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A Simulation Study on Tests of Hypotheses for Fixed Effects in Mixed Models for One-Way ANOVA under the Violation of the Equal Variances Assumption of the Treatment Groups with and without Missing Data

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Abstract. This article considers the analysis of experiment of one-way completely randomized design (one-way ANOVA) that is frequently used in every discipline. We investigate a common problem that is data collected in practice usually violate parametric assumptions to some degree. We concentrated our attention on ANOVA when the equal variances assumption for the treatment groups is violated. We investigate the performance of a general linear fixed effects model approach (GLM procedure of the SAS System) in analyzing one-way ANOVA under the violation of only one assumption that is heterogeneous variances. Also, we investigate the performance of a general linear mixed effects model approach (MIXED procedure of the SAS System) in analyzing one-way ANOVA under the violation of only one assumption that is heterogeneous variances as alternative to GLM procedure of the SAS System. The main result of our article is that the general linear mixed effects model approach can be recommended to be used in case of the suspicion of the violation of the equal variances assumption specially in case of unbalanced data where the general linear fixed effects model approach showed serious departures upward from the nominal level.

Keywords: One-Way ANOVA, GLM procedure, MIXED procedure, Kenward-Roger method, Restricted maximum likelihood (REML).

1. Introduction

This article considers the analysis of experiment of one-way completely randomized design (one-way ANOVA) that is frequently used in every discipline. Sir R. A. Fisher[1], explained the relationship between the mean, the variance, and the normal distribution as follows: "The normal distribution has only two characteristics, its mean and its variance. The mean determines the bias of our estimate, and the variance determines its precision". When the variances of treatment groups are unequal, the comparison may be invalid. In this article, we investigate the performance of a general linear fixed effects model approach (GLM procedure of the SAS System) in analyzing one-way ANOVA under the violation of only one assumption that is the equal variances assumption (heterogeneous variances). This approach is the traditional approach that is usually used in the analysis of ANOVA. Also, we investigate the performance of a general linear mixed effects model approach (MIXED procedure of the SAS System) in analyzing one-way ANOVA under the violation of only one assumption that is heterogeneous variances. We used the general linear mixed effects model approach to analyze one-way ANOVA under the violation of only one assumption that is the equal variances assumption (heterogeneous variances) as alternative to the general linear fixed effects model approach where the general linear mixed effects model approach has the ability to accommodate the violation of the equal group variances. The performance of the two approaches compared in both cases of balanced and unbalanced data.

The model fit by the GLM procedure (the general linear fixed effects model approach) is[2],

$$\mathbf{y} = \mathbf{X}\beta + \mathbf{e}$$

where

$\mathbf{X}$ = $N \times p$ design matrix for fixed effects.

β = $p \times 1$ vector of fixed effects parameter.

$\mathbf{e}$ = $n \times 1$ vector of residuals.

For the usual general linear fixed effects model, it is assumed $\mathbf{y} \sim N(\mathbf{X}\beta, \sigma^2\mathbf{I})$. GLM procedure uses method-of-moments to estimate the variance component. The mixed effects linear model extends the general linear fixed effects model approach by allowing a more general specification of covariance matrix of the vector of Y. The model fit by the MIXED procedure (the general linear mixed effects model approach) is[3,4].

$$\mathbf{y} = \mathbf{X}\beta + \mathbf{Z}\gamma + \mathbf{e} \tag{1.1}$$

where:

β = $p \times 1$ vector of fixed effects parameter.

γ = $q \times 1$ vector of random effects parameter.

$\mathbf{e}$ = $n \times 1$ vector of residuals.
$\mathbf{X}$ = $n \times p$ design matrix for fixed effects.
$\mathbf{Z}$ = $n \times q$ design matrix for random effects.

$$\gamma \sim N(\mathbf{0}, \mathbf{G}),\ \mathbf{e} \sim N(\mathbf{0}, \mathbf{R}),$$
$$\mathbf{y} \sim N(\mathbf{X}\beta, \mathbf{V}), \text{ and } \mathbf{V} = \mathbf{ZGZ}' + \mathbf{R}.$$

The general linear fixed effects model is a special case of the general linear mixed effects model with $\mathbf{Z} = \mathbf{0}$ (which means $\mathbf{Z}\gamma$ disappears from the model (1.1)) and $\mathbf{V} = \mathbf{R} = \sigma^2\mathbf{I}$. MIXED procedure lets us specify various covariance structures for $\mathbf{G}$ and $\mathbf{R}$ matrices. When $\mathbf{V}$ is known, the best linear unbiased estimators (BLUE) of estimable functions $\mathbf{h}'\beta$ of the fixed effects in (1.1) are given by

$$\mathbf{h}'\hat{\beta} = \mathbf{h}'(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y}, \tag{1.2}$$

$$\text{with } \operatorname{var}(\mathbf{h}'\hat{\beta}) = \mathbf{h}'(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}\mathbf{h}. \tag{1.3}$$

In most applications $\mathbf{V}$ is unknown. Therefore, it is estimated from the data where estimators based on (1.2) are not generally BLUE[5]. Various procedures proposed for testing hypotheses on fixed effects in mixed models with unknown $\mathbf{V}$, most of which assume that $\mathbf{V}$ is estimated by the REML method[6-8]. The resulting estimates of fixed effects are often referred to as empirical BLUE (eBLUE)[5]. Standard error estimates based on (1.3) are biased downwards when $\mathbf{V}$ replaced by its estimate[9]. Fixed effects are estimated based on (1.2), with $\mathbf{V}$ replaced by a plug-in restricted maximum likelihood (REML) estimates. Null hypotheses of the form $H_0 : \mathbf{h}'\beta = 0$ are tested by

$$F = \frac{\hat{\beta}'\mathbf{h}[\mathbf{h}'(\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-}\mathbf{h}]^{-1}\mathbf{h}'\hat{\beta}}{rank\ (h)} \sim F_{(rank(\mathbf{h}),\upsilon)} \tag{1.4}$$

when *rank* ($\mathbf{h}$) > 1. In general, the test statistics in (1.4) only have approximate *F – distribution.* The approximate denominator degree of freedom υ of *F – distribution* can be determined using one of the four different methods implemented in MIXED procedure of SAS System. The four methods of the approximations are residual method, containment method (this is the default in MIXED), extended Satterthwaite[10] method of Giesbrecht and Burns[7] and Fai and Cornelius[6], and Kenward-Roger[8] method.

2. Methodology

The study considered the one-way completely randomized design. The design consists of three treatment groups with both equal and unequal number of replications. The goal of the study is to compare the empirical Type I error rate and the empirical power for the two approaches under the two situations of existence and non existence of the violation of the equal variances assumption in both cases of balanced and unbalanced data. Unbalancedness (Missing Data) was generated by randomly dropping certain number of observations. In order to accomplish the goals of this study, it was necessary to design a simulation study of one-way ANOVA data. The following model reflects the experiment of one-way completely randomized design:

$$y_{ij} = \mu_i + \varepsilon_{ij} \ , \text{ where } i = 1,2,3 \text{ and } j = 1,2,\ldots,n \ . \tag{2.1}$$

Multivariate normal data were generated according to model (2.1). There were 60 scenarios to generate data involving one covariance structure with 10 settings of covariance matrix parameter values and three different sample sizes (n = 3, 5, and 10 replications per treatment group). The covariance structure was a completely general (unstructured) covariance matrix parameterized directly in terms of variances and covariances. The variances are constrained to be nonnegative and the covariances are all equal to zero. The 10 settings of covariance matrix parameter values can be classified into two classes of covariance matrix setting. The first class has equal variances for the treatment groups and the second class has unequal variances for the treatment groups. The 10 settings are given in Table 1.

Table 1. The ten settings of covariance matrix parameter values used in the simulation.

Class	Setting no.	Covariance matrix	Class	Setting no.	Covariance matrix
1	1	$\begin{bmatrix} 10 & 0 & 0 \\ 0 & 10 & 0 \\ 0 & 0 & 10 \end{bmatrix}$	2	6	$\begin{bmatrix} 10 & 0 & 0 \\ 0 & 10 & 0 \\ 0 & 0 & 100 \end{bmatrix}$
1	2	$\begin{bmatrix} 25 & 0 & 0 \\ 0 & 25 & 0 \\ 0 & 0 & 25 \end{bmatrix}$	2	7	$\begin{bmatrix} 10 & 0 & 0 \\ 0 & 20 & 0 \\ 0 & 0 & 30 \end{bmatrix}$
1	3	$\begin{bmatrix} 50 & 0 & 0 \\ 0 & 50 & 0 \\ 0 & 0 & 50 \end{bmatrix}$	2	8	$\begin{bmatrix} 10 & 0 & 0 \\ 0 & 30 & 0 \\ 0 & 0 & 90 \end{bmatrix}$
2	4	$\begin{bmatrix} 10 & 0 & 0 \\ 0 & 10 & 0 \\ 0 & 0 & 50 \end{bmatrix}$	2	9	$\begin{bmatrix} 10 & 0 & 0 \\ 0 & 40 & 0 \\ 0 & 0 & 160 \end{bmatrix}$
2	5	$\begin{bmatrix} 10 & 0 & 0 \\ 0 & 10 & 0 \\ 0 & 0 & 75 \end{bmatrix}$	2	10	$\begin{bmatrix} 5 & 0 & 0 \\ 0 & 25 & 0 \\ 0 & 0 & 125 \end{bmatrix}$

For each scenario, we simulated 5000 datasets. SAS (Version 8.02) PROC IML code was written to generate the datasets. A (n) 3 × 1 vectors of multivariate normal were generated using SAS's NORMAL function[11]. Denoted the vector:

$$\mathbf{y}_j = \begin{bmatrix} y_{1_j} \\ y_{2_j} \\ y_{3_j} \end{bmatrix} \sim N_3 \left(\begin{bmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \end{bmatrix} ; \Sigma = \begin{bmatrix} \sigma_1^2 & 0 & 0 \\ 0 & \sigma_2^2 & 0 \\ 0 & 0 & \sigma_3^2 \end{bmatrix} \right) ; \; 1,2,\ldots,n$$

After the simulated data sets were generated, the simulated data sets were analyzed using both the two approaches in order to evaluate the performance of the two approaches. Kenward-Roger method was used for computing the denominator degrees of freedom for the tests of fixed effects from all the analyses with the PROC MIXED procedure for the following reasons: 1) Kenward and Roger[8] found good performance of their method across a number of design, 2) Guerin and Stroup[12] recommended using the Kenward-Roger method as standard operating procedure, and 3) One of our previous simulation study was in good agreement with findings of the previous authors. In our investigations, the evaluation of the analysis was in terms of control of Type I error, and the power. Type III sums of squares and its associated statistics were used in the analysis that is corresponds to Yates' weighted squares of means analysis. In case of a valid alternative hypothesis, the values of fixed effect used under the alternative are summarized in Table 2.

Table 2. Marginal means in case of validity of the alternative hypothesis.

Levels of treatment effect	Marginal mean
1	–3
2	0
3	3

It may be of interest to note that the following commands represent a traditional analysis of one-way completely randomized design by using the general linear fixed effects model approach (PROC GLM of the SAS System).

```
PROC GLM DATA = DAT1;
        CLASS    TREATMENT;
        MODEL  Y = TREATMENT;
        RUN;
```

Also, it may be of interest to note that the following commands represent the analysis of one-way completely randomized design under the violation of equality of variance by using the general linear mixed effects model approach (PROC MIXED of the SAS System).

```
PROC MIXED DATA = DAT1;
        CLASS    TREATMENT;
        MODEL  Y = TREATMENT / DDFM = KR;
        REPEATED  / GROUP = TREATMENT;
        RUN;
```

Note that TREATMENT identifies the treatment groups and Y identifies the response variable[13].

3. Results

3.1 Results Under the Null Hypothesis

Due to space limitations, we present only part of the total simulation results of the 60 scenarios. The complete results are available from the author upon request. Table 3 summarizes results of the average of the empirical Type I error rate across the first class of the investigated settings of covariance matrix, when data are simulated under the null hypothesis and no assumption violations are existed, for the two approaches with the three different sample sizes in both cases of balanced and unbalanced data. Table 4 summarizes results of the average of the empirical Type I error rate across the second class of the investigated settings of covariance matrix, when data are simulated under the null hypothesis and the equal variances assumption is violated, for the two approaches with the three different sample sizes in both cases of balanced and unbalanced data. Table 3 indicates that although the nominal level was controlled well with the two approaches for both the cases of balanced and unbalanced data, slight downward departures were observed with the general linear mixed effects model approach for balanced data case particularly for small sample size. Table 4 indicates that the general linear mixed effects model approach provided the best control of the nominal error probability for both cases of balanced and unbalanced data. On the other hand, the general linear fixed effects model approach shows serious upward departures and it is getting worse for the unbalanced data case. As expected, control of the nominal error probability improved with increasing sample size for the balanced data case.

3.2 Results Under the Alternative Hypothesis

In order to help in the interpretation of empirical power results, the noncentrality parameter for each effect is reported. The noncentrality parameter was computed by $\beta'\mathbf{h}(\mathbf{h}'(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}\mathbf{h})^{-1}\mathbf{h}'\beta$ for each simulation run and average across runs. Table 5 reports the average of the noncentrality parameter across the first class of the investigated settings of covariance matrix, when data are simulated without violation of any assumption, for the two approaches with the three different sample sizes in both cases of balanced and unbalanced data.

Table 3. Average of the empirical Type I errors across the first class of the investigated covariance settings for F-test under the null hypothesis (nominal Type I error = 0.05).

Effect	Sample size: 3			
	Balanced data		Unbalanced data	
	PROC GLM	PROC MIXED	PROC GLM	PROC MIXED
Treatment	0.0482	0.0238666	0.0478	0.0518
	Sample size: 5			
Treatment	0.0492	0.039	0.05	0.0408
	Sample size: 10			
Treatment	0.0476	0.0464	0.0488	0.0452

Table 4. Average of the empirical Type I errors across the second class of the investigated covariance settings for F-Test under the null hypothesis (nominal Type I error = 0.05).

Effect	Sample size: 3			
	Balanced data		Unbalanced data	
	PROC GLM	PROC MIXED	PROC GLM	PROC MIXED
Treatment	0.0811142	0.0403714	0.1235142	0.0527142
	Sample size: 5			
Treatment	0.0742285	0.0459714	0.1380571	0.0527142
	Sample size: 10			
Treatment	0.0679714	0.0492571	0.1275428	0.0503142

Table 5. Average of the Noncentrality Parameter (NCP) across the first class of the investigated covariance matrix settings.

Effect	Sample size: 3			
	Balanced data		Unbalanced data	
	PROC GLM	PROC MIXED	PROC GLM	PROC MIXED
Treatment	7.3931907	11.489411	7.448789	15.351142
	Sample size: 5			
Treatment	8.1769216	9.7156072	6.5162515	12.920849
	Sample size: 10			
Treatment	12.503809	13.495347	10.280901	11.762313

Table 6 reports the average of the noncentrality parameter across the second class of the investigated settings of covariance matrix, when data are simulated with the violation of the equal variances assumption, for the two approaches with the three different sample sizes in both cases of balanced and unbalanced

Table 6. Average of the Noncentrality Parameter (NCP) across the second class of the investigated covariance matrix settings.

Effect	Sample size: 3			
	Balanced data		Unbalanced data	
	PROC GLM	PROC MIXED	PROC GLM	PROC MIXED
Treatment	6.6450683	10.502715	10.14615	19.59795
	Sample size: 5			
Treatment	6.7539962	8.3582622	10.061416	19.683221
	Sample size: 10			
Treatment	8.250965	10.044385	9.1920511	9.3716447

data. Table 7 summarizes results of the average of the empirical power across the first class of the investigated settings of covariance matrix, when data are simulated without violation of any assumption, for the two approaches with the three different sample sizes in both cases of balanced and unbalanced data. Table 8 summarizes results of the average of the empirical power across the second class of the investigated settings of covariance matrix, when data are simulated with the violation of the equal variances assumption, for the two approaches with the three different sample sizes in both cases of balanced and unbalanced data. Table 7 shows that the empirical powers of the balanced data case were similar for the two approaches. Also, it showed that the empirical powers of the unbalanced data case were higher for the general linear fixed effects model approach comparing to the general linear mixed effects model approach due to their higher Type I error rates. As expected, the empirical power improved with increasing sample size for both approaches in both cases of balanced and unbalanced data.

Table 7. Average of the empirical power across the first class of the investigated covariance matrix settings of F-Test under the alternative hypothesis.

Effect	Sample size: 3			
	Balanced data		Unbalanced data	
	PROC GLM	PROC MIXED	PROC GLM	PROC MIXED
Treatment	0.1997333	0.0898666	0.1614666	0.0821333
	Sample size: 5			
Treatment	0.3756666	0.307	0.2477333	0.1853333
	Sample size: 10			
Treatment	0.6370666	0.6113333	0.5452666	0.5063333

Table 8. Average of the empirical power across the second class of the investigated covariance matrix settings for F-Test under the alternative hypothesis.

Effect	Sample size: 3			
	Balanced data		Unbalanced data	
	PROC GLM	PROC MIXED	PROC GLM	PROC MIXED
Treatment	0.1670571	0.0828857	0.2093142	0.0669428
	Sample size: 5			
Treatment	0.2927142	0.2732285	0.3496857	0.1389714
	Sample size: 10			
Treatment	0.4518571	0.5193428	0.4650285	0.40080

Finally, Table 9 shows the rejection rate of testing the homogeneity of variances for the treatment groups using the likelihood ratio test for the ten investigated covariance matrix settings. Table 9 (The first covariance class) indicates that although the control of the nominal error probability improved with increasing the sample size for both cases of the balanced and unbalanced data, slightly more departures upward were observed with the case of the unbalanced data comparing to the case of the balanced data. On the other hand, Table 9 (The second covariance class) indicates that although the empirical powers improved with increasing the sample size for both cases of the balanced and unbalanced data, the empirical power was higher for the case of the balanced data as compared with the case of the unbalanced data.

4. Conclusion

In our simulation, we considered one-way completely randomized design (one-way ANOVA), looking at the performance of two approaches that are a general linear fixed effects model approach and a general linear mixed effects model approach with different settings of the covariance matrix. The main result of our article is that overall, the general linear mixed effects model approach provided the best control of the nominal Type I error rate. Thus, this approach can be recommended to be used with the suspicion of the violation of the equal variances assumption specially in case of unbalanced data where the general linear fixed effects model approach showed serious departures upward from the nominal level. These results are in good agreement with the theory that suggests accommodating the violation of the equal variances assumption in the analysis. In addition, our power analysis showed that power was larger when the Type I error rate was on the liberal side. Thus, differences in power among the approaches were mainly due to differences in Type I error control. The power differences between the effects can be explained mainly by differences in

Table 9. The rejection rate of testing the homogeneity of variances for the treatment groups using the likelihood ratio test for the ten investigated covariance matrix settings (nominal Type I error = 0.05).

Cases of data	Sample size: 3									
	Covariance settings									
	The first covariance class			The second covariance class						
	Cov - 1	**Cov - 2**	**Cov - 3**	**Cov - 4**	**Cov - 5**	**Cov - 6**	**Cov - 7**	**Cov - 8**	**Cov - 9**	**Cov - 10**
Balanced	0.0848	0.0848	0.0848	0.2086	0.301	0.3652	0.1216	0.236	0.3456	0.4322
Unbalanced	0.0938	0.094	0.0938	0.1782	0.2282	0.2726	0.1186	0.2072	0.2776	0.3378
Cases of data	Sample size: 5									
	Covariance settings									
	The first covariance class			The second covariance class						
	Cov - 1	**Cov - 2**	**Cov - 3**	**Cov - 4**	**Cov - 5**	**Cov - 6**	**Cov - 7**	**Cov - 8**	**Cov - 9**	**Cov - 10**
Balanced	0.0614	0.0614	0.0614	0.373	0.5408	0.6552	0.1454	0.4376	0.6394	0.8778
Unbalanced	0.686	0.686	0.0686	0.2698	0.3904	0.4478	0.1356	0.3418	0.4938	0.6166
Cases of data	Sample size: 10									
	Covariance settings									
	The first covariance class			The second covariance class						
	Cov - 1	**Cov - 2**	**Cov - 3**	**Cov - 4**	**Cov - 5**	**Cov - 6**	**Cov - 7**	**Cov - 8**	**Cov - 9**	**Cov - 10**
Balanced	0.0592	0.0592	0.0592	0.711	0.8778	0.944	0.2756	0.8152	0.9542	0.9896
Unbalanced	0.0632	0.0632	0.0632	0.5396	0.7272	0.8298	0.2338	0.6872	0.8748	0.9462

the noncentrality parameter. Further simulation need to be performed for this design to see if the main results of our article stay the same under the violation of other assumptions.

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دراسة بطريقة المحاكاة عن اختبارات الفروض لتأثيرات ثابتة باستخدام النموذج المخلوط لتحليل التباين ذي الاتجاه الواحد عندما يكون شرط تَسَاوي التباين لمجموعات المعالجات غير متحقق في حالة وجود وعدم وجود مشاهدات مفقودة

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المستخلص. تهتم هذه الورقة العلمية بدراسة واحد من أهم التصاميم في مجال تصميم التجارب الإحصائية من حيث كثرة استخداماته في جميع مجالات العلوم، وهو التصميم العشوائي الكامل ذو الاتجاه الواحد. تتركز دراستنا حول مشكلة عادةً ما يتكرر حدوثها عند جمع البيانات في المجالات التطبيقية، وهي عدم تحقق الاشتراطات المعلمية لنموذج هذا التصميم إلى حد ما. وتم التركيز - خاصة - على شرط واحد فقط من ضمن الاشتراطات، وهو تَسَاوي التباين لمجموعات المعالجات. هدف الدراسة هو مقارنة أداء كل من طريقة النموذج الخطي للتأثير الثابت، وطريقة النموذج الخطي للتأثير المخلوط في تحليل هذا التصميم عندما يكون شرط تَسَاوي التباين لمجموعات المعالجات غير متحقق. وقد أوضحت النتائج أنه يمكننا أن نوصي باستخدام طريقة النموذج الخطي للتأثير المخلوط كبديل لطريقة النموذج الخطي للتأثير الثابت في حالة عدم تحقق هذا الشرط، ويكون ذلك ضروريًا في حالة وجود مشاهدات مفقودة، حيث إن طريقة النموذج الخطي للتأثير الثابت أظهرت بُعداً ملحوظًا بزيادة عن المستوى المتعارف عليه لاحتمال الوقوع في خطأ من النوع الأول في هذه الحالة.