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Comparing frequentist and bayesian approaches in AMMI analysis in a simulated scenario

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ABSTRACT:*The Additive Main Effects and Multiplicative Interaction (AMMI) model is useful for studying patterns of genotype responses between environments in agronomic assays. The main objective of this work was to compare the Frequentist-AMMI and Bayesian- AMMI approaches and to highlight the main differences that arise between these analysis procedures. For that, a simulated scenario was considered in which 9 genotypes were evaluated in 14 environments. The results showed the great flexibility of the Bayesian method to incorporate inference to the model parameters, especially those that describe the genotype interaction by environments in the biplot graphic.*

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I. INTRODUCTION

The linear-bilinear model of Additive Main Effects and Multiplicative Interaction(AMMI) is used to analyze data organized in a double entry table in which the interaction between two factors is important for the study. In this sense, AMMI found great applicability in the final stages of plant breeding in which, as a rule, different genotypes are evaluated in various environments composing a bidirectional set of multi-environmental trials (MET). MET data are fundamental for the analysis of the genotype environment interaction (GEI), which imposes great difficulties on the breeder's work in the identification, selection and recommendation of superior genotypes.

In the AMMI analysis, first the main effects are adjusted by least squares, and then the estimates of the bilinear terms of the model are obtained by the singular value decomposition (DVS), applying the matrix of non-additivity errors to the main effects. The DVS makes it possible to simplify the data, and takes into account the principle of parsimony, capturing the pattern of the original data by an approximation of a smaller dimension matrix [5-6]. Another prerogative over bilinear models is the possibility of directly accessing genotypic adaptability and stability through biplot graphical representation [7,11].

Currently, has been observed an increase in the application of the Bayesian paradigm to the analysis of linear-bilinear models, especially to the AMMI model. The first work on this topic was proposed by [25], which showed how to conduct the adjustment of the AMMI from the Bayesian perspective by sampling the parametric values using the Markov Chain Monte Carlo (MCMC). Since then, appear important contributions to the method [4,10,14-17,22-23,28].The main objective of this article is to compare the frequentist-AMMI with the Bayesian-AMMI in a simulated scenario.

II. MATERIAL AND METHOD

The set of simulated data for this work was produced from Gaussian distributions. Wherein, the stable genotypes were generated with averages centered on zero and small variability, whereas for the unstable genotypes, it considered an average other than zero and high variance. Altogether 9 (G) genotypes (4 stable and 5 unstable) were generated in 14 (E) environments. The design considered was randomized blocks.

The AMMI model in vector notation can be written by:

$$\mathbf{y} = \mathbf{X}_1\boldsymbol{\beta} + \mathbf{Z}\mathbf{g} + \sum_{k=1}^{t} \lambda_k diag(\mathbf{Z}\boldsymbol{\alpha}_k)\mathbf{X}_2\boldsymbol{\gamma}_k + \boldsymbol{\varepsilon} \qquad (1)$$

where $\mathbf{y}$ is the vector containing n phenotypic responses; $\boldsymbol{\beta}_{l\times 1}$ and $\mathbf{g}_{r\times 1}$ are vectors of main effects of environments and genotypes, respectively, with $l = c \times b$ (c the number of environments and b the number of

blocks) and r number of genotypes, or cultivars, evaluated. The λ_k factor is the k-th singular value and $\boldsymbol{\alpha}_k$ and $\boldsymbol{\gamma}_k$ are the respective genotypic and environmental singular vectors. The matrices $\mathbf{X}_1$, $\mathbf{Z}$ and $\mathbf{X}_2$ are the design and $\boldsymbol{\varepsilon}$ is the experimental error vector such that $\boldsymbol{\varepsilon} \sim N(\mathbf{0}, \mathbf{I}\sigma_e^2)$; where $\mathbf{0}$ is the null vector, $\mathbf{I}$ the ide identity matrix (n x n) and residual variance.

The model (1) is subject to orthonormality restrictions in relation to the singular vectors $\left(\boldsymbol{\alpha}_k\boldsymbol{\alpha}_k = \boldsymbol{\gamma}_k\boldsymbol{\gamma}_k = 0\right)$ and $\left(\boldsymbol{\alpha}_k\boldsymbol{\alpha}_{k'} = \boldsymbol{\gamma}_k\boldsymbol{\gamma}_{k'} = 1;\ k \neq k'\right)$, as well as the relation of order of the singular values $\left(\lambda_1 > \lambda_1 > \cdots \lambda_t\right)$ being $k = \{1,2,\cdots,t\}$ with $t = \min\{\text{r}-1, \text{c}-1\}$.

The prior distributions used in this approach are the same as those found in [15]:

$\boldsymbol{\beta} \mid \boldsymbol{\mu}_{\boldsymbol{\beta}}, \sigma^2_{\boldsymbol{\beta}} \sim N\left(\boldsymbol{\mu}_{\boldsymbol{\beta}}, \sigma^2_{\boldsymbol{\beta}}\right); \sigma^2_{\boldsymbol{\beta}} \to \infty$ equivalent $\boldsymbol{\beta} \sim$ constant;

$\boldsymbol{g} \mid \boldsymbol{\mu}_g, \sigma^2_g \sim N\left(\mathbf{0}, \mathbf{I}\sigma^2_g\right)$; in which $\sigma^2_g \sim \dfrac{1}{\sigma^2_g}$;

$\lambda_k \mid \mu_{\lambda_k}, \sigma^2_{\lambda_k} \sim N^+\left(\mu_{\lambda_k}, \sigma^2_{\lambda_k}\right); \sigma^2_{\lambda_k} \to \infty$ in which $\lambda_k \mid \mu_{\lambda_k}, \sigma^2_{\lambda_k} \sim$ constant;

$\alpha_k \sim$ uniform spherical on the correct space;

$\gamma_k \sim$ uniform spherical on the correct space;

$\sigma^2_e \sim \dfrac{1}{\sigma^2_e}$.

The likelihood function is given by:

$$L(\boldsymbol{\theta} \mid \mathbf{y}) = \frac{1}{(2\pi)^{\frac{n}{2}} \left|I\sigma_e^2\right|^{\frac{1}{2}}} \exp\left\{-\frac{1}{2\sigma_e^2}(\mathbf{y}-\boldsymbol{\theta})^{\bullet}\ (\mathbf{y}-\boldsymbol{\theta})\right\} \qquad (2)$$

on what $\boldsymbol{\theta} = \mathbf{X}_1\boldsymbol{\beta} + \mathbf{Z}\mathbf{g} + \sum_{k=1}^{t} \lambda_k diag(\mathbf{Z}\boldsymbol{\alpha}_k)\mathbf{X}_2\boldsymbol{\gamma}_k + \boldsymbol{\varepsilon}$

The joint posterior distribution is obtained by combining likelihood with the joint prior densities, being written as:

$$p(\boldsymbol{\Phi} \mid \mathbf{y}) \propto p\left(\mathbf{y} \mid \boldsymbol{\theta}, \sigma^2_e\right) p\left(\mathbf{g} \mid \boldsymbol{\mu}_g, \sigma^2_g\right) p\left(\boldsymbol{\beta} \mid \boldsymbol{\mu}_{\beta}, \sigma^2_{\beta}\right) p\left(\sigma^2_g \mid v_g, S^2_g\right) p\left(\sigma^2_e \mid v_e, S^2_e\right) \times$$

$$\times \prod_{k=1}^{t} p\left(\lambda_k \mid \boldsymbol{\mu}_{\lambda_k}, \sigma^2_{\lambda_k}\right) p(\boldsymbol{\alpha}_k)\, p(\boldsymbol{\gamma}_k)$$

on what $\boldsymbol{\Phi} = (\boldsymbol{\alpha}, \boldsymbol{\gamma}, \boldsymbol{\lambda}, \mathbf{g}, \boldsymbol{\beta}, \sigma^2_g, \sigma^2_e)$

The conditional posterior distributions are obtained from (3) by algebraic calculations under the hypotheses assumed for the hyperparameters and are as follows:

$$\boldsymbol{\beta} \mid \cdots \sim N\left[\left(\mathbf{X}_1^{\bullet}\,\mathbf{X}_1\right)^{-1}\mathbf{X}_1^{\bullet}\ (\mathbf{y} - \mathbf{Z}\mathbf{g} - \boldsymbol{\Theta}), \left(\mathbf{X}_1^{\bullet}\,\mathbf{X}_1\right)^{-1}\sigma^2_e\right];\ \boldsymbol{\Theta} = \sum_{k=1}^{t} \lambda_k diag(\mathbf{Z}\boldsymbol{\alpha}_k)\mathbf{X}_2\boldsymbol{\gamma}_k.$$

$$\mathbf{g} \mid \cdots \sim N\left[\left(\mathbf{Z}^{\bullet}\,\mathbf{Z} + \mathbf{I}\frac{\sigma^2_e}{\sigma^2_g}\right)^{-1}\mathbf{Z}^{\bullet}\ (\mathbf{y} - \mathbf{X}_1\boldsymbol{\beta} - \boldsymbol{\Theta}), \left(\mathbf{Z}^{\bullet}\,\mathbf{Z} + \mathbf{I}\frac{\sigma^2_e}{\sigma^2_g}\right)^{-1}\sigma^2_e\right]$$

$\sigma^2_g \mid \ldots \sim \text{Scaled} - \chi^{-2}\left[n_g, \mathbf{g}^{\bullet}\,\mathbf{g}\right]$.

$\sigma^2_e \mid \ldots \sim \text{Scaled} - \chi^{-2}\left[n, (\mathbf{y}-\boldsymbol{\theta})^{\bullet}\ (\mathbf{y}-\boldsymbol{\theta})\right]$.

$$\lambda_k \mid \cdots \sim N^+\left[\left(\boldsymbol{\phi}_k^{\bullet}\,\boldsymbol{\phi}_k\right)^{-1}\boldsymbol{\phi}_k^{\bullet}\,\boldsymbol{\Delta}_{k'}, \left(\boldsymbol{\phi}_k^{\bullet}\,\boldsymbol{\phi}\right)^{-1}\sigma^2_e\right]$$

being $\boldsymbol{\Delta}_{k'} = \mathbf{y} - \mathbf{X}_1\boldsymbol{\beta} - \mathbf{Z}\mathbf{g} - \sum_{k' \neq k}^{t} \lambda_{k'} diag(\mathbf{Z}\boldsymbol{\alpha}_{\mathbf{k}'})\mathbf{X}_2\boldsymbol{\gamma}_{\mathbf{k}'}$ e $\boldsymbol{\phi}_k = diag(\mathbf{Z}\boldsymbol{\alpha}_k)\mathbf{X}_2\boldsymbol{\gamma}_k$

$p(\boldsymbol{\alpha}_k \mid \text{others}) \propto exp\left\{k\boldsymbol{\alpha}_k^{\bullet}\ \boldsymbol{\Lambda}_{\boldsymbol{\alpha}_k}^{\bullet}\ (\mathbf{y} - \mathbf{X}_1\boldsymbol{\beta} - \mathbf{Z}\mathbf{g})\right\}$, $\boldsymbol{\Lambda}_{\boldsymbol{\alpha}_k} = diag\left(\mathbf{X}_2\boldsymbol{\gamma}_k\right)\mathbf{Z}$ e $k = \lambda_k / \sigma^2_e$;

$p(\boldsymbol{\gamma}_k \mid \text{others}) \propto exp\left\{k\boldsymbol{\gamma}_k^{\bullet} \ \boldsymbol{\Lambda}_{\gamma_k}^{\bullet}\left(\mathbf{y}-\mathbf{X}_1\boldsymbol{\beta}-\mathbf{Z}\mathbf{g}\right)\right\}$, $\boldsymbol{\Lambda}_{\gamma_k} = diag\left(\mathbf{Z}\boldsymbol{\gamma}_k\right)\mathbf{X}_2$.

The densities of the singular vectors are proportional to a Von Mises-Fisher (VMF) which is a spherical distribution [13]. However, these vectors are distributed only in a restricted subspace, as they must be orthogonal to the other vectors. Sampling with correct space is performed from auxiliary variables in the corrected subspace using orthogonal transformation [12,25]. More details on algebraic calculations, as well as on the sampling process can be found in [15].

Conditional densities are all known and allow direct sampling. Thus, a Gibbs sampler was used, whose steps are described by [22].The convergence of the chains was monitored by the criteria of [8,19], implemented in the Bayesian Output Analysis (BOA) package[24].

Point estimates were obtained by means of the generated MCMC chains. Regions of Highest Posterior Density (HPD) were built for univariate parameters. For genotypic and environmental scores, bivariate regions with 95% credibility were incorporated by the method of [9].

The selection of the model in the classical approach was performed by the Fr test [1]. All analyzes of this work were performed with the software R [18].

III. RESULTS AND DISCUSSION

Initially, a joint analysis of variance was performed for groups of experiments and the results are shown in Table 1. As can be seen, the effects of genotypes and interaction are significant according to the F test applied at the level of 1% significance. As the GEI is significant, general conclusions about the simulated genotypes cannot be made and they must be evaluated within each environment. Therefore, the application of the AMMI model is justified.

Table1 -Table of joint analysis of variance for groups of experiments.

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
Enviroment	13	259.4	19.958	1.7295	0.1094
Blocks (Env.)	28	323.1	11.539	0.9720	0.5104
Genotype	8	1092.3	136.537	11.5002	<0.0001*
Env. x Gen.	104	13908.4	133.735	11.2642	<0.0001*
Residuals	224	2659.4	11.873	-	-

*: significant effect by the F test at the level of 1% probability

Table 2 is presented the adjustment of the AMMI model. As possible to observe, the first two terms explain about 70% of the total GEI variation. According to the Fr test, the AMMI-5 model would be the one to be selected to analyze the data.

Table 2 -Summary of adjustment of the AMMI model for fixed effects and result of the model selection according to the Fr test.

	Perc. %	Cum. Perc%	Df	Sum Sq	Mean Sq	Fr value	Pr(>F)
AMMI1	45.17	45.17	84	6282.327	90.786	7.646	<0.0001*
AMMI2	25.57	70.74	66	3556.884	61.654	5.193	<0.0001*
AMMI3	14.45	85.20	50	2010.065	41.182	3.468	<0.0001*
AMMI4	8.23	93.43	36	1145.042	25.391	2.138	0.0004*
AMMI5	4.04	97.47	24	561.702	14.682	1.236	0.212
AMMI6	1.84	99.30	14	255.636	6.910	0.582	0.878
AMMI7	0.48	99.78	6	66.565	5.030	0.423	0.863
AMMI8	0.22	100.00	0	30.185	0	0	1.00

*: significant effect by the Cornelius' Fr test at the level of 1% probability

The AMMI-2 biplot is shown in Figure 1. The interpretations are based on the properties of the internal product between the markers in the main plane determined by the first two main components (PC1 and PC2). Points further away from the origin indicate that the associated genotypes (or environments) have more

expressive contributions to the effect of the interaction whereas those located close to the origin are characteristic of stable genotypes (or environments), that is, they have little contribution to GEI.

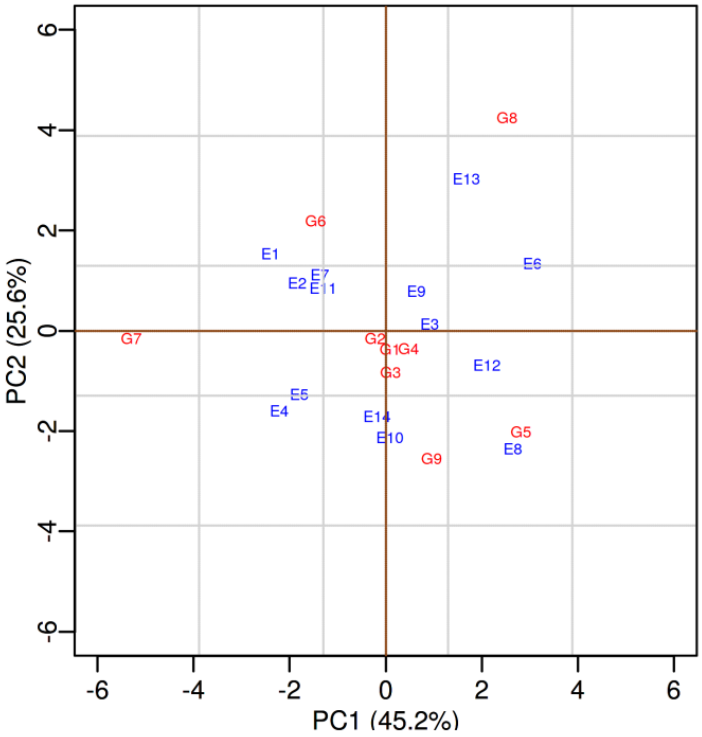

Fig. 1 -AMMI-2 biplot for genotypic and environmental scores from the simulated data set.

Genotypes G7 and G8, together with environments E6, E8 and E13, are those with the greatest contributions to GEI. On the other hand, the environments E3 and E9 and the subgroup of genotypes {G1, G2, G3, G4} have few contributions to the effect of the interaction, since they are closer to the origin.

Acute angles indicate specific adaptability between genotypes and environments; obtuse angles indicate unfavorable combinations (lack of adaptation) and right angles declare that that specific combination did not contribute to GEI. The following positive combinations between genotypes and environments can be suggested: G8 to subgroup {E6, E13}; subgroup of genotypes G5 to the environmental subgroup {E8, E12}; G6 to the subgroup {E1, E2, E7, E11}; G7 to the subgroup {E4, E5} and G9 to the subgroup {E10, E14}. Stable genotypes {G1, G2, G3, G4}, in turn, have wide adaptation.

For the application of the Bayesian paradigm, Markov chains were generated with 85,000 iterations, discarding the first 5,000 and thinning every 10, leaving 8,000 observations for the sampling process. Good convergence properties were obtained from the criteria of [8,19]. Figure 2 presents graphs of the traces of the components of variance, whose behaviors corroborate the results of the criteria used for monitoring convergence.

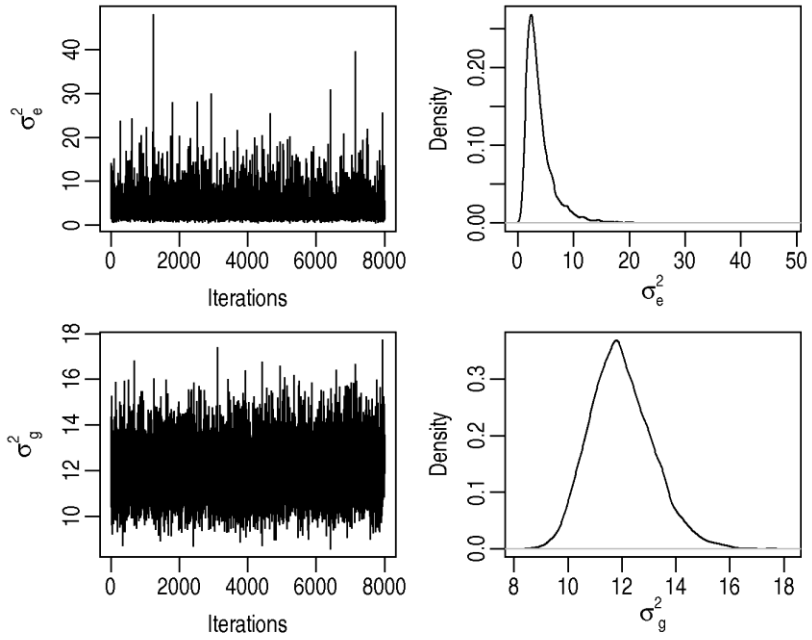

Fig. 2 -Traces and densities of the chains generated by the posterior of the components of variance

Table 3 shows the posterior means together with the HPD credibility regions of the singular values and components of variance and the solutions of the frequentist-AMMI model. There is a clear shrinkage effect of Bayesian predictions compared to DVS solutions of conventional AMMI model, which is more marked from the sixth component. This fact has been observed in different studies [4,12,15,22]. According to [12]bayesian predictions, from non-informative priors, correct the bias of the OLS estimates, as well as those obtained by the shrinkage estimators described by [2-3]. The shrinkage method proposed by [22], in the Bayesian context, offers even more shrinking estimates than the fixed effects shrinkage method or the method applied in this study.

Table 3 - Estimates of the ordinary least squares (OLS), the posterior mean, standard deviation and credible intervals (95%) for the singular values

Parameters	OLS estimates	Mean	Standard deviation	Lower Limit	Upper Limit
λ_1	45.7614	44.9449	2.0152	41.1218	49.0659
λ_2	34.4329	33.4402	2.0414	29.5273	37.4566
λ_3	25.8847	24.6668	2.0569	20.3300	28.3938
λ_4	19.5366	18.0013	2.1017	13.7973	21.9857
λ_5	13.6833	11.6555	2.2409	7.2938	16.1089
λ_6	9.2310	5.3473	2.7231	0.0103	9.6459
λ_7	4.7104	1.8618	1.4896	0.0000	4.8035
λ_8	3.172	0.8163	0.8504	0.0000	2.5616
σ^2_g	-	3.1548	2.8142	0.6982	0.6982
σ^2_e	-	11.8849	1.1584	9.8856	14.3549

A means along with regions of credibility at 95% probability for the main effect of genotypes are shown in Figure 3. The means are ranked from left to right and intersections between the intervals indicate similar effects between the respective genotypes. It is possible to highlight that the G2 and G9 genotypes have statistically positive effects.

Here, another difference is highlighted in relation to the fixed AMMI, the genotypes were treated as random. In the Bayesian perspective, all parameters are treated as random variables. Assuming genotypes to be

random provides more accurate estimates [20]. In the classic AMMI analysis, on the other hand, all effects are taken as fixed.

As the simulated set for this analysis is balanced, there were no differences regarding the ranking of OLS estimates from the AMMI-frequentist analysis (data not shown).

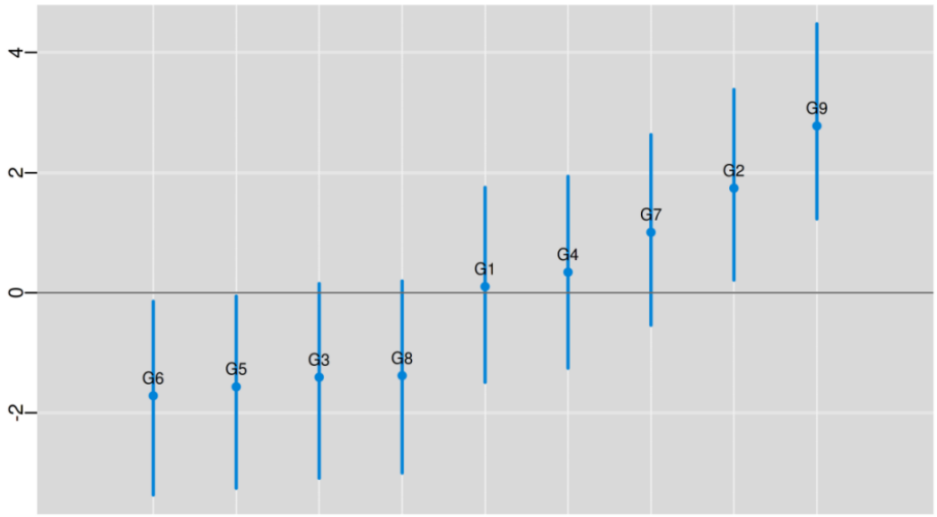

Fig. 3 -Posterior means and HPD regions, at 95% credibility, for genotype main effects.

In terms of selection, it is still necessary to carry out an assessment regarding stability and adaptability. The biplot of the posterior estimates is shown in Figure 4. This is perhaps the most striking difference (to be considered in this work) between frequentist-AMMI and Bayesian-AMMI, which is the flexibility to incorporate inference into the biplot. Bayesian-AMMI provides a direct parametric method to incorporate inference to the biplot by building regions of credibility to genotypic and environmental scores. This has been one of the major limitations with respect to classic biplot analyzes that, in most cases, do not consider any uncertainty measures regarding the plotted scores [27]. In addition, frequentist methods used for such purposes are susceptible to criticism for using restrictive assumptions such as asymptotic normality of individual scores, or even problematic computational procedures in non-parametric methodologies [26,15].

Bivariate regions were built at a 95% credibility level. Regions that include the origin of the biplot indicate that the respective genotypes (or environments) do not effectively contribute to interaction and were not plotted to simplify possible interpretations. Positions and overlaps of the regions in the biplot (determined by the first two main axes) are used to identify separable subgroups of genotypes and environments related to the effect of GEI, as well as to suggest adaptability of genotypes to specific environments. The same pattern determined by the frequentist biplot can be observed in the posterior biplot, with the difference that the latter allows to separate subgroups of genotypes and environments (with the same pattern in relation to GEI) using levels of credibility.

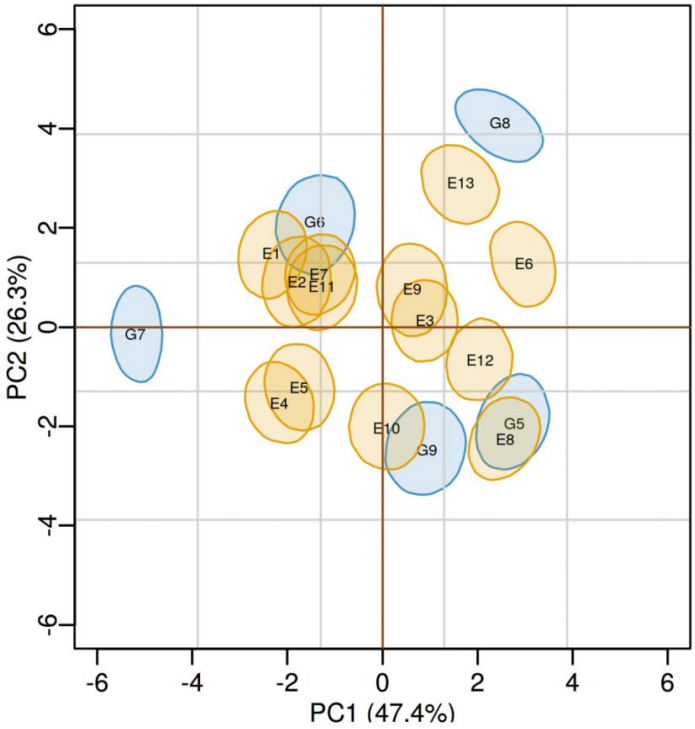

Fig. 4 - Bivariate regions, at 95% credibility, for genotypic and environmental scores on the AMMI-2 biplot.

Combining the information in Figure 3 with the biplot shown in Figure 4, it can be concluded that G2 is stable and, therefore, widely adapted and recommended. On the other hand, G9 contributes to interaction and suggests adaptability for the E10 and E8 environments. The other unstable genotypes have no interest in yield, and for two of them there are significantly negative main effects. An exception would be G7, whose effect would not be statistically different from the general average, but it has a great GEI effect and suggests adaptation for both the subgroup {E1, E2, E7, E11} and for E4 and E5.

Although not addressed here, the Bayesian methodology still offers the recognized advantages of treating unbalanced data and with heterogeneity of variance and the possibility of using information in addition to that present in the experimental data as demonstrated in recent works [17,21,23]. This also poses problems for analyzes that consider effects as fixed.

IV. CONCLUSION

Bayesian analysis allows inference to be directly incorporated to all parameters of the AMMI model by means of joint posterior distribution. It specially offers a flexible parametric method to incorporate uncertainty into the biplot. Such information made it possible to make more critical decisions in relation to the purely descriptive method of the frequentist biplot.

As observed, the information obtained from the regions of the posterior credibility for the genotype effects and GEI interaction, made it possible to analyze the stability and declare which genotypes and / or environments are significantly stable. Bayesian-AMMI also makes it possible to separate genotypes and environments into homogeneous subgroups with the same interaction patterns using levels of credibility.

Notwithstanding all these advantages, the referred method is still little used and more work, such as the one presented here, is necessary to publicize the method in order to make it a popular tool in the analysis of MET data.

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