Principal components analysis of the chemical attributes of the soil of a preserved Cerrado fragment

The number of studies on the importance of Cerrado soil to biogeochemical cycles is growing, with this being the focus of most research in the Cerrado biome. The objective of this research was to verify the correlation among different chemical attributes of the soil in a Cerrado fragment located in Mãe Bonifácia Park, in Cuiabá, Mato Grosso (MT), Brazil, using principal components analysis. For this study, five soil samples were collected at 0-10 cm depth monthly from August 2015 to July 2016. After the collection and identification of the soil, chemical analyses were performed to determine the following chemical characteristics of the soil: organic matter (OM), base saturation (V%), sum of bases (SB), cation exchange capacity (CTC), pH, and concentrations of H⁺, Al³⁺, Ca²⁺, Mg²⁺, K⁺, P, S, Cu, Mn²⁺, Mg²⁺, Zn, Fe²⁺ and B³⁺. The soil was characterized as acidic, which is typical for Cerrado soils, although some chemical elements were found in high concentrations. After the analysis of principal components, it was possible to reduce the seventeen original variables to four principal components that represented 88.86% of the total variation of the data. In which the first main component explained 41.18%, the second component explained 28.39%, the third 11.29% and the fourth explained 7.98%. Based on this analysis, it was identified that the chemical attributes such as the sum of base (SB), organic matter (OM), cation exchange capacity (CTC), calcium (Ca²⁺), saturation (V%) and pH represented the greater data variance.

Keywords: Biogeochemical; Soil chemistry; Mãe Bonifácia Park.

Análise de componentes principais dos atributos químicos do solo de um fragmento preservado de Cerrado

É crescente os estudos relacionados a importância do solo do Cerrado para os ciclos da natureza, tendo este importante papel nas funções ecossistêmicas como, por exemplo, os ciclos biogeoquímicos. O objetivo desta pesquisa foi verificar a correlação entre atributos químicos do solo de um fragmento de Cerrado localizado no parque Mãe Bonifácia, em Cuiabá-MT, por meio da técnica de análise de componentes principais. Para esse estudo foram coletadas cinco amostras de solo com profundidade de 0-10 cm, mensalmente no período de agosto de 2015 a julho de 2016, totalizando 12 coletas. Após a coleta e identificação, realizou-se a análise química para determinação dos seguintes atributos do solo (MO, V%, SB, CTC, pH, H⁺, Al³⁺, Ca²⁺, Mg²⁺, K⁺, P, S, Cu, Mn²⁺, Mg²⁺, Zn, Fe²⁺ e B³⁺). Observou-se que o solo é caracterizado como ácido, típico dos solos do Cerrado, entretanto alguns atributos tiveram uma concentração elevada. Após a análise de componentes principais, conseguiu-se reduzir as dezessete variáveis originais para quatro componentes principais que representaram 88,86% da variação total dos dados. Em que a primeira componente principal explicou 41,18%, a segunda componente explicou 28,39%, a terceira 11,29% e a quarta explicou 7,98%. Com base nessa análise, identificou-se que os atributos químicos como a soma de base (SB), matéria orgânica (MO), capacidade de troca catiônica (CTC), cálcio (Ca²⁺), saturação (V%) e o pH representaram a maior variância dos dados.

Palavras-chave: Biogeoquímico; Química do solo; Parque Mãe Bonifácia.

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INTRODUCTION

The intervention of man in any natural ecosystem causes modifications to the physical and biological environment that can cause the quality of the environment to degrade (BRANCO et al., 1999). Eventually, the microbial transformations and different chemical reactions occurring in the soil can be altered, depending on the types of anthropogenic activities enacted (THEODORO et al., 2003).

Soil can be defined as a mixture of inorganic and organic materials formed by a series of intemperic processes operating on the Earth's surface, which cause the decomposition of primary rocks and minerals through the action of physical, chemical, and biogenic weathering (HUNT, 1972). The soil is the main substratum on which plants develop, and on which all living terrestrial organisms depend. It is one of the main environmental compartments receiving many pollutants that, when deposited randomly, can contribute to the progressive degradation of terrestrial, aquatic, atmospheric, and biological environments (MANAHAN, 1999).

In addition, the soil contributes to the cycling of nutrients, which is of paramount importance to the maintenance of life within ecosystems. Indeed, these are interrelated processes in which chemical elements, including all of the elements essential to life, are used in successive periods of energy fixation and circulate through the biosphere in characteristic ways, from the environment to organisms and vice versa (ODUM, 2013).

The soil quality of the Cerrado is an important factor that determines the characteristic vegetation types found in this ecosystem. The soil is deep, well-drained, and subjected to intense weathering and leaching, which makes it acidic, nutrient-poor, and contain high levels of iron and aluminum (GOMES et al., 2000). Despite the high acidity and low fertility of its soil, the Cerrado is threatened because it is the main agricultural frontier of Brazil due to its proximity to major consumer centers, flat topography, and satisfactory road structure (KER et al., 1992).

The use of land in the Cerrado is always questionable, as negative impacts caused by the misuse of the soil reduce the area that can be preserved for agricultural use, which thus requires the use of large amounts of fertilizers and pesticides to increase the limited productive capacity there. In conjunction with habitat loss and anthropogenic climate change, these activities are changing the natural nutrient cycling in this region every day.

In addition to the anthropization and intensive use of the soil of the Cerrado for agricultural production, other environmental factors can accelerate the degradation process. For example, rainfall concentrations vary throughout the year, which produces interannual variations in vegetated surfaces; for instance, in dry periods there is a great loss in leaf area (NOVAIS et al., 2018), with a risk of burning, favoring periodic spatial and temporal modifications in the albedo (NOVAIS et al., 2015, NOVAIS et al., 2016) and soil moisture and, consequently, variability in some physicochemical processes in the soil and the atmosphere of the region (BARROS et al., 2010).

Such soil properties as variation in soil texture, moisture retention, and chemical properties like pH

and aluminum content determine the distributions of different tree species in the Cerrado (SOUZA et al., 2007; ASSIS et al., 2011). Soil moisture variation, for example, can cause variations in physical, chemical, and biological processes that alter soil characteristics, such as redox potential, pH, and the content and oxidation state of iron and manganese (PEZESHKI et al., 2012), among other nutrients. The effects of these disturbances on soil properties and the microbial community can interfere with the regeneration capacity of the forest or mediate the introduction of other plants to the area (MOREIRA et al., 2004).

Thus, the objective of this study was to assess the correlations among different chemical attributes of the soil in a Cerrado fragment located in the city of Cuiabá, Mato Grosso (MT), Brazil, by means of using principal components analysis (PCA).

MATERIALS AND METHODS

Study Area

The municipality of Cuiabá has an area of 3,224.68 km², of which 254.57 km² (7.89%) is urban and 2,970.11 km² (92.1%) (JOAQUIM et al., 2018). It is located at an altitude of 165 m above sea level (a.s.l.), within the geomorphological province called the Cuiabana Depression. The regional climate is Aw, according to the Köppen climate classification system, and is characterized by being hot and humid with rains in summer and a dry season in winter, with distinct seasons (wet and dry) and an annual accumulated of 1,400 mm year⁻¹ (ALVARES et al., 2013).

In this context, the area of study is located, the Mãe Bonifácia Urban Park (Figure 1) under the geographical coordinates 15 ° 34'44"S and 56 ° 05'016 " 'W, with 77.16 hectares of area, and altitude between 164m and 195m (Pacheco et al., 2018) which over the years was surrounded by the expansion of the neighborhoods surrounding it (SOUZA et al., 2020).

Figure 1: Location map of Mãe Bonifácia urban park in Cuiabá-MT, Brazil. **Fonte:** Adapted from Novais et al. (2018).

According to Andrade et al. (2016) the park is a remnant fragment of the Cerrado in its natural form, that is, without alterations resulting from relevant anthropogenic activities, having its biophysical

characteristics preserved. The soil of the region is predominantly of the Type Concretary Cambic Alic (SCCa), characterized by being mineral soil, well drained, of medium depth, with the presence of iron concretions along the profile in an amount greater than 50% of the volume (SEPLAN, 2001).

Data collect

To cover the seasonal variability on the variables under study, 12 collections were made over a year, starting in August / 2015 and ending in July / 2016. Five collection points were established, forming a polygon defined as follows: with distances of 10.97 m between points 1 and 2, 15.30 m between points 2 and 3, 8.60 m between points 3 and 4, 6.60 m between points 3 and 4, and 7.53 m between points 5 and 1, ending the polygon.

Organic matter was removed from the soil surface before each collection, according to Arruda et al. (2014), remove leaves, sticks and other things remains from the soil surface that may compromise the quality of the sampling. The samples were taken from the first 10 centimeters of soil using an auger, weighing approximately 1kg each (LEMOS et al., 1996). According to Arruda et al. (2014), states that it is necessary for samples to be taken uniformly in volume and depth. Thus, after collection, the samples were placed in identified plastic bags and stored in a refrigerated environment.

After sampling, the soil samples were sent to the laboratory for chemical analyses of their CaCl_2 , phosphorus (P), potassium (K^+), calcium (Ca^{2+}), magnesium (Mg^{2+}), aluminum (Al^{3+}), hydrogen (H^+), zinc (Zn^{2+}), copper (Cu^{2+}), iron (Fe^{3+}), manganese (Mn^{2+}), boron (B^{3+}), and sulfur (S^{2-}) content, and their pH was also determined.

The above chemical and granulometric analyses were performed according to the EMBRAPA (1999) methodology by the laboratory in the city of Cuiabá, where the pH was determined in CaCl_2 (ratio 1:2.5) and P, K, Zn, Cu, Fe, and Mn were extracted with Mehlich-1 ($0.0125 \text{ mol L}^{-1}$ of H_2SO_4 and 0.05 mol L^{-1} of HCl) and quantified as follows: P was quantified by photocolormetry, K using a flame photometer, and micronutrients by atomic absorption spectrophotometry. Exchangeable Al, Ca, and Mg were extracted with 1 mol L^{-1} KCl, Al and H were extracted with a 0.5 mol L^{-1} calcium acetate solution with a pH of 7 and titrated with $0.0606 \text{ mol L}^{-1}$ NaOH, and S and B were extracted by turbidimetry in barium sulphate or in hot water, respectively, and both were quantified by photocolormetry.

The sum of bases (SB), base saturation (V%), and cation exchange capacity of the soil at a pH of 7 (CTC) were calculated through the sorption complex analysis.

The soil chemical parameters were chosen because they are typically reported for Cerrado soils (LOPES et al., 1977; FURLEY et al., 1988; HAASE, 1999; LILIENFEIN et al., 2003; SOUZA et al., 2007; VOURLITIS et al., 2011; WANTZEN et al., 2012).

Statistics

For the multivariate statistical analysis of correlations among soil properties, principal components analysis (PCA) was used. PCA is a multivariate statistical technique that consists of transforming a

multidimensional set of original variables into another set of variables of the same dimensionality, called principal components (VARELLA, 2008).

The principal components identified by PCA are presented in descending order of importance, i.e. the first PC explains the maximum possible proportion of the variation in the original data, the second the maximum possible proportion of variation not yet explained by the first component, and so on, while the last component will make the least contribution to explaining the total variation in the original data (JOHNSON et al., 1998; MORRISON, 2003).

With this analysis it is possible to identify the attributes that have the greatest contribution to the composition of the studied soil. The correlation matrix was used to assess dependency, so that each variable has the same weight in obtaining the components. Then, the correlation matrix was submitted to principal component analysis, which allows transforming a set of data, initially correlated, into a new set of uncorrelated variables (NOGUEIRA et al., 2014).

The variables that will be generated are called CP (main component) and have statistical independence, that is, they are not correlated. Each CP is estimated with the purpose of retaining, in order of estimation, the total variation contained in the initial data. That is, the first main components contain most of the total variability of the data (SOUZA, 2000; REGAZZI, 2001; MANLY, 2008). ACP can be given by Equation 1.

$$Z_i = a_{1i}X_1 + a_{2i}X_2 + \dots + a_{ni}X_n \quad (1)$$

Where: Z_i is the i -th main component, a_{ji} are the coefficients of the main component, X_j is the value of the j -th variable and n is the number of variables (MANLY, 2008; DOMINICK et al., 2012).

All observed variables were standardized and included in the main component performance score equations. The standardization of variables is performed by the value of the variable minus the average of the group of variables assessed divided by the standard deviation, called the standard score or z-score (SILVA et al., 2015). According to equation 2:

$$Z = \frac{\text{value of the variable} - \text{average}}{\text{standard deviation}} \quad (2)$$

The eigenvalues obtained by principal component analysis were subjected to Varimax rotation, this method was developed by Kaiser in 1958. According to Johnson et al. (1998), it uses the rotation of factors to improve the interpretation of results, without changing the matrix of correlation and much less the specific variances, thereby improving the distribution of the percentage of explanation of the variance between the components.

For statistical analysis, the SPSS Statistic 21® software was used in the Principal Component Analysis (ACP) calculations, in the various calculations (eigenvalues, loads, commonality and correlation matrix).

RESULTS AND DISCUSSION

Figure 2 shows the average of the principal chemical parameters of the soil. The highest values of P, H, Fe and M.O occurred in August 2015. The concentrations of K and Ca increased over time, while those of P, H, Cu and M.O tended to decrease. Ja Zn, Mn and S did not vary their concentrations on average.

The highest values of P, H, Fe and M.O occurred in August 2015. The concentrations of K and Ca increased over time, while those of P, H, Cu and M.O tended to decrease. Ja Zn, Mn and S did not vary their concentrations on average.

Figure 2: Principal soil chemical parameters of a Cerrado fragment.

The concentrations of organic matter decrease with time since the experiment started in August, a dry period for the Brazilian savannas, with leaves falling in the deciduous forests.

The principal components analysis (PCA) grouped all of the soil chemical attributes examined (17 original variables) into four main factors, as presented in table 1.

Table 1: Eigenvalues and accumulated percentage of the total variance explained by main component (CP) of the Cerrado fragment.

Components	Eigenvalues	Variance %	Cumulative %
1	7.002	41.186	41.186
2	4.827	28.396	69.582
3	1.921	11.298	80.879
4	1.357	7.985	88.864
5	0.731	4.302	93.166
6	0.505	2.968	96.134
7	0.307	1.805	97.938
8	0.165	0.973	98.912

9	0.112	0.657	99.568
10	0.6	0.351	99.919
11	0.014	0.081	99.919

Extraction method: analysis of the main component.

The PCA was overall able to explain 88.86% of the total variance in the data. This agreed with results of Johnson et al. (1998), who stated that a minimum percentage of the total variance explained close to 80% is needed to determine the appropriate number of principal components for a given dataset, while Hair et al. (2006) suggests 60%.

The first principal component explained 41.18% of the total variation in the data, and thus can be considered the repository of the most important information concerning the relations among the different soil variables tested, their eigenvalues are presented in Table 1. The second component explained 28.39% of the variation, followed by the third that explained 11, 29% and the fourth 7.98%. Together they explained approximately 88.84% of the total variance of the chemical attributes present in the soil of the Cerrado fragment.

The sedimentation curve can be seen in Figure 3, in which a decay is perceived up to the fourth eigenvalue, becoming almost parallel to the abscissa axis, then falling again. In this case, only one or two components could be retained, however we opted for a greater explanation of the accumulated variance of the data, thus analyzing 4 main components.

Figure 3: Sedimentation curve of the main components for the Cerrado fragment.

The literature indicates that the researcher can use the accumulated variance criterion to determine the number of factors that must be extracted. Hair et al. (2006) suggest the 60% level as being acceptable. We used the criterion of Kaiser (1958) and the first fourth components were retained, reducing from 17 to 4.

The correlation between the original variables and the main components is called loading. These provide an indication of how important the original variables are for the formation of the main components. Therefore, loadings close to 1 indicate that this variable is important in the formation of the main component,

while loadings close to zero indicate that the variable is not important in the formation of the main component (GOMES et al., 2000).

Table 2 shows the loadings of the main components for each of the 17 variables. For each variable, the highest loading was selected, in absolute value, to understand which or which variables are most important in the formation of each of the first 4 components.

Table 2: Principal component analysis (PCA) of soil chemical variables in the Cerrado fragment.

	Components			
	1	2	3	4
P	-0.263	0.002	0.179	0.858
K ⁺	0.658	-0.121	-0.487	0.319
Ca ²⁺	0.926	0.201	-0.189	-0.160
H ⁺	-0.390	0.853	0.159	0.287
MO	0.086	0.947	0.157	0.235
Zn ²⁺	0.617	0.594	0.358	0.215
Cu ²⁺	-0.155	0.140	0.890	-0.059
Fe ²⁺	-0.047	-0.006	0.756	0.454
Mn ²⁺	0.276	-0.345	0.064	-0.607
B	0.175	-0.909	-0.052	0.127
S	-0.084	-0.803	0.249	0.225
Mg ²⁺	0.895	0.088	0.268	-0.114
Al ³⁺	-0.930	0.153	0.211	0.232
CTC	0.079	0.938	0.163	0.259
SB	0.977	0.144	-0.074	-0.110
V (%)	0.914	-0.290	-0.137	-0.192
pH	0.914	-0.277	-0.112	-0.253

Extraction method: Principal component analysis.

Rotation method: Varimax with Kaiser normalization.

Figure 4 shows the graphical representations of the loadings of the first two components. In addition, the values corroborate with the results found in table 2.

Figure 4: Graphical representation of the loadings of the first two main components.

Based on the data in Table 2 and using equation (2), the mathematical model of equation (1) used for the scores of the main components (CP1, CP2) was estimated, corresponding to approximately 69.58% of the total variation. as can be seen in equations 3 and 4.

According to equation (3) the main values that were associated in the first component that presented

a positive contribution between the attributes were:

$$CP1 = -0.263 * (P) + 0.658 * (K+) + 0.926 * (Ca^{2+}) + 0.617 * (Zn^{2+}) + 0.89 * (Mg^{2+}) - 0.930 * (Al^{3+}) + 0.977 * (SB) + 0.914 * (V\%) + 0.914 * (pH) \quad (3)$$

$$CP2 = 0.853 * (H+) + 0.947 * (MO) - 0.909 * (B) - 0.803 * (S) + 0.938 * (CTC) \quad (4)$$

The soil of the study area was characterized by its strong acidity, with an average pH value of 4.75 in $CaCl_2$. The soil's sum of bases (SB), base saturation (V%), and concentrations of calcium (Ca^{2+}), magnesium (Mg^{2+}), potassium (K+), and zinc (Zn^{2+}) were all positively correlated within the first principal component, while the aluminum (Al^{3+}) concentration was correlated negatively with the other variables in the first component (Table 2). These findings agreed with the results of Vourlitis et al. (2013), who evaluated the fertility of the Cerrado soil.

Based on the PCA results, when the soil's capacity to retain cations increased, there was a simultaneous increase in its SB (Table 2). In the system under study this was likely mainly due to the increased presence of Ca^{2+} in the sortative complex (VALADÃO, 2015), as suggested by the relationships among variables within the first principal component. As the soil exchange complex grows richer in bases, especially with Ca^{2+} , the pH rises, which neutralizes Al^{3+} (VALADÃO, 2015). The pH influences the solubility, solution concentration, and ionic forms of the nutrients in the soil and consequently their absorption and use by plants.

The second component explained 28.39% of the total variation in the data (Table 1) and contained mainly positive eigenvalues for the variables hydrogen (H+), organic matter (OM) and cation exchange capacity (CTC) (Table 2). The increase in CTC as a function of OM indicated by this positive correlation likely occurred due to the generation of negative charges by the break in the C chains that form the radicals R-COH (carboxyl) and R-OH (hydroxyl) on the surfaces of OM (RAIJ, 1991). Further, H^+ (hydrogen) content is already known to be an essential mediator of the survival of organic matter in the soil (EBELING et al., 2008).

Boron and sulfur concentrations were correlated negatively (Table 2) with the other variables in the second component. This result is directly related to the mineralization of organic matter in the soil. Which is lower during drier periods and also to the decreased adsorption of this nutrient during such periods since it occurs through mass flow (MALAVOLTA et al., 1985).

The third principal component comprised the micronutrients copper and iron which together explained 11.29% of the variation in the data (Table 1) and were positively correlated with one another (Table 2). This correlation is related to several metabolic activities in plants, as Cu and Fe participate in the formation of several enzymes (e.g. catalase, peroxidase, cytochrome oxidase, and xanthine oxidase), and are also indispensable in the processes of respiration photosynthesis, N_2 fixation and electron transfer through cycling between Fe^{2+} and Fe^{3+} (GUERINOT et al., 1994; MARENCO et al., 2009).

The fourth and last principal component represented 7.98% of the total variation in the data (Table 1) and comprised the main nutrients phosphorus (P) and manganese (Mn) which were negatively correlated with each other (Table 2). This may be related to the fact that the soil availability of manganese is reduced

by increased pH as well as high levels of organic matter, phosphorus, copper, and zinc, which result in elemental complexation (RAIJ, 1991).

CONCLUSIONS

In view of the results obtained the analysis of main components proved to be effective. Thus, fewer variables were necessary to explain the total variation without significant loss of information. Therefore, the principal component analysis reduced the 17 original variables (MO, V%, SB, CTC, pH, H^+ , Al^{3+} , Ca^{2+} , Mg^{2+} , K, P, S, Cu, Mn^{2+} , Mg^{2+} , Zn^{2+} , Fe and B) for four main components that represented 88.86% of the total data variation.

The first component explained 41.18%. The pH contributed significantly to the variables of the first component. The second component explains 28.39% of the total variation. In the third component formed by the micronutrients copper and iron. The variation was explained by 11.29%. The fourth component explained 7.98% of the total variance, corresponding to the elements phosphorus and manganese.

Attributes such as base sum (SB), organic matter (OM), cation exchange capacity (CTC), calcium (Ca^{2+}), saturation (V%) and pH represented most of the data variance.

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