

Prediction of coffee sensory attributes using near-infrared spectroscopy

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ABSTRACT

Cup tasting is the traditional method for evaluating coffee beverage quality. However, sensory analysis has several limitations, including subjectivity, high costs and the challenge of establishing desirable limits for different quality attributes. Therefore, this study aimed to predict coffee sensory attributes based on near-infrared (NIR) spectra of roasted and ground coffee samples. For that, an experiment was conducted during the 2020-2021 harvest season in the Zona da Mata region of Minas Gerais State, Southeastern Brazil, involving seven arabica coffee fields. A total of 180 coffee samples were harvested, processed, and evaluated through sensory analysis following the Specialty Coffee Association protocol. Subsequently, regression models using NIR spectra (1000 to 2500 nm) coupled with Partial least squares (PLS) and PLS-OPS (ordered predictors selection) were developed. The PLS-OPS models yielded the best results, with correlation coefficients (r^2) ranging from 0.78 to 0.82 and prediction errors (RMSEP) between 0.15 and 0.13 for aftertaste, overall perception, body, and balance. While predictions for aroma, flavor, and acidity require further improvement, the other attributes showed performance comparable to more complex analytical techniques. These findings demonstrate that NIR spectroscopy, combined with advanced chemometric modeling, offers a promising, cost-effective alternative for predicting coffee sensory quality.

Key words: *Coffea arabica* L.; cup quality analysis; digital agriculture; proximal sensing.

1 INTRODUCTION

Coffee is the second most traded commodity worldwide and is produced in over 50 countries. Brazil is the world's largest coffee producer and exporter, responsible for approximately one-third of global output (United States Department of Agriculture - USDA, 2023a). Despite this, only 34% of the current Brazilian production is consumed domestically, emphasizing its strategic importance as an export commodity. In the 2023-2024 season, Brazil is expected to produce, consume, and export 66.4, 22.6, and 43.8 million 60 kg bags (USDA, 2023b). Such facts solidify the Brazil's position as a major producer and exporter of commodity coffee.

Despite the primary focus on commodity coffee production, since the mid-2000s, in the third wave of coffee, Brazilian producers have increasingly directed their attention towards producing specialty coffees, characterized by their high quality and distinctiveness (Boaventura et al., 2018; De Araújo et al., 2021). In this wave, specialty coffee is considered an artisanal product as complex as wine (Guimarães; Gonzaga de Castro Júnior; Carvalho de Andrade, 2016). Moreover, certain producers have recognized that specialty coffee can guarantee higher profit margins, enabling them to become less dependent on international commodity prices (Boaventura et al., 2018; Guimarães et al., 2019). This is particularly attributed to the significant impact of coffee beverage quality on price setting and export potential.

Specialty coffees are distinguished by their superior beverage quality, which results from complex interactions among the environment, plant genetics, crop management, harvest, and post-harvesting practices (Cheng et al., 2016; Läderach et al., 2011; Silva Neto et al., 2018; Silva et al., 2014). Specifically, the primary factors influencing coffee quality include fruit ripeness at harvest, edaphoclimatic conditions, planting altitude, the microbiome of plants and fruits, genotypes, and post-harvest practices (Decazy et al., 2003; Oliveira Aparecido et al., 2018; Silva Oliveira et al., 2021; Veloso et al., 2020; Worku et al., 2018).

Due to the economic significance of specialty coffee, its evaluation plays a pivotal role in quality control, valuation, and product enhancement. At present, beverage quality is evaluated through sensory analysis, commonly known as cup tasting, conducted by professional coffee tasters, referred to as "Q-Graders" (Di Donfrancesco; Gutierrez Guzman; Chambers, 2014). This analysis encompasses various attributes (e.g., flavor, aroma, and acidity) discerned by senses and assessed organoleptically by cuppers (Santos et al., 2012; Tolessa et al., 2016). Then, the quality attributes are graded following specific protocols such as those of the Specialty Coffee Association (SCA) (SCA, 2021).

However, this methodology is inherently subjective, expensive, time-consuming, requires trained cuppers, which impedes the efficient execution of routine analysis, and poses

challenges when processing numerous samples during the peak of coffee harvesting (Craig et al., 2018; Feria-Morales, 2002). These limitations underscore the need for faster and more reliable alternatives to assess the sensory quality, and other attributes present in coffee beans. Spectroscopic methods in the near-infrared (NIR) range serve as prime examples of fast, reliable, chemical-free, and cost-effective techniques that have found widespread application in assessing food quality attributes (Mutz et al., 2023; Nicolai et al., 2007; Wang et al., 2015).

Recent studies have demonstrated the potential of NIR spectroscopy for coffee analysis across various domains including sensory attribute prediction (Baqueta; Coqueiro; Valderrama, 2019; Ribeiro; Ferreira; Salva, 2011; Tolessa et al., 2016), chemical property estimation (Caporaso et al., 2018; Levate Macedo et al., 2021; Pizarro et al., 2007), adulteration detection (Correia et al., 2018; Winkler-Moser et al., 2015), roasting process monitoring (Bertone et al., 2016; Catelani et al., 2018), determination of geographical origin (Baqueta et al., 2023; Medina et al., 2017), as well as defect detection (Abadi et al., 2015).

Most of these studies underscore the potential of NIR spectroscopy for assessment of coffee sensory attributes. Despite this, the high spectral resolution of NIR spectra often yields numerous variables, many of which may be irrelevant or redundant, thereby making data processing time-consuming and potentially compromising results (De Paulo et al., 2023; Forina et al., 2004). Consequently, variable selection becomes crucial to identify the spectral data most correlated with the attribute of interest. In this sense, ordered predictors selection (OPS) has proven to be an important methodology for variable selection (Teófilo; Martins; Ferreira, 2009). The core of OPS is to rearrange the data matrix in order of importance. This occurs through an informative vector, whose aim is to identify spectral variables with the highest correlation with the corresponding property vector (De Paulo et al., 2023; Teófilo; Martins; Ferreira, 2009).

OPS has been widely used to process different types of NIR data sets (Assis et al., 2017; Vieira et al., 2021), including coffee samples (Ribeiro; Ferreira; Salva, 2011; Ribeiro; Salva; Silvarolla, 2021). Based on these studies, the application of OPS holds promise in significantly reducing the dataset, thereby enhancing the interpretability and predictive capacity of partial least squares (PLS) models. Notably, only one study has coupled PLS with OPS for coffee sensory attributes prediction. Ribeiro, Ferreira and Salva (2011) developed regression models for body, flavor, cleanliness, and overall quality prediction using PLS and OPS. Despite the accurate predictions of scores conferred by cuppers, these authors worked with a limited dataset of coffee samples. In view of the aforementioned, this study aimed to predict coffee sensory attributes using NIR spectra of roasted and ground coffee samples.

2 MATERIAL AND METHODS

2.1 Study area

The study was conducted in seven arabica coffee (*Coffea arabica* L.) fields situated in the municipalities of Paula Cândido and Araponga, within Minas Gerais State, Southeastern Brazil (Figure 1). The climate in this region is classified as humid subtropical (CWA), characterized by dry winters and hot summers according to the Köppen-Geiger classification (Alvares et al., 2013).

The characterization of the arabica coffee fields is presented in Table 1. The study area encompasses different coffee cultivars, with each field exhibiting distinct areas, plant densities, and terrain characteristics.

2.2 Field data collection and processing

Coffee samples, each composed of three kilograms of cherry fruits, were harvested on different dates between April and June during the 2020-2021 season (Table 2). To ensure representative sampling across the fields, an irregular sampling grid was established based on the fruit load in each coffee field. The sampling points were designated by three plants situated adjacent to one another within the same cultivation row. Subsequently, the coffee fruits were manually harvested from eight plagiotropic branches, with two branches selected randomly from each plant quadrant in the middle third of the plants. Lastly, georeferencing of the sampled points was conducted using a topographic GNSS (Global Navigation Satellite System) receiver (model: ProXT, Trimble Inc., Sunnyvale, CA, USA).

After the harvest, the coffee samples were pulped using a mechanical device (Model: DMMP - 04, Pinhalense, São Paulo, Brazil) with continuous water flow, and subsequently were dried in a mechanical dryer equipped with a gas burner, as previously detailed (Silveira et al., 2016). The drying air temperature was maintained between 35 and 40 °C until the coffee samples reached 12% moisture content. The sample moisture content monitoring was performed using a digital grain moisture meter (Model: G650, Gehaka, São Paulo, Brazil). After drying, the coffee samples remained with endocarp (parchment) and were packed in kraft paper bags for storage until further processing. Lastly, the samples were hulled using a portable device (Model: DRC-1 830, Pinhalense, São Paulo, Brazil), packed in plastic bags, and stored until sensory analysis.

2.3 Sensory analysis using the SCA protocol

Coffee sensory attributes were evaluated following the protocol developed by the Specialty Coffee Association (SCA) (SCA, 2021). Three Q-Grader certified tasters conducted the sensory evaluation. Initially, the coffee



Figure 1: Location of the coffee fields in the Zona da Mata region of Minas Gerais State, Southeastern Brazil.

Table 1: Characteristics of the arabica coffee fields used in this study.

Field	Area (ha)	Cultivar	Density (Plants ha ⁻¹)	Average Terrain Slope (%)	Average Altitude (m)
1	1.53	Catucai Saulo	8000	30.13 ± 10.10	863.39 ± 9.58
2	0.86	Catucai	8000	42.00 ± 19.47	838.74 ± 8.37
3	0.75	Geisha	3400	18.28 ± 6.02	923.58 ± 2.03
4	0.81	Catuai MG44	3800	23.53 ± 7.69	704.51 ± 3.96
5	2.57	Catuai MG44	3800	24.02 ± 8.78	703.59 ± 6.32
6	0.56	Red Catuai	4000	10.16 ± 5.65	772.29 ± 1.19
7	0.88	Red Catuai	4000	12.45 ± 5.15	762.81 ± 1.56

Table 2: Harvesting dates and the number of samples collected on each coffee field.

Field	Date		Samples per harvest			Total (n = 180)
1	21/05/2021	7	-	-	-	7
2	21/05/2021	8	-	-	-	8
3	27/05/2021	22	-	-	-	22
4	06/04, 12/04, and 19/04/2021	6	14	11	-	31
5	08/04, 14/04, 21/04, and 27/04/2021	10	16	10	20	56
6	19/05 and 25/05/2021	22	8	-	-	30
7	01/06/2021	26	-	-	-	26

n, refers to the number of samples.

samples were roasted at 190-210 °C for 9 to 12 minutes using a sampling roasting machine (Model: Probat Leogap TP2, Curitiba, Brazil). Next, the coffee samples were ground to a medium particle size using an electric grinder (Model: Bunn GVH-37, Springfield, Illinois, USA). The tasting process involved five cups per sample, with each taster conducting one evaluation per sample.

Following the cupping protocol proposed by the SCA, the evaluation focused on the attributes of Aroma, Flavor, Aftertaste, Acidity, Body, Balance, Overall cup perception, and the Final Score. The attributes Sweetness, Clean cup, and Uniformity were omitted from this study, as all samples, irrespective of coffee cultivars, received the same score. The SCA protocol uses a 16-point scale, allowing for quarter-point (0.25) increments between numeric values ranging from 6 to 9. Theoretically, this scale spans from 0 to 10 points, with the lower end representing scores below specialty grade (SCA, 2021). After assessing all attributes, tasters assign a final score, with 100 points being the maximum attainable score for a coffee sample. These scores reflect the overall quality of the beverage, with samples achieving a final score of 80 points or higher being classified as specialty coffee (SCA, 2021).

2.4 NIR spectra measurement

Coffee NIR spectra were acquired subsequent to processing and sensory analysis. Roasted and ground coffee samples (20 g per sample) were placed in black plastic lids, and absorbance spectra were recorded using a spectroradiometer (model: ASD FieldSpec PRO 4, Analytical Spectral Devices, Inc., Boulder, Colorado, USA) with spectra ranging from 350 to 2500 nm. The device exhibited a spectral resolution of 3 nm for the range 350–1000 nm and 8 nm for the range 1001–2500 nm. Despite that, the spectral data output resolution was 1 nm since the device automatically interpolated the data to achieve this resolution.

To obtain the absorbance spectra of the roasted coffee samples, a contact probe (also from Analytical Inc.) equipped with a built-in light source (6.5 W halogen lamp) and a 2-cm-diameter circular viewing window was attached by a fiber-optic cable to the spectroradiometer (Figure 2). For precise positioning of the spectroradiometer relative to the sample, the probe was vertically fixed to a black chamber featuring a hole on its top with the same diameter as the spectroradiometer probe, allowing it to fit snugly into the chamber. The hole in the black chamber was sealed by the structure of the contact probe, which had a rubber ring on its base to prevent light entry. Subsequently, the probe was positioned on top of the plastic lid containing the coffee, and five measurements per sample were conducted. The spectroradiometer was calibrated after every three samples using a white spectralon plate. Finally, the average values of the five readings were computed to generate a representative spectral signature for each sample. For this study, the spectra were limited to the NIR region between 1000 and 2450 nm.

2.5 Data Analysis

2.5.1 Predicting coffee sensory attributes using NIR spectra

Initially, the spectra were organized in a matrix of independent variables (X), with rows representing the 180 spectra of the coffee samples and columns representing the 1451 wavelengths (1000 to 2450 nm). The dependent variable vector (y) consisted of the results from the cup quality analysis for each sensory attribute. Before analysis, the data was divided into calibration (n = 126, 70%) and validation (n = 54, 30%) datasets using the Kennard-Stone algorithm (Kennard; Stone, 1969). The calibration dataset was used to optimize model parameters, including data preprocessing, the number of latent variables (LVs), and the selection of optimal wavelengths. The validation dataset was then used to evaluate the model's ability to predict new samples.

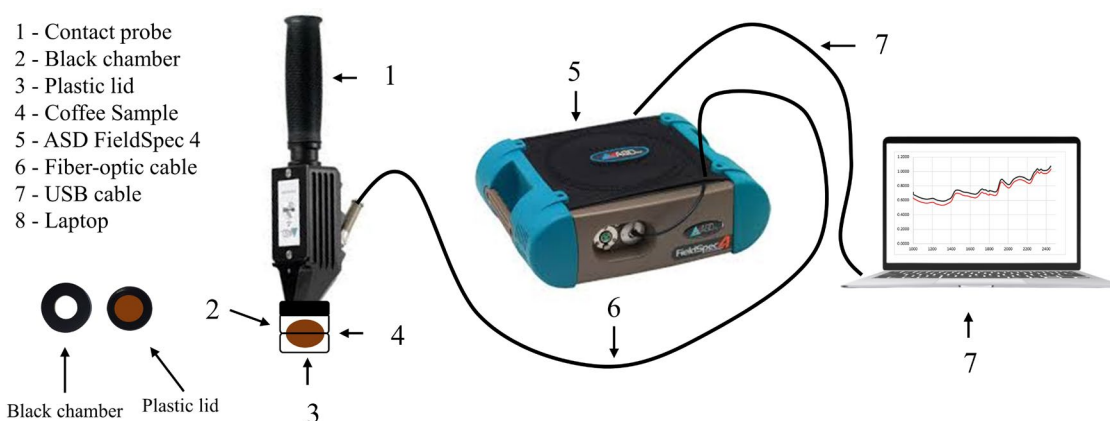


Figure 2: Laboratory experiment set up used to acquire the absorbance spectra of the roasted coffee samples.

The training process was conducted in two steps. First, various preprocessing strategies were applied to the raw spectra to transform the data, extract useful information, and eliminate data artifacts such as noise, baseline drift, and slope, thereby developing models with reliable performance for predicting unknown samples (Corrêdo et al., 2021; Oliveri et al., 2019). The preprocessing methods that yielded the best performance for model prediction were as follows: smoothing and mean centering for aroma; asymmetric least squares (AsLS) and autoscaling for flavor; robust normal variate (RNV) and normalization for aftertaste; net analytical signal (NAS) and detrending for acidity; NAS and smoothing for body and balance; AsLS and NAS for overall perception; and detrending and NAS for the final score.

Additionally, a preliminary data overview was performed using principal component analysis (PCA) to identify outliers in the training and testing datasets. The combination of Q-residuals and the Hotelling statistics (T^2) ellipse at a 5% significance level was used to detect and remove outliers from the dataset (Xu et al., 2018). Then, the PLS regression method was employed to determine the number of latent variables (LVs) for the prediction models using the entire spectra (1000 to 2450 nm). The optimal preprocessing techniques and the number of LVs were selected based on the lowest root mean square error of cross-validation ($RMSE_{cv}$) value, and the highest coefficient of correlation (r_{cv}). Random cross-validation was conducted with a 10-fold split.

For the second step, the ordered predictors selection (OPS) method was utilized to select the most predictive wavelengths. These selected wavelengths were then used to develop new prediction models. In this method, an informative vector is created, containing information from the best independent variables for prediction. The variables were selected based on the absolute values of this informative vector (Teófilo; Martins; Ferreira, 2009). Subsequently, the original independent variables were arranged in decreasing order of magnitude, with higher absolute values indicating greater importance to the response variable.

Initially, the algorithm selected a subset of variables, which were then used to build and evaluate the first model. Subsequently, new independent variables (windows) were added to the first model, creating new models until all variables were considered. The performance of these models was obtained during each evaluation and stored for later comparison. Among the subsets of selected variables (initial window and its extensions), the one with the lowest $RMSE_{cv}$ was selected. This study utilized a new version of the OPS that includes three approaches for variable selection: AutoOPS, feedOPS, and iOPS.

AutoOPS is an automated method designed to select variables by utilizing different informative vectors and their combinations. Differently, the FeedOPS applies feedback in

the OPS algorithm, allowing pre-selected variables to be re-evaluated in a new selection run until specific criteria are met. Lastly, iOPS applies OPS to subdivisions of the full array, called OPS intervals. Each interval undergoes variable selection using AutoOPS or feedOPS to reduce variables. Intervals with selected variables are merged into a new matrix, where further variable selection occurs with a predetermined window and increment. AutoOPS (or feedOPS) is then applied to the new array to determine the optimal set of variables (Roque et al., 2019; Wang et al., 2023). Specific details about the processes and foundations of these OPS versions are provided elsewhere (Roque et al., 2019; Teófilo; Martins; Ferreira, 2009). Finally, the performance of the PLS-OPS models was assessed using the root-mean-square-error of the prediction ($RMSE_p$) and the coefficient of correlation of the prediction (r_p). All algorithms were written in Matlab environment, version 2018a (Mathworks, Inc, Natick, Massachusetts, USA).

3 RESULTS

3.1 Descriptive statistics of the coffee quality attributes

The SCA protocol includes eleven key attributes for coffee beverage quality assessment. This study focused on eight of them: aroma, flavour, aftertaste, acidity, body, balance, overall perception, and final score. Mean scores for these attributes, as evaluated by the Q-Graders, served as dependent variables in the PLS regression models construction. Table 3 provides a summary of the statistics for all sensory attributes evaluated. Before characterizing the data, an outlier analysis was conducted on the dataset. This was achieved using PCA in combination with Q-residuals versus leverage and Hotelling statistics. Consequently, different samples were identified as outliers for each quality attribute and subsequently removed from the dataset. The number of outliers ranged from 20 to 25 among the sensory attributes. This discrepancy arose because the analysis was performed individually for each attribute.

Regarding the descriptive statistics, the minimum and maximum values fell within the range of 6 to 9 on the quality scale, indicating specialty grade for the evaluated samples. The maximum value for the final score was 85, classified as excellent quality, while the minimum value was below specialty quality at 72.4 points. However, considering the average values, the coffee beverages were classified as very good quality, with the final score exceeding 80 points, the threshold for this classification (SCA, 2021). Lastly, despite using five coffee cultivars in the sensory analysis, the variability (coefficient of variation) observed in the different quality attributes was low, ranging from 2.20% for the final score to 3.79% for overall perception.

Table 3: Descriptive statistics of the coffee sensory attributes.

Quality Attribute	Average $\pm$ SD	Minimum	Maximum	CV (%)	n
Aroma	7.44 $\pm$ 0.24	6.88	8.25	3.27	155
Flavour	7.34 $\pm$ 0.23	6.83	8.00	3.12	155
Aftertaste	7.06 $\pm$ 0.26	6.50	7.67	3.68	156
Acidity	7.29 $\pm$ 0.24	6.83	7.88	3.25	159
Body	7.17 $\pm$ 0.24	6.58	7.83	3.37	159
Balance	7.19 $\pm$ 0.24	6.58	7.83	3.45	157
Overall Perception	7.16 $\pm$ 0.27	6.50	7.88	3.79	160
Final Score	80.58 $\pm$ 1.77	72.40	85.00	2.20	158

SD, Standard deviation; CV, Coefficient of variation; n, Number of samples.

3.2 Spectral characterization of the coffee cultivars

The samples analyzed in this study exhibited a similar shape to the typical raw spectra of roasted coffee documented in the literature (Craig *et al.*, 2014; Ribeiro; Ferreira; Salva, 2011). The spectra of the five cultivars displayed significant similarity, discernible primarily by slight variations in absorbance ($\log(1/R)$ intensity) across the entire spectral range (Figure 3). The shape of the spectra was predominantly influenced by water absorption bands, notably in the regions from 1440 to 1460 nm (1st overtone of O–H stretching) and from 1920 to 1950 nm (combination bands of O–H stretching and O–H deformation) (Craig *et al.*, 2014). Consequently, the absorption of chemical compounds associated with the sensory attributes was likely diminished in comparison to the water-related bands in both regions.

The regions between 1720–1760 nm (1st overtone of C–H and S–H) and 2300–2350 nm (C–H + C–C combination bands) have been previously associated with lipid content, whereas the range from 2100–2140 nm (N–H combination bands) was linked to carbohydrates, chlorogenic acids, and proteins (Craig *et al.*, 2014; Ribeiro; Ferreira; Salva, 2011). However, these regions comprise distinct bands that cannot be individually characterized due to the overlap of overtones and combination bands.

3.3 Performance of the PLS and PLS-OPS regression models

The PLS and PLS-OPS models were calibrated and validated for the eight sensory attributes. Model selection was based on the lowest number of LV's and RMSE values, and in the highest coefficient of correlation (r) between the observed and predicted data. The PLS-OPS models demonstrated a slight improvement in prediction performance across all sensory attributes, except for aroma, which was better modeled using PLS with the full spectra (1000 to 2450 nm) (Table 4). Among the attributes evaluated, aftertaste was the most precisely predicted by PLS-OPS in both cross-validation (RMSE_{CV} : 0.15 and r_{CV} : 0.68)

and prediction steps (RMSE_p : 0.13 and r_p : 0.82). Conversely, the prediction model for aroma showed the lowest performance (RMSE_{CV} : 0.15 and r_{CV} : 0.48; RMSE_p : 0.13 and r_p : 0.68).

Among the OPS versions used, both the AutoOPS and feedOPS presented the lowest error in the cross-validation (RMSE_{CV}) for all sensory attributes. Subsequently, the variables selected by these methods were used to build the PLS models. Both versions selected different subsets of wavelengths for each sensory attribute from the initial 1451 variables (1000–2450 nm) (Table 4). Due to the extensive data volume, which varied among sensory attributes, the selected variables were grouped into spectral regions and/or specific wavelengths and included in the supplementary material of this manuscript. In summary, the OPS versions selected 9 regions for building the aroma model, 9 for flavor, 26 for aftertaste, 13 for acidity, 24 for body, 1 for balance, 25 for overall perception, and 22 for the final score. It is important to clarify that this manuscript does not intend to compile all spectral regions contributing to the prediction of each sensory attribute. Instead, it aims to illustrate the general spectral regions selected, consistent with the literature. Furthermore, the OPS variable subset selection relied on statistical criteria (*e.g.*, VIP values, correlation and regression coefficients, etc.) rather than spectroscopy or chemical considerations, leading to some differences from literature-reported spectral regions.

Nevertheless, for all quality attributes, the selected variables were distributed throughout the entire spectra (1000–2450 nm). Notably, a majority of the spectral regions and/or wavelengths (50 regions encompassing all attributes) were concentrated within the range of 2000 to 2500 nm (combination bands region). This region is recognized for exhibiting absorption peaks for aromatic compounds, caffeine, chlorogenic acids, proteins, lipids, and carbohydrates, all of which are relevant to the studied quality attributes (Baqueta *et al.*, 2023; Barbin *et al.*, 2014; Craig *et al.*, 2014; Ribeiro; Ferreira; Salva, 2011).

When comparing the number of latent variables (LVs) included to build the regression models, both the PLS

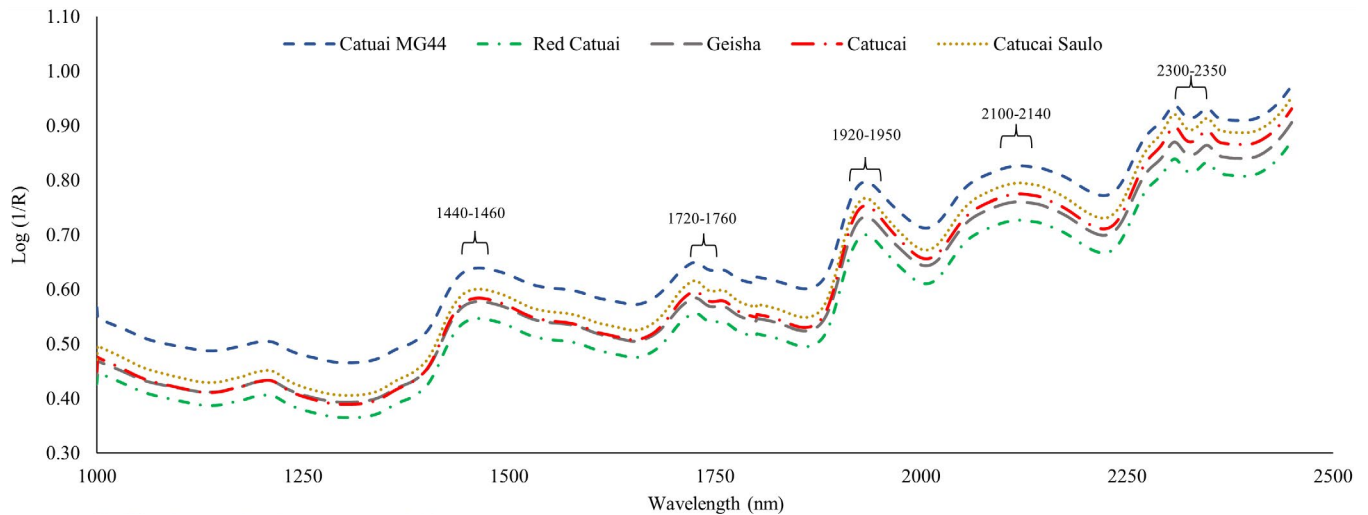


Figure 3: Average absorbance spectra in the NIR region obtained from the roasted coffee samples.

Table 4: Results of the coffee sensory attributes prediction using the PLS regression models with all variables (1000 to 2450 nm) and those selected by the PLS-OPS models.

Attribute	Model	Variables	LV	RMSE _c	r _c	RMSE _{cv}	r _{cv}	RMSE _p	r _p
Aroma	PLS	1451	10	0.13	0.63	0.15	0.41	0.12	0.69
	PLS-OPS ¹	260	10	0.13	0.64	0.15	0.48	0.13	0.68
Flavour	PLS	1451	15	0.06	0.95	0.15	0.65	0.15	0.72
	PLS-OPS ²	760	14	0.06	0.94	0.14	0.68	0.15	0.73
Aftertaste	PLS	1451	12	0.14	0.75	0.18	0.54	0.15	0.76
	PLS-OPS ²	100	12	0.12	0.80	0.15	0.68	0.13	0.82
Acidity	PLS	1451	10	0.13	0.74	0.17	0.51	0.15	0.70
	PLS-OPS ²	660	9	0.13	0.72	0.16	0.58	0.14	0.73
Body	PLS	1451	10	0.15	0.68	0.18	0.48	0.16	0.73
	PLS-OPS ²	180	10	0.15	0.67	0.17	0.54	0.15	0.79
Balance	PLS	1451	12	0.13	0.74	0.16	0.55	0.15	0.74
	PLS-OPS ¹	1400	12	0.13	0.74	0.16	0.57	0.14	0.78
Overall	PLS	1451	8	0.14	0.76	0.19	0.55	0.16	0.74
	PLS-OPS ¹	120	8	0.14	0.76	0.18	0.62	0.14	0.80
Final Score	PLS	1451	5	0.91	0.72	1.06	0.60	0.98	0.74
	PLS-OPS ¹	580	5	0.90	0.72	1.00	0.64	0.95	0.75

¹ and ², refer to the OPS versions: AutoOPS and feedOPS; LV, Number latent variables; RMSE_c, RMSE_{cv}, and RMSE_p refer to the root mean square error in the calibration, cross-validation, and prediction steps; r_c, r_{cv}, and r_p refer to the coefficient of correlation in the calibration, cross-validation, and prediction steps.

and PLS-OPS models used the same number of LVs, except for flavor and acidity, which differed among models. The performance of the regression models ranged from moderate (Aroma) to satisfactory (Aftertaste and Overall perception) when compared to previous studies outlined in the discussion section. Lastly, scatterplots of the predicted vs. measured sensory attributes are presented in Figure 4. Both calibration and validation sets were included to illustrate that the samples fell within the same range, regardless of the coffee cultivars.

4 DISCUSSION

4.1 Applicability of NIR spectroscopy for coffee sensory quality prediction

Coffee sensory analysis is a complex and subjective process where Q-graders distinguish quality attributes using their senses. Due to individual preferences, results can be inconsistent, making it challenging to define desirable

limits for attributes like acidity, flavor, sweetness, and body (Agnoletti et al., 2022; Pereira et al., 2020). Therefore, employing instrumental methods and statistical modeling is recommended to achieve faster and unbiased results. This study utilized PLS and PLS-OPS regression models to predict eight sensory attributes using the NIR spectra of roasted coffee samples.

The study showed promising results for the final score and individual sensory attributes such as aroma, flavor, aftertaste, acidity, body, balance, and overall perception. Baqueta et al. (2019) reported correlation coefficients (r_p) and prediction errors (RMSE_p) of 0.75 and 0.16 for aroma, 0.77 and 0.13 for flavor, 0.80 and 0.28 for body, and 0.73 and 0.16 for overall quality using NIR spectroscopy with PLS on commercial coffee varieties. In contrast, we found lower correlation values, particularly for aroma (r_p : 0.69 and RMSE_p: 0.12). Nonetheless, the prediction errors were smaller, and the other attributes showed correlation values above 0.7, indicating satisfactory results (Santos et al., 2019).

Tolessa et al. (2016) evaluated the same quality attributes as this study, except for balance, and reported higher performance for overall perception (r_p : 0.90 and RMSE_p: 0.22) and final score (r_p : 0.90 and RMSE_p: 1.04). Conversely, their results for aroma (r_p : 0.01 and RMSE_p: 0.40), flavour (r_p : 0.59 and RMSE_p: 0.29), aftertaste (r_p : 0.72 and RMSE_p: 0.27), and body (r_p : 0.72 and RMSE_p: 0.24) were lower compared to our study's findings, regardless of the model used (PLS or PLS-OPS). In a recent study, Agnoletti et al. (2022), utilized

chromatographic analysis along with PLS and GA-SVR (Genetic Algorithm with Support Vector Regression) to predict scores for aroma, aftertaste, acidity, body, balance, and overall perception. The prediction performance varied among quality attributes and was generally lower than in this study, except for aroma and body.

Table 5 presents a compilation of studies that attempted to predict coffee sensory attributes, showing a range of performance outcomes based on the analytical techniques used. The performance (r_p and RMSE_p) obtained in this study is consistent with those reported in the scientific literature for spectroscopy-based methods. Only one study reported higher prediction performance when specifically using NIR and the PLSR technique (Ribeiro; Ferreira; Salva, 2011).

Despite the varying analytical techniques used to gather chemical information for predictions, the differences in the prediction performance (r_p and RMSE_p) values across these studies were minimal. This consistency reinforces the effectiveness of PLS regression with variable selection methods in predicting coffee sensory attributes. Furthermore, the differences in model performance could be attributed to several factors, such as the number of samples used for calibration and validation, scanning procedures, multivariate methods, narrow value ranges, and especially the low variability in scores among different coffee cultivars. In this study, although the spectra of the five cultivars differed in absorption intensity, the quality attributes showed low variability (Table 3 and Figure 3), which affected model performance.

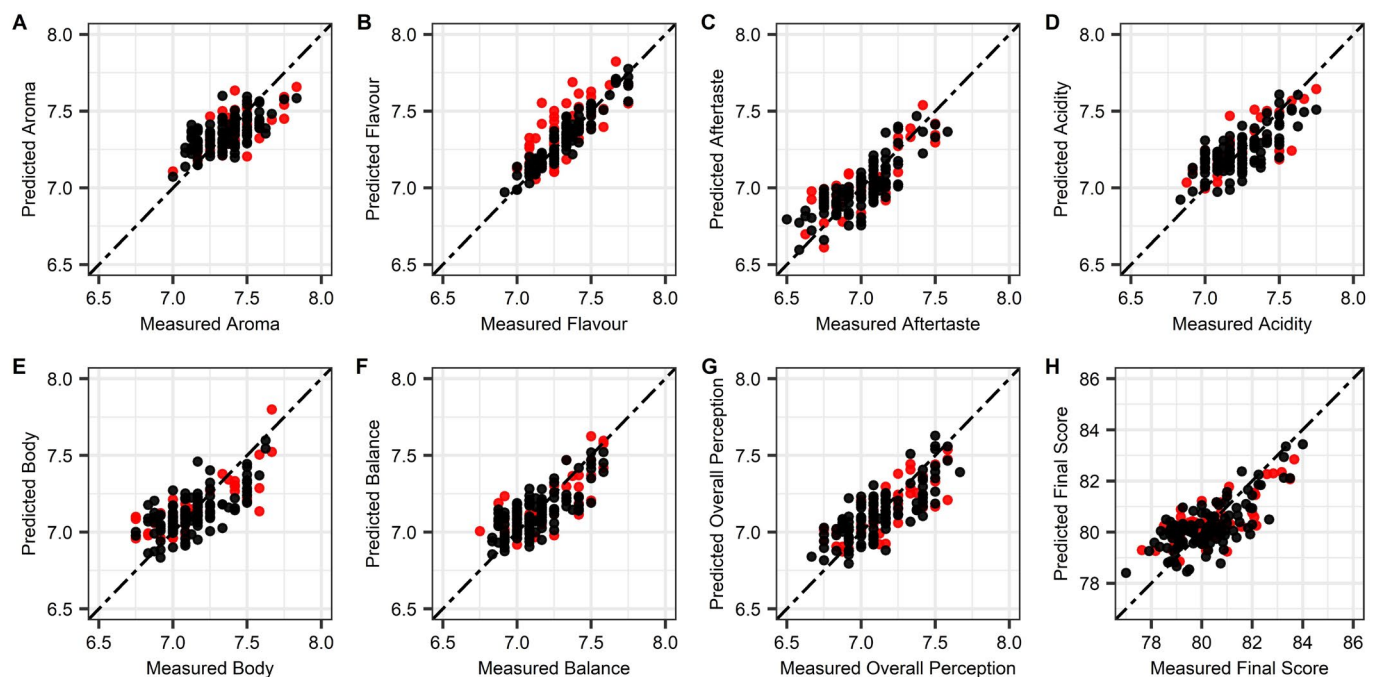


Figure 4: Scatterplots of predicted versus measured values of the coffee sensory attributes. A 1:1 line (grey, dashed) is provided for reference. Black and Red dots refer to the calibration and validation datasets.

Table 5: Compilation of distinct analytical methods used to predict coffee sensory attributes.

Instrument	Modelling method	Attributes	Sample preparation	N	Performance (r_p and RMSE _p)	Reference
FT-NIR	PLSR	aroma, flavour, aftertaste, acidity, body, overall perception, and final score	Direct read from roasted and ground coffee	86	0.59 – 0.90 1.04 – 0.22	(Tolessa et al., 2016)
HS-SPME-GC/MS	PLSR, SVR and SVR-GA	aroma, aftertaste, acidity, body, balance, and overall perception	Chromatographic analysis of roasted and ground coffee	40	0.18 – 0.85 0.42 – 0.20	(Agnoletti et al., 2022)
NIR	PLSR-OPS	flavour, acidity, body, and overall perception	Direct read from roasted and ground coffee	51	0.83 – 0.93 0.42 – 0.25	(Ribeiro; Ferreira; Salva, 2011)
NIR	PLSR	aroma, flavor, acidity, body, overall perception	Direct read from roasted and ground coffee	217	0.73 – 0.80 0.28 – 0.11	(Baqueta; Coqueiro; Valderrama, 2019)
FTIR	PLSR	final score	Direct read from roasted and ground coffee	56	0.94 – 0.97 0.99 – 0.23	(Belchior et al., 2019)
FTIR and NIR	PLSR	aroma and final score	Direct read from roasted and ground coffee	56	0.97 – 0.99 0.52 – 0.23	(Belchior; Botelho; Franca, 2022)
NIR	PLSR and PLSR-OPS	aroma, flavour, aftertaste, acidity, body, Balance, overall perception, and final score	Direct read from roasted and ground coffee	180	0.69 – 0.82 0.98 – 0.12	This study

FT-NIR, Fourier-transform near-infrared; HS-SPME-GC/MS, Headspace solid-phase micro-extraction gas-chromatography-mass spectrometry; NIR, Near-infrared; FTIR, Fourier-transform infrared; PLSR, Partial least square regression; OPS, Ordered predictors selection; SVR, Support vector regression; GA, Genetic algorithm; N, Number of samples; r_p and RMSE_p, coefficient of correlation and root mean square error of the prediction.

The PLS-OPS models effectively reduced the number of variables and computational cost while increasing prediction performance compared to the PLS models. For all attributes, the selected variables were distributed across the entire spectral range (1000–2450 nm). This is because the compounds influencing coffee sensory attributes are absorbed throughout the whole spectrum (Belchior et al., 2020). This study did not aim to establish a relationship between sensory attributes and the spectra of chemical compounds in coffee samples. Therefore, only a brief description of relevant spectral regions and sensory attributes that match previous studies is presented.

For example, the spectral regions from 1552 to 1556 nm (1st overtone C-H), 1988 to 2082 nm (1st overtone of C=O and O-H combination bands), and 2246 to 2394 nm (O-H and CH + CH combination bands) were linked to organic and chlorogenic acids and used to predict beverage acidity (Ribeiro; Ferreira; Salva, 2011). The influence of these acids is due to their decomposition during roasting and the impact of the resulting products on compounds that affect acidity (Esteban-Díez; González-Sáiz; Pizarro, 2004). In this study, the selected spectral regions for acidity prediction covered the entire spectrum, with the majority of variables ranging from 2009 to 2084 nm and 2138 to 2414 nm.

This study identified spectral regions that coincided with previous research for flavor (1830–2060 and 2180–2250 nm), aftertaste (1722–1724 nm), and body (1721–1731, 1938–1939, 1966–1971, 2309–2314, and 2399–2401 nm) (Supplementary Table). Many of these spectral regions are closely related to the NIR spectra of trigonelline, chlorogenic acids, coffee

lipids, pure caffeine, 5-caffeoylquinic acid, cellulose, sucrose, and casein, which influence the scores for flavor, acidity, body, and overall perception (Ribeiro; Ferreira; Salva, 2011).

Given that the selected spectral regions were distributed across the entire spectrum, it is challenging to specify and describe the chemical compounds influencing each quality attribute precisely, as their absorption peaks are close to each other. Additionally, the PLS-OPS technique selects variable subsets using a combination of statistical parameters, such as VIP values and correlation coefficients (Teófilo; Martins; Ferreira, 2009), which do not always correlate directly with the chemical compounds responsible for the sensory attributes.

Finally, the complexity of coffee as a matrix, influenced by multiple variables during production phases (*e.g.*, cultivation, harvesting, post-harvesting, and extraction of sensory properties) (Belchior et al., 2019), makes it difficult to establish a linear relationship between the spectra and the sensory attributes. Future research should include data from more coffee varieties with a wider range of sensory attribute values and explore other modeling techniques to address these complexities.

5 CONCLUSIONS

This study demonstrated the effectiveness of NIR spectroscopy with PLS and PLS-OPS for predicting eight coffee sensory attributes. PLS-OPS models performed best for aftertaste, overall perception, body, and balance, with the correlation coefficients (r_p) ranging from 0.78 to 0.82 and prediction errors (RMSE_p) from 0.15 to 0.13. However,

improvements are still needed for prediction of aroma, flavor, and acidity. Despite this, the performance achieved was comparable to results from more complex analytical methods.

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7 AUTHOR'S CONTRIBUTIONS

Conceptual idea: Martins, R.N.; Pinto, F.de.A.C.; de Queiroz, D.M.; Côrredo, L.de.P.; Methodology design: Martins, R.N.; Pinto, F.de.A.C.; Cardoso, W.J.; Teófilo, R.F.; Data collection: Martins, R.N.; Portes, M.F.; Data analysis and interpretation: Martins, R.N.; Cardoso, W.J.; Teófilo, R.F.; Côrredo, L.de.P., and Writing and editing: Martins, R.N.; Pinto, F.de.A.C.; de Queiroz, D.M.; Côrredo, L.de.P.; Cardoso, W.J.; Portes, M.F.; Valente, D.S.M.; Teófilo, R.F.

8 DATA AVAILABILITY STATEMENT

Data available upon request to authors.

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