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Case study of modeling covariance between external factors and sensory perception of coffee

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ABSTRACT

Analysis and inference of sensory perceptions in coffee beverages are complex due to numerous random causes intrinsic to productivity, preparation, and especially consumer and/or taster subjectivity. In this context, latent variables often composed of a combination of other observed variables are discarded from conventional analyses. Following this argument, this study aimed to propose a model of structural equations applied to a database, geographical indication of coffees in Serra da Mantiqueira, with a methodological contribution characterized by inclusion of a treatment effect, contemplated by different altitudes at which coffees were produced. From the methodology used, a covariance structure was estimated, and used in another statistical methodology to discriminate the effects. It is concluded that the proposed model proved to be advantageous for allowing the analysis of the relationship of latent variables, production and environmental variations, which are not considered in a sensorial analysis, and showed that, in fact, they influence the sensorial perception, for the coffees produced in the Serra da Mantiqueira region. The correlation structure generated from the covariance matrix adjusted by the model resulted in estimates that could be used in other statistical methodologies more appropriate to discriminate the effects, exemplifying the use of principal components.

Key words: Latent variable; adjusted goodness-of-fit (AGFI); altitude; goodness-of-fit (GFI).

1 INTRODUCTION

Coffee is a very popular drink in several countries around the world, distinguished by being a natural product with different aromas and pleasant flavors. Among the most cultivated species, Arabica (*Coffea arabica L.*) stands out, from which the cultivars have the potential to be classified as special (Ramos et al., 2016). Specialty coffees are of great importance in the economic scenario, and their sensory quality is appreciated by the productive sector and the market. Coffee beverage quality is defined by a chain of processes that, in short, involves planting and environmental variations. These external factors contribute to the quality of the drink, which in turn is mainly evaluated by several sensory attributes, especially flavor and acidity. These characteristics are the most appreciated by consumers who present a lower or higher degree in relation to their sensory perception.

Sensory perception discrimination arouses consumer interest in knowing more technical information when purchasing a particular coffee. Santos, Cirillo and Guimarães (2021) highlighted studies in the United States and Canada, corroborated by Quintão and Brito (2016) and Quintão, Brito and Belk (2017a, 2017b), which identified heterogeneous communities of specialty coffee consumers in those countries, that is, coffees with high scores in international competitions. Thus, those authors subdivided such consumers into three categories, which are associated in their level of expertise with conceptual and perceptual knowledge of the product.

The understanding of consumer segments has increased in interest, mainly due to a growing number of consumers, mainly young people. This group has increasingly hung out at coffee shops that offer coffees with distinct flavors and intense aromas, resulting in pleasant drinks. It is also noted that the consumer who appreciates quality beverages is curious about technical issues, such as the degree of roasting, preparation, origin and certifications, since genetic, environmental and cultural factors understand the quality of the coffee, to be mentioned by the methods harvesting, processing, storage, twisting and grinding, which can directly affect the final quality of the coffee and the sensory attributes of the drink

Regarding consumption forecasting, a research on market trends by the Brazilian Association of Coffee Industry showed that coffee consumption increased by 3.5% from 2016 to 2017 (Sociedade Nacional de Agricultura - SNA, 2018). This fact reflects that coffee connoisseurs continue to increasingly consume the product. It has been consumed in the most different ways as coffee quality has increased in Brazil.

With all these arguments in mind and emphasizing the subjectivity of each consumer, evaluations of quality and aptitude are limited to univariate or multivariate statistical methodologies, as they account only mean and/or individual answers obtained by variables observed during the of the experiment. In this study, consumer subjectivity is contextualized by covariance structure modeling. It includes latent variables defined as “constructs” that involve characteristics related to external factors. These, in turn, are defined by the latent variables management, environmental description, and sensory perception specification. The composition of these constructs through some observed variables, as well as the formalization of a hypothetical model, are described in a diagram illustrated in methodology.

Thus, our objective was to evaluate a case study considering representative samples from several specialty coffee plantations. The samples were identified by geographic coordinates, variables related to planting areas, and pest control performed. In short, this study aimed to propose the use of structural equations to model the covariance of coffee quality sensory perception (flavor and acidity) with the altitudes where they were produced.

2 MATERIAL AND METHODS

2.1 Experiment characterization

The database used to formulate a structural equation model corresponded to part of the data from the project "Identity and Traceability", which geographically identified coffees in the region of Serra da Mantiqueira (Borém, 2020). In this project, the samples of coffee (*Coffea arabica* L.) were collected over three consecutive seasons (2010/11, 2011/12, and 2012/13) from commercial plantations on farms located in the municipality of Carmo de Minas, Minas Gerais State, Brazil.

The selected study area has a location delimited by the geographic coordinates 22°07'21" south latitude and 45°07'45" west longitude, and a territorial extension of 32,332 ha.

The coffee field environment was stratified into different altitude categories. All collection points were georeferenced. Figure 1 describes the variables used in this study.

2.2 Structural model specification

Figure 1 displays the structural equation model formulated based on the data obtained, with the factors specified by constructs that define the latent variables (not observed, characterized by ellipses): production, environmental variations, and sensory perceptions these being formed by combinations of observed variables (characterized by rectangles).

The relationship that explains these trends is given by a set of equations, which determine the causality between attributes (observed variables) and latent variables, as described in Equations (1), (2) and (3) (Bollen; Noble, 2011):

$$\eta = B\eta + \Gamma\xi + \zeta \tag{1}$$

$$X = \Lambda_x \xi + \delta \tag{2}$$

$$Y = \Lambda_Y \eta + \varepsilon \tag{3}$$

Wherein: $\eta_{(m\times 1)}$ represented the vector of endogenous latent variables; $\xi_{(n\times 1)}$ the vector of exogenous latent variables; $\zeta_{(m\times 1)}$ the vector of structural errors; $\mathbf{B}_{m\times m}$ the matrix of coefficients that relates the endogenous latent variables, and, lastly, $\Gamma_{(m\times r)}$ the matrix of coefficients that relates the exogenous latent variables with the endogenous latent variables.

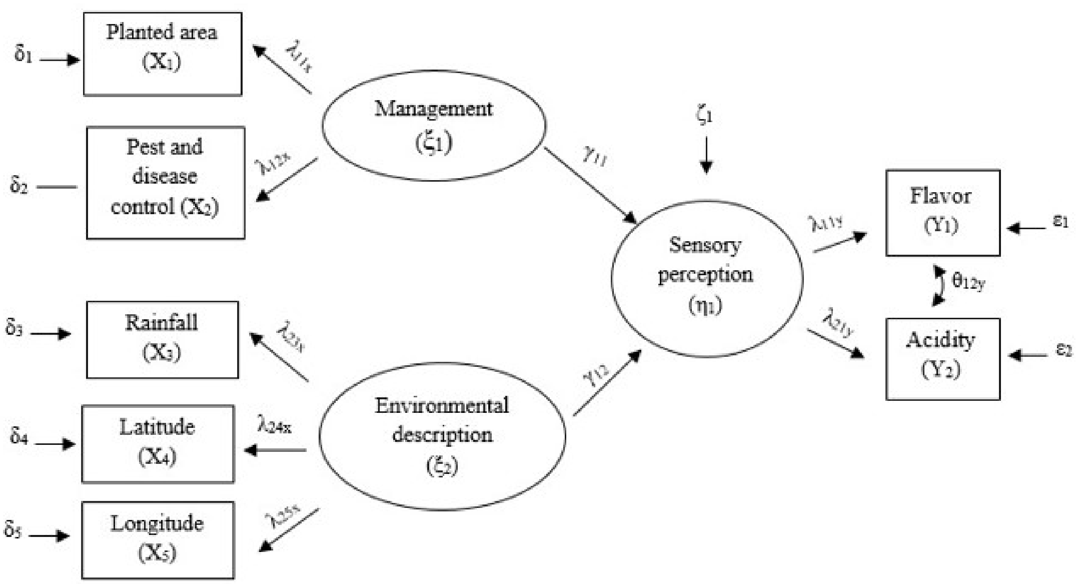

Figure 1: Path diagram for sensory analysis of specialty coffees.

Note: The rectangles X and Y refer to the indicator variable; one-sided arrows represent causal effects; bilateral arrows represent correlation among indicator variables; the ellipses h_1,x_1, and x_2 represent the latent variables.

The relationship between endogenous latent variables and observed variables y_j (j=1,2) was determined by the matrix of coefficients $\Lambda_{y(p\times m)}$, given the measurement error represented by $\varepsilon_{(p\times 1)}$. Equation (3) refers to the measurement model **X** that relates the observed variables x_k (k=1...5) to the latent variable. The relationship between the exogenous latent variable and the observed variables was specified through the matrix of coefficients $\Lambda_{x(q\times r)}$. Finally, the measurement error represented by the vector $\delta_{(q\times 1)}$.

Mathematically, the diagram in Figure 1 is represented by the matrix equations described by Hampton (2015). Thus, for Equation (1), it can be described in a matrix according to the following relationship given in (4):

$$[\eta_1] = [y_{11} \quad y_{12}]\begin{bmatrix}\xi_1\\ \xi_2\end{bmatrix} + [\zeta_1] \tag{4}$$

Wherein: the constructs defined by the endogenous (η_1) and exogenous (ξ), latent variables, hypothetically, representing the constructs sensory perceptions, environmental variations, and production.

The linear relationships between these variables are described in (2) and (3), respectively, in a matrix they are defined by Equation (5) and (6):

$$\Lambda_x = \begin{bmatrix}\lambda_{11} & 0\\ \lambda_{12} & 0\\ 0 & \lambda_{23}\\ 0 & \lambda_{24}\\ 0 & \lambda_{25}\end{bmatrix};\ \delta = \begin{bmatrix}\delta_1\\ \delta_2\\ \delta_3\\ \delta_4\\ \delta_5\end{bmatrix} \qquad \begin{bmatrix}x_1\\ x_2\\ x_3\\ x_4\\ x_5\end{bmatrix} = \begin{bmatrix}\lambda_{11} & 0\\ \lambda_{12} & 0\\ 0 & \lambda_{23}\\ 0 & \lambda_{24}\\ 0 & \lambda_{25}\end{bmatrix}\begin{bmatrix}\xi_1\\ \xi_2\end{bmatrix} + \begin{bmatrix}\delta_1\\ \delta_2\\ \delta_3\\ \delta_4\\ \delta_5\end{bmatrix} \tag{5}$$

$$\Lambda_y = \begin{bmatrix}\lambda_{12}\\ \lambda_{21}\end{bmatrix};\ \varepsilon = \begin{bmatrix}\varepsilon_1\\ \varepsilon_2\end{bmatrix} \qquad \begin{bmatrix}y_1\\ y_2\end{bmatrix} = \begin{bmatrix}\lambda_{12}\\ \lambda_{21}\end{bmatrix}[\eta_1] + \begin{bmatrix}\varepsilon_1\\ \varepsilon_2\end{bmatrix} \tag{6}$$

In certain situations, environmental variation is predictable through plant genotype, product origin, cultivation method, and processing. However, there may be temperature fluctuations in plants exposed to sun and rainfall. A joint analysis of all these factors in a precise way makes it difficult to determine a single cause. Thus, it is justified to consider it as a latent variable.

The correlation matrix estimation corresponding to the hypothetical model (Figure 1) was performed following the procedure defined by McDonald and Hartmann (1992), respecting the relationship: $\mathbf{v} = \mathbf{A}\mathbf{v} + \mathbf{u}$, which is expressed by the set of linear regressions, represented in the diagram by arrows. Thus, **v** refers to the vector formed by observed and latent variables; **A** is the matrix of regression coefficients specified by the factor loadings obtained in the model fit; and **u** is the vector of errors estimated by least squares method. Then the covariance matrix on the hypothetical model (Figure 1) is obtained by Equation (7):

$$\hat{\Sigma}_\theta = J(I_a - A)^{-1}P[(I_a - A)^{-1}]^t J^t \tag{7}$$

2.3 Incorporation of design with treatment effect given by different altitude categories and adaptation of goodness of fit indices

Given the covariance matrix postulated by model (7) and the sample covariance matrix S, without considering the repetitions of variables, the inclusion of repetitions was done by defining the ratio t = k/r, wherein k = p+q and represents the sum of p endogenous variables with q exogenous variables, of the r repetitions. Thus, when the number of repeated observed variables is fixed (t), the mean for each variable will be obtained as a function of the number of repetitions r. Following this procedure, through the altitude classes, five treatments were determined, described in Table 1.

Table 1: Treatments used in the experimental design based on altitude.

Treatment	Altitude
T1	900 m – 1,000 m
T2	1,000 m – 1,100 m
T3	1,100 m – 1,200 m
T4	1,200 m - 1,300 m
T5	1,300 m – 1,400 m

Once the treatments were determined, the matrix T described in (8) was generated, known as matrix of the means of the repeated observed variables, as written below:

$$\boldsymbol{T} = \begin{pmatrix}\bar{t}_{11} & \bar{t}_{21} & | & \bar{t}_{11} & \bar{t}_{21}\\ \vdots & \vdots & | & \vdots & \vdots\\ \bar{t}_{15} & \bar{t}_{25} & | & \bar{t}_{15} & \bar{t}_{25}\end{pmatrix}_{5\times 4} \tag{8}$$

Using the matrix T as a reference, each treatment mean was corrected as a function of the general mean of each variable, as recommended by Konishi (2015), resulting in the matrix M given in (9), as follows:

$$M = \begin{pmatrix}\bar{t}_{11} - \bar{x}_{1.} & \bar{t}_{21} - \bar{x}_{2.} & | & \bar{t}_{11} - \bar{y}_{1.} & \bar{t}_{21} - \bar{y}_{2.}\\ \vdots & \vdots & | & \vdots & \vdots\\ \bar{t}_{15} - \bar{x}_{1.} & \bar{t}_{25} - \bar{x}_{2.} & | & \bar{t}_{15} - \bar{y}_{1.} & \bar{t}_{25} - \bar{y}_{2.}\end{pmatrix}_{5\times 4} \tag{9}$$

Afterwards, the singular value decomposition was applied, wherein $\mathbf{M}=\mathbf{UDV}^T$, with $\mathbf{U}$ and $\mathbf{V}$ being orthogonal matrices, whose columns are formed, respectively, by their eigenvectors $\mathbf{MM}^T$ and $\mathbf{M}^T\mathbf{M}$. The covariance matrix, considering the repetitions in the observed variables, will be determined by $\sum\mathbf{U}=\mathbf{UU}^T$.

Goodness-of-fit index (GFI) measures the quantity of relative covariance in a sample **(S)** predicted by the model's covariance matrix (. Then, the adjusted goodness-of-fit index (AGFI) was proposed to better adapt the GFI to the degrees of freedom and number of variables observed, which are usually above 0 and equal at most 1.

Both GFI and AGFI were improved by incorporating the covariance matrix, which represents information from observed variable repetitions. To do so, we considered the formulations obtained by the ordinary least squares (OLS), as given in equations (10) and (11).

$$GFI_{(OLS)} = 1 - \frac{tr\left[\left((\boldsymbol{S} + \Sigma_U) - \hat{\boldsymbol{\Sigma}}_\theta\right)^2\right]}{tr[(\boldsymbol{S} + \Sigma_U)^2]} \tag{10}$$

$$AGFI_{(OLS)} = 1 - \left[\frac{k(k+1)}{2gl_p}\right]\left[1 - GFI_{(OLS)}\right] \tag{11}$$

Wherein: $\hat{\boldsymbol{\Sigma}}_\theta$is the population covariance matrix of the proposed model; $\boldsymbol{S}$ is the sample covariance matrix; $\boldsymbol{S}+\hat{\boldsymbol{\Sigma}}_\theta$ is the covariance matrix with repetition and treatment effects (experimental); $tr(.)$ is the trace operator; p is the number of endogenous observed variables (Y); q is the number of exogenous observed variables (X); and gL_p is the degree of freedom of the proposed model.

For comparative purposes, a principal component analysis is presented later, considering the usual correlation, with the representative correlation of the model in which the repetition structure is incorporated (Figure 1).

For the model covariance matrix, data analysis was performed using Lavaan package (Rosseel, 2012) of R software, version 4.1.2 (R Development Core Team, 2021). A routine was developed in the same software to obtain modified goodness of fit indices.

3 RESULTS

In accordance with the proposed method, the validation of the proposed structural model, which justifies the inclusion of repetitions and treatments, is given in a comparative way to the conventional fit. Table 2 describes the results of the validation process.

The results in Table 2 show that, in all situations, the inclusion of repetitions improved the quality of the fit indices evaluated. However, when considering only 2 repetitions, the fit can be considered moderate, therefore, if the objective is to model the covariance requiring a minimum number of repetitions, still without loss of generality, one can consider fitting the model to be adequate.

Table 2: Estimates of goodness-of-fit indexes (GFI and AGFI) to validate the structural equation model with the inclusion of a fully randomized design and altitude ranges defined as treatments, in estimates of different numbers of repetitions.

Amounts to estimate the number of repetitions		Index estimates	
Number of repetitions		With repetitions	Without repetitions
$GFI_{(OLS)}$	2	0.6087	0.1988
	5	0.6129	0.2125
	10	0.7769	0.6852
	20	0.9417	0.8977
$AGFI_{(OLS)}$	2	0.5616	0.1027
	5	0.5665	0.1779
	10	0.7501	0.5848
	20	0.9023	0.8329

To illustrate, here it comes the application of a principal components analysis, with description of the main result, to be verified in the percentage of the explanation of the sample variation, given by the principal components (Figures 2-4). For such application, we considered the correlation matrices generated from () to 2, and 20 replications defined, respectively in matrices (12) and (13).

$$R_\theta = \begin{bmatrix} 1.000 & & & & & & \\ -0.347 & 1.000 & & & & & \\ -0.106 & -0.041 & 1.000 & & & & \\ 0.142 & 0.179 & -0.176 & 1.000 & & & \\ -0.092 & -0.026 & 0.127 & -0.079 & 1.000 & & \\ -0.142 & -0.025 & 0.151 & -0.103 & 0.919 & 1.000 & \\ -0.144 & 0.126 & -0.002 & 0.382 & -0.016 & 0.004 & 1.000 \end{bmatrix} \tag{12}$$

$$R_\theta = \begin{bmatrix} 1.000 & & & & & & \\ -0.327 & 1.000 & & & & & \\ -0.193 & -0.012 & 1.000 & & & & \\ 0.222 & 0.105 & -0.199 & 1.000 & & & \\ -0.082 & -0.121 & 0.058 & -0.091 & 1.000 & & \\ -0.117 & -0.104 & 0.113 & -0.110 & 0.928 & 1.000 & \\ -0.115 & 0.287 & -0.061 & 0.558 & -0.083 & -0.067 & 1.000 \end{bmatrix} \tag{13}$$

Considering the restitution of sample variability in the first two components (Figures 2-4), the inclusion of latent variables and design structure to estimate the correlation matrix (R_θ) promoted an accumulation of 65.64%. Increasing the number of repetitions, such accumulation went to 56.42%. In both situations, there is an advantage in the application of principal components analysis, in which, considering only the sample correlation matrix (R), the accumulation was 52.73%.

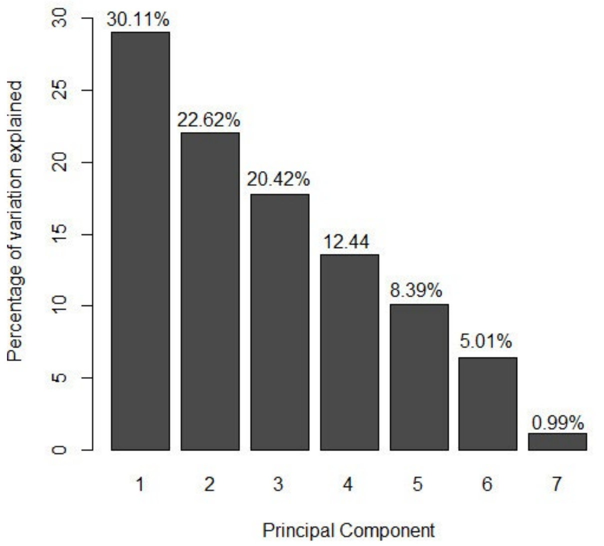

Figure 2: Percentage of sample variation explained by components with usual correlation matrix.

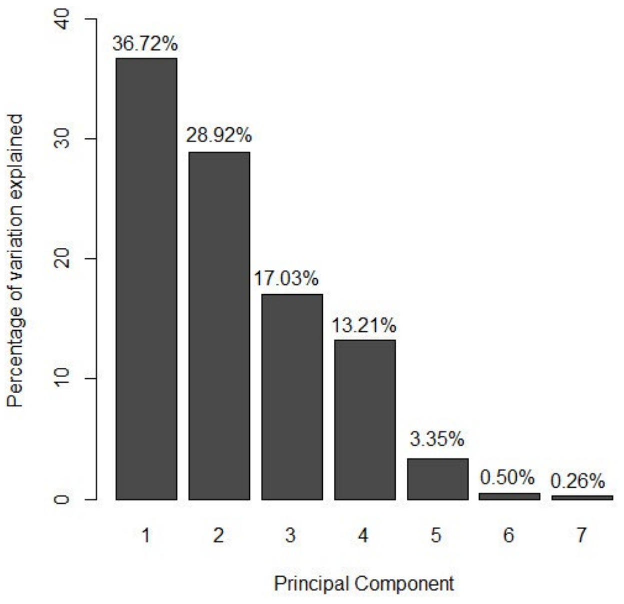

Figure 3: Percentage of sample variation explained by components with correlation matrix R_θ and with 2 repetitions for treatment.

4 DISCUSSION

The justifications for selecting the variables that form each construct that modeling of the covariance structure (7), imposed by the model (Figure 1), represented by the latent variables, are given below. Rainfall is one of the climatological factors that most contribute to coffee production during the phenological phases. It is therefore used to geographically order suitable, restricted, and unsuitable areas for cultivation. Currently, regions with restricted water availability, but which adopt the practice of supplementary irrigation, have stood out both in productivity and in coffee beverage quality (Barbosa et al., 2012). However, Weldemichael and Teferi (2020) reported that, among the most frequently mentioned environmental factors, rainfall is considered a negative factor for coffee quality.

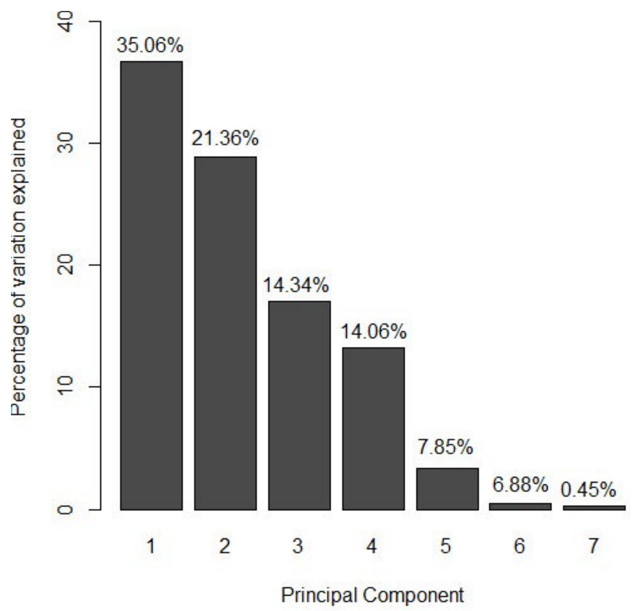

Figure 4: Percentage of sample variation explained by components with correlation matrix R_θ and with 20 repetitions for treatments.

Coffee beverage acidity may or may not be a desirable attribute, and it depends on the predominant acid in it. A pleasant acidity develops a vibrant flavor in coffee beverages, increasing sweetness perception and giving it a fresh fruit taste. Overall, low-acid coffee beverages do not have a high sensory score (Specialty Coffee Association of America - SCAA, 2008). Moreover, pulped coffees often show different sensory attributes from dry-processed coffees, such as more a pronounced acidity (Elhalis; Cox; Zhao, 2023).

Flavor is the main and most important criterion for evaluating coffee quality (Córdoba et al., 2021). Its analysis reflects a combination of all perceptions observed in the tasting. Flavor scores denote the intensity, quality, and complexity of the combination of taste and aroma of beverages (Malta el al., 2013).

Since the inclusion of repetitions provided an improvement in the quality indices evaluated. This fact suggests that, by not considering information from the treatments (i.e., ranges of altitudes) a false interpretation can be induced, as well as an underestimation of the proximity of covariance matrices between sampled data and the model, as the indexes are formulated following that reasoning.

In general, an increase in the number of repetitions improved the estimation of the indices. In this sense, according to the criterion established by Jöreskog and Sorbom (1986), estimates of GFI above 0.90 are considered excellent fit. Therefore, for the application proposed in this study, 20 repetitions of the variables observed for each altitude range may be recommended, given the hypothetical model (Figure 1) that justifies the covariance modeling.

After obtaining the model-adjusted covariance matrix ($\boldsymbol{\Sigma}_{\theta}$), including information on the repetitions of treatments (altitudes), the user can use it in different data analysis methods involving dimension reduction, thus, for example, principal component analysis, biplots, multidimensional scaling, discriminant analysis, in short, techniques that presuppose, as data entry, the covariance matrix.

5 CONCLUSIONS

The covariance matrix modeling proposed in this study, as a case study, proved to be advantageous for allowing analysis of the relationship among latent variables disregarded in sensory analysis. The proposed method allows the incorporation of environmental variables, such as altitudes, to be considered as repetitions of the observed variables.

The model-adjusted covariance matrix correlation structure generates more promising estimates when principal component analysis is used. Therefore, such a recommendation tool can be used in other dimensionality reduction techniques.

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7 AUTHORS' CONTRIBUTIONS

MR: wrote the manuscript and performed the experiment; MAC: supervised the experiment and co-work the manuscript, and FMB: review and approved the final version of the work; MAC: conducted all statistical analyses.

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