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Within and among farm variability of coffee quality of smallholders in southwest Ethiopia

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Abstract

The biophysical drivers that affect coffee quality vary within and among farms. Quantifying their relative importance is crucial for making informed decisions concerning farm management, marketability and profit for coffee farmers. The present study was designed to quantify the relative importance of biophysical variables affecting coffee bean quality within and among coffee farms and to evaluate a near infrared spectroscopy-based model to predict coffee quality. Twelve coffee plants growing under low, intermediate and dense shade were studied in twelve coffee farms across an elevational gradient (1470–2325 m asl) in Ethiopia. We found large within farm variability, demonstrating that conditions varying at the coffee plant-level are of large importance for physical attributes and cupping scores of green coffee beans. Overall, elevation appeared to be the key biophysical variable influencing all the measured coffee bean quality attributes at the farm level while canopy cover appeared to be the most important biophysical variable driving the above-mentioned coffee bean quality attributes at the coffee plant level. The biophysical variables driving coffee quality (total preliminary and specialty quality) were the same as those driving variations in the near-infrared spectroscopy data, which supports future use of this technology to assess green bean coffee quality. Most importantly, our findings show that random forest is computationally fast and robust to noise, besides having comparable prediction accuracy. Hence, it is a useful machine learning tool for regression studies and has potential for modeling linear and nonlinear

multivariate calibrations. The study also confirmed that near-infrared spectroscopic-based predictions can be applied as a supplementary approach for coffee cup quality evaluations.

Keywords: coffee quality, near-infrared spectroscopy (NIRS), random forest, PERMANOVA

1. Introduction

Coffee is one of the most important global commodities providing livelihood opportunities to millions of people in the global South (Legesse, 2020; Davis *et al*. 2019; Ovalle-Rivera *et al*. 2015). In addition to being an important cash crop to farmers in Ethiopia, it generates about a quarter of the country's export earnings (Legesse, 2020). Quality is becoming paramount in the global coffee market. Coffee quality is about having desirable characteristics such as clean in its appearance and good cupping scores (Carvalho *et al*. 2020). High-quality coffee shows little or no physical defects, for instance, broken beans, insect damage, and other foreign materials such as seeds of shade trees black beans, immature beans, and floaters and, when roasted, have a distinctive character in the cup and high cup tasting scores.

Green been coffee quality is a complex characteristic that depends on a series of pre-harvest factors that might vary either within or among farms. Some of the pre-harvest factors that vary within farms include microclimate, soil physicochemical properties, shade, age and variety of the coffee tree. Factors that vary among farms include growing elevation and macroclimate, agronomic practices and coffee variety (Getachew *et al*. 2022; Sarmiento-Soler *et al*. 2022). Variation in soil characteristics and fertilization can be situated at both levels. Harvesting and processing conditions can also be considered important factors influencing coffee quality. Elevation and shade cover play an important role through temperature, availability of light and water, especially during the seed ripening period (DaMatta *et al*. 2018, Sarmiento-Soler *et al*. 2022). Microclimate has a strong influence on flowering, bean expansion, and ripening (Borem *et al*. 2020, Hameed *et al*. 2020). Elevation is the major driving factor of climatic and edaphic factors at larger spatial scales. Shade tree canopy cover, on the other hand, modulates macroclimatic trends through its effect on microclimate. Cool climates (higher elevations, with at least intermediate canopy cover) had a high potential to produce coffee beans possessing superior total preliminary quality, higher caffeine,

total chlorogenic acid (CGA) contents, and trigonelline concentrations (Worku *et al*. 2018; Tolessa *et al.* 2017; paper in-press). Water deficits, on the other hand, during the coffee fruit expansion and filling period caused appreciable productivity loss and decreased bean quality (Kath *et al*. 2020; Semedo *et al*. 2018). In terms of soil characteristics, is especially soil pH associated with the acidity of coffee, body and cup cleanness. More soil nitrogen increased the caffeine content, resulting in a more bitter taste of the brew (Yadessa *et al*. 2020; Clemente *et al*, 2015). Hence, assessing the importance and variations of these biophysical variables at a larger-scale across elevational gradients among coffee farms and the variations among coffee trees within the farms across a canopy cover gradient and their associated effect on coffee bean quality is very critical. Interestingly, assessing the relative importance of within farm variability and variability among farms has rarely been quantified in smallholder coffee farms. The existence of such inter-and intra-farm variability could have a direct implication on input allocation, agronomic management decisions and the productivity of these systems (Trevisan *et al*. 2021; Monteiro *et al*.2020; Sida *et al*. 2020). Although several studies highlighted the effects of these variables on coffee bean quality, their relative importance has not yet been quantified, and documenting such differences may help to improve agronomic management decisions.

Coffee quality assessment is a key step in price setting to determine its export potential in coffee-producing countries. Thus, accurate quality assessment is of major importance to many coffee producers, roasters, and distributors. For each coffee bean shipment, further characterization is required to verify if it attains the required quality (Dos Santos *et al*. 2016). Coffee bean quality is mainly described by its physical attributes (mainly determined by bean length, diameter, and hundred bean mass), raw and cup quality attributes (Cheng *et al*. 2016; Dos Santos *et al*. 2016). The raw quality assessment evaluates defects that are manually separated and counted according as primary and secondary defects and odor. Primary defects include full black, full sour, fungus presence, foreign matter, insect damage, dried cherry, any mimic seed and soil presence whereas secondary defects include partial black, partial sour, floater, immature, etc. Cup or sensory quality, determine the desirability of a coffee for consumption (Tolessa *et al*. 2018; Teklu *et al*. 2011). These quality attributes, such as cup cleanness, acidity, body, and flavor can be distinguished by sensory organs and are assessed by professional cup tasters based on established procedures. In

Ethiopia, cupping score analysis enables experts to evaluate the preliminary cup assessment, which is used to group coffee into different specialty categories (Ribeiro *et al*. 2021; Levate Macedo *et al*. 2020; Okubo *et al*. 2019; Tolessa *et al*. 2016). Coffee beans graded from grade one to three are grouped into specialty coffee and these three categories are further classified into different specialty grades, which are called: Q1, Q2, and commercial type. In this particular study, our focus is mainly on total preliminary and specialty quality and bean physical attributes.

Though standardized, methods of assessing coffee quality are prone to subjective judgments in addition to being costly and time-consuming. An alternative technique is use of Near-Infrared Spectroscopy (NIRS). NIRS technology-based sorting and grading systems for various aspects of food quality and safety are widely used. NIRS analysis is rapid, requires limited sample preparation, reduces costs of chemicals, and also multiple components can be determined on the same sample from a single measurement. NIRS analyses integrated to chemometrics have been proposed as an analytical methodology to characterize food (Al-Harrasi *et al*. 2020; Genisheva *et al*. 2018), medicine (Kucharska-Ambrożej *et al*. 2020; Calvo *et al*. 2018) and coffee samples (Souza *et al*. 2022; Ribeiro *et al.* 2021; Zhu *et al.* 2021). Their use has been considered to distinguish coffee origin (Adnan *et al.* 2020; Giraudo *et al.* 2019*;* Dos Santos *et al*. 2014*),* assess the quality of coffee beans (Tolessa *et al*. 2016; Esteban-Diez *et al*. 2004), caffeine content (Ayu *et al*. 2020; Budiastra *et al*. 2018; Zhang *et al*. 2017; Pizarro *et al*. 2007) and lipids (Caporaso *et al*. 2018) as well as to measure sugars content, roasting degrees and moisture (Levate Macedo *et al*. 2021). NIRS, specifically for coffee, has been successfully applied to coffee analysis, including determination of geographical origin (Giraudo *et al*. 2019), estimation of its chemical properties (Caporaso *et al*. 2018; Ayu *et al*. 2020), roasting process monitoring (Yergenson *et al*. 2020; Catelani *et al*. 2018; Bertone *et al*. 2016), adulteration detection (Chakravartula *et al*. 2022; De Carvalho Couto *et al*. 2021; Correia *et al*. 2018), and sensory analysis (Ribeiro *et al*. 2011).

Nowadays, combination of multivariate calibration methods with spectroscopic data has allowed the analysis of complex spectra of multi-component system. A vast range of linear and non-linear computational methods is used for modeling these systems. Among them, random forest (RF) and partial least square regression (PLSR) are useful when non-linear or high-dimensional

relationships exist in the dataset. RFs are known as a flexible approach to capture non-linear relationships in high-dimensional data by learning a multitude of decision trees. Furthermore, they can be used to rank the predictors according to their importance to obtain accurate predictions. PLSR can cope with multidimensional data, and can eliminate multicollinearity problems by generating latent variables (components) from the covariance matrix of dependent and independent variables (Tyralis *et al*. 2019).

Here we compile a database of 12 coffee trees selected across a gradient of open to dense canopy cover within each of 12 farms selected across an elevational gradient from 1470 m to 2325 m above sea level. This resulted in a total of 12 trees times 12 farms, that is, 144 coffee trees, specifically designed to quantify among and within farm variability, and assess the relative importance of the biophysical drivers of this variability. All farms were of the semi-plantation coffee production type. Our response variables were the cupping scores and physical bean attributes and NIRS spectra of the green coffee beans. We specifically addressed the following three important questions:

i) How much green coffee bean quality variation is there among and within coffee farms?

ii) What is the relative importance of biophysical drivers (type and degree of canopy cover, soil temperature and moisture) for green bean coffee quality?

iii) Can NIR spectra of green coffee beans be used to predict cupping scores?

2. Methodology

In this section, we give an overview of the methods used in this study. In section 2.1 the data acquisition is described in detail. Section 2.2 treats the preprocessing techniques that are required to analyze the near infra-red spectroscopic (NIRS) data. The statistical machine learning methods used to analyze the data are discussed in section 2.3.

2.1 Data acquisition

We describe all aspects related to the data acquisition. Two main types of data were acquired: biophysical variables related to the selected coffee trees and NIRS data from their coffee beans.

Study area: The study was conducted in the Goma and Gera districts of Jimma Zone in southwestern Ethiopia (7°37'48'' – 7°56'37''N latitude and 36°13'41'' – 36°39'17''E longitudes) on 12 coffee farms (Table 1 and Fig. 1). The region is characterized by a humid and warm subtropical climate with a yearly rainfall between 1500 and 2000 mm. The main rainy season is from May to September (monomodal rainfall) accounting for about 85% of the annual rainfall and coffee cultivation in the region is entirely rain-fed. Differences in temperature vary throughout the year with a mean monthly temperature between 13°C and 26°C. The bulk of coffee growing soils in the region are classified as Eutric Nitisols, which are deep, red, and well-drained soils with a clay content of more than 30% and a pH (measured in H_2O) between 4.2 and 6.2 (Muleta *et al*. 2008, Dubale, 1996).

Coffee farms selection and characterization: The study covered agroforestry sites distributed across the landscape, comprising an area of approximately 50 by 50 km. To encompass a natural temperature gradient, 12 coffee farms were selected across elevational gradients ranging between 1470 m – 2325 m asl. All the selected coffee farms are categorized as a semi-plantation coffee production system, with high anthropogenic disturbances resulting in a relatively species poor canopy consisting of tree species such as *Albizia schimperiana*, *Albizia gummifera* and *Croton macrostachyus*. Mulching and organic fertilizers are a commonly used soil fertility management strategies. To avoid spatial autocorrelation, the selected farms were at least 3-4 km apart.

Within each farm, sampling was conducted in 30 x 30 m area (sampling coffee plants consistently positioned inside the plantation to avoid edge effects) in which 12 individual coffee trees were selected. Shade tree canopy cover was measured for each selected coffee tree. Four coffee trees were sampled under each of the following canopy cover categories: light (<35% canopy cover), intermediate (35-65%) and dense shade levels (>65%). Accordingly, a total of 144 coffee trees were sampled from 12 coffee farms. All the measurements and data provided in this manuscript (shade tree canopy cover, soil moisture content, and soil temperature) are at the individual coffee tree-level with n = 144 whereas soil chemistry is at the coffee farm level.

Biophysical variables: The following biophysical variables were measured to describe elevation, shade tree canopy cover, soil temperatures and moisture, and soil properties per individual coffee trees. The variables are used to determine coffee quality (both cupping scores and NIR spectra).

i) Elevation

The elevation of each coffee farm was measured with a GPS (Garmin-60, Kansas, USA).

ii) Shade tree canopy cover

Shade tree canopy cover over each coffee tree was quantified using a convex spherical crown densiometer (Forest densiometers, Model A, Bartlesville, Oklahoma, USA). The densiometer is made of a small wooden box with a convex mirror consisting of a grid of squares; shade tree canopy cover is then calculated as the proportion of 96 points that was intersected by vegetation times 1.04. The densiometer was held at breast height and the observer's head was reflected from the edge of the mirror just outside the box. The curved mirror reflects the canopy above. Above the canopy of each sampled tree using a ladder all the time, two counts were recorded and their mean was used.

iii) Soil temperature, moisture and chemical characteristics

a) **Soil temperature**: To quantify the temperatures in each coffee farm, soil temperatures were recorded at one-hour intervals for a 10 months period (February 2020 to November 2020, i.e., period from coffee flowering to harvest) using miniature temperature sensors (type HOBO 8K Pendant Temperature/Alarm Data Logger – UA-001–08, Onset Computer Corporation, Bourne, MA, USA) buried in the soil at 10 cm depth and 40 cm distance from the coffee tree trunk at all 144 coffee plants. We could not measure air temperatures due to theft of visible devices. To ensure the best representation of temperature experienced by the coffee plant, the daily minimum, mean and maximum soil temperature values were computed. From the daily data, monthly mean, minimum and maximum temperatures of the period February - November 2020 were used for further analyses.

b) **Soil moisture (gravimetric method)**: Surface mineral topsoil (0-10 cm) was sampled in the dry season at the start of the coffee flowering season in February 2020 to reflect the weather-independent water status of the site (rough farm ranking, independent from rainfall) using a core sampler after removing the surface litter and plant debris at three locations per coffee tree (10 cm away from the stem in three directions). The samples were taken during the measurement of the canopy cover. These three samples were pooled into one sample for soil moisture content and nutrient analysis. The mass of the fresh soil samples was recorded using a balance immediately after sampling. The samples were oven-dried at 65°C for 48 hrs (Robertson *et al*. 1999), after which the dry mass was recorded immediately to determine gravimetric soil moisture content. Finally, the percent soil moisture was computed as (fresh soil mass – dry soil mass)/dry soil mass) x 100).

c) **Soil chemical characteristics**: An oven-dried sub-sample was used for the measurements of pH, soil organic carbon, total N, Olsen-P, exchangeable Ca, Mg and K (Table 1). All the soil samples were dried to a constant weight at 65°C for 48 h, ground and sieved over a 2 mm mesh. The pH (in H_2O) of the soil was measured using a calibrated glass electrode (model Ross sure-flow 8172 BNWP, Thermo Scientific Orion, USA). Soil organic C and total N, were measured using a CNS elemental analyser with a thermal conductivity detector in a (vario Macro Cube, Elementar, Uberlingen, Germany). Soil total Ca, K and Mg were measured by atomic absorption spectroscopy (Varian SpectrAA-220, USA) after complete destruction of the soil samples with $HClO_4$ (65%), HNO_3 (70%) and H_2SO_4 (98%) in Teflon bombs for 4 h at 150°C. Exchangeable K^+, Ca^{2+}, Mg^{2+}, Na^+ and Al^{3+} concentrations were measured by atomic absorption spectroscopy after extraction in 0.1 M $BaCl_2$ (NEN 5738:1996).

Coffee berry sampling and measurements: All fully ripe, red colored coffee berries were hand-picked once at peak harvest between early October and early November 2020 from each individual coffee tree using local coffee bags. Berries were harvested first from lower elevation sites followed by the higher elevation sites. The berries were dry processed, i.e. sun-dried (on raised beds with a mesh wire) immediately after harvest (harvesting was in the morning and drying started in the afternoon). The berries were returned back to the bags before sunset and stored in clean rooms (to

prevent any spoilage), and returned back to the raised beds in the morning until the green beans attained 11.5% moisture content measured using a coffee moisture tester (mini GAC, Dickey - John, USA). The berries were regularly turned to maintain uniform drying. The dried coffee berries were dehusked using a coffee hulling machine (coffee huller, McKinnon, Scotland) at Jimma University, cleaned and stored at room temperature in separate labeled bags for analysis.

For cup quality (60% of the total preliminary quality), green coffee bean samples were evaluated for cup quality attributes by a panel of three internationally trained, experienced and certified Q-grade cuppers at the Ethiopian Commodity Exchange (ECX) center based in Jimma town. Acidity, body, cup cleanness and flavor were assessed in accordance with the standard method (ECX, 2011). This Q-grade standard method involves Q-certified cuppers, i.e., cuppers licensed by Specialty Coffee Association (SCA) Coffee Quality Institute (CQI). The cuppers were trained in descriptive sensory analyses in using a sensory lexicon of cup quality (Di Donfrancesco *et al*. 2014). Accordingly, aroma, flavor, acidity, body, uniformity, cup cleanness, overall preference, aftertaste, balance and sweetness were each rated on a scale from 0 to 10. This total preliminary assessment was used to classify the coffee samples into different quality grades. According to ECX (2011), dry-processed coffee samples were categorized into different quality grades based on total preliminary assessment and classified as: 91-100 (grade 1), 81-90 (grade 2) and 71-80 (grade 3) whereas the specialty coffee achieving scores between 85-100 are classified as specialty 1 (Q_1) and 80-84 is specialty 2 (Q_2), and Q_3 (commercial type) (https://sca.coffee/research/protocols-best-practices).

Roasting, grinding and brew preparation was standardized. A roaster equipped with a cooling system, in which air was forced through a perforated plate, capable of roasting up to 500 g of coffee beans, was used for roasting the coffee beans. An amount of 100 g green beans was used for each sample and the beans were put into the roasting machine with six cylinders (Probat, 4 Barrel Roaster, Germany) and were carefully roasted for 7-8 minutes to medium roast at temperatures of 200˚C. The roasted bean samples were ground to a medium level using a Guatemala SB electrical grinder that was cleaned well after each sample. The medium roasted coffee was tipped out into a cooling tray and allowed to cool down for 4 minutes rapidly by

blowing cold air through it. Then, eight gram of coffee powder was put into a 250 mL cup and 5 cups per sample were used. Next, 125 ml boiled water (93˚C) was poured onto the ground coffee, followed by stirring the content to ensure the homogeneity of the mixture. Then, the cups were filled with an additional 125 mL and left to settle. After three minutes, the floaters were skimmed, and the brew was ready for cup tasting. Finally, the five prepared cups were tasted by three professional Q-grade cuppers operating in ECX. Each panelist gave their independent judgment using a cupping form and the average score of the three cuppers was used for analysis. Total preliminary quality is the sum total of raw bean quality (primary defects, secondary defects, and odor) and cup quality attributes (acidity, body, flavor, and cup cleanness), whereas specialty quality is the sum total of ten cup quality attributes (aroma, flavor, aftertaste, acidity, body, balance, overall, cup cleanness, sweetness, and uniformity).

Scanning of coffee bean samples with NIR spectroscopy and spectral data acquisition

Approximately 50 g of each dried and grounded green coffee bean sample was placed into a glass Petri dish (diameter = 2 cm, depth = 1 cm). Samples in the Petri dish were pressed gently and levelled by a spatula, which was necessary as the bean powder surface ensures maximum diffuse reflection and high signal-to-noise ratio. A Fourier Transform-NIR spectrometer (Tango, Brucker, Belgium) was used to obtain coffee bean spectra. Green coffee samples were ground to a size smaller than 5 mm and 15-20 g of each sample was used for analysis. The samples were irradiated with tungsten (5V/7W) as source of near infrared light and the spectra measurements were performed at room temperature. The coffee bean samples were scanned in diffuse reflectance mode using a Compact NIR spectrophotometer (Tec5 Technology for spectroscopy, Germany) and the reflectance was detected by an Indium Gallium Arsenide (InGaAs) diode. This generated NIR spectra data consist of two lists of numbers (wavenumber and its associated reflectance). Each spectrum had 1898 data points in the wavenumber range of 3952 to 11540 cm-1 (867 to 2530 nm) with data spacing of 4 cm^{-1} for a total of 144 bulk coffee bean samples (Appendix Fig. S1).

2.2 NIRS data preprocessing and analysis

Preprocessing of NIR spectra is an essential component of multivariate data calibration. Its primary goal is to remove unwanted information such as spectra noise, and scattering effect that are not

related to the variables (properties) of interest. Furthermore, we also apply outlier detection, spectra trimming and optimal wavelength selection through a PCA analysis.

Spectra preprocessing: A variety of mathematical spectra pre-processing were tested in order to improve model robustness and prediction accuracy. Several pre-processing methods such as spectra normalization, de-trending (DT), standard normal variate (SNV), vector normalization, spectra derivatives, multiplicative scatter correction (MSC), orthogonal signal correction (OSC) and combinations of them have been investigated in several studies. Generally, with a well-tested pre-processing steps, the performance of the model can be greatly improved. These mathematical pre-processed methods strongly depend on a given dataset, and no universal solution could be found. However, certain preprocessing techniques were selected following the best results of (Jiao *et al*. 2020; Dotto *et al*. 2018; Nawar *et al*. 2017; Knox *et al*. 2015; Peng *et al*. 2014; Cambule *et al*. 2012; Knox *et al*. 2012).

Among the extensively reviewed prepressing techniques, Savitzky-Golay smoothing, multiplicative scatter correction, and standard normal variate were found to be a better preprocessing algorithms for preprocessing of our raw spectra, and all three of them were examined in two models. Besides, these mathematical pre-processed algorithms were widely used in reflectance spectroscopy methods in many literatures (Bian *et al*. 2021; Ren *et al*. 2021; Jiao *et al*. 2020; Nawar *et al*. 2017). The details of these preprocessing algorithms are put in the appendix word file 1.

Outlier detection in pre-processed NIR spectra: This was performed using the 25^{th} and 75^{th} percentile by checking outliers in NIR spectra using the quantile() function from the package "ggstatsplot". The suspected outliers were detected using the interquartile range (IQR). Finally, the subset() function from the same package was used to eliminate outliers. Accordingly, five rows from the dataset were detected as outliers and subsequently omitted (Bello *et al*. 2020).

Spectra trimming: this is a procedure where wavelength ranges with high signal-to-noise ratio are removed. This is to specify the wavelength regions of interest without any standard procedures

(Wadoux *et al*. 2021; Ng *et al*. 2018). This is because, the spectra measurements below 720 nm and above 2500 nm do not contain much useful information since they are at the boundary of the range recorded by the sensor. Hence, NIR spectra within a range of 720–2500 nm was retained for further spectra processing, which has brought the number of data points per spectrum to p = 1884.

Optimal wavelength selection: As the complete spectra contains redundant information as indicated in Appendix Fig S1, this would result in complex, unstable, and inaccurate models. Hence, optimal wavelength selection is generally used to identify those wavelengths that capture a large part of the information present in the spectra (Mishra *et al*. 2021; Rodriguez-Pulido *et al*. 2013). We performed a PCA analysis showing that the first component explained 97.8% of the variability present in the whole spectra. The wavelengths corresponding to the peaks from the loading plot of the first component were selected as the optimal wavelengths (Appendix Fig S3) (Mishra *et al*. 2021; Rodriguez-Pulido *et al*. 2013). In this way, 87 wavelengths were selected and used to infer the final model. An excel containing all the selected wavelengths using the PCA loading method can be found in the Appendix table 1.

2.3. Statistical data analysis

We introduce the statistical machine learning methods that are used for data analysis.

Variable importance: For data visualization and to detect multicollinearity among the biophysical variables, PCA was employed. The PCA provides a set of explanatory orthogonal vectors by projecting similar variables in the two-dimensional space and subsequently variables closer to each other indicates the high correlation. Accordingly, Tmin (minimum temp) was omitted from the analysis and the remaining predictor variables were considered for variable selection procedures (Janitza *et al*. 2018; Wright *et al*. 2017). Likewise, as elevation is the natural driving factor for other biophysical variables, it was also omitted from the analysis. Based on this, permutation-based variable importance was used to estimate the influence of a given variable in a model prediction and ultimately estimate its relative importance for the coffee quality and hundred bean mass. This technique assigns a score to input variables based on how useful they are at predicting a target variable (Probst, 2018; Wright *et al*. 2017). Here only random forest was used for

classification and ranking candidate biophysical variables based on the variable importance using varImp package (Probst, 2019). A higher score means that the specific variable will have a larger effect on the model that is being used to predict a certain variable. By looking at the variable importance, we can easily decide which variables to possibly drop because they do not contribute much to the prediction process. The method for calculating permutation accuracy importance was applied in R using the ranger package (Janitza *et al*. 2018; Wright *et al*. 2017).

Permutational Multivariate Analysis of Variance (PERMANOVA): The proportion of variance explained by the individual coffee trees and coffee farms was performed using geometric partitioning of variance in a multivariate data analysis technique to examine whether the variability observed in physical coffee bean quality and cupping scores is between the individual coffee trees or coffee farms and to quantify the proportion of variance explained by each of them. To this end, a variance partitioning approach was adopted in the multivariate domain (Behrens *et al*. 2018; Anderson, 2005). This relied on a PERMANOVA model, featuring the Manhattan distance matrix among observations (i.e. cupping scores) as the dependent matrix and coffee trees and farms as a fixed and random variable, respectively. PERMANOVA was chosen because it generates a geometric partitioning and extends the analysis much broader, allowing rigorous meaningful analysis of high-dimensional systems having variables with extremely non-normal or over dispersed behavior. It is not restricted by distributional assumptions and can accommodate heterogeneity within-group dispersions than the classical ANOVA. The model was based on $1x10^5$ permutations and the breakdown of the variance among coffee trees and farms was carried out by evaluating the marginal effect of each of them in the full model. In doing so, the share of the coffee farms and coffee trees was examined through linear mixed effect models for the total preliminary and specialty quality, and hundred bean mass. The estimation of the variance function, its partition among the two, and how each of them affects cupping scores and hundred bean mass was then performed according to the approach of Hoffman (2021). The permutational multivariate analysis of variance was carried out using *"*variancePartition*" and* "vegan" package.

Random forest and partial least square regression to predict coffee quality based on NIR spectra data: A two-dimensional data matrix consisting of pre-processed spectra (as independent

variables) and measured cupping scores (total preliminary and specialty quality) as dependent variable was created from the 139 coffee bean samples (as 5 of the rows were outliers and subsequently removed). For the purpose of coffee quality prediction random forests (RF) and partial least square regression (PLSR) were tested.

Both PLSR and RF models were chosen because they are more powerful than the conventional regression models for modeling complex and non-linear data in a high-dimensional and hierarchical fashion. PLSR can cope with multidimensional data, and can eliminate multicollinearity problems by generating latent variables (components) from the covariance matrix of dependent and independent variables. Hence, PLSR is recommended as one of the best performing calibration techniques for spectral data (Kuang *et al*. 2015). RF, on the other hand, uses an ensemble of a large number of decision trees by offering sufficient accuracy, simple implementation, and high robustness (Tyralis *et al*. 2019). The algorithm is a model ensemble method constructed based on combining several decisions by the regression and classification trees. Two key parameters need to be taken into account: one is the number of the decision trees and the other is the number of sampled variables for building a decision tree. RF has the capability of ranking the importance of variables by their importance (Janitza *et al*. 2018). The method could be briefly summarized in three steps: (1) the Bagging method to generate T subsets of training data randomly; (2) each training sample is employed to generate the corresponding decision trees randomly choosing m attributes from M attributes as the split attributes set of the current node prior to select attributes on each non-leaf node, and split the node in the best split way among the M attributes; (3) each tree grows sufficiently without pruning, and was used to test the corresponding category from the test set. Finally, the majority vote of the decision trees was used to make an ensemble classification decision (He *et al*. 2022; Khan *et al*. 2022; Asadi *et al*. 2021; Ao *et al*. 2019).

Model validation and evaluation: To validate the RF and PLSR for coffee quality prediction, a leave-one-out cross-validation (LOOCV) procedure was performed. In each run, one sample was left out to test the models while the other samples are used to train and calibrate the models. Training and calibration involved a randomly split into calibration (n=112) and prediction (n=27)

samples. For the PLSR the number of latent variables were optimized during this calibration step. For the RF, we optimized the number of sampled variables (over a range of 2 to 87) and the minimum size of terminal nodes (over the values 1,5 or 10) while the number of trees was held fixed at 500 (Tridawati *et al*. 2020; Wadoux *et al*. 2019; Freeman *et al*. 2016). The process of LOOCV was repeated until every sample is left out once. The implementation was performed with the R environment for statistical computing using the packages 'caret' and 'randomForest' (Kuhn and Johnson, 2013).

In both RF and PLSR models, four statistical metrics: correlation coefficient (r), coefficient of determination (R^2), root mean square error (RMSE), and residual predictive deviation (RPD) were used to evaluate the predictive performance of the models according to the classification criteria of Viscarra *et al*. (2009). The coefficient of determination (R^2) reflects the percentage of variance in the response variable that is accounted for by the explanatory variables. An R^2 value between 0.5-0.65 indicates that more than half of the variance in the response variable is accounted for by the explanatory variable. R^2 value in the range of 0.66-0.81 indicates approximate quantitative predictions whereas the R^2 value in the range of 0.82-0.9 reveals a good prediction. Calibration models possessing an R^2 value above 0.91 are considered excellent (Nakagawa *et al*. 2017). RMSE allows to measure how far the predicted values deviate from the observed values in a regression analysis. The larger the difference, the larger the gap between the predicted and observed values. The smallest RMSE value is usually related to the optimal calibration model and the better a model is able to fit the data. RPD takes both the prediction error and the variation of observed values into account, hence providing a metric of model validity that is more objective than RMSE and more easily comparable across model validation studies. The greater the RPD, the better the model's predictive capability (Nakagawa *et al*. 2017; Kapper *et al*. 2012).

RPD is defined as the standard deviation of the measured value divided by the RMSE of the predicted values (Kapper *et al*. 2012; Guy *et al*. 2011). It is calculated as follows:

$$RPD = \frac{SD}{\mathrm{RMSE}}$$

where SD is the standard deviation of the measured value and RMSE is the standard error of prediction. In general, when RPD≥2, it indicates that the model works well and can be used for

462 quantitative analysis and evaluation (Kapper *et al*. 2012). Models estimations were computed
463 using PLSR and RF along with four statistical metrics: correlation coefficient (r), coefficient of
464 determination (R^2), root mean square error (RMSE), and residual predictive deviation (RPD)
465 according to the classification criteria of Viscarra *et al*. (2009). Generally, a good model prediction
466 corresponds to high R^2, r, and RPD, and low RMSE values. Finally, scatter plots showing the
467 relationship between the spectra data and cupping scores were generated using the best model. For
468 all statistical procedures, R-4.1.2 software (R Core Team, 2022) was used.
469

470 ## 3. Results

471 Descriptive statistical results of soil chemistry, moisture and temperature in the twelve coffee
472 farms are shown in Table 1. The coefficients of variation (CV) of soil chemistry, moisture and
473 temperature showed that among all the measured soil chemical variables, Olsen-P had the highest
474 CV (63.7%), particularly in the coffee farm with elevation 2325 m asl followed by soil
475 exchangeable K (62.7%) at coffee farms situated at 2027 m asl elevation. Likewise, Olsen-P had
476 the next highest CV (60.0%) at the coffee farm situated at the elevation of 1774 m asl, as compared
477 to other measured soil parameters. In contrast, soil C at the coffee farm situated at the elevation of
478 1650 m asl had the lowest CV (0.1%), showing that this soil chemical variable is more homogenous
479 than other soil chemical variables in the study sites. CV values of soil moisture content showed
480 inconsistent values across elevational gradients.
481

482 ### 3.1. The relationship between elevation and canopy cover on coffee quality attributes

483 Elevation significantly ($p<0.05$) affected all the three coffee bean quality attributes (total
484 preliminary quality, specialty quality, and hundred bean mass). An interaction effect of elevation
485 and canopy cover significantly influenced total preliminary quality and hundred bean mass but not
486 the specialty quality (Fig. 2 and Appendix table S1). A clear relationship of hundred bean mass
487 with elevation and shade canopy cover was observed, confirming that a greater hundred bean mass
488 was produced in response to increasing elevations, at intermediate and dense shade levels (Fig. 2
489 and Appendix table S1). Under conditions of light shade levels (10-35%) and intermediate shade
490 levels (35-65%), hundred bean mass increased with elevation (Fig. 2 and Appendix table S1).
491 However, a decreasing trend in hundred bean mass was observed under dense shade (>65% shade

level) when elevation keep increasing. Dense shaded conditions and the low temperatures at higher elevations may not improve the growth potential and quality of the beans, however, dense shaded environments at warmer environments of the low elevations show an increased trend in bean mass. Our study confirmed that higher elevations with cooler climates (>1900 m) with intermediate shade cover (35-65%) showed a higher potential to produce green coffee beans having superior total preliminary quality (Fig. 2 and Appendix table S1). The results further support that coffee cup quality attributes are more sensitive to temperature changes than to other farm management practices, possibly due to the fact that cup quality attributes such as flavor, taste, aroma and body are temperature-dependent. Coffee beans from higher elevations had a greater specialty quality as compared to coffee beans grow in warmer climates (Fig. 2 and Appendix table S1). Shade cover affected the total preliminary quality and it had no effect on specialty quality. This confirms that shade drives the physical bean quality (raw value) much more than the sensory attributes. In other words, poor management of shade at a given elevation will have a negative impact on the potential to produce qualitative coffee.

3.2. Quantifying the proportion of variance explained by coffee trees and coffee farms

The permutational multivariate analysis of variance (PERMANOVA) depicted significant differences in coffee quality among coffee farms and between the individual coffee trees (model residuals). In terms of the breakdown of the total variance in total preliminary quality, a linear mixed model depicted a substantial contribution of individual coffee trees (73%) while only 17% was explained by the coffee farm (Fig. 3a). In the specialty quality, the model depicted large contribution of the individual coffee trees (96%), and only 4% by the coffee farms (Fig. 3a). Similarly, for hundred bean mass, the model depicted a substantial contribution of individual coffee tree (76.6%) and coffee farms (23.4%) (Fig. 3a).

Meanwhile, the biophysical variables contributed differently for the coffee quality attributes. Canopy cover contributed 9.6%, 4.2% and 22.4% for total preliminary quality, specialty quality and hundred bean mass, respectively. Soil moisture contributed 0.1%, 0.2% and 2.7% for total preliminary quality, specialty quality and hundred bean mass, respectively. Tmax (max temperature) contributed 2.1%, 2.3% and 0.2% for total preliminary quality, specialty quality and

hundred bean mass, respectively. Tmean (mean temperature) contributed 0.1% each for total preliminary quality, specialty quality and hundred bean mass, respectively (Fig. 3b).

3.3. Establishing a relationship between NIRS and cup quality

The outcomes of the examined models in the estimation of coffee quality and their performance assessment using different statistical metrics are presented in Table 2. Both RF and PLSR models were tested, optimized and compared to each other. A good model prediction corresponds to high R^2, r, and RPD, and low RMSE values. As can be seen from table 2, the performance of the models without the spectra preprocessing was low, and spectral data preprocessing could significantly improve the performance of the two models. Therefore, preprocessing of the raw spectral data is an important first stage before any regression model is established as it improves the prediction. In addition, compared with the single preprocessing method, the combination of different preprocessing methods can greatly improve the performance of the model. Accordingly, the results suggest that the RF model has a better predictive power as compared to PLSR for both training and testing datasets at a specified preprocessing algorithms for both total preliminary and specialty quality as indicated in (Table 2 and Fig. 4). Moreover, RF model showed a higher R^2 and lower RMSE values as compared to PLSR in the estimation of total preliminary and specialty quality, which demonstrated that it has satisfactory estimative capability in coffee quality assessment. RPD in total preliminary and specialty quality was also found to be superior in RF model (Table 2).

3.4. Quantifying the relative importance of biophysical variables on measured and predicted coffee quality

By applying random forest models, the main important biophysical variables influencing coffee quality were identified. The measured relative importance of the investigated variables derived from the RF model as shown in Fig. 5 differed among the different coffee cupping scores. As presented in the figure, the order of importance of the variables to total preliminary and specialty quality and NIRS is: canopycover>soilmoisture>Tmean>Tmax, in which the first three explained 31.8 - 40%, 27.4 – 33.3% and 19.2%, respectively, of the variation in the data. On the other hand, the order of importance of the variables to hundred bean mass is:

canopycover>Tmean>soilmoisture>Tmax, in which the first three explained 32.4%, 29.3% and 22.2%, respectively, of the variation in the data (Fig. 5). Similarly, the order of importance of the variables to NIRS is as follows: canopycover>soilmoisture>Tmean>Tmax, in which the first three of them contributed 37.7%, 28.2% and 22.4%, respectively for the variations. Hence, the biophysical variables affecting coffee cupping (total preliminary and specialty quality) appeared to be the same for the NIR spectra.

4. Discussion

4.1. Intra-farm variability is larger than the inter-farm variability

Our findings indicate that elevation is the key biophysical variable influencing all the measured coffee bean quality attributes (hundred bean mass, total preliminary and specialty quality) at the farm level (Fig 2 and Appendix table 1) while canopy cover was the most important biophysical variable driving the coffee bean quality attributes and NIRS at the plant level (Fig 3).

Most importantly, the results show the existence of high variability between coffee plants within a farm, as evidenced from the variance partitioning procedures in permutational multivariate analysis of variance in a linear mixed model. The magnitude of variability observed within a coffee farm is far larger than the variability among coffee farms in terms of the measured coffee bean quality attributes. The order of importance of the variables to total preliminary and specialty quality was found to be in order of canopycover>soilmoisture>Tmean>Tmax. This means that conditions varying at the coffee plant-level might be of greater importance for influencing hundred bean mass and cupping scores when considering the farm-level as a whole. The potential explanations for this huge intra-farm variability could be due to various reasons: variation in genetic structure of the coffee plants (there is definitely an inherent variation in growth rate among coffee plants due to the variation in resource use (for instance, nutrient capture, transport and utilization efficiency, water use efficiency, light use efficiency), individual leaf trait variability like SLA due to the variation in genetic structure of the coffee plants, disease sensitivity of the individual coffee plants); the way how the coffee plants were obtained (if not all, most coffee plants of the smallholders are reared from seeds by natural means, and this could be a potential

584 explanation for the huge intra-farm variability). Variation will become high in the case of sexually
585 reproduced plants especially if it is reared by natural selection); poor and inconsistent farm
586 management practices within a farm (for instance, no definite spacing between plants and rows in
587 smallholder coffee farms unlike that of the plantations); age of the coffee plants (although an effort
588 was made to consider coffee trees aged between 6 and 10 years old, we still believe that age
589 matters).
590
591 Although significant variability has been documented in many African smallholder production
592 systems, agronomic research for development generally ignores such variability in the decision-
593 making process and programs (Oyinbo *et al*. 2019; MacCarthy *et al*. 2018). Incorporating this
594 variability in agronomic decision-making to minimize its effect requires systematic quantification
595 of the variability. However, quantifying intra-farm variability has been a challenge so far and
596 operationalizing this variability in agronomic decision-making is even more challenging (Sida *et*
597 *al*. 2021; Trevisan *et al*. 2021; Van Loon *et al*. 2019).
598
599 Most of the observed variation (more than 75%) is due to unmeasured variation or residuals. This
600 implies that a large proportion of the variation in coffee cupping scores is to be explained by other
601 plant-level factors such as the specific nutrient levels, coffee tree pruning, fruit thinning, rate,
602 method and timing of fertilizer application, age of the coffee trees, shade tree species, cultivar
603 characteristics, and disease sensitivity of the individual coffee trees. Besides, the variance
604 partitioning procedures have shown that the total preliminary and specialty quality, and hundred
605 bean mass, were driven by the shade tree canopy cover (30-46% variability), which reflects that
606 canopy cover at the coffee plant-level is more important for explaining variation for green bean
607 quality. Hence, based up on the local conditions and the requirements, smallholder coffee farmers
608 can manage their shade tree canopy cover to optimize their coffee quality.
609
610 In addition, Olsen-P had the highest CV (63.7%), particularly in the coffee farm with elevation
611 2325 m asl followed by soil exchangeable K (62.7%) at coffee farms situated at 2027 m asl
612 elevation. It is interesting to notice that, unexpectedly, soil available P content (in this case, Olsen-
613 P) was higher at higher elevations compared to the lower and mid-elevations. The most likely

reason for this could be differences in local environmental conditions mainly soil characteristics such as weathering and/or litter quality. We still believe that more samples would have improved the accuracy of the fluctuation in P concentrations. Consequently, more data would be necessary to test this hypothesis.

4.2. Importance of the biophysical variables for coffee cupping scores and NIRS

The results of the random forest model indicated that canopy cover, soil moisture and mean soil temperature were identified as the key variables affecting total preliminary and specialty quality, and hundred bean mass at a coffee-tree level. Large number of studies have shown that shade percentage, soil moisture and temperature affect coffee cupping scores. At the local scale, canopy cover is the main determinant of microclimate temperature and radiation. Shade canopy cover provides a means to keep coffee plants closer to their ideal temperature ranges (18˚C-21˚C) and prevent damage from extreme minimum and maximum temperatures and drought (Nesper *et al*. 2017, Somporn *et al*. 2012). Numerous studies have shown that there was a significant positive correlation between coffee quality and shade tree canopy cover as well as soil moisture and significant negative correlation between coffee quality and temperature (Bosselmann *et al*. 2009; Avelino *et al*. 2007; Leonel and Philippe, 2007). A decline in soil temperature were recorded with elevation, implying that the spatial distribution of soil temperatures is controlled mainly by elevation (Navarro-Serrano *et al*. 2020). Although soil temperatures can be affected by the interaction of multiple local factors such as shade canopy cover, mulching and irrigation, elevation was found to be the main driving variable for the changes in soil temperatures (Getachew *et al*. 2022; paper in-press; Onwuka and Mang, 2018; Barman *et al*. 2017).

Likewise, DaMatta *et al*. (2018) reported that coffee plants tolerated higher temperatures when ample water was supplied. A study from Southwest Ethiopia demonstrated that coffee trees grown under open shade conditions produced beans of lower acidity, body and flavor as compared to the coffee plants grown under dense shade (Bote, 2016). On the other hand, higher bean size and mass were obtained when shade canopy cover increased. Shade promotes slower and more balanced fruit maturation by the mother plant, thus yielding a better-quality product than unshaded coffee plants (Barbosa *et al*. 2012; Geromel *et al*. 2008; Leonel and Philippe, 2007). These previous

findings further support that coffee cup qualities are more sensitive to temperature changes, possibly due to the fact that formation of biochemical precursor molecules responsible for cup quality attributes such as flavor, taste, aroma and body are temperature dependent. Meanwhile, Bertrand *et al*. 2012 demonstrated that mean soil temperature during coffee bean development influenced acidity, fruity character and flavor. Silva *et al*. (2005) reported that temperature was likely the most important factor to bring variations in coffee cup quality from the southwest region of Ethiopia. Our results thus corroborate that the physical attributes and cupping scores are more temperature driven. Altitude and shade cover management is therefore important to enhance the potential to bring good coffee beans to the market.

4.3. Comparison of the two models for the quantitative prediction of coffee cupping scores

Based on two of the tested models (RF and PLSR), the effects of different preprocessing methods were examined. The pre-processing of spectral data can remove the influence of irrelevant information on our spectra and ultimately improved the robustness and accuracy of the models. As can be seen from table 2, RF and PLSR models produced different outputs when different preprocessing methods were used separately or in combination. When the spectra were completely not preprocessed, R^2 was only 0.56 and 0.52, and RMSE was 0.87 and 1.92 in PLSR and RF, respectively in specialty quality. After application of Savitzky-Golay smoothing, multiplicative scatter correction, and standard normal variate, the R^2 was raised to 0.87, while RMSE was reduced to 0.26 when RF was used. Therefore, the performance of the RF model without preprocessing was obviously low, and spectral data preprocessing could significantly improve the performance of the model. In addition, compared with the single preprocessing method, the combination of different preprocessing methods was of great help to the performance.

Referring to Table 2 again, the RMSE of the RF for total preliminary quality was 0.55, which represented the lowest error of prediction when Savitzky-Golay smoothing, multiplicative scatter correction and standard normal variate preprocessing methods were applied. The R^2 is 0.83, indicating that the RF model can predict the data reasonably better (Barea-Sepulveda *et al*. 2022, Anderson *et al*. 2020; Zhang *et al*. 2020; Ghasemi and Tavakoli, 2013). Most importantly, the RPD of random forest was 3.87, whereas the RPD of PLSR was 1.41 for the total preliminary quality when the same preprocessing methods were utilized. The RF thus performed well (Barea-

Sepulveda *et al*. 2022, Anderson *et al*. 2020). Given these findings, a simultaneous application of spectral preprocessing methods (Savitzky-Golay smoothing, multiplicative scatter correction and standard normal variate) in conjunction with the RF model better predicted the coffee cup quality.

Several studies have reported that the performance of different tree-based models including RF can vary from study to study, thus there is no general best modelling technique for predicting coffee quality (NS Akbar *et al*. 2020; Martinez-Santos *et al*. 2021). Moreover, it has been suggested that the predictive power of the modelled output is also the result of the research design, preprocessing methods and input variables (Vargas and Hanandeh, 2021; Naccarato *et al*. 2016; Aertsen *et al*. 2010). Overall, near-infrared spectroscopic based predictions of green bean quality can be utilized to complement cupping evaluations conducted by humans, and most importantly, to increase the throughput of the cupping evaluations.

Limitations and way forward

Our results show the existence of high variability among coffee plants within farms, which can be as high as 73%. Although we have quantified the magnitude and distribution of the inter-and intra-farm variability in smallholder coffee farms, a couple of questions remain unaddressed in our study. We were limited to disentangle the drivers of some relationships in this work because of data limitations such as coffee cultivar characteristics (as there is definitely an inherent variation in growth rate among coffee plants due to the variation in resource use), disease sensitivity of the individual coffee trees, limited soil moisture data, plant nutrient levels, etc. Most importantly, our study is also a relatively a short-term study and this again calls for caution for generalizing our results and long-term investigations are necessary.

Conclusion

The main contribution of this work is the assessment of the spatial variability of coffee quality in response to different biophysical drivers. Our study showed the existence of large within farm variability, indicating that conditions varying at the coffee plant-level are of importance for improving the physical attributes and cupping scores of green coffee beans, and hence documenting such differences may help to improve agronomic decision-making processes. However, quantifying the factors responsible for the large within farm variability is much more

challenging than identifying and measuring among-farm variability. Understanding, quantifying, and managing within farm variability is crucial to improve to improve nutrient use efficiency, water availability, pruning, pest and disease control, etc. Meanwhile, the overall biophysical variables responsible for the coffee cupping scores and NIRS were identified and quantified, which are fundamental to improving coffee quality. Overall, elevation was the key variable driving biophysical variable influencing all the measured coffee bean quality attributes (hundred bean mass, total preliminary and specialty quality) at the farm level while canopy cover was the most important biophysical variable driving the coffee bean quality attributes and NIRS at the shrub level. Accordingly, canopy cover appeared to be the main controlling variable for the variation in total preliminary and specialty quality, and hundred bean mass, followed by soil moisture and soil temperatures. On the other hand, NIRS was confirmed to be a good approach in estimating the cupping scores. However, the developed NIRS models need to be tested further on data from other Ethiopian regions to ensure the models' stability and accuracy.

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Data availability: The datasets and R-code analyzed during the current study will be made available after publication via an online repository such as figshare.

Declarations

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