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On the accuracy of threshold genomic prediction models for leaf miner and leaf rust resistance in arabica coffee

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Abstract

Obtaining resistance cultivars for leaf miner and leaf rust are the main important strategy of Brazil's national coffee breeding program. The narrow genetic basis, and founder effect consequences, lead to challenges in quantifying and detecting genetic diversity for these traits. Biotechnology tools allied with classical breeding strategies are powerful in detecting variability and deploying a precision selection. The selection based on the genetic merit of an individual obtained from thousands of single nucleotide polymorphism effects is known as genomic selection. The ordinal scale principally makes the resistance evaluation of the leaf rust and leaf miner of the score, categorizing the phenotypes following the discrete (ordinal) distribution. Hence, this distribution can be better analyzed by threshold models. Our goals were to optimize genomic prediction models for coffee resistance to leaf rust and leaf miner via threshold models and compare pedigree and genomic relationship matrices to underlying prediction models. We have observed that the genomic model with the genomic relationship matrix performed better for all scenarios. For the traits with at least five degrees of scores, the threshold models performed better, whereas for a trait with ten degrees of scores, we see no advantage to using a threshold model for genomic prediction.

Keywords Coffea arabica · Leucoptera caffeella · Hemileia vastatrix · Bayesian generalized mixed models

Introduction

The coffee breeding programs in Brazil aim to aggregate value to the final product and reduce the costs of production, especially by selecting resistant cultivars to the main coffee pests and diseases in the country: coffee leaf miner (*Leucoptera coffeella* Guérin-Ménéville) and coffee leaf

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rust (*Hemileia vastatrix* Berk. et Br.) (Zambolim 2016; Dantas et al. 2021). Breeding methods such as pedigree and backcrossing have been used to transfer leaf rust and leaf miner resistance alleles from diploid species like *Coffea canephora* (Fazuoli et al. 2018b, a), *C. liberica* (Fazuoli et al. 2019), and *C. racemosa* (Carvalho 1988; Mendonça et al. 2016) to tetraploid *C. arabica* cultivars.

Arabica coffee (*Coffea arabica*) is the only allotetraploid species of the gender *Coffea*, with a well-described, narrow genetic basis (Lashermes et al. 2009). Traditionally, phenotypic selection coupled with a long testing phase has been performed, ultimately resulting in low rates of genetic gain. However, molecular markers allied to classical breeding can speed up selection and increase these rates. To this end, genomic selection (GS), which stands for the prediction of the genomic breeding values using the effect of hundreds to thousands of single-nucleotide polymorphisms (SNPs) distributed across the genome (Meuwissen et al. 2001), has been used with success in different animal and vegetal species. In coffee, recent studies proved its potential for other agronomical traits (Ferrão et al. 2017, 2019; Sousa

et al. 2019), although investigations addressing pests and diseases predictions are lacking.

The sources of resistance to coffee leaf miner from crosses between C. racemosa and C. arabica credited the resistance to two different genes (Guerreiro-Filho et al. 1999). Afterward, a differential gene expression study revealed a complex response between plant and insect resistance interaction, suggesting a pool of four main genes with an active metabolic pathway (Cardoso et al. 2014). Furthermore, coffee leaf rust resistance is achieved by a range of genes that can be annulated by virulence genes of the pathogen in whole or in part (Bettencourt and Rodrigues 1988). Finally, some interspecific crosses (C. arabica x C. canephora) were performed to access the incomplete resistance of H. vastatrix in C. arabica, which produced hybrids such as Icatu with a quantitative response of resistance (Zambolim 2016). Furthermore, the lower genomic heritability found for leaf miner resistance and leaf rust resistance (0.30 and 0.31 respectively) reflects the complexity of the genetic control as demonstrated in the study conducted by Sousa et al. (2019).

The evaluation of traits such as leaf rust (Eskes and Toma-Braghini 1981) and leaf miner (Guerreiro Filho et al. 1999) are mainly obtained by an ordinal degree of a visual score, which categorizes the phenotypes and the data set collected by using a discrete (ordinal) distribution. Theoretically, GS models have first proposed for quantitative traits with a normal (Gaussian) distribution (Meuwissen et al. 2001). Nevertheless, categorical response traits do not usually follow the assumption of normally distributed phenotypes.

The phenotyping is carried by the practitioner, who categorizes the observed data by a degree of a score, which does not necessarily represent the actual scale of the biological event. Data transformations are used to facilitate the statistical analysis of categorical traits (also known as threshold traits), although scaling the data can lead to the following complications: (i) the variance changes differently relative to the population mean changes, (ii) the selection response comes to be symmetric in negative and positive directions bringing bias in the selection response, and (iii) the non-additive effects are strongly affected by the scale transformation (Falconer and Mackay 1960). In this sense, threshold mixed models have been applied to analyze the categorical traits by presupposing an underlying continuous distribution of phenotypes that design a normal distribution liability, a consistent approach to obtaining accurate and better-predicted results (Gianola 1982; Mrode 2014).

The expansion of threshold models has been proposed to be used in GS models. (Kizilkaya et al. 2011) expanded the Bayes C methodology for keratoconjunctivitis (caused by *Moraxella bovis* bacterial) with a degree of score evaluation in beef cattle. Wang et al. (2013) expanded the Bayesian GS models for threshold models originating Bayes-TA, Bayes-TB, and Bayes-TCpi with simulated data. Kizilkaya et al. (2014) reported a simulation study comparing predictions performed via Bayes-Cpi and Bayes-TCpi for categorical and ordinal data, concluding that threshold models performed better in a genomic prediction context for small training sets. Finally, Montesinos-López et al. (2015) proposed the threshold genomic best linear unbiased predictor (TGBLUP) with genotype-by-environment (GE) interaction to evaluate maize lines for cercosporiosis (caused by *Cercospora zea-maydis*) by the ordinal categorical degree of score. Overall, these studies represent a significant advance in GS research associated with non-Gaussian responses.

Frequently, perennial crops are evaluated across several years, and the interaction between genotypes-by-years can be regarded in the model. Typically, C. arabica genotypes are tested in multiple trials for three or four consecutive harvests to capture spatial and temporal variations (Guerreiro Filho et al. 2018). The extension of GBLUP to accommodate genotype-by-environment (GE) interactions under a Gaussian process, but using covariance functions based on genetic similarities, was initially proposed by Jarquín et al. (2014) Herein, we propose to use the flexibility of the TGBLUP to include GE interaction effects, but in the context of categorical responses. Thus, the objectives of this study are to (i) optimize genomic prediction models for coffee resistance to leaf rust and leaf miner via threshold models; and (ii) contrast pedigree prediction and genomic relationship prediction for implementation of genomic selection in a coffee breeding program.

Material and methods

Plant material and phenotyping

The plant material used in this study consisted of 596 arabica coffee plants which come from nine progenies, five from self-pollination, and four from open pollination, with a single check (Catuaí Vermelho IAC 99) (Table S1). These progenies were obtained from a breeding program started in the seventies from an interspecific biparental cross between species of C. arabica (cultivar Blue Mountain, 2n = 4x = 44) where the geographical origin is Ethiopia, and C. racemosa (cultivar IAC1195, 2n = 2x = 22) with geographical origin in Mozambique, both from the African continent (Davis et al. 2006) (Supplementary Figure S1). The racemosa coffee introduced resistance genes to leaf miner in the population. During the crossing generations, an arabica cultivar resistant to the leaf rust race two was included in the genealogy, specifically with the plant H4782-7-882 (Icatu Vermelho) (Supplementary Figure S1). The population was tested following a randomized complete block design (RCBD), nine replications, and evaluated in the 2011 and 2012 field

seasons, considering one plant per plot. The selection unit was the coffee tree. The experiment was conducted at the Agronomic Institute of Campinas, at the Experimental Center "Santa Elisa," Brazil, SP (22°51'S, 47°04'W). The evaluations of resistance were:

- (i) Leaf miner (*Leucoptera coffeella*) reaction was evaluated in conditions of natural infestation of the insect on the field in periods of high incidence. The first evaluation (LM1) was carried out in April/May and the second in September/October (LM2). Since these evaluation periods were held during distinct plant phenology stages, we considered these evaluations as two different traits. The evaluations were visually performed using an ordinal scale of 1 to 5 based on attack severity, where 1 to 0–10% leaf attack; 2 to 11–25% leaf attack; 3 to 26–50% leaf attack; 4 to 51–75% leaf attack; and 5 to 76–100% leaf attack (Guerreiro Filho et al. 1999). Plants classified with 1 were considered resistant.
- (ii) Leaf rust reaction type (LR1) was evaluated in the natural infestation conditions for leaf rust (Hemileia vastatrix) on the field. The month of disease infestation was June/July. The ordinal visual scale of score ranged from 1 to 5, where 1=plants without lesions; 2=few chlorotic lesions without spores and without defoliation; 3= few pustules with spores and low defoliation; 4= generalized pustules with spores and defoliation; and 5= generalized pustules with many spores and marked defoliation (Eskes and Toma-Braghini 1981). Plants classified 1 and 2 were considered resistant and others, susceptible to coffee leaf rust.
- (iii) Leaf rust lesion density (LR2) was evaluated in the same reaction type conditions but considering the whole plant's aspect. The visual ordinal scale of score ranged from 1 to 10, where 1 = Absence of sporulating lesions; confirmation necessary by pushing aside branches of the lower canopy and more detailed observation of the branches inside the shrub; 2 = Presence of one diseased branch at first look on any side of the shrub. Pushing aside of lower canopy branches may be necessary for confirmation. On detailed observation, more than one diseased branch may be found; 3 to 9 = These values represent a gradual increase in the number of diseased branches per tree, seen at first look. Value 8 corresponds with an average attack on susceptible coffee cultivars in Brazil at harvest time; 10=This scale value indicates the maximum of disease incidence, corresponding to the level of disease of the very susceptible Harar coffee type in Brazil at harvest time. Normally, susceptible cultivars may drop leaves before reaching this level. Therefore, an S value associated with intensive leaf

shedding should be scored as a 10, than 50% of all lesions (Eskes and Toma-Braghini 1981).

The Pearson's correlation between the score scale from each evaluated trait was calculated with the function *pair*. *panels* from psych (Revelle 2015) R package, which generated the histograms and linear regression plots of all combinations.

Genotyping

All 596 coffee plants were genotyped using DNA from young healthy leaves. The DNA extraction was performed following the CTAB protocol (Doyle and Doyle 1987). Genotyping-by-sequencing (GBS) was performed using an Illumina-HiSeq 2500 with 48 pooled genotypes per lane. The sequenced libraries were built following the protocol proposed by (Elshire et al. 2011), with DNA samples digested using the Pst1 enzyme. The arabica coffee reference genome (assembly Cara_1.0) was used to align the reads (assembly Cara_1.0-https://www.ncbi.nlm.nih.gov/ genome/?term=txid13443[orgn]) with bowtie two aligner (Langmead and Salzberg 2012). The single-nucleotide polymorphism (SNP) calling was performed in FreeBayes software (Garrison and Marth 2012) as diploid species, considering a diploid-like meiotic behavior of arabica coffee. A total of 120,617 genetic variants were called. Missing data were imputed using the default settings implemented in the Beagle 5.0 software (Browning et al. 2018). Loci were filtered by applying the following criteria: maintaining only biallelic markers, removing sites with a minor allelic frequency (MAF) lower than 5%, keeping markers with a call rate of at least 80%, and using the VCFtools software (Danecek et al. 2011). Also, the linkage disequilibrium pruning of markers with pairwise correlation (r^2) higher than 0.99. The final molecular marker matrix obtained with 4666 SNPs was used in a genomic prediction analysis.

Regression models applied to genomic prediction

In this study, we compare different kernels as a relationship matrix. First, we use the numerator relationship matrix (A) composed of the (Wright 1917) coefficient of relationship between genotypes, as proposed by Henderson (1976), known as the pedigree relationship matrix, with squared dimension of number of evaluated genotypes. Second, the genomic relationship matrix (G), with the same dimension of the A matrix, was computed following the formula: $G = \frac{Z'Z}{2\sum p_k(1-p_k)},$ where pk is the allele frequency (VanRaden 2008). The kernels were computed using the AGHmatrix R package (Amadeu et al. 2016). We compared the predictive performance considering the scenarios: (i) pedigree relationship matrix (A) or genomic relationship matrix (G); and (ii) predictive models fitted assuming a normal (gaussian) distribution for the response variables or assuming an ordinal distribution (threshold models). The models followed the single-step approach, where predictions are performed by using a linear mixed model as ABLUP with pedigree matrix (A), and GBLUP with the genomic relationship matrix (G) (Misztal et al. 2009). The genomic estimated breeding values (GEBV) considering a Gaussian distribution for the response variable was obtained following the model:

$$y_{ijk} = \mu + b_k + h_j + g_i + g_{hij} + e_{ijk}$$
(1)

where y_{ijk} is the phenotypic scale of score for each trait, μ is the overall mean, b_k is the fixed effect of kth block, h_j is the fixed effect of the *j*th year, g_i is the random effect of genotypes with $g_i \sim N(0, G_0 \sigma_a^2)$ where G_0 is either a pedigree matrix (A) or a genomic relationship matrix (G), gh_{ij} is the random effect of the interaction between genotypes and years, with $gh_{ij} \sim N(0, I_H^{JxJ} \otimes G_0 \sigma_t^2)$, and e_{ijk} is the random effect of the residual, with $e_{ijk} \sim N(0, I\sigma_e^2)$, and $\sigma_a^2, \sigma_t^2, \sigma_e^2$ are the variance components of the respective effects.

For responses with a non-gaussian distribution, we used a threshold (cumulative *probit*) model. Results were compared to traditional gaussian models. In this context, threshold models can be applied for categorical scale data and described as the distribution definition, the linear predictor, and the link function (Montesinos-López et al. 2015).

Distribution

The distribution for the observed response variable follows $(y_{Cijk}|b, h, g) \sim \text{Multinomial}(N_{ijk}, \pi_{Cijk})$, where N_{ijk} is the sample size of observations, π_{Cijk} is the probability of occurrence of each class by observation with $\sum \pi_{Cijk} = 1, C$ is the observed categories number, *b* is the fixed effect of the block, *h* is the fixed effect of years, and another distribution of the models is *g* with $g \sim N(0, G_0)$, where G_0 is the variance–covariance matrix of the effect of the genotype.

Linear predictor

 $\eta_{Cijk} = \gamma_C + x_{ijk}^T b + x_{ijk}^T h + z_{ijk}^T g + z_{ijk}^T g h$, where η_{Cijk} is the Cth link for the fixed and random effects combination, γ_C is the intercept (threshold) for the Cth link, and x_{ijk}^T and z_{ijk}^T are the incidence vector corresponding to fixed and random effects, respectively. To fully specify the model, a total of C - 1 link function is required.

Link function

The cumulative distribution function of a standard normal distribution (probit link) was used as $\eta_{(C-1)ijk} = \phi^{-1}(\pi_{(C-1)ijk})$, which produces the area under the theoretical Gaussian slope. This link function is normally used when the data set is classified in more than one category.

The theory behind threshold models supposes a theoretical normal distribution under the process to scale an observed category. It produces a normal distribution variable called "*liabilities*," with $\varepsilon_{ijk} \sim N(0, 1)$ (Gianola 1982). An expansion of GBLUP was proposed by called threshold genomic best linear unbiased predictor (TGBLUP), which implies the same flexibility of the traditional GBLUP to use genetic kernels and expand for interaction effects kernels in the model (Montesinos-López et al. 2015). In this context, we suggested the single-step TGBLUP as the following latent variable model:

$$l_{ijk} = b_k + h_j + g_i + gh_{ij} + e_{ijk}$$
(2)

where l_{iik} is the "liability" or the latent variable with the distribution of the corresponding random effects that give the observed categorical phenotypes given a probit link function, b_k is the fixed effect of kth block, h_i is the fixed effect of the *j*th year, g_i is the random effect of genotypes with $g_i \sim N(0, G_0 \sigma_a^2)$ where G_0 is the pedigree matrix A or the genomic relationship matrix G, gh_{ii} is the random effect of the interaction between genotypes and years, with $gh_{ii} \sim N(0, I_H^{JxJ} \otimes G_0 \sigma_t^2)$, and e_{iik} is the random effect of the residual, with $e_{ijk} \sim N(0, I\sigma_e^2)$, and $\sigma_a^2, \sigma_t^2, \sigma_e^2$ are the variance components of the respective effects with σ_e^2 fixed to one, to correspond to the unobservable latent variable. All Bayesian models and genetic parameters were fitted in the BGLR package in R (Pérez and de Los Campos 2014), with the number of iterations of 30,000, burn-in of 1000, and a thin of 10. The data set used in this study is available in the Mendeley Data repository (Carvalho et al. 2020).

Predictive ability evaluation

The validation was performed using the typical random repeated sample method, in which the data set was randomly split into two parts, 70% for training and 30% for testing. This procedure was replicated fifty times. We accessed the predictive abilities by measuring the *Pearson's Product Moment* correlation $\hat{r}_{(\hat{y}y)}$ between the predicted estimated breeding value (\hat{y}_i) of the testing population and the corresponding phenotypic value (y_i) for genotypes. Goodness-of-fitness was measured considering the deviance information criterion (DIC), which is the Akaike information criterion (AIC) in a Bayesian model selection context (Spiegelhalter

et al. 2002). The model with lower DIC is preferred, which means better adjustment. The DIC was estimated for the tested models using the A or G matrix for gaussian or ordinal distributions. The reliability was measured following the equation: $r^2 = 1 - \frac{(SE)^2}{\sigma_g^2}$; where *SE* is the average standard error from each predicted value and σ_g^2 is the genetic additive variance (Isik et al. 2017).

Results

Phenotypic data, correlation, adjusted model, and reliability

The phenotypic data were visually evaluated in field trials (Fig. 1). The frequency of scores is around the middle of the scale for each trait. LR2 was assessed on a score scale

with ten levels, the double of levels compared with other traits with a segregation behavior divided between the ordinal scale scores. The raw data are separated by progenies, and the frequency of the score scale is shown for each trait (Supplementary Figure S2). The progeny one is the check (Catuaí Vermelho IAC 99), with scores concentrated in high scale levels. We can see a clear segregation pattern in the other progenies, with most of the scores grouped in the middle of the scale. Progenies 2, 5, and 8 have a small frequency of low levels for LM1 (Supplementary Figure S2 A and B). For LR1, just the progenies 2 and 7 did not show plants with low scores, but any progenies have the lowest score 1 (Supplementary Figure S2 C). For the LR2, the only progeny showing the lowest score on the scale is progeny 5 (Supplementary Figure S2 D).

The pairwise correlations were positive and statistically significant (p value < 0.05) (Fig. 2). The scale of scores related to leaf miners presented a medium



Fig. 1 The frequency distribution degree of a score of raw phenotypic data for A leaf miner—LM1, B leaf miner—LM2, C leaf rust—LR1, and D leaf rust—LR2



Fig. 2 The correlation between traits: leaf miner—LM1, leaf miner—LM2, leaf rust—LR1, and leaf rust—LR2, with histogram distribution on diagonal, linear relation in the bottom of the matrix, and the

cate the level of significance equal to 0.1%

Table 1 Deviance information criterium (DIC) measured for LM1 leaf miner 1, LM2—leaf miner 2, LR1—leaf rust 1, and LR2—leaf rust 2, in the models of ordinal distribution and Gaussian distribution with A (pedigree matrix), G (genomic relationship matrix) matrix

DIC	Gaussian		Ordinal	
	A	G	A	G
LM1	2203.37	2138.75	1904.53	1864.41
LM2	2516.15	2406.21	2424.23	2296.68
LR1	1969.35	1956.89	1739.13	1720.07
LR2	3628.01	3623.29	4718.05	4659.71

 Table 2
 Reliability measured for LM1—leaf miner 1, LM2—leaf miner 2, LR1—leaf rust 1, and LR2—leaf rust 2, in the models of ordinal distribution and Gaussian distribution with A (pedigree matrix), G (genomic relationship matrix) matrix

Pearson correlation in the top of the matrix where the asterisks indi-

r^2	Gaussian		Ordinal	
	A	G	A	G
LM1	0.79	0.74	0.65	0.58
LM2	0.68	0.63	0.29	0.31
LR1	0.82	0.79	0.59	0.57
LR2	0.90	0.88	-0.60	-0.31

correlation (0.42), while the scores related to leaf rust showed a higher correlation (0.63). On the other hand, the leaf miner and leaf rust resistance showed a low correlation with each other, ranging from 0.17 to 0.29 (Fig. 2). The linear regression of data between pairs of traits present at the bottom of the diagonal shows a no linearity relation between traits (Fig. 2), just for LR1 and LR2 has slight linearity relation.

The model adjustment for the gaussian and threshold model was compared. Based on the DIC, we also compared the mixed models using pedigree and genomic information (Table 1). Comparing the A and G matrix, DIC is slightly lower for models with the G matrix, suggesting a better goodness-of-fit statistic. The comparisons between models under different distribution assumptions showed a lower DIC value for the ordinal distribution for LM1, LM2, and LR1. For LR2, the traditional gaussian model had a lower DIC and hence a better goodness-of-fit statistic.

Similarly, different models' reliability was measured, comparing the kernels A and G (Table 2). Contrasting A and G kernels, the reliability was higher for the A than the G kernel. Looking at the distributions, the Gaussian had higher reliability than the Ordinal. Therefore, reliabilities ranged from 0.58 to 0.79 for LM1, 0.29 to 0.68 for LM2, 0.57 to 0.82 for LR1. For the LR2, the better results for reliability were for Gaussian distribution with 0.88 and 0.90 for G and A kernels, respectively.

Single-step predictive ability

The pedigree relationship matrix (A) and the genomic relationship matrix (G) were represented by a heatmap of all genotypes, divided between progenies (Supplementary Figure S3). Almost the same number of genotypes represented each progeny. In the pedigree heatmap (Supplementary Figure S3 A), the progenies 6, 7, 8, 9, and 10 are closest to each other, even though they came from different plants of self-pollination (Supplementary Figure S1). The progeny 8 was the most endogamic, which was obtained from a two-generation of self-pollination. Progenies 8 and 4 have a slight correlation as the progenies 6 and 3. It occurs because progenies 4 and 3 were open pollination from the plants, which originated progenies 8 and 6 from self-pollination, respectively. Progeny 2 is the most unrelated compared with others. Considering the genomic relationship heatmap (Supplementary Figure S3 B) is possible to see a slightly closer pattern from the pedigree heatmap with other resolution. We can see that the progenies are more related than as shown in the pedigree heatmap.

The best resolution of the genomic matrix in defining the realized pedigree impacted the predictive performance. The predicting ability for all tested scenarios ranged from 0.15 to 0.71 (Fig. 3). We observed that predictive abilities computed using genomic information (G matrix) were higher for all traits than the pedigree matrix (A matrix). Considering the G matrix, for LM1, the ordinal models have a slightly better predictive ability than Gaussian models with a value of 0.57. Considering the LM2 and LR1, the differences considering the distributions do not appear considering two numbers of decimal points, with values of 0.46 and 0.62 for the G matrix, respectively. Finally, for LR2, the gaussian models presented a better predictive ability than the ordinal distribution (Fig. 3).

Discussions

Coffee breeding programs addressing resistance to pests and diseases are based on introducing a new genetic source of resistance into the breeding routine. To this end, the main approach to monitor genetic progress is evaluating the agronomic traits using field trials and visual ordinal scales. This kind of evaluation is useful and practical for the field, facilitating the evaluator's work. Even though the degree of score facilities measurements, the response variable does not follow the traditional assumption of normality (Gaussian distribution), rendering traditional mixed model methods (as the GBLUP model) statistically not appropriate. Such properties as selection invariance and the ability to maximize the probability of correct pairwise ranking do not hold categorical traits considering best linear unbiased predictor (BLUP) (Fernando et al. 1983), which can be expanded to GBLUP. Despite the nonnormality of the data set, a biological event of resistance to have an implicit normal distribution, which can be evaluated with threshold models as proposed by (Gianola 1982). Considering the model's predictive ability, we compare the GBLUP and TGBLUP with the A and G matrix for all categorical resistance traits, fitting the model (Montesinos-López et al. 2015).



Fig. 3 Predictive ability divided by tested scenarios: A: pedigree matrix, G: genomic relationship matrix, Gaussian: models of normal (gaussian) distribution, Ordinal: models of ordinal distributions. The error bar indicates the standard deviation from the mean

Phenotypic data and estimation of genetic parameters

We observed that the frequency of each class of visual score is associated with the segregation pattern observed in the breeding population (Fig. 1). Specifically, the pattern revealed a low number of plants resistant to LM1, LM2, and LR2. For LR1, for example, no resistant plants were observed, and few plants presented the degree of score two (moderately resistant). The frequency of scores divided by progenies for each trait shows the resistance difference between progenies (Supplementary Figure S2). For LM1, the bests progenies with resistance score one is numbers 2, 5, and 8. Regarding the LM2, no progenies are represented in the degree of score one, which means no full resistant plants for this trait, but 5, 8, and 9 are the bests progenies with scores two (medium resistance).

The traits of leaf miner resistance were evaluated during two different periods of the year, LM1 during April/May and LM2 during September/October. Both periods were considered the infestation peak in coffee species (Souza et al. 1998). In the first evaluation, almost all plants were in fruiting maturation, while in the second most of the plants were in the flowering stage (Meireles et al. 2009). Between LM1 and LM2, the resistance signal captured by the degree of score can be related not just to the phenology stages but the infestation peak of the leaf miner, which corroborates with the medium correlation of the traits (Fig. 3). The leaf rust traits signal, captured by the degree of a score, follows almost the same pattern between them, which corroborates the high values of the correlation of LR1 and LR2 (Fig. 3).

We observed important differences in the estimation of reliability values regarding the different modeling approaches tested in this study. For LM1, LM2, and LR1 traits, in which the degree of scores ranges from 0 to 4 and presents a better DIC for the ordinal models, the gaussian models resulted in higher values of reliability. Reliability measures how distant the true value is from the estimated value, with values close to 1 means high proximity. Also, reliability has close relation with accuracy (Mrode 2014). For example, the accuracy values previously reported by Sousa et al. (2019) for leaf miner and leaf rust resistance are close to the values reported in this study considering the ordinal data. This comparison reveals that the gaussian models might inflate the reliability values, unless for the LR2, which has a score ranging from 0 to 9.

Single-step genomic prediction

The predictive ability follows the same pattern for all traits, with higher predictive ability of models with the G matrix than with the A matrix. Similar results were also reported by Clark et al. (2012) when using a deep pedigree and a shallow

pedigree compared with the genomic relationship matrix. The differences in predictive ability observed between models with A and G corroborates the identifiable differences between heatmaps (Supplementary Figure S3), i.e., the information captured by the A matrix is not the same as for the G matrix. Additionally, the ability to capture the Mendelian sampling by the G matrix seems to play an important role determining its higher predictive ability compared to A matrix, even when deep pedigrees are utilized.

Comparisons between the Gaussian and threshold models for LM1 revealed a slightly better prediction for ordinal distribution. Otherwise, for LM2 and LR1, both distribution models showed similar values. The LR2 trait performed better for Gaussian distribution. The predictive ability for leaf rust and leaf miner was higher (0.26 and 0.18, respectively) than as Sousa et al. (2019) found in arabica coffee. Ferrão et al. (2019) found 0.50 on average of predictive ability for leaf rust in robusta coffee, considering different environments and populations with varying maturation periods, corroborates our results. Such as simulated by Wang et al. (2013), traits with categorical, ordinal data fit better in threshold models than considering a Gaussian model. The same authors discuss the advantage of the threshold models, which accordingly, more levels of scale score (more than eight), the similar is the predictive ability between the threshold models and the Gaussian models; these results corroborate our results. Even though our predictive ability is the same for the Gaussian and threshold models considering LM2 and LR1, the model fitness and the reliability results are more reasonable when considering the threshold models than the Gaussian models. Finally, traits with a non-normal distribution can be better evaluated using generalized linear mixed models with an adequate distribution, which follow the statistical assumptions and perform reliable results.

Conclusions

Genomic prediction for leaf miner and leaf rust in which the resistance is evaluated considering the degree of a score, threshold models are a reliable approach that must be considered when the score scale follows at least five levels. However, for those traits with ten levels in a degree of a score, Gaussian distribution models perform as well as the threshold ones. Moreover, models with genomic relationships perform better than pedigree, even with a deep pedigree.

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Data Availability https://data.mendeley.com/datasets/whtnz2w7t9.

Declarations

Ethical approval This article does not include studies about humans or animals performed by any of the authors.

Conflict of interest The authors declare no conflict of interest.

Data archiving statement All files are available from the Mendeley database (https://doi.org/10.17632/whtnz2w7t9.2 https://data.mende ley.com/datasets/whtnz2w7t9/2).

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