COMPARISONS BETWEEN METHODS OF ESTIMATION OF THE RANDOM STANDARD DEVIATION IN FACTORIAL EXPERIMENTS WITH TWO LEVELS BY FACTOR AND WITHOUT REPEAT

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▪ ABSTRACT: To obtain the estimate of random variance in complete and fractional factorial experiments with two levels per factor evaluated without repetition, Hamada and Balakrishnan (1998) provide a list of several methods. Thus, based on this review, the objective of the present study was to compare the estimates of standard deviations with only influences of random causes according to four methods: de Lenth (1989), Juan and Pena (1992), Dong (1993) and without any restriction on data, here called total standard deviation. For this, a normal random variable with 10.000 values was simulated, whose simulation was repeated 16 times. Subsequently, they were replaced in each of the 16 data sets, 0%, 1%, 2%, 3% and 4% of the random values by outliers in order to break the simulated variable randomness. Based on the estimate of the mean absolute percentage error (MAPE) obtained in relation to the parametric random standard deviation, it was concluded, through regression analysis, that it increased due to the increase in the percentage of substitution of random values for outliers, with the exception of that obtained according to the method of Juan and Pena (1992). Even so, for data sets with up to 3.68% outliers, the best methods for estimating the random standard deviation (σ_{random}) were those of Lenth (1989) and Dong (1993), as they provided the lowest estimates MAPE. Above this percentage and up to 4% of outliers, the method of Juan and Pena (1992) proved to be better. However, as the highest MAPE estimate provided by the three estimation methods was very low (4.00%), and yet, as the differences observed between them were practically negligible, it was concluded that the three methods provided good estimates of σ_{random} and that, consequently, can be recommended to estimate the mean square of the residue in complete and fractional factorial experiments with two levels per factor and with individual observations per treatment. On the other hand, the total standard deviation method was unable to avoid the effect of non-randomness on the estimate of the σ_{random}.

▪ KEYWORDS: Residue, random variance; outliers.

1 Introduction

When complete and fractional factorial experiments with two levels per factor are planned without repetition, the main effects and those of interactions of different orders

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can be tested if their estimates are considered as values of a normal random variable. In such cases, the variance analysis has, when all effects are considered in the model, zero degree of freedom for the residue. Therefore, it is not possible to obtain the mean squared residues (MSR).

In a review work, Hamada and Balakrishnan (1998) presented a summary of 24 methods proposed between 1959 and 1996 to estimate the random standard deviation (σ_{random}), that is, a standard deviation that behaves as the square root of MSR, in complete and fractional factorial experiments with two levels per factor and with individual observations per treatment. In addition, interpretations were also presented about them through a study by data simulation. Subsequently, Ye *et al.* (2001) proposed a modification in one of these methods, in the case of Lenth (1989), because they consider it as simple and efficient.

The main and precursor idea for the emergence of all 24 methods of estimation of σ_{random} was based on the occurrence of zero degree of freedom for the residue due to the absence of repetition of factorial experiment treatments, and, consequently, the impossibility of its attainment through this basic principle.

In the area of statistical process control, Mahmoud *et al*. (2010), Saleh *et al*. (2015) and Soube et al. (2020) also presented new methodologies for estimating the random variability of the process through the construction of control charts.

Those of Lenth (1989), Juan and Pena (1992) and Dong (1993) were selected of the methods reviewed by Hamada and Balakrishnan (1998), in order to verify their efficiencies when estimating, also, the σ_{random}, but from a non-variable obtained from data sets with individual observations and without considering experimental designs. As the method of Lengh (1989) has been very disseminated in the analysis of factorial experiment without repetitions and in statistical software, the purpose was to use similar and newer methods. Despite the previous review about the subject, a detailed conclusion has not yet been observed, nor according to the imposition tested in the present work.

2 Purposes

The purpose of this work was to compare the quality estimate of the σ_{random} by the methods of Lenth (1989), Juan and Pena (1992), Dong (1993) and without any restrictions to the data, here called total standard deviation, of a non-random variable imposed by the presence of *outliers*. Consequently, the purpose was to recommend at least one of them to obtain MSR estimate in complete and fractional factorial experiments with two levels per factor and with individual observations per treatment.

3 Methods of estimation

3.1 Lenth

Lenth (1989) presented a relatively simple methodology, which consists of obtaining an estimate Lenth of the σ_{random}, defined as pseudo-standard error (PSE):

$$s_{random} = PSE = 1.5 \times Md|\hat{e}_j|, \text{ para j = 1, 2, ..., } m \leq n. \quad (1)$$

In order to obtain PSE, first the following quantity is obtained:

$$s_0 = 1.5 \times Md|\hat{e}_i|, \text{ para i = 1, 2, ..., } n. \quad (2)$$

As it is possible to observe, the difference between the equations of PSE and of the s_0 is only in the calculation of the median (Md), being:

$$|\hat{e}_j| = |\hat{e}_i| 2.5 s_0, \quad (3)$$

where $|\hat{e}_j|$ – vector that contains only the m absolute estimates of the effects to be used in the calculation of the PSE and $|\hat{e}_i|$ = vector that contains all n absolute estimates of the effects to be tested.

In other words, in the equation of the PSE, the median will be lower or, at most, equal to that used in the s_0, as it removes the most expressive and possibly non-random absolute effects. For this reason, PSE is used as the estimate of the σ_{random}.

As can be seen, PSE is obtained based only and absolute estimates of effects that are less than $2.5s_0$. This means, therefore, that, at most, *n* absolute estimates are used to obtain them. According to Lenth (1989), PSE is consistent with σ_{random} only when there are no significant effects, that is, when H_{0i}: $e_i = 0$ hypothesis is not rejected. Otherwise, it overestimates it.

3.2 Juan and Pena

Juan and Pena (1992) proposed an alternative method to that of Lenth (1989), in which, initially, the median of all n estimates of absolute effects, called MAD_0 is calculated. After, another MAD_0 is calculated as the median of the estimates of absolute effects less than $wMAD_0$, according to a constant $w > 2$. The process of calculating the MAD_0 and obtaining estimates of absolute effects less than $wMAD_0$ continues until the MAD_0 value does not change. Finally, the last MAD_0 value is defined by $IMAD_0$.

$$s_{random} = s_{IMAD} = \frac{IMAD_0}{a_w}, \quad (4)$$

where a_w – correction factor.

In order to have a better estimate, Juan and Pena (1992) recommended $w = 3.5$ e $a_w = 0.6578$.

3.3 Dong method

Dong (1993), in competition with the method of Lenth (1989), proposes the following estimate of the σ_{random}:

$$s_{random} = s_{Dong} = \sqrt{\frac{\sum_{j=1}^{m} \hat{e}_j^2}{m}} \quad (5)$$

where $|\hat{e}_j| = (|\hat{e}_i| 2.5 s_0)$ – vector that contains only m absolute estimates of the effects to be used in calculation of the s_{Dong} (j = 1, 2, ..., m ≤ n); $s_0 = 1.5 \times Md|\hat{e}_i|$; $|\hat{e}_i|$ - vector that contains all n e absolute estimates of the effects to be tested (i = 1, 2, ..., n) and Md - median.

3.4 Normal probability plots of effects

For the construction of the normal probability ploto f the effects, consider the estimates of the effects $\hat{e}_1, \hat{e}_2, ..., \hat{e}_n$ arranged in ascending order; for each estimate $\hat{e}_i$, there is an accumulated distribution function F($\hat{e}_i$) (theoretical). Consequently, there is a corresponding z_i value of the standardized normal distribution, given by;

$$z_i = \frac{\hat{e}_i - 0}{s_{random}}, \quad (6)$$

where $F(\hat{e}_i) = F(z_i) = P(Z \leq z_i) = \Phi(z_i), para\ i = 1,2, \ldots, n.$

In this case, the median position method can be used to calculate the cumulative distribution function S($\hat{e}_i$) (empirical), as follows:

$$S(\hat{e}_i) = \frac{i - 0,3}{n + 0,4}. \quad (7)$$

The z_i' value associated to $S(\hat{e}_i)$ is obtained by:

$$z_i' = \Phi^{-1}[S(\hat{e}_i)], \quad (8)$$

where $(\hat{e}_i) = S(z_i') = P(Z \leq z_i') = \Phi(z_i'), parai = 1,2, \ldots, n.$

In this way, the normal probability plot of the effects can be constructed by representing, on the x axis, the estimates $\hat{e}_i{}'$s and, on the y axis, the linearized accumulated probabilities or the values (scores) of Z. If the plotted points (z_i' *vs.* $\hat{e}_i$) in the graph are located approximately along a straight line (z_i *vs.* $\hat{e}_i$), the graph will indicate that the estimates of the effects are likely to be values of a normal random variable with zero average; systematic deviations from it indicate estimates other than zero.

The rejection of H_{0i}: $e_i = 0$ occurs when you have $|\hat{e}_i| \geq$ ME (margin of error), at the level of significance α, where:

$$ME = t_{\alpha/2,n/3} \times s_{random}. \quad (9)$$

where $t_{\alpha/2,n/3}$ - student's t-distribution value with n/3 degrees of freedom that leaves a $\alpha/2$ probability at the tail end to the right.

4 Methods

4.1 Data simulation

In order to compare the four methods of estimation of the σ_{random}, a normal random variable was Y (μ = 87.5; σ^2 = 8.125) with 10000 values was chosen arbitrarily and simulated, whose stimulation was repeated 16 times, being: σ_{random} = 2.85. Subsequently, in each of the 16 data sets 100 (1%), 200 (2%), 300 (3%) and 400 (4%) random values of Y were replaced by the same and respective quantities of *outliers*, with the aim of breaking their randomness. In addition, the 16 data sets with 10000 simulated random values were maintained.

The *outliers* were added unilaterally to the right, considering them as all those greater that:

$$q_3 1.5 a_{iq}, \quad (10)$$

where q_3 - quartile 3 and a_{iq} - interquartile range.

In order to obtain them, a new simulation was performed under normal distribution with μ = 87.5 + 6σ = 104.6 and σ^2 = 8.125 of 400 values. And after the confirmation of being *outliers*, the first 100, 200, 300 and 400 replaced the last 100, 200, 300 and 400, respectively, in the original data sets.

Therefore, a total of 80 data sets were generated with five percentage were generated, in total, 80 data sets with five percentages of substituting random values for *outliers*: 0%, 1%, 2%, 3% and 4%.

For the verification of the normality of Y, the Kolmogorov-Smirnov test was applied at 5% significance, with the aim of confirming normal randomness in data sets without *outliers* and, non-randomly, in those with substitutions of random values for *outliers*. The choice of the Kolmogorov-Smirnov test was due to the sample containing an excessive number of 10000 values.

4.2 Estimation methods

The estimate of the σ_{random} was done by four methods in each of the 80 data sets, separately, that is, in 16 data sets with different percentages of substitution of random values for *outliers*.

4.2.1 Lenth

According to the method of Lenth (1989), the estimate of the σ_{random} of the variable Y was obtained by:

$$s_{random} = PEP = 1.5 \times Md|y_j - \bar{y}| \quad (11)$$

where $|y_j - \bar{y}| = (|y_i - \bar{y}|2.5s_0)$; $s_0 = 1.5 \times Md|y_i - \bar{y}|$; $|y_i - \bar{y}|$ is vector that contains all the absolute deviations of the values in relation to the average of the variable Y (i = 1, 2, ..., 10,000) and Md - median.

4.2.2 Juan and Pena

The method of Juan and Pena (1992) provided the following estimate of the σ_{random} variable Y:

$$s_{random} = s_{IMAD} = \frac{IMAD_0}{0.6578}. \quad (12)$$

In order to obtain it, the first step was to calculate MAD_0 as the median of the 10,000 absolute deviations of the Y values in relation to their mean. After, another MAD_0 was calculated as the median of the absolute deviations less than $3.5 \times MAD_0$. And so, successively, until obtaining the value of $IMAD_0$, in other words, the value of MAD_0 that has not changed.

4.2.3 Dong

According to the method of Dong (1993), the estimate of the σ_{random} of the variable Y was given by:

$$s_{random} = s_{Dong} = \sqrt{\frac{\sum_{j=1}^{m}\left(y_j - \bar{y}\right)^2}{m}} \quad (13)$$

where $|y_j - \bar{y}| = (|y_i - \bar{y}|2.5s_0)$; $s_0 = 1.5 \times Md|y_i - \bar{y}|$; $|y_i - \bar{y}|$ is vector that contains all the absolute deviations of the values in relation to the variable mean Y (i = 1, 2, ..., 10.000 e j = 1, 2, ..., m ≤ 10.000) e Md - median.

4.2.4 Total standard deviation

The fourth method, called the total standard deviation, provided the following estimate of the σ_{random} of variable Y:

$$s_{random} = s_T = \sqrt{\frac{\sum_{i=1}^{10.000}(y_i - \bar{y})^2}{10.000 - 1}} \quad (14)$$

This method was used only to serve as a reference for the control of non-randomness by the other three previous methods, since it will only be efficient when all values are random from the same probability distribution.

4.3 Normal probability plot

Based on the best or one of the best methods of estimation of the σ_{random}, normal probability plots were constructed for the data sets with 1%, 2%, 3% and 4% of the random values replaced by *outliers*.

In order to construct the normal probility plot of deviations of the Y values from their mean (i = 1, 2, ..., 10.000), the theoretical and empirical cumulative distribution functions were considered, as follows:

$$F(y_i - \bar{y}) = \Phi(z_i) \quad (15)$$

$$S(y_i - \bar{y}) = \frac{i - 0{,}3}{n + 0{,}4} = \Phi(z'_i) \quad (16)$$

The deviations $(y_i - \bar{y})$ were represented on the x axis and the scores (z_i e z'_i) on the y axis, being:

$$z_i = \frac{y_i - \bar{y}}{s_{random}} = \Phi^{-1}[F(y_i - \bar{y})] \quad (17)$$

$$z'_i = \Phi^{-1}[S(y_i - \bar{y})] \quad (18)$$

where $\frac{\sum_{i=1}^{10.000} y_i}{10.000}$.

Thereby, if the points plotted on the graph are located approximately along a straight line, the graph will have indicated that the deviations were probably values of a normal random variable with zero mean, that is, $y_i - \bar{y} = 0$; the systematic deviations from it will have indicated deviations other than zero, in other words, $y_i - \bar{y} \neq 0$.

4.4 Statistical analysis

In order to evaluate the quality of the estimate σ_{random}, the mean absolute percentage error (MAPE) were estimated according to the four methods studied and five percentages of replacement of the random values by *outliers* as

$$MAPE = \frac{1}{16}\sum_{r=1}^{16}\left|\frac{\sigma_{random} - s_r}{\sigma_{random}}\right| \times 100 = \frac{1}{16}\sum_{r=1}^{16}\left|\frac{2.85 - s_r}{2.85}\right| \times 100. \qquad (19)$$

The MAPE values shot the absolute differences between the random standard deviations estimated by the four methods and the σ_{random}. For a good method of estimation, it is expected that all 16 differences are equal to zero.

According to the obtained MAPE values in each of the four methods of estimation separately, linear regression analysis was performed as a function of the percentages of substitution of random values for *outliers*, whose regression coefficients were tested, separately, by Student t test at 5% significance, after performing the regression analysis of variance. The largest regression model adopted was given by:

$$ep_k = \beta_0 + \beta_1 p_k + \beta_2 p_k^2 + \varepsilon_k, \qquad (20)$$

where k = 1, 2, 3, 4 e 5; ep_k – observed value of the MAPE at level k; p_k – percentage of substitution of random values by *outliers* at level k (0, 1, 2, 3 e 4); β_0 – constant of regression; β_1 e β_2 – regression coefficients and ε_k – regression error associated with the observed value ep_k, being that $\varepsilon \sim N(0; \sigma_i^2)$.

In order to evaluate the quality of the estimate of the σ_{random}, the MAPE regression analysis was used as a function of the percentages of substitution of random values for *outliers*, this is because the MAPE (dependent variable Y) measures, in percentage and absolute, the error estimate. The percentages of *outliers* represent quantitative levels of the independent variable X. Consequently, the absence of the effect of X on Y or, otherwise, the lower this effect, the better the efficiency of the estimation method.

All statistical analyzes were performed using R (R CORE TEAM, 2020).

5 Results and Discussion

According to the Kolmogorov-Smirnov test, it was confirmed that normal randomness occurred ($P > 0.05$) only in the 16 data sets without outliers. In the other sets with 1%, 2%, 3% and 4% substitution of random values for *outliers*, it was concluded that the variables did not behave ($P < 0.05$) in a random way. This implied that in these 64 data sets with *outliers*, the total standard deviation was not constituted only by the random fraction and that, consequently, the methods of Lenth (1989), Juan and Pena (1992) and Dong (1993) should estimate smaller standard deviations, as they try to separate and include only the random part of this data.

In fact, despite the increase in the percentage of substitution of random values for *outliers*, it provided an increase ($P < 0.05$) in the MAPE, according to the estimation methods of Lenth (1989), Dong (1993) and the deviation- standard, it was practically mitigated by the first two. In addition, the increase in this percentage did not change (P >

0.05) the estimate of the σ_{random} by the method of Juan and Pena (1992). Thus, the following regression models are adjusted, for $0 \leq p_k \leq 4$ (Figures 1 and 2):

$\acute{e}p_k = 1.2673 - 0.4134^{*}p_k + 0.2770^{*}p_k^2$ ($R^2 = 0.82$), for the method of Lenth (1989);

$\acute{e}p_k = 3.47$, for the method of Juan and Pena (1992);

$\acute{e}p_k = 1.4011 - 0.4291^{*}p_k + 0.2674^{*}p_k^2$ ($R^2 = 0.77$), for the method of Dong (1993); and

$\acute{e}p_k = 1.1373 + 18.8409^{*}p_k - 0.8868^{*}p_k^2$ ($R^2 = 0.93$), for the total standard deviation.

*: significant by Student's t test ($P < 0.05$).

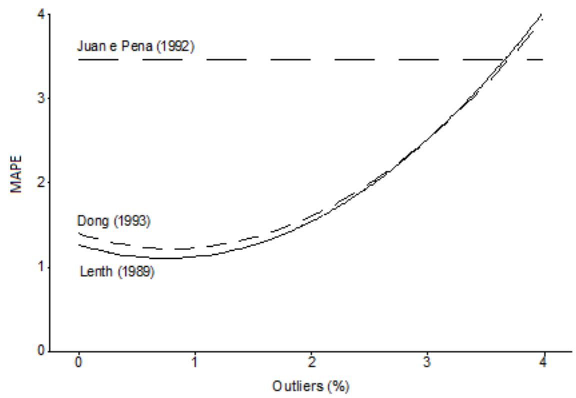

Figure 1- MAPE estimates provided by the methods of Lenth (1989), Juan e Pena (1992) and, Dong (1993).

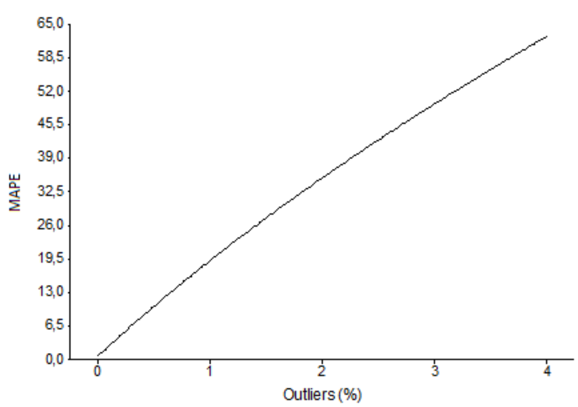

Figure 2 - MAPE estimates provided by the total standard deviation method.

As already mentioned, the total standard deviation method was the only one that failed to avoid the effect caused by the percentages of substituting random values for *outliers.* Consequently, it was unable to avoid the effect of non-randomness, being indicated, therefore, only when all the variables evaluated are considered random. According to their results, MAPE estimates have increased a lot, that is, from 0.74% (without the presence of *outliers*) to 62.59% (4% of *outliers*), approximately.

Lawson (2008) reports that discrepant values can be the main impediment to invalidating the variability estimate. Thus, the use of a method that minimizes the effect of the non-randomness of the data set will provide a more correct estimate of the σ_{random}. This means, therefore, that in the presence of *outliers*, the total standard deviation method should be avoided.

The methods of Lenth (1989) and Dong (1993), on the other hand, proved to be the same and very sensitive in detecting the presence of *outliers* and, consequently, in estimating more adequately the σ_{random}, up to approximately 3.68% of them. Without the presence of *outliers*, the average MAPE estimate provided by the two methods was 1.34%. And for 4% of *outliers*, from 4.00%.

On the other hand, the method of Juan and Pena (1992), although not influenced by the percentage of substitution of random values for *outliers*, it provided an estimate of MAPE slightly higher and equal to 3.47%. For this reason, it was also very sensitive in detecting the presence of *outliers* and appeared to be relatively better than the two previous methods, only when 3.68% to 4% of *outliers* occurred in the data set.

However, in practical terms, the differences between the estimates of σ_{random} observed between the methods of Lenth (1989), Juan and Pena (1992) and Dong (1993) with up to 4% *outliers*, were considered irrelevant, given the highest MAPE estimate caused by them was approximately 4.00%.

Consequently, the results obtained in the present work guarantee, as a good recommendation, the three methods reported, historically and in short, by Hamada and Balakrishnan (1998).

Based on the estimate of σ_{random} by the method of Lenth (1989), normal probability plots were constructed for data sets with 1%, 2%, 3% and 4% of the random values replaced by *outliers*, which revealed the presence, most of the *outliers* distanced from the straight line (Figure 3).

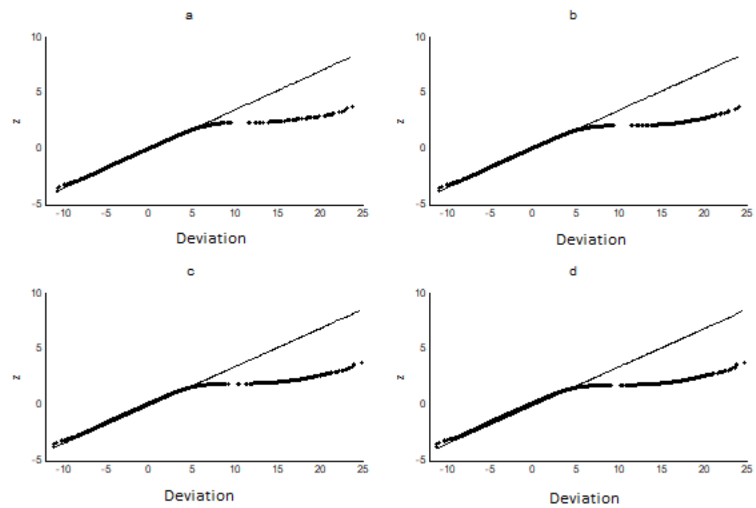

Figure 3 - Normal probability plots of deviations of Y values from their average, for data sets with 1% (a), 2% (b), 3% (c) and 4% (d) replacement of random values by *outliers*.

Conclusions

The methods of Juan and Pena (1992) and Dong (1993), although newer, were not more efficient than the method of Lenth (1989).

The methods of Lenth (1989), Juan and Pena (1992) and Dong (1993) show the same and adequate efficiency in estimating the random standard deviation of a non-random variable as a function of the presence of *outliers*.

The methods of Lenth (1989), Juan and Pena (1992) and Dong (1993) are recommended to provide the estimate of the mean square of the residue in complete and fractional factorial experiments with two levels per factor and with individual observations per treatment.

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- *RESUMO: Para obter a estimativa da variância aleatória em experimentos fatoriais completos e fracionados com dois níveis por fator avaliados sem repetições, Hamada e Balakrishnan (1998) fornecem uma lista de vários métodos. Assim, com base nessa revisão, o objetivo do presente trabalho consistiu em comparar as estimativas dos desvios-padrão com apenas influências das causas aleatórias de acordo com quatro métodos: de Lenth (1989), de Juan e Pena (1992), de Dong (1993) e sem nenhuma restrição aos dados, aqui denominado de desvio-padrão total. Para isso, foi simulada uma variável aleatória normal com 10.000 valores, cuja simulação foi repetida 16 vezes. Posteriormente, foram substituídos em cada um dos 16 conjuntos de dados, 0%, 1%, 2%, 3% e 4% dos valores aleatórios por outliers com o objetivo de quebrar a aleatoriedade da variável simulada. Com base na estimativa do erro percentual médio absoluto (EPMA) obtida em relação ao desvio-padrão aleatório paramétrico, concluiu-se, por meio da análise de regressão, que ela aumentou em função do aumento do percentual de substituição dos valores aleatórios por outliers, com exceção à obtida de acordo com o método de Juan e Pena (1992). Mesmo assim, para conjuntos de dados com até 3,68% de outliers, os melhores métodos de estimação do desvio-padrão aleatório ($\sigma_{aleatório}$) foram os de Lenth (1989) e de Dong (1993), por terem fornecido as menores estimativas do EPMA. Acima desse percentual e até 4% de outliers, o método de Juan e Pena (1992) mostrou-se ser melhor. No entanto, como a maior estimativa do EPMA proporcionada pelos três métodos de estimação foi muito baixa (4,00%), e ainda, como as diferenças observadas entre eles foram, praticamente, desprezíveis, concluiu-se que os três métodos forneceram boas estimativas do $\sigma_{aleatório}$ e que, consequentemente, podem ser recomendados para estimar o quadrado médio do resíduo em experimentos fatoriais completos e fracionados com dois níveis por fator e com observações individuais por tratamento. Por outro lado, o método do desvio-padrão total não conseguiu evitar o efeito da não aleatoriedade sobre a estimativa do $\sigma_{aleatório}$.*

- *PALAVRAS-CHAVE: Resíduo, Variância aleatória, outliers.*

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