Acta Scientiarum
http://periodicos.uem.br/ojs
ISSN on-line: 1807-8664
Doi: 10.4025/actascitechnol.v46i1.59135

STATISTIC

Simulation of robust adaptive regression multi-level models for quality analysis of special coffees in cold storage

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ABSTRACT. Numerous factors contribute to specialty coffee quality, storage and cooling conditions. We may therefore assume that sensory evaluation results can be corrupted by measurement errors, especially when cuppers are not trained, leading to occurrence of observation outliers. Therefore, this study aimed to propose simulation scenarios considering parametric values of multilevel model fit with robust adaptive regressions to the presence of outliers in a real experiment with processed and unprocessed coffee beans stored at different times and temperatures. In this context, we considered computationally simulated scenarios in which sensory scoring errors can be made at L = 5 and 10 units. The proposed method was feasible for the sensory scoring of an experiment of coffee storage conditions and cooled environments. This is because it included robust characteristics of samples evaluated with up to 30% of outliers.

Keywords: processed coffee; simulation; outliers; sensory analysis.

Received on May 10, 2021.
Accepted on December 16, 2022.

Introduction

Attention to coffee beans is indeed one of the criteria for producing high-quality coffee for international markets. However, it is not only restricted to genetic, environmental, and technological factors (Borém et al., 2020), or absence of defects (Brighenti & Cirillo, 2018), but also storage conditions. This is because color, flavor, and aroma may change when coffee beans are stored for long periods under unfavorable environmental conditions (Borém et al., 2019).

Studies have shown reductions in the initial quality of coffee beans stored at high temperatures for relatively long periods (Coradi, Borém, & Oliveira, 2008). In addition to physical changes, chemical changes may occur, such as loss of sugars due to increased bean respiration, especially when associated with high temperatures (Alves et al., 2017).

In this context, alternative procedures to reduce bean deterioration due to unfavorable temperature and relative humidity conditions have been used for packaging and storage. Therefore, these new methods and statistical models have contributed to improve storage conditions aimed at preserving quality of processed and unprocessed coffee beans.

As an example, Abreu et al. (2017) applied a simultaneous response optimization technique to determine the best time and storage condition combination for conservation of *Coffea arabica* L. fruits harvested at cherry stage, processed by wet and natural routes, and dried until reaching 11% water content. Part of the beans was processed, and the other part was only processed after storing for 3, 6, and 12 months under two ennvironment conditions: cooled air at 10°C with 50% relative humidity and 25°C with no humidity control. The authors concluded that an adequate storage time for natural coffee is about seven months and three months for pulped coffee when kept at 10°C.

Among storage conditions, cooling is one of the most effective to preserve the initial quality of agricultural products (Rigueira, Lacerda Filho, Volk, & Cecon, 2009). According to Ferreira et al. (2016), results may be unreal (outliers) due to accuracy and precision of sensory characteristics, especially when the final score is validated by a probabilistic model. This is one of the main criteria to classify a coffee as special due to influence of storage and cooling conditions. It is then corroborated by subjective factors, ability, and sensory memory of each cupper and/ or consumer.

Such heterogeneity has been explored in probabilistic models and approaches that are robust to such discrepant observations. Potential errors that may arise from sensory analysis can be defined as follows: (a) errors of expectation, which occur when cuppers have some previous knowledge of coffee preparation and/ or samples, and (b) stimulus errors, which occur when samples are not presented in a consistent manner (Lim, 2011). Faced with these errors and undesirable effects, sensory experiment results may be affected by observations classified as 'outliers'. Thereby, inappropriate treatment of these observations results in imprecise and incoherent analyses (Cirillo et al., 2019).

In this context, different methods and new statistical modeling techniques have been employed, Santos, Cirillo, and Guimarães (2021) used adaptive regressions in structural equation models to determine different profiles of specialty coffee consumers. Through this methodological approach, the authors built an index to validate descriptive variables used to compose constructs and determine profiles among consumers (Santos & Cirillo, 2021). In this line, Resende, Cirillo, and Borém (2020) had presented an index to validate preferences for specialty coffees by different groups of consumers. They built the index using principal component analysis, regression models, and computationally intensive tests and concluded that it was suitable since it discriminated specialty coffees produced at different altitudes. It had been previously confirmed by Liska et al. (2015) and Oliveira et al. (2019) who considered automatic classification methods with automated models by machine learning to evaluate different groups of consumers. Likewise, Alves et al. (2017) proposed a methodological procedure to discriminate coffees in blends of different varieties. These authors observed that the proposed method was efficient since untrained consumers could detect differences between blends and pure coffees.

Outliers can substantially influence sensory analysis results. One of their sources may be changes in physiological properties with storage conditions and temperature. This problem can be controlled by random or hierarchical models. In this sense, Pereira et al. (2017) used hierarchical cluster analysis to analyze data and observed interaction effect between Q-graders, as well as morning and afternoon coffee tasting. Their results indicate that cuppers are fully capable of evaluating coffees despite variances in their perceptions of attributes defining the best coffees.

Regression methods have been used to assess maintenance of initial coffee bean quality as a function of post-harvest storage time. Nonlinear trajectories between predicted and new measures have been observed to validate the adopted experimental design structure, such as intraclass correlation coeficient. However, these models, known as multilevel models (Durrant, Vassalo, & Smith, 2018), are fragile given an excessive number of outliers, that is, contrasting responses concerning the mean of evaluations. Such a deficiency implies that robust procedures for outliers are to be incorporated into these models (Torti, Perrotta, Atkinson, & Riani, 2012). However, the theoretical formalization with a mathematical basis becomes complex and unfeasible to be implemented in practice.

Our study was carried out based on this complexity and maintenance of the sensory quality of cooled coffee beans. Regarding discrepant results, our study aimed to build an adaptive multilevel model incorporated with robust regression estimates obtained by least trimmed squares (LTS) and least median of squares (LMS) methods (Muhlbauer, Spichtinger, & Lohmann, 2009). The model was validated by Monte Carlo simulation, with parameters being defined by the analysis of a factorial experiment on special coffee beans conditioned by the following factors: how beans were stored (intact or peeled), coffee scores at the beginning of storage, storage air temperature, and sampling time during storage.

Methodology

The methodological structure used in this study is described in the following sections: data structure, model simulation under the experimental conditions used for cooling specialty coffee beans, and incorporation of adaptive regressions.

Data structure

Data used in the model were obtained from an experiment at the Central Seed Analysis Laboratory of the Department of Agriculture, Federal University of Lavras, Lavras - Minas Gerais State, Brazil. The experiment compared specialty coffees with different quality scores and stored for different periods in environments at different temperatures. The model estimates were later used as parameter values in simulations.

Stored, processed and unprocessed, pulped cherry coffee beans of three different quality grades were used in this study. Four factors were considered: processing, initial quality, and storage temperature and period, as detailed below:

- Processing: it refers to how coffee beans were stored, that is, intact (with parchment) or processed (without parchment, i.e., peeled);

- Initial quality: coffee scores at the beginning of the experiment by sensory analysis made according to the cupping protocol of the Specialty Coffee Association of America (SCAA);
- Storage temperature: in a controlled temperature room (at 10°C) or room without temperature control (average of 25°C);
- Storage period: time at which samples were taken for sensory quality analysis throughout the 12 months of storage in both environments, which were: 1 – zero months, 2 – three months, 3 – six months, 4 – nine months, and 5 – twelve months.

A multilevel model was fit to each coffee type, following three hierarchies, as shown in Figure 1, wherein: t_{ijk} refers to the time factor (level 1), X_{jk} refers to the temperature (level 2), and W_k refers to the coffee quality (level 3).

Model simulation under the experimental conditions used for cooling specialty coffee beans

Following the hierarchical structure in Figure 1, the multilevel model was fit to actual data, assuming random intercept and slope. Thus, a response referring to the sensory score (y_{ijk}) was obtained as a function of the components η_{ijk} and γ_{ijk}, which refer to terms with fixed and random effects, respectively.

$$\hat{y}_{ijk} = \hat{\eta}_{ijk} + \hat{\gamma}_{ijk} \quad (1)$$

$$\hat{\eta}_{ijk} = \hat{\beta}_{0k} + \hat{\beta}_{1k_{(Q)}} \quad (2)$$

$$\hat{\gamma}_{ijk} = \hat{\beta}^{*}_{0jk} + \hat{Z}_{ij}Q_k + \hat{Z}^{*}_{ij}T_{jk} \quad (3)$$

In Equation 2, intercept and slope coefficients refer to the initial scores given for quality level (Q). Similarly, random intercept ($\hat{\beta}^{*}_{0jk}$) and random slope ($\hat{Z}_{ij}$ and $\hat{Z}^{*}_{ij}$) $coefficients$ in Equation (3) are associated with the factors quality (Q) and period (T), respectively, wherein k = 1,..., 3 and j = 1 and 2. After fitting the model, such specifications allowed us considering model estimates as parametric values of the experiment via Monte Carlo simulation (Table 1 and 2) so that simulated responses were consistent with the specified experimental conditions of cooling of specialty coffees.

Maintaining the assumption that assessments may be susceptible to measurement errors at L = 5 and 10 units, plus or minus, compared to the actual observed score, we incorporated several process-controlled outliers (Equation 4) by arbitrary specification, using parameter α, which are interpreted as mixing probabilities and set at 0.10, 0.20, and 0.30 (Equation 4).

$$y^{*}_{ijk} = u\alpha + (1-\alpha)u, \quad (4)$$

where: $u \sim U(0.1)$ and $0 \le \alpha \le 1$.

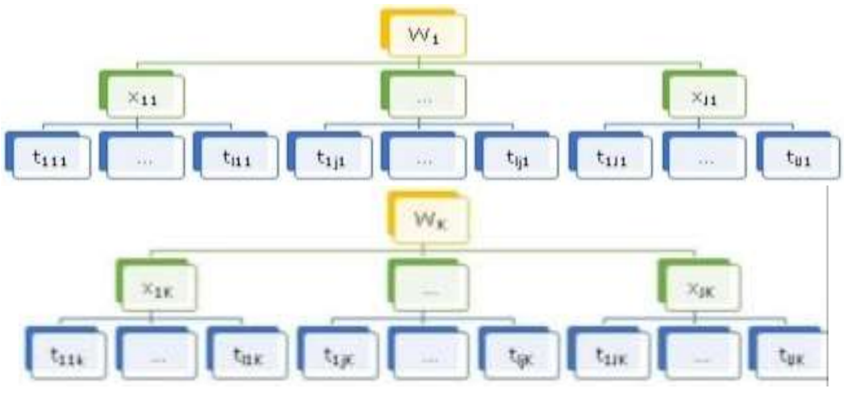

Figure 1. Scheme of hierarchies in a 3-level multilevel hierarchical (MLH) model.

Table 1. Parametric values estimated with actual data and used in simulations to evaluate performance of the adaptive regressions applied to processed coffees due to different measurement errors and number of outliers.

Random effect estimate			
Factor	Coefficient	Variance	Standard deviation
Period	Intercept	2.3410	1.5301
	Slope	0.0000090820	0.0030140
Temperature	Intercept	3.6130	1.9008
	Slope	0.00016310	0.0127
Residual	-	2.0200	1.4246

Table 2. Parametric values estimated with actual data and used in simulations to evaluate performance of the adaptive regressions applied to unprocessed coffees due to different measurement errors and number of outliers.

Random effect estimate			
Factor	Coefficient	Variance	Standard deviation
Period	Intercept	1.6525	1.2854
	Slope	0.035150	0.1874
Temperature	Intercept	2.2491	1.4996
	Slope	0.016760	0.1294
Residual	-	1.7862	1.3364

Therefore, the following rule was adopted: $\{u > \alpha y^*_{ijk} = y_{ijk} - L;\ u < \alpha y^*_{ijk} = y_{ijk}$.

Least trimmed squares (LTS) and least median of squares (LMS) regressions were fit assuming a fixed effect between variables. It was done because of outlier incorporations into the simulated sample. The fitted regressions are represented in Equation 5 and 6:

$$y^*_{ijk} = \hat{\beta}_{0k(LMS)} + \hat{\beta}_{1k(LMS)}Q, \quad (5)$$

$$y^*_{ijk} = \hat{\beta}_{0k(LTS)} + \hat{\beta}_{1k(LTS)}Q. \quad (6)$$

Incorporation of adaptive regressions

Adaptive regressions in this study were implemented by combining random coefficients (intercept and slope), which were estimated between multilevel regressions fitted by restricted maximum likelihood method (REML) and LMS and LTS robust regressions for fixed effects, according to Equation 7 and 8.

$$\hat{\beta}_{0(ADPT)} = w\hat{\beta}_{0(REML)} + (1 - w)\hat{\beta}_{0(a = 1)} \quad (7)$$

$$\hat{\beta}_{1(ADPT)} = w\hat{\beta}_{1(REML)} + (1 - w)\hat{\beta}_{1(a = 1)} \quad (8)$$

However, w was originally interpreted as a residual perturbation parameter. It was estimated by graphically inspecting arbitrary values (between 0.05 and 0.5) assigned as a function of prediction error. This error was obtained after fitting the complete model (Equation 9) for the ith epoch effect (i = 1,...,5). Coefficients referring to intercepts and slopes, estimated in fixed, random, and adaptive effects approaches, and identified in the subscript indices, were included.

$$y^*_{ijk} = \hat{\beta}_{0(ADPT)} + \hat{\beta}_{0(Ti\,/\,random)} + \hat{\beta}_{0(Fixed)} + \hat{\beta}_{1(Fixed)}Q_i + \left(\hat{\beta}_{1(ADPT)} + \hat{\beta}_{1(Qi/\,random)}\right).T_i \quad (9)$$

Adaptive regression coefficients were formed considering two relationships regarding the confounding of robust regressions with outlier detection. Thus, a random number u was generated so that if $u \geq w$, then $\beta_{0(ADPT)} = \beta_{0(a = 1)}$, otherwise $\beta_{0(ADPT)} = \beta_{0(MV)}$, with $\beta_{0(a = 1)}$ and $\beta_{1(a = 1)}$ being the intercept and slope coefficient estimates, respectively, obtained by the robust LMS method, while for the LTS method, a = 2 was assumed.

Finally, the procedure was performed by developing functions and a script for data entry and simulation, using the R software (R Core Team, 2020).

Results and discussions

Random and fixed coefficients (Table 1 and 2, respectively) were estimated considering hierarchical structure and sensory evaluations. And then they were used as parametric values for simulations to build adaptive regressions.

Experimental conditions refer to preset factor levels for model fit, that is, they are not merely arbitrary. As previously highlighted, estimates were considered as parametric values for reproduction of 1000 experiments on sensory scoring, which were altered by L = 5 and 10 units, suggesting measurement errors in evaluations. Thus, intraclass correlation was estimated considering actual data on coffee processing or non-processing and an adaptive multilevel structure.

Model simulation considering measurement error in assessments of sensory scores specified in L = 5 units

Performance of robust LMS and LTS regression estimators was evaluated before analyzing adaptive model estimates to determine the best value for mixing probability (w) and thus minimize error. In this sense, different proportions of outliers were fixed, representing the average of observations affected by measurement errors, defined at 10, 20, and 30%. Figure 2 and 3 show the results using as reference data on processed and unprocessed coffees, respectively. Therefore, a measurement error of up to L = 5 units was considered.

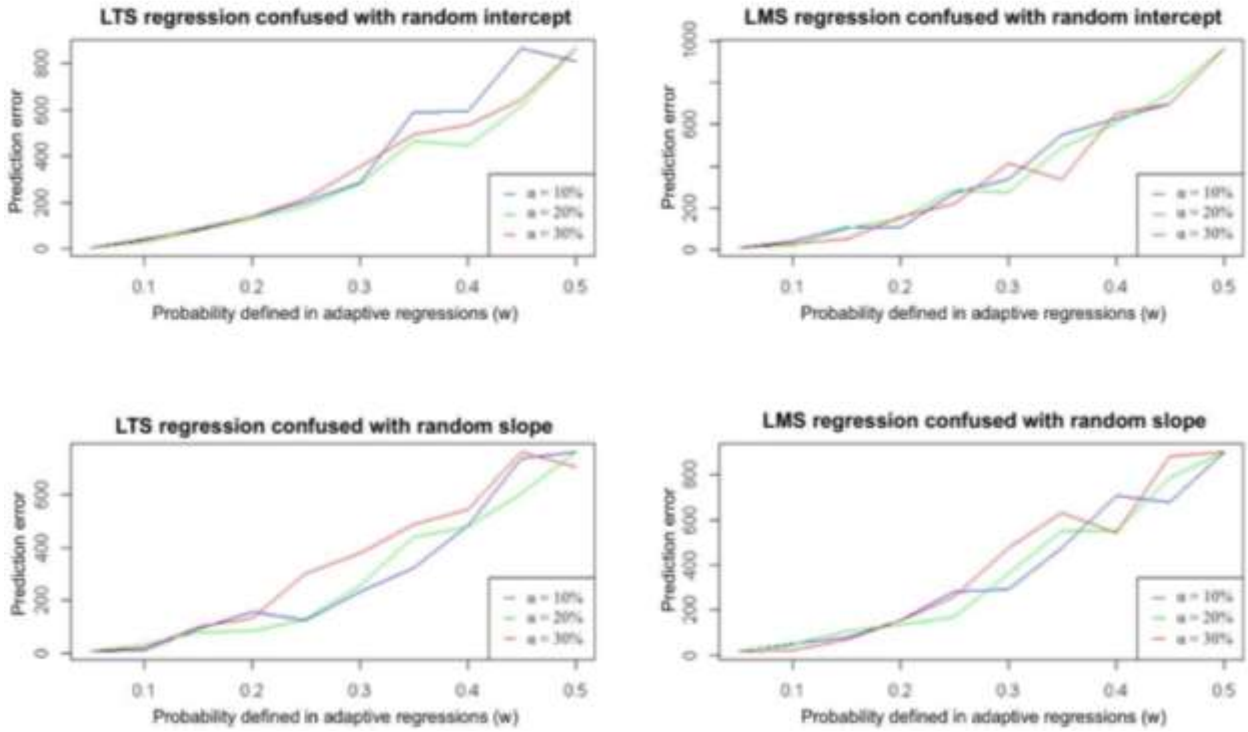

Figure 2. Performance of LTS and LMS regressions in processed coffees considering a measurement error of *L* = 5 units.

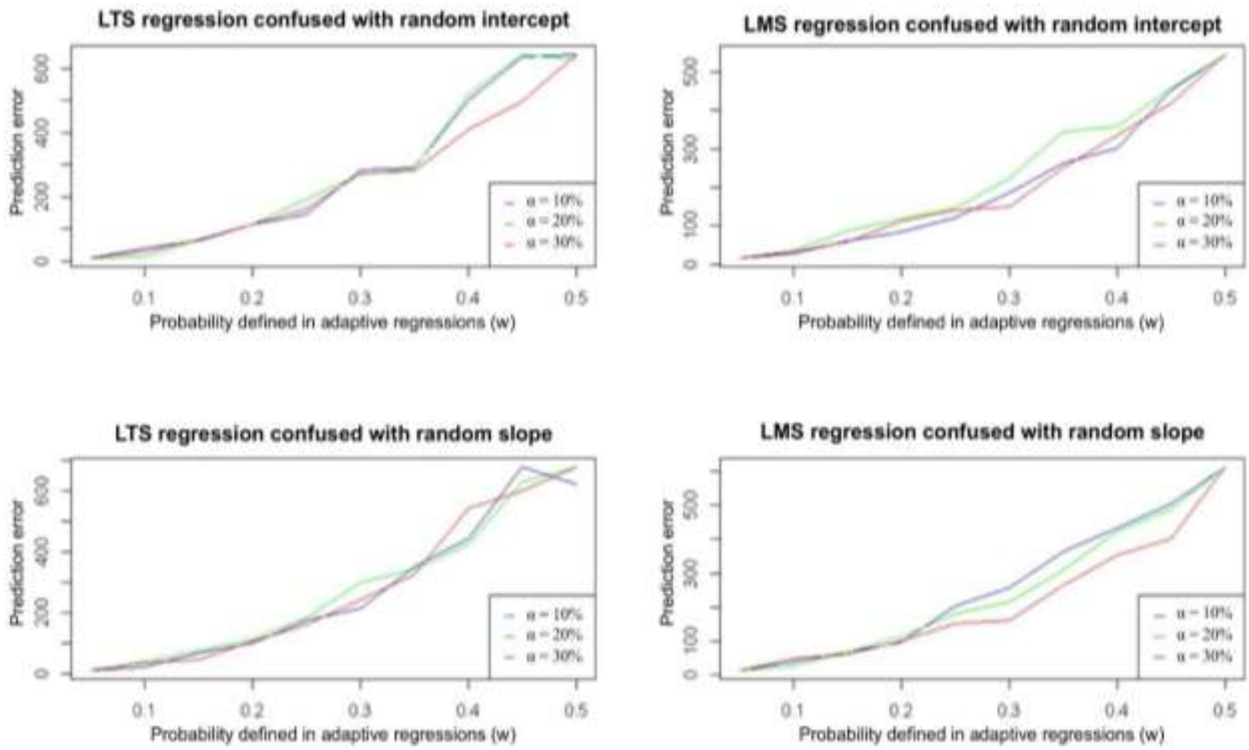

Figure 3. Performance of LTS and LMS regressions in unprocessed coffees considering a measurement error of *L* = 5 units.

Results in Figure 2 allowed us to infer that confusion of robust regression fixed estimates by LMS and LTS methods with random intercept and then random slope, as a function of a sequence of w values, were conclusive to inspect the value to be considered to compose adaptive regressions. In this context, when assuming w ⩽ 0.10, the experimental error is minimized, regardless of the number of outliers. Therefore, in practice, this modeling is justified, including percentages of outlier observations of up to 30% (α = 0.30). Results were similar between LMS and LTS methods, with small oscillations attributed to the Monte Carlo error.

Considering the same evaluation scenarios, Figure 3 shows the results for unprocessed coffees. They indicate a behavior similar to that of processed coffees ($w \leq 0.10$). However, in general, curves for different percentages of outliers were more homogeneous, and discrepancies between numbers of outliers were not noticeable for this scenario of evaluation.

The results shown in Table 3 and 4 are in accordance with the simulated results, in which w = 0.05 was selected to compose the multilevel model with adaptive regressions. Variantions in processed coffees were, in general, lower than in unprocessed coffees. Therefore, processed coffee results were more accurate in terms of predictions by the fitted model.

Fixed effect estimates for data considering a specification error in scores at L = 5 units (Table 3) showed that intercept contribution to both processed and unprocessed coffees was little in terms of the model predictive power, given a p-value > 0.05. Conversely, slope coefficient estimates (p-value < 0.05) resulted in a higher influence on the model predictive power. Therefore, the null hypothesis that this parametric value is null must be rejected.

Model simulation considering measurement error in assessments of sensory scores specified in L = 10 units

Some results and interpretations regarding the simulated data are similar to the previous subsections, considering an error of up to L = 10 units.

Contamination by outliers was homogeneous among processed coffee samples. It can be observed by the small differences between graphs when w varied, except for a few points whose discrepancy is attributed to random effects. Therefore, experimental errors did not increase as a function of the proportion of outliers that the sample had when the robust estimation methods LMS and LTS were used. Furthermore, both estimation methods had no significant differences between them. Furthermore, experimental error is lower for higher contributions of robust estimators to the model, therefore, w must be 0.10 or lower.

Figure 4 shows no significant graphic differences, thus experimental error increased gradually as w increased, regardless of the number of outliers. Thus, the estimation methods of very robust regression (LMS and LTS) resisted up to 50% of outliers (Torti et al., 2012).

Moreover, the robust estimators showed no discrepancy for prediction errors; however, the mixture coefficient w had a difference between its values, thus $w \leq 0.10$ resulted in smaller prediction errors compared to other mixture probabilities (w) (Figure 5).

Table 3. Estimates for random effects considering a measurement error of L = 5 units.

Factor	Coefficient	Variance	Standard deviation
		Unprocessed coffee	
Period	Intercept	2.8016	1.6738
	Slope	0.00030440	0.017450
Temperature	Intercept	3.9413	1.9852
	Slope	0.00018450	0.013580
Residual		2.0200	1.4246
		Processed coffee	
Period	Intercept	0.85810	0.92635
	Slope	0.00012740	0.011290
Temperature	Intercept	0.21660	4.6545
	Slope	0.0021990	0.046900
Residual	-	1.9920	-

Table 4. Estimates for fixed effects considering a measurement error of L = 5 units.

Coefficient	Estimate	Standard deviation	t-value	p-value
		Unprocessed coffee		
Intercept	9.0227	10.5923	0.8520	0.275
Slope	0.81460	0.12520	6.5070	0.0485
		Processed coffee		
Intercept	17.0464	6.2762	2.7160	0.1106
Slope	0.71641	0.071690	9.993	0.0317

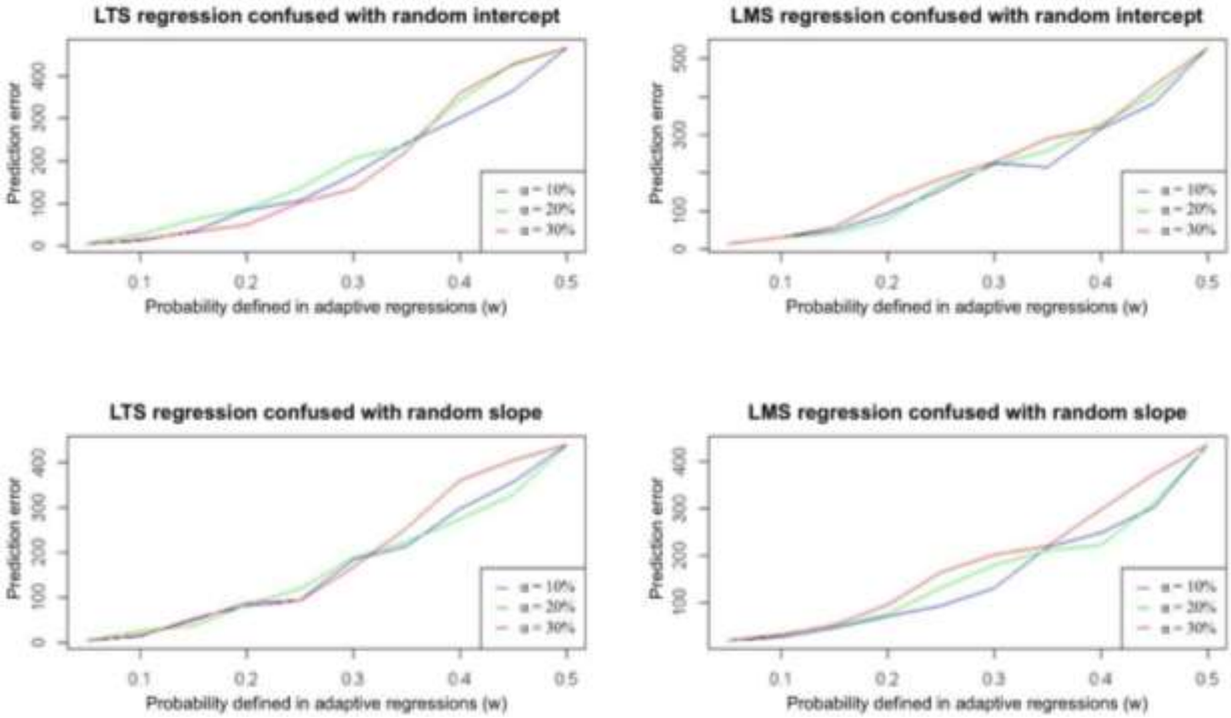

Figure 4. Performance of LTS and LMS regressions in unprocessed coffees considering a measurement error of L = 10 units

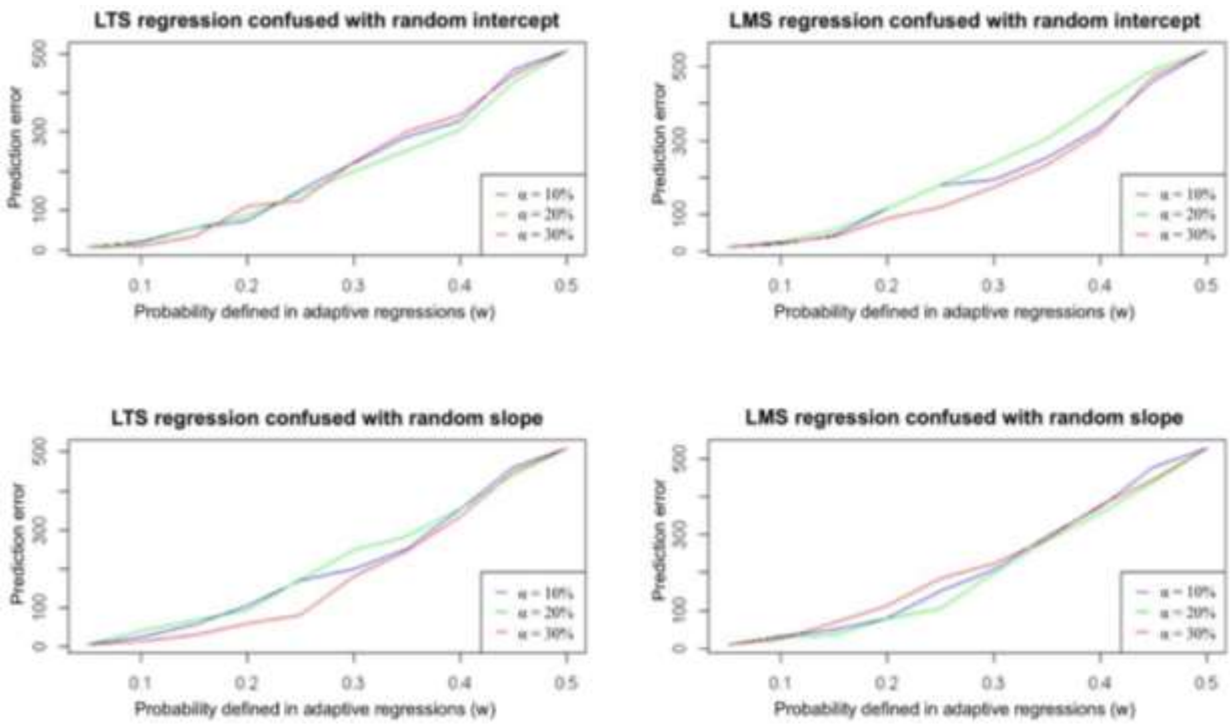

Figure 5. Performance of LTS and LMS regressions in processed coffees considering a measurement error of L = 10 units.

Table 5 and 6 show the estimates of random and fixed effects, respectively, considering a model with a random intercept and slope with three levels.

The variance in processed coffee coefficients was lower than that in unprocessed coffee ones. Additionally, the residual of processed coffees was also lower than that of unprocessed coffees. Therefore, processed coffee results achieved a higher statistical credibility regarding the hypothesis test.

Intercept and slope had relevant contributions to the model predictive power ($p < 0.05$) (Table 6). Therefore, these coefficients differed from zero, given the specification error in the scores (L = 10 units) when considering the fit to the unprocessed coffee data. Thus, the parametric value for these terms includes a non-null value. Such an effect was confirmed only for slope in terms of processed coffee estimates.

Estimates of intraclass correlation coefficients for adaptive models regarding the original model

Multilevel models were fitted in different hierarchies preliminary to the simulation to determine which would be the best structure to justify such an approach. Estimates of intraclass correlation coefficients were used as shown in Table 7. This coefficient is a statistical tool used to verify the joint homogeneity of data and is interpreted as a variance ratio (Shrout & Fleiss, 1979).

Table 5. Estimates for random effects considering a measurement error of L = 10 units.

Factor	Coefficient	Variance	Standard deviation
		Unprocessed coffee	
Period	Intercept	3.1426	1.7727
	Slope	0.0010156	0.031870
Temperature	Intercept	4.2665	2.0655
	Slope	0.00021710	0.014740
Residual		3.2064	1.7906
		Processed coffee	
Period	Intercept	1.9410	1.3932
	Slope	0.000017830	0.0042230
Temperature	Intercept	3.3280	1.8241
	Slope	0.00013830	0.011760
Residual	-	2.0940	1.4472

Table 6. Estimates for fixed effects considering a measurement error of L = 10 units.

Coefficient	Estimate	Standard deviation	t-value	p-value
		Unprocessed coffee		
Intercept	3.8453	10.6814	0.36000	0.039
Slope	0.82260	0.12390	6.6420	0.0475
		Processed coffee		
Intercept	12.3556	6.4055	1.9290	0.1522
Slope	0.71800	0.072740	9.8820	0.0321

Table 7. Estimates of intraclass correlation coefficients considering sensory score and measurement error of 5 units, obtained by robust adaptive model estimates (with w = 0.05).

Intraclass correlation coefficients for the simulated model on measurement error of 5 units			
	Period	Temperature	Quality
Models with random intercept and fixed slope			
Processed	32.94%	40.99%	26.05%
Unprocessed	43.21%	33.54%	23.24%
Models with random intercept and slope			
Processed	27.73%	7.12%	65.15%
Unprocessed	31.12%	29.40%	38.47%
Intraclass correlation coefficients for the simulated model on measurement error of 10 units			
	Period	Temperature	Quality
Models with random intercept and fixed slope			
Processed	37.25%	23.67%	39.08%
Unprocessed	35.80%	24.83%	39.37%
Models with random intercept and slope			
Processed	20.74%	42.98%	36.28%
Unprocessed	30.88%	37.95%	30.99%
Intraclass correlation coefficients considering the original data			
	Period	Temperature	Quality
Processed	29.35%	45.31%	25.33%
Unprocessed	29.40%	39.47%	31.12%

The coefficients in Table 7 showed that, when considering a three-level structure, the evaluation of sensory scores that most corroborate justifying a multilevel model had greater emphasis on processed coffee data, considering a sensory measurement error of up to L = 5 units (65.15%). In this sense, the scores were homogeneous in terms of hierarchy, but heterogeneous among them, having as reference intraclass correlation coefficients. Therefore, the higher the intra-quality correlation, the higher the dependence between sensory score responses. In conclusion, building a model that respects data aggregation structure is plausible.

Similarly, the same observations can be followed for unprocessed coffee, but this model does not ensure significant information gains due to the low intraclass correlation coefficients (below 40%).

Conclusion

An adaptive regression applied to LMS and LTS robust estimation methods and maximum likelihood estimator are feasible for samples with a high proportion of outliers (up to 30%), allowing analysis with a relatively low experimental error in term of contamination.

Given the experimental conditions mentioned, the evaluation of sensory scores that most corroborate justifying a multilevel model through intraclass correlation coefficients can be verified when considering parametric values referring to the fit of processed coffee data for a measurement error of up to $L = 5$ units (65.15%).

Acknowledgments

The authors would like to thank the *Conselho Nacional de Desenvolvimento Científico and Tecnológico* - CNPq for the financial support through research grant (project n° 140242/2019-8) and the *Coordenação de Aperfeiçoamento de Pessoal de Nível Superior* (Capes).

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