= interaction effect of i^{th} level of factor A (variety) and k^{th} level of factor C (row spacing). BC_{jk} Interaction effect of j^{th} level of factor B (seed rates) and k^{th} level of factor C (row spacing).
ABC_{ijk} Interaction effect of i^{th} level of factor A (variety), j^{th} level of factor B (seed rates) and k^{th} level of factor C (row spacing).

ε_{ijk} Is the random error associated with observing y_{ijk} and assumed iid~$N(0,\sigma^2)$.

Hypothesis Testing

H_o: $\mu = o$ versus H_a: $\mu \neq o$

H_o: $A_i = o$ versus H_a: $A_i \neq o$

H_o: $B_j = o$ versus H_a: $B_j \neq o$

H_o: $AB_{ij} = o$ versus H_a: $AB_{ij} \neq o$

H_o: $C_k = o$ versus H_a: $C_k \neq o$

H_o: $AC_{iK} = o$ versus H_a: $AC_{ik} \neq o$

H_o: $BC_{jK} = o$ versus H_a: $BC_{jk} \neq o$

H_o: $ABC_{ijK} = o$ versus H_a: $ABC_{ijk} \neq o$

Parameters Estimation

Inferences on specific factor effects requires the estimation of the parameters of ANOVA models such as blocks, treatments, interactions, error and total are given below (Robert, et al., 2003);

Correction Factor (CF) = $\frac{y_{...}^2}{n} = n\bar{y}_{...}^2$ (2)

where n is the total number of observation

Total Sum of Square (TSS) = $\sum_i \sum_j \sum_k (y_{ijk} - \bar{y}...)^2$ (3)

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Sum of Square A (SSA) = $\frac{\sum_i y_{i..}^2}{bcr} - CF$ (4)

Sum of Square B (SSB) = $\frac{\sum_j y_{.j.}^2}{acr} - CF$ (5)

Sum of Square C (SSC) = $\frac{\sum_k y_{..k}^2}{abr} - CF$ (6)

Sum of Square of AB (SSAB) = $\frac{\sum_i \sum_j y_{ij.}^2}{cr} - CF - SSA - SSB$ (7)

Sum of Square AC (SSAC) = $\frac{\sum_i \sum_k y_{i.k}^2}{br} - CF - SSA - SSC$ (8)

Sum of Square BC (SSBC) = $\frac{\sum_j \sum_k y_{.jk}^2}{ar} - CF - SSB - SSC$ (9)

Sum of Square ABC (SSABC) = $\frac{\sum_i \sum_j \sum_k y_{ijk}^2}{r} - CF - SSA - SSB - SSC - SSAB - SSAC - SSBC$ (10)

Sum of Square Error (SSE) = $TSS - SSA - SSB - SSC - SSAB - SSAC - SSBC - SSABC$ (11).

Yates' Algorithm

Frank Yates created an algorithm to easily find the total factorial effects that are easily programmable in excel. While the algorithm is fairly straightforward, it is also quite tedious. Computer methods are used almost exclusively for the analysis of fractional design. However, Yates' algorithm is modified for use in the 3^{k-1} factorial design. The Yates' algorithm procedure is given in Table 2.

The treatment combinations are written down in standard order; that is, the factors are introduced one at a time, each level being combined successively with every set of factor levels above it in the table. (The standard order for a 3^3 design would be 000, 100, 200, 010, 110, 210, 020, 120, 220, 001 . . .). The Response column contains the total of all observations taken under the corresponding treatment combination. The entries in column (1) are computed as follows. The first-third row of the response column consists the sums of each of the three sets of values. The fourth, fifth and sixth row of the response column is the sixth minus the fourth observation in the same set of three. This operation computes the linear component of the effect. The seventh, eighth and ninth row of the response column is obtained by taking the sum of the seventh and ninth values minus twice the eighth in the set of three observations. The Effects column is determined by converting the treatment combinations at the left of the row into corresponding effects. That is, 10 represent the linear effect of A, A_L, and 11 represent the AB_{LXL} component of the AB interaction. The entries in the Divisor column are found from 2^r3^tn where *r* is the number of factors in the effect considered, *t* is the number of factors in the experiment minus the number of linear terms in this effect, and *n* is the number of replicates. For example, B_L has the divisor $2^1 \times 3^1 \times 4 = 24$. The sums of squares are obtained by squaring the element in column (2) and dividing by the corresponding entry in the Divisor column.

Table 1: ANOVA for 3^3 Factorial Design

Source of Variation	Degree of Freedom	SS	Mean Sum of Square	F-Value
A	a-1	SSA	MSA = $\frac{SSA}{df(A)}$	$F_A = \frac{MSA}{MSE}$
B	b-1	SSB	MSB = $\frac{SSB}{df(B)}$	$F_B = \frac{MSB}{MSE}$
C	c-1	SSC	MSC = $\frac{SSC}{df(C)}$	$F_C = \frac{MSC}{MSE}$
AB	(a-1)(b-1)	SSAB	MSAB = $\frac{SSAB}{df(AB)}$	$F_{AB} = \frac{MSAB}{MSE}$
AC	(a-1)(c-1)	SSAC	MSAC = $\frac{SSAC}{df(AC)}$	$F_{AC} = \frac{MSAC}{MSE}$
BC	(b-1)(c-1)	SSBC	MSBC = $\frac{SSBC}{df(BC)}$	$F_{BC} = \frac{MSBC}{MSE}$
ABC	(a-1)(b-1)(c-1)	SSABC	MSABC = $\frac{SSABC}{df(ABC)}$	$F_{ABC} = \frac{MSABC}{MSE}$
ERROR	abc(r-1)	SSE	MSE= $\frac{SSE}{df(ERROR)}$	
TOTAL	(n-1) or (abcr-1)	SST		

Table 2: Standard Tables for Yates Algorithm

Treatment combination	Response	Column1	Column2	Effects	Divisor	Sum of Square
00	-	-	-			$\frac{(column2)^2}{divisor}$
10	-	-	-	2^1x3^1x4	A_L	$\frac{(column2)^2}{divisor}$
20	-	-	-	2^1x3^2x4	A_Q	$\frac{(column2)^2}{divisor}$
01	-	-	-	2^1x3^1x4	B_L	$\frac{(column2)^2}{divisor}$
11	-	-	-	2^2x3^0x4	AB_{LXL}	$\frac{(column2)^2}{divisor}$
21	-	-	-	2^2x3^1x4	AB_{QXL}	$\frac{(column2)^2}{divisor}$
02	-	-	-	2^1x3^2x4	B_Q	$\frac{(column2)^2}{divisor}$
12	-	-	-	2^2x3^1x4	AB_{LXQ}	$\frac{(column2)^2}{divisor}$
22	-	-	-	2^2x3^2x4	AB_{QXQ}	$\frac{(column2)^2}{divisor}$
						$\frac{(column2)^2}{divisor}$

Table 3: ANOVA for Yates' Algorithm

Source of Variation	Sum of Square	Degree of Freedom	Mean Square	F_o	P-value
$A=A_L$ x A_Q		2	$\frac{SSA}{2}$	$\frac{SSA}{SSE}$	
$B=B_L$ x B_Q		2	$\frac{SSB}{2}$	$\frac{SSB}{SSE}$	
$AB=AB_{LxQ} + AB_{QxQ}$		4	$\frac{SSAB}{4}$	$\frac{SSAB}{SSE}$	
Error		27	$\frac{SSE}{27}$		
Total		35	$\frac{SST}{35}$		

The Sum of Squares column now contains all of the required quantities to construct an analysis of variance table if both of the design factors A and B are quantitative.

Covariance Structures

The covariance are the mean value of the product of the deviations from their respective means, as mention above the covariance structures used are First order auto-regressive (AR(1)), Compound symmetry (CS), Huynh-Feldt (HF), Heterogeneous first order auto-regressive (ARH(1)).

First Order-Auto-regressive (AR (1))

This is a first-order autoregressive structure with homogenous variances. The correlation between any two elements is equal to rho for adjacent elements, ρ^2 for elements that are separated by a third, and so on. ρ is constrained so that $-1<\rho<1$ (Chan, 2004).

$$\sigma^2\begin{bmatrix} 1 & \rho & \rho^2 & \rho^3 \\ \rho & 1 & \rho & \rho^2 \\ \rho^2 & \rho & 1 & \rho \\ \rho^3 & \rho^2 & \rho & 1 \end{bmatrix}$$

Compound Symmetry (CS)

This structure has constant variance and constant covariance (Chan, 2004).

$$\sigma^2\begin{bmatrix} 1 & \rho & \rho & \rho \\ & 1 & \rho & \rho \\ & & 1 & \rho \\ & & & 1 \end{bmatrix}$$

Huynh-Feldt (HF)

This is a "circular" matrix in which the covariance between any two elements is equal to the average of their variances minus a constant. Neither the variances nor the covariances are constant (Gurbuz, *et al*., 2003).

$$\begin{bmatrix} \sigma_1^2 & \frac{\sigma_1+\sigma_2}{2}-\lambda & \frac{\sigma_1+\sigma_3}{2}-\lambda & \frac{\sigma_1+\sigma_4}{2}-\lambda \\ & \sigma_2^2 & \frac{\sigma_2+\sigma_3}{2}-\lambda & \frac{\sigma_2+\sigma_4}{2}-\lambda \\ & & \sigma_3^2 & \frac{\sigma_3+\sigma_4}{2}-\lambda \\ & & & \sigma_4^2 \end{bmatrix}$$

Heterogenous First Order-Auto-regressive (ARH (1))

This is a first-order autoregressive structure with heterogeneous variances. The correlation between any two elements is equal to ρ for adjacent elements, ρ^2 for two elements separated by a third, and so on. ρ is constrained to lie between –1 and 1 (Verkebe & Molenberghs, 1997).

$$\begin{bmatrix} \sigma_1^2 & \sigma_1\sigma_2\rho & \sigma_1\sigma_3\rho^2 & \sigma_1\sigma_4\rho^3 \\ & \sigma_2^2 & \sigma_2\sigma_3\rho & \sigma_2\sigma_4\rho^2 \\ & & \sigma_3^2 & \sigma_3\sigma_4\rho \\ & & & \sigma_4^2 \end{bmatrix}$$

Goodness of Fit Criteria

Information criteria are used when comparing different models for the same data. Akaike's information criterion (AIC) and Bayesian information criterion (BIC) was used in this study to determine the most suitable covariance structure for model approach. The smaller the goodness of fit criterion (AIC, BIC) is better in SPSS and MINITAB packages (Littell, et al., 1996). The test for goodness of fit determines whether a set of observed data conforms to a specified probability distribution.

Akaike Information Criterion (AIC)

Akaike information criterion is a measure of the goodness of fit or a test for goodness of fit of an estimated statistical model (Littell, *et al*., 1996). The formula for the criterion is given as follow:

$$AIC = 2l + 2d \qquad (12)$$

Where

l is the log likelihood evaluated at the parameter estimates or restricted log-likelihood maximum value and **d** is parameter number.

Bayesian Information Criterion (BIC)

The Bayesian Information Criterion (BIC) or Schwarz Bayes Information Criterion (SBC) is a criterion for model selection among a finite set of models. It is based in point of the likelihood function and it is closely related to Akaike Information Criterion (AIC). In facts, Akaike was so impressed with Schwarz's Bayesian formalism that he developed his own Bayesian formalism, now often referred to as the ABIC for "Akaike Bayesian Information Criterion" (Littell, et al., 1996). The formula for the BIC is given as

$$BIC = -2\ln L + k\ln(n) \quad (13)$$

Where L is the restricted log-likelihood maximum value k is the parameter number and n is the observation number under the assumption that the model errors or disturbances are independent and identically distributed (iid) according to a normal distribution and that the boundary condition that the derivative of the log likelihood with respect to the time variance is zero.

$$BIC = n.\ln(\hat{\sigma}_e^2) + k.\ln(n) \quad (14)$$

Explanatory variables increase the value of BIC. Hence, lower BIC implies either fewer explanatory variables, more strongly than those the Akaike information criterion, though it depends on the size of n and relative magnitude of n and k. (Bhat & Kumar, 2010).

Where

$\hat{\sigma}_e^2$ is the error variance and the error variance in this case is defined as

$$\hat{\sigma}_e^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \hat{x}_i)^2 \quad (15)$$

One may point out from probability theory that $\hat{\sigma}_e^2$ is a biased estimator for the true variance σ^2. Let $\hat{\sigma}_e^2$ denote the unbiased form of approximating the error variance. It is defined as

$$\hat{\sigma}_e^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \hat{x}_i)^2 . \quad (16)$$

Additionally, under the assumption of normality the following version may be more tractable

$$BIC = X^2 + k.\ln(n) \quad (17)$$

Note that there is a constant added that follows from transition from log-likelihood to X^2; however, in using the BIC to determine the "best" model the constant becomes trivial given any two estimated models, the model with the lower value of BIC is the one to be preferred. The BIC is an increasing function of σ_e^2 and an increasing function of k. that is, unexplained variation in the dependent variable and the numbers of

Tests for Normality

An assessment of the normality of data is a pre-requisite for many statistical tests, as normal data is an underlying assumption in parametric testing. There are two methods

of assessing normality, graphically and numerically.
In this paper graphical method will be used as a means of assessing normality.

Software for the Analysis

As stated earlier, the MINITAB version 16.2 and SPSS latest version software were used for the analysis of the research and the software were designed to handle many statistical analyses. The package series were used to test for the best covariance structure using some selected criteria and many other related statistical test in the data set. It is also used to plot the graph of the normality and nature of the trend. Two goodness of fit were used to assess the best covariance structure stated earlier.

Results

Table 4 summarizes the results of yield using ANOVA which indicates that seed rates and row spacing applied gives a better yield than the varieties, all the interaction produces a better yield as such irrigation scheme which improved modern yield in the stated conditions above gives more yield and save cost, provided the assumption are made and satisfied.
Table 5 shows the summary of selected covariance structures using goodness of fit criterion as an indicator of finding the best covariance structure, the structure which least criterion is the best. Therefore, table 5 indicates AR (1) as the best covariance structure, followed by ARH (1) and HF. This suggests that modern improved seed rates and varieties gives more yield or produces more output. In general, the result shows that there is significant improvement using new seed rates.
Table 4 shows that two factors are significant. That is factor A and factor C are significant, F_{cal} at df (2, 243) is greater than F_{tab} at df (2, 243), $\alpha = 0.05$ and P-value is less than 0.05 at both factor A and C. But P-values is greater than 0.05 in factor B which indicates that is not significant, at df (2, 243), $\alpha = 0.05$, also P-values is less than 0.05 in all the interactions, which shows that there are significant different between the interactions A*B, A*C, B*C at df (4, 243), $\alpha = 0.05$ and A*B*C at df (8, 243), $\alpha = 0.05$. Hence, it can be concluded that the yield of seed rates, row spacing and varieties have different effects at different levels which indicates that there is significant different in yield between different factors, that is if P-values are less than 0.05 it shows that there is significant different in the yield.

Multilevel Factorial Design

Table 4: ANOVA for Yield, Using Adjusted SS for Test

SOURCE	DF	Seq SS	Adj SS	Adj MS	F	P
SEED RATES	2	377931	377931	188966	5.76	0.004
VARIETIES	2	31517	31517	15759	0.48	0.619
ROW SPACING	2	204013	204013	102006	3.11	0.047
SEED RATES *VARIETIES	4	644273	644273	161068	4.91	0.001
SEED RATES*ROW SPACING	4	362224	362224	90556	2.76	0.029
VARIETIES*ROW SPACING	4	685262	685262	171315	5.22	0.000
SEED RATES*VARIETIES*ROW SPACING	8	758717	758717	94840	2.89	0.004
Error	243	7978319	7978319	32833		
Total	269	1.1E+07	1.1E+07			

S = 181.198   R-Sq = 27.75%   R-Sq(adj) = 20.02%

Table 5: Criteria Results for Comparing Covariance Structures

	COVARIANCE STRUCTURES			
Information criteria	CS	HF	AR (1)	ARH (1)
AIC	3553000	3546000	3279000	3546000
BIC	3921000	3859000	3295000	3859000

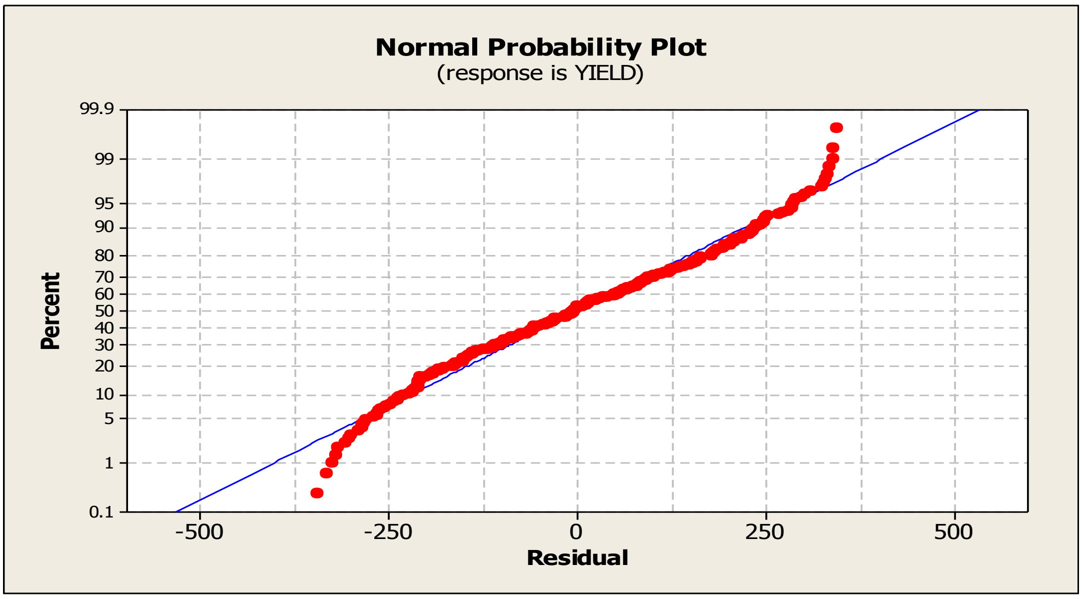

Figure 1: Normal Probability

Figure 1 indicates that the distribution of residuals is normal, because, from the figure you can see that the residuals resemble a straight line therefore the normality assumption hold.

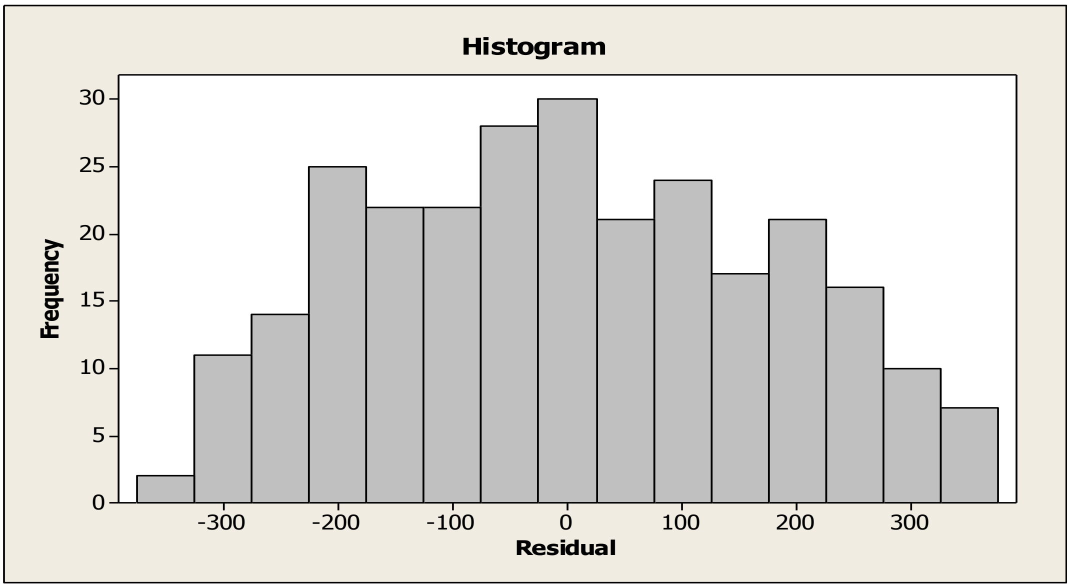

Figure 2: Histogram

Figure 2 show that the plots are independence since both of them do not reveal any pattern. Therefore, the independence assumption is satisfied.

Y_{ijk}=

$$\mu + A_i + B_j + AB_{ij} + C_k + AC_{ik} + BC_{jk} + ABC_{ijk} + \varepsilon_{ijk} \quad (18)$$

In addition, R^2 is moderately ok which explained the variability of the data.

Table 5 shows the information criteria for different covariance structure in mixed model approach. According to AIC and BIC fitting criteria, First Order Auto-regressive (AR (1)) has the best covariance structure (it has the smaller value on both AIC and BIC), then followed by Huynh-Feldt (HF) and Heterogeneous first-order Auto-regressive ARH(1). (AR (1)) is the best covariance structure among the four selected structures and hence is the most fitted and accepted in this work and the work related to this type.

Discussion

In this paper, the set of data used was tested for adequacy and found to satisfy the assumption of normality, independence and homogeneity. 3^3 multilevel full factorial design analysis shows that two factors A and C are significance while the other factor B is not significance, because the P-values of factors A and C are less than 0.05 while the P-values of factor B is greater than 0.05. Null hypothesis indicates that the hypothesis should be rejected for factors A and C and conclude that there is significance difference between the yields. Coefficient of determination (R^2) also indicates that the analysis is satisfied, because R^2 explained the variability of the data.

According to information criteria AIC and BIC, First Order Auto-regressive (AR(1)) was the best covariance structure (since it is the one that provide the smaller value on both the AIC and BIC) then followed by Huynh-feldt (HF) and Heterogeneous first order autoregressive ARH (1). (AR(1)) gave information about bread wheat yield in seed rates, row spacing and varieties

Conclusion

This paper is concerned with determining the best covariance structure in seed rates, row spacing and varieties (V1, V2 and V3) of the bread wheat yield. Full factorial design method allow a large number of variables to be investigated in a compact trial, enable outliers in the data to be identified and provide detailed process knowledge. R^2(adj) penalizes the statistic as extra variables in the model. With regard to covariance structures, first order auto-regressive (AR(1)) was found to be the best covariance structure defining yield of bread wheat as a function of seed rates, row spacing and varieties.

The model and different covariance structures studied here shows that there are indeed tangible benefits gained. These benefits can result in the better yield at the same time contribute to knowledge

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