Cleberton Correia Santos
(Organizador)

# Estudos Interdisciplinares nas Ciências e da Terra e Engenharias 5

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Cleberton Correia Santos
**(Organizador)**

# Estudos Interdisciplinares nas Ciências Exatas e da Terra e Engenharias 5

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## APRESENTAÇÃO

O livro "Estudos Interdisciplinares nas Ciências Exatas e da Terra e Engenharias" de publicação da Atena Editora apresenta em seu 5º volume 37 capítulos com temáticas voltadas à Educação, Agronomia, Arquitetura, Matemática, Geografia, Ciências, Física, Química, Sistemas de Informação e Engenharias.

No âmbito geral, diversas áreas de atuação no mercado necessitam ser elucidadas e articuladas de modo a ampliar sua aplicabilidade aos setores econômicos e sociais por meio de inovações tecnológicas. Neste volume encontram-se estudos com temáticas variadas, dentre elas: estratégias regionais de inovação, aprendizagem significativa, caracterização fitoquímica de plantas medicinais, gestão de riscos, acessibilidade, análises sensoriais e termodinâmicas, redes neurais e computacionais, entre outras, visando agregar informações e conhecimentos para a sociedade.

Os agradecimentos do Organizador e da Atena Editora aos estimados autores que empenharam-se em desenvolver os trabalhos de qualidade e consistência, visando potencializar o progresso da ciência, tecnologia e informação a fim de estabelecer estratégias e técnicas para as dificuldades dos diversos cenários mundiais.

Espera-se com esse livro incentivar alunos de redes do ensino básico, graduação e pós-graduação, bem como outros pesquisadores de instituições de ensino, pesquisa e extensão ao desenvolvimento estudos de casos e inovações científicas, contribuindo na aprendizagem significativa e desenvolvimento socioeconômico rumo à sustentabilidade e avanços tecnológicos.

Cleberton Correia Santos

## SUMÁRIO

# CAPÍTULO 27

# MULTISCALE SPATIAL INFLUENCE ON METABOLITES IN JABUTICABA

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**ABSTRACT:** Jabuticaba seeds make up agroindustrial residues, despite its chemical composition with potential biological activity. Multivariate variograms were indicates a spatial chemical structure in seed metabolites, as well as the environmental factors responsible for them. A spatial dependence between the nutrients of the seeds and soils of the fruit origin was observed, suggesting a phenotypic response of the metabolites to the environmental sources of these nutrients. Moran's eigenvector maps (MEM) allowed the modeling of the spatial influence at fine and broad distances in the study area, and controlled the spatial variance not explained by seed ($Mn^{2+}$, $Cu^{2+}$) and soil ($Mn^{2+}$).

**KEYWORDS:** *Myrciaria cauliflora*, chemical composition, spatial variation, multivariate geostatistics

**RESUMO:** Sementes de jabuticaba compõem resíduos agroindustriais, apesar de sua composição química com potencial atividade biológica. Variogramas multivariados indicaram uma estrutura química espacial para metabólitos de sementes, bem como os fatores ambientais responsáveis por ela. Uma dependência espacial foi observada entre nutrientes das sementes e dos solos de origem dos frutos, sugerindo uma resposta fenotípica dos metabólitos às fontes ambientais desses nutrientes. Os mapas de autovetores de Moran (MEM) permitiram modelar a influência espacial a curtas e longas distâncias, na área de estudo, controlando a variância espacial não explicada pelos nutrientes da semente ($Mn^{2+}$, $Cu^{2+}$) e do solo ($Mn^{2+}$).

**PALAVRAS-CHAVE:** *Myrciaria cauliflora*, composição química, variabilidade espacial, geoestatística multivariada.

## 1 I INTRODUCTION

Natural processes occur in a particular spatial location that can be represented by geographic coordinates, which can be used to evaluate the trends of response variables, as a function of latitude and longitude of the sampling sites, represented by polynomial functions adjusted by means of polynomial regression. These models allow us to find the structure of the variables in the environment and the tendencies of spatial structures to be linear, cubic, third order or higher, in a simple and powerful way. However, these polynomial functions are appropriate for phenomena that occur on a large scale, and for those of small scale, techniques using eigenfunctions are more appropriate (LEGENDRE & LEGENDRE, 2012), since they allow to represent structures at all distances between sites collection.

Eigenfunctions are families of multiscale methods for multivariate responses. The technique consists of constructing eigenvectors of spatial matrices and using them as predictors in linear models. Some of these eigenvectors were originally called PCNM (Principal Coordinates of Neighbor Matrices) and now called dbMEM (distance-based Eigenvector Maps), and included within MEM, i.e. Moran's Eigenvector Maps (DRAY et al., 2006). They are able to identify the scale in which spatial correlation occurs, which allows the elaboration of models that can be decomposed into different scales, facilitating the interpretation and understanding of the relations between response and explanatory variables.

Dray et al. (2006) found an algebraic formulation for the construction of MEM that allowed the construction of the two matrices: a) a connectivity matrix (B), represented by any type of graph, but often using minimum spanning tree algorithms, Gabriel graphs and Delaunay triangulation, among others, of the spatial coordinate points; b) an array of weights (A) that translates a notion of distance between neighboring samples but which can be replaced by different relations, such as similarity, which establishes exchanges of matter or energy between neighbors with greater or lesser ease.

MEN allowed the study of spatial (and temporal) structure in different fields and for the most part, use binary eigenfunctions or transformations at geographic distances. Once the trend of the variables in space is found, it is possible to use this information in multivariate techniques such as clustering (HCA), canonical redundancy analysis (RDA), and partitioning of the total variation by pRDA of the set of response variables as a function of environmental spatial predictors.

Geostatistics provides other proposals for spatial variance analysis, for example, in the construction of variograms. In these graphical tools, the ordinate is represented by the semivariance, $\gamma(h)$, and the abscissa by the distances between the collection sites, called classes (lag). Semivariance is the measure of the distance-dependent sample variance and indicates the spatial correlation between the samples. These tools are widely used and can be modeled in linear, exponential, spherical and Gaussian formats, mainly. The variograms can be uni or multivariate, the latter being described by Wagner (2004), in the proposition of multiscale ordination methods (MSO). These methods integrated well-known ordination techniques (PCA, RDA) into the classical variograms with statistical significance tests using Monte Carlo permutations. Thus, variograms matrices were used as geostatistical extensions of MSO, allowing the integration of spatial structures of a wide variety of processes and at different levels of organization.

In recent work (SANTOS et al., 2019), the dynamics of the metabolites of the seeds and peels of jabuticaba fruits resulted from abiotic factors, including mineral nutrients from fruit's parts and soil. In order to associate the chemical variability and geographic scale of sampling sites, the aims were to evaluate the presence of spatial correlation and to apply spatial representation models with MEM eigenfunctions and multiscale techniques by means of multivariate variograms, allowing to evaluate the dependence of the geographical scale on the variability of the metabolites from jabuticaba fruits.

## 2 I MATERIAL AND METHODS

In the spatial analyzes, the first two RDA axes were used to represent the chemical variability, since it summarizes the multidimensional chemical information in the samples at the collection sites (PEREIRA et al., 2017; SANTOS et al., 2019). RDA can also provide the main variance fractions explained by the predictors selected among seed ($Mn^{2+}$ and $Cu^{2+}$) and peels ($Mn^{2+}$ and P) of fruit origin and soil ($Mn^{2+}$) nutrients, in addition to spatial predictors based on MEM. In this work three classes of MEM were obtained (Table 1), according to a strategy defined by Legendre & Legendre (2012).

In the first two classes a connectivity matrix (B) define vertices of triangles without the inclusion of new locations (Delaunay triangulation). The third class uses the concept of distance around a point, which identifies pairs between sampling points from a multivariate variogram of the response matrix. The absence of weighting or the inverse weighting of the Euclidean distance define the weight matrix (A).

| Classes | Matrices | | MEM Properties |
|---|---|---|---|
| | Connectivity (B) | Weight (A) | |
| 1 | Neighborhood based on Delaunay triangulation | all 1 | Binary and based on the topology and with influence only of B |
| 2 | | $f_2=1-(d/d_{max})^a$ | Weighted by the inverse of the power of Euclidean distance (nonlinear) |
| 3a | Distance based on multivariate variogram | all 1 | Based on the multivariate variogram with influence only of B |
| 3b | | $f_2=1-(d/d_{max})^\alpha$ | Weighted by the inverse of the power of Euclidean distance (nonlinear) |

Table 1. Classes of Mohan's Eigenvectors Maps (MEM).

The significant MEMs of each class were selected by an automatic selection procedure, retaining those of the lowest value of the corrected Akaike information criterion (AICc). The selected MEMs were incorporated into the explanatory matrix containing the nutrients of the parts of the fruits and the soil's origin. The RDA of the best model was based on the values of variance inflation factor (VIF) and adjusted coefficient of determination ($R^2_{adj}$).

RDA results were used in the construction of variograms to estimate the magnitude of the spatial dependence between the sampling sites. The variance was estimated using semivariance, γ(h), where n(h) is the number of pairs in the distance classes h; $Z_x$ and $Z_{x+h}$ are values of the chemical parameters in the positions x and x+h, respectively:

$$\gamma(h) = \frac{1}{2n(h)} \Sigma_{x=1}^{n} (Z_x - Z_{x+h})^2$$

The number of classes (h = 8) was determined by Sturge's rule, which avoids arbitrary inflation of spatial variation explained as a function of class size.

Most models begin with a value of semivariance above zero, called a nugget ($C_o$). If there is spatial autocorrelation, the semivariance increases with the distance intervals (class) until reaching its maximum, known as sill ($C_o$+C). The variance between the nugget and sill is called partial sill (C) and corresponds to the part of the variance explained by the spatial structure. The ratio C/($C_o$+C) determines the spatial autocorrelation force (structural variance, *Q*). The range estimate the scale at which spatial dependence occurs. The parameters nugget, range, *Q* and $R^2_{adj}$ were obtained from the theoretical model with best fit based on automatic selection with cross-validation parameters as validation strategy. All the data were investigated for anisotropy. The distribution of the chemical parameter ($Z_x$) was expressed by means of a linear interpolation map (kriging) that provides the best estimate that minimizes the prediction error variations for the response variables.

Multiscale analysis (WAGNER, 2004) was used to model spatial structures at various scales. In these cases, semivariance multiple comparisons were performed by Bonferroni correction (k' = 0.05/n, where n is the number of classes and k' the adjusted significance) avoiding the increase of the type I error. Envelopes describing the confidence limits around the mean semivariance were used to assess the scale independence over the distance. Prior the analysis, the response matrix was transformed to log(x+1), centered on the mean and detrended in relation to the geographic coordinates, while the explanatory matrix was autoscaling. For the calculations were used the packages $GS^+$ (Geostatistics for the Environmental Sciences, version 10.0, Gamma Design, Michigan, 2014) and R (R Foundation for

Statistical Computing, version 3.4.3, Vienna, 2017).

## 3 I RESULTS AND DISCUSSION

The correlation between the Euclidian distances (ED) of the response matrix and the geographic distance between the samples indicated a strong association between the two matrices, suggesting a spatial influence on the chemical variability. The distance values varied from 0.4 (6.1 m) between samples 1 and 3 of S1 soil, to 17.3 (1457.6 m) between sample 3 of soil S3 and sample 1 of soil S5. The lowest ED of the metabolites was for seed samples with small geographical distances, while the highest were observed among the geographically distant sites. This result was confirmed by Mantel test (R = 0.950, $p$ = 0.001, 999 permutations), while peels metabolites did not present any significant correlation (R = -0.112, $p$ = 0.818), evidencing the absence of spatial autocorrelation. However, the tests were based on linear strategies, not eliminating nonlinear models of spatial influence on the peel metabolites.

The construction of eigenfunctions for the three classes of MEM led to eigenvalues selected by the lowest value of AICc (LEGENDRE & LEGENDRE, 2012). The MEM of each class composed, with the seed nutrients ($Mn^{2+}$, $Cu^{2+}$) and the fruit cultivation soil ($Mn^{2+}$), the explanatory matrix for new RDA. The most representative set of MEM resulted from the RDA with the lowest VIF values and of the higher $R^2_{adj}$ for the data of the seeds (Table 2).

| Classes | Matrices | | MEM | RDA | |
|---|---|---|---|---|---|
| | Connectivity (B) | Weight (A) | | VIF* | $R^2_{adj}$ |
| 1 | Delaunay triangulation | 1 | 2; 4; 8 | 9.1 | 0.900 |
| 2 | | $f_2=1-(d/d_{max})^a$ | 1; 4 | 6.2 | 0.880 |
| 3a | Multivariate variogram | 1 | 1; 8 | 11.9 | 0.959 |
| 3b | | $f_2=1-(d/d_{max})^\alpha$ | 2; 14 | 15.4 | 0.933 |

Table 2. Selected MEM based on $AIC_c$ criterium. *Highest VIF-value in RDA.

The analysis of the previous criteria led to the model represented by MEM1 and MEM8 (class 3a). The other two models were discarded because of a high value of VIF (class 3b) or because it presented a low $R^2_{adj}$ value (class 2), compared to that of class 3a. MEM represent a spectral decomposition of the spatial relations between the observations in all possible ranges of variation. Thus, they represent different spatial scales and those of class 3a suitably modeled the space between the samples to broad (MEM1) and fine (MEM8) scales (Figure 1).

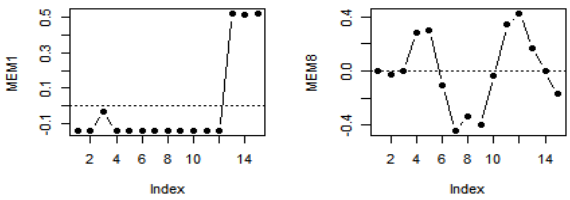
| Class (MEM) | Eigenvectors of Sampling Sites (Index) |
|---|---|
| 3a (1; 8) |  |



Figure 1. MEM eigenvectors according to selected class 3a.

The RDA1 was responsible for 52.2% of the explained variation ($F = 2.0$, $p = 0.001$) and separated the seeds from the S5 soil (Figure 2), mainly due to the low $Mn^{2+}$, moisture, insoluble fibers and ash contents, and accumulation of monomeric sugars (glucose and fructose) and citric acid. These characteristics are strongly associated with MEM1, emphasizing that RDA1 is linked to the variability of primary metabolites, which operates mainly on a long scale of geographical distance between samples.

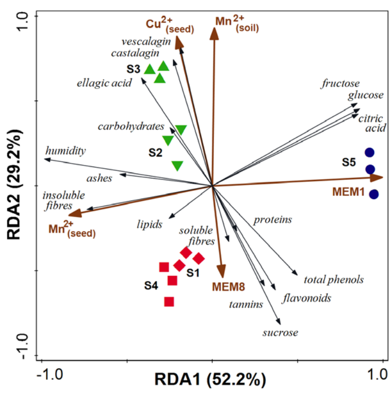




Figure 2. RDA triplot of seed metabolites in sampling sites (S1-S5) with explanatory variables.

On the other hand, RDA2 (29.2%, $F = 3.5$, $p = 0.001$) is mainly associated with the variability of special (secondary) metabolites between short-distance sampling sites (S1-S4), correlated to MEM8. Seeds of the poor soils in $Mn^{2+}$ (S1 and S4) accumulated mainly polyphenols (phenols, flavonoids and total tannins) and sucrose, while seeds rich in $Cu^{2+}$ and originated from soil rich in $Mn^{2+}$ (S2 and S3) showed highest contents of ellagic acid and ellagitannins (vescalagin and castalagin), especially in the S3 orchard. The influences of descriptors were quantitatively assessed using the variation partitioning by pRDA (Table 3) in four sets: seed nutrients ($Mn^{2+}$, $Cu^{2+}$), soil ($Mn^{2+}$), broad (MEM1) and fine (MEM8) spatial scales.

| Effects and Variables | Covariables | Variation Fraction | $R^2_{adj}$ (%) | *F* | *P* |
|---|---|---|---|---|---|
| Total effect | | | | | |
| Nutrient*, soil§ and spatials^z | | **[a-o]** | **95.9** | 66.2 | 0.001 |
| Partial effects | | | | | |
| Nutrient | Soil, spatials | [a] | 18.8 | 26.2 | 0.001 |
| Nutrient | | **[aeghklno]** | **60.8** | 11.9 | 0.001 |
| Soil | Nutrient, spatials | [b] | 5.8 | 15.2 | 0.001 |
| Soil | | **[befiklmo]** | **21.4** | 4.8 | 0.007 |
| Spatial (broad) | Nutrient, soil, spatial (fine) | [c] | 22.9 | 56.7 | 0.001 |
| Spatial (broad) | | **[cfgjlmno]** | **48.1** | 14.0 | 0.001 |
| Spatial (fine) | Nutrient, soil, spatial (broad) | [d] | 1.3 | 4.0 | 0.005 |
| Spatial (fine) | | [dhijkmno] | 4.7 | 1.7 | 0.179 |
| Joint effects | | | | | |
| Nutrient and soil | | **[e]** | **14.1** | | |
| Soil and spatial (broad) | | [f] | 1.4 | | |
| Nutrient and spatial (broad) | | **[g]** | **35.2** | | |
| Nutrient and spatial (fine) | | [h] | 0.5 | | |
| Soil and spatial (fine) | | [i] | -0.3 | | |
| Spatials | | [j] | -2.3 | | |
| Nutrient, soil and spatial (fine) | | [k] | 7.7 | | |
| Nutrient, soil and spatial (broad) | | [l] | -7.0 | | |
| Soil and spatials | | [m] | 6.3 | | |
| Nutrient and spatials | | [n] | -1.8 | | |
| Nutrient, soil and spatials | | [o] | -6.6 | | |
| Residuals | | **[p]** | **4.1** | | |

Table 3. Variation partitioning by pRDA of the seed metabolites with MEM.

*from seeds ($Cu^{2+}$ e $Mn^{2+}$); §($Mn^{2+}$); ^zMEM1 (fine) e MEM8 (broad).

The mineral nutrients of seeds and soil explained ca. 73% of the variability of the seed metabolites, with 24% of this fraction without spatial influence (fractions [a]+[b]). The spatial structure was mainly due to the long-distance component (MEM1) (48.1%). The contribution to short distances (MEM8) was only 4.7%, and not significant, despite its small and without any overlap, but with significant contribution for the variance explained ([d] = 1.3%, $p < 0.005$). The fraction [g] (35%) represented a strong spatial component that is jointly explained by the seed nutrients and MEM1 variation.

There is also some variation explained by the spatial variables independently of the environment (mineral nutrients). This variation is represented by the fractions [c], [d] and [j], which together explain 21.9% of the variation, which may be associated to unmeasured environmental variables, such as the effective luminous intensity in the orchards, which are spatially structured and can be influences chemical plasticity (MIEHE-STEIER et al., 2015). In turn, thin spatial structures are often associated with spatial autocorrelation of biotic origin, such as competition, intra and interspecific interaction. The spatial variables presented a nonzero intersection, despite the fact that they are orthogonal ([j] = -2.3%; [j+m+n+o] = -4.4%). This occurs because of the nutrients are not orthogonal to the MEM.

In order to better describe the spatial structure, the variograms were obtained from the two first RDA axes. The use of variograms is very important in chemistry of natural products, although scarcely studied and restricted to polyphenols and essential oils (BALUJA et al., 2012, VILELA et al., 2013). The nugget effect allows information on sources of error in the measurements or in the presence of undetected variations in the vicinity of samples. In addition, the variogram evaluates the spatial dependence by nugget/sill ratio and the effective range of spatial autocorrelation, both used in management and conservation of populations (VILELA et al., 2013).

In this study, Gaussian and spherical models were modeled for the variograms of RDA1 and RDA2, respectively (Table 4), confirming the spatial chemical structure and discarding the random distribution of the seed metabolites at the sampled sites.

| Response Variable | Model | Nugget | Sill | Range (m) | *Q* (%)* | $r^2$ | RSS§ | MCD (m)$^z$ |
|---|---|---|---|---|---|---|---|---|
| RDA1 | Gaussian | 0.005 | 0.159 | 1401.2 | 96.8 | 0.914 | 4.5E-5 | 508.6 |
| RDA2 | Spherical | 0.001 | 0.563 | 135.0 | 99.8 | 0.207 | 0.966 | 50.5 |

Table 4. Variogram parameters modeled for seed metabolites of *M. cauliflora* fruits.

*Structural variance; §residual sum of square; $^z$mean correlation distance (3/8 × range × *Q*)

The results showed that at least 97% of the total variance of the seed metabolites are spatially structured. On the other hand, the proportion of the nugget effect was higher in RDA1 (3.2%) than in RDA2 (0.2%), which reflects the greater spatial dependence of latter (99.8%). The range of variograms decreased from RDA1 (1401.2 m) to RDA2 (135.0 m), similarly to the mean spatial correlation distance (MCD), about 10 times between the two response variables. The MCD informs about the distance of the spatial dependence and indicated a decrease in size of geographical area that presents similar content among special metabolites. Thus, the variability in the content of metabolites such as lipids, proteins, sugars, with the exception of sucrose, citric acid and fibers occurred at longer distances than those involving polyphenols (phenols, flavonoids, tannins, ellagic acid, vescalagin and castalagin).

These results confirm the changes in the spatial chemical pattern, not only between the biosynthetic routes (primary and special metabolism), but also between different classes of the same metabolic route (polyphenols). Qualitative and quantitative changes such as polyphenols may provide a constitutive defense against herbivores or an induced response to herbivore damage, attracting predators or parasites (JURGENS et al., 2006).

The predictive maps (Figure 3) were based on adjusted models for each RDA axis by ordinary kriging. All maps showed higher variation among samples with certain similarities in the spatial patterns of two well differentiated areas: an area with high variation, mainly of primary metabolites (RDA1), along the South-North direction (S5) and another (West-East) with greater complexity of special metabolites (RDA2). The models were validation by cross-validation, with intercept close to zero (0.01 for both RDA 1 and RDA2), high $r^2$ values (0.980 and 0.932) and low standard error (0.15 and 0.27, respectively).

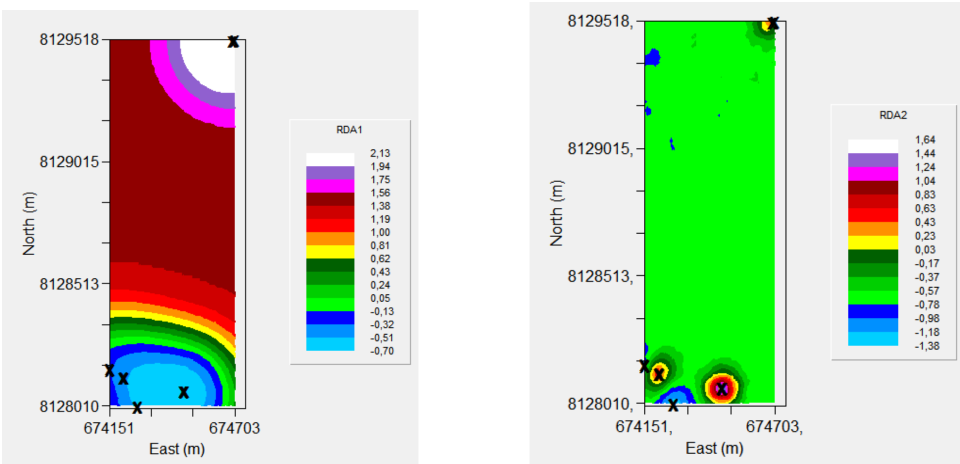



Figure 3. Spatial distribution maps of the jabuticaba metabolites according to the adjusted models from RDA1 (A) and RDA2 (B).

Unlike the genetic diversity, the description of chemical spatial structure has been little studied (ALI et al., 2010; VILELA et al., 2013; ZAOUALI et al., 2008). These studies have focused on spatial autocorrelation approaches, which do not always correctly estimate the variation explained by spatial structures. Thus, spatial chemometric methods using variograms can be used as additional tools to establish *in situ* conservation areas or *ex situ* conservation areas important for conservation and management strategies.

Although very useful, the above approach has the drawback of being restricted to a univariate analysis. A solution to this problem was the development of a multivariate variograms methodology (WAGNER, 2004), which combines ordination (PCA, RDA) with variograms, i.e multiscale ordination (MSO). MSO allows to perform three main diagnoses: 1. stationarity, that is, if the mean and variance remain constant throughout the study area; 2. absence of spatial correlation of the regression residuals, that is, the regression coefficients of the RDA can be interpreted, since the residuals are spatially independent; 3. dependence of the spatial correlation structure with the scale, that is, the regression coefficients will only be valid if the spatial correlation structure is invariant-scale (correlation between the response and explanatory variables does not depend on the scale).

In this study, MSO was performed initially by decomposition of the eigenvalues from the response matrix (seed metabolites) without conditioning, that is, a PCA was applied obtaining the total variance in the classes h (Figure 4A). Each point in the variogram represents the sum of all contributions of chemicals to spatial covariance, weighted over all pairs of samples within the respective distance class, and plotted as mean of distance between pairs.

The total variance showed a strong increase with the distance and the spatial autocorrelation in three classes was statistically significant, which violates the assumption of stationarity along the distance h. When the metabolites are conditioned by the nutrients of seed ($Cu^{2+}$, $Mn^{2+}$) and soil ($Mn^{2+}$), the eigenvalues of the RDA are partitioned into the classes (Figure 4B).

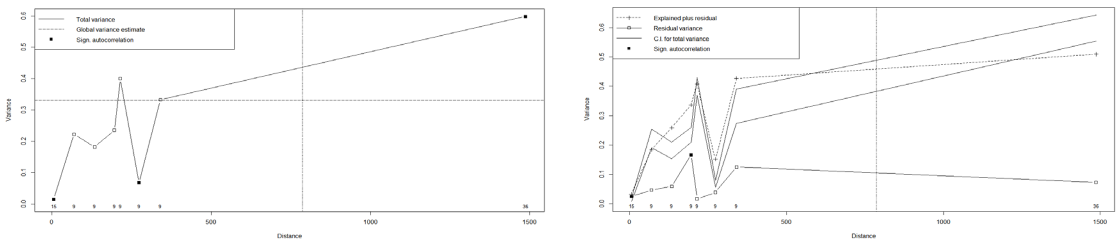



Figure 4. Multivariate variogram of the total variance of (A) seed metabolites (response matrix) and (B) metabolites explained by seed and soil nutrients.

The residual variance showed spatial autocorrelation in the lowest (distance < 5.6 m) and fourth classes (195.6 m). Among these classes and above the latter, RDA residues were spatially independent. Moreover, when the correlations between the RDA matrices do not vary with the scale, the sum of the explained variance and the residual remains within the envelope (5% probability). In the Figure 4B all classes go beyond the envelope, except for the fifth class, and it cannot be assumed that the metabolites are implicitly scale-invariant. In an attempt to control this regionalization of variables caused by spatial autocorrelation, MSO was performed with the introduction of MEMs into the set of explanatory variables initially formed by nutrients (Figure 5A). The results showed that the model controlled the regional spatial scale, although there is a significant spatial autocorrelation in the residuals at short distances (5.6 m), in addition to exceeding the envelope in the first and sixth (273.1 m) classes. An explanation for the short spatial autocorrelation, captured by the pRDA (fraction [d], Table 3), would be the genotypic similarity between neighboring trees, which could create a spatial structure regardless of environmental conditions (COVELO et al., 2011). This situation is possible because autocorrelation on a fine scale is strongly associated with phenotypic characteristics of individuals (ANDREW et al., 2007). Finally, the RDA was carried out with the explanatory variables of nutrients, now controlled by the spatial structure, using the MEM as covariables. Figure 5B shows that the MEM controlled the problem of scale dependence, so that the model was adequate for the nutritional variables of the seed and soil.

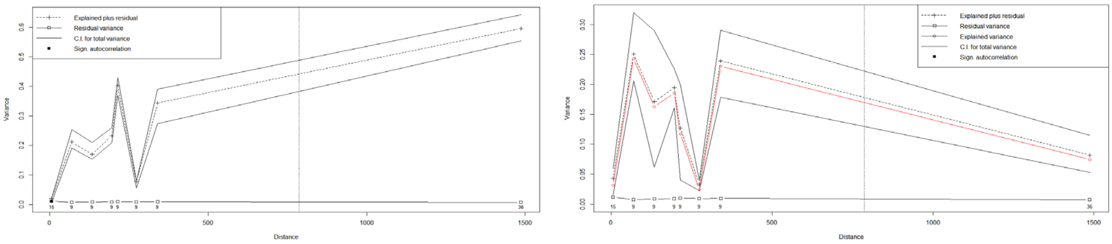



Figure 5. Multivariate variogram of metabolites explained by (A) seed and soil nutrients, and MEM an (B) after removal of spatial structure explained by MEM.

In the multivariate variogram there is no spatial autocorrelation in the regression residuals (RDA), and the explained plus residual variance, after elimination of the spatial structure by the MEM, remains within the confidence interval of total variance throughout the scale, including first and sixth classes. In addition, MEM also removed the trend of total variance gradient in the present metabolites, resulting in an expected globally oscillating empirical variogram. Thus, MEM variables were able to control the spatial variance in the metabolites of jabuticaba seeds, not explained by the predictive variables represented by the nutrients of seed and soil.

## 4 I CONCLUSIONS

The concentration of nutrients in plant tissues reflects both genotypic and phenotypic variation and environmental availability may increase the concentration within the individual, especially when another nutrient becomes limiting. In this study, a significant spatial correlation between nutrients of jabuticaba seeds to different soils were observed, suggesting a phenotypic response to the environmental sources these nutrients.

Several processes can create the same pattern of spatial structure, such that only their identification is insufficient to elucidate the mechanism that generates variability in space. The MEM not only allowed the modeling of spatial variability of seed metabolites, but also identified scales at short or long distances, and confirmed that chemovariations were not only invariant, but according to assumptions of stationarity and independence of residues.

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