Technical Notes

ANISOTROPIC GEOSTATISTICAL MODELING OF CARBON DIOXIDE EMISSIONS IN THE BRAZILIAN NEGRO BASIN, PANTANAL SUL

GEOPANTANAL, v. 40, Número Especial, p. 227-238, agosto 2015.

INTRODUCTION

Currently the cycle of carbon dioxide, CO_2 , has been methodically studied for researches on environmental science disciplines. Mainly because CO_2 is one of the gases in the Atmosphere that has been considered responsible for what is now called the "Greenhouse Effect". The other gases are Methane (CH₄), Nitrous oxide (N₂O), Chlorofluorocarbons (CFCs), Hydro-fluorocarbons (HFCs), and Sulfur hexafluoride (SF₆).

The Greenhouse gases absorb part of the infrared radiation reflected by the Earth's surface, preventing it from escaping into space. Thus the surface of the Earth is being heated because of the Greenhouse Effect, causing global warming with a direct effect on climate change on our planet (SHAH, 2014).

The CO_2 is sequestered from the Atmosphere only by the absorption of the other two reservoirs: oceans and terrestrial biomass. The main sources of net CO_2 emissions to the Atmosphere are deforestation and industrial activities that burn fossil fuels. The soils around the globe have also increased their emissions of carbon dioxide in recent years. The increasing temperatures are likely to cause a net release of carbon dioxide from soils by triggering microbes to speed up their respiration of plant debris and other organic matter (BOND-LAMBERTY, 2010).

Studies of the global CO₂ balance show that the emission is increasing while its sequestration is decreasing in recent years. So, methodologies which allow spatial modeling the CO₂ reservoirs are important, including sequestration and emission values influenced both by anthropogenic and natural phenomena. The results of these studies allow decision taking to mitigate the damaging effects of this phenomenon on our planet.

Modeling of natural variables, such as temperature, soil properties, CO₂ and others, requires the use of appropriated methods in order to obtain reliable representations for the spatial variability of the property in study. A relevant question for modeling natural variables is to consider its spatial behavior, i.e., how such property values change in the geographic space. By definition, isotropic are those phenomena evenly propagated in all spatial directions. The isotropy is a rare feature observed in natural properties. The most common and frequent is the presence of anisotropy, characterized by the asymmetrical spread of the property in space, being more intense in one direction and less in the other directions (CAMARGO et al., 2001). Therefore, in order to model the anisotropy and to reconstruct the spatial distribution of natural variables from a set of sample data, it is important that the model correctly represents its spatial autocorrelation structure. In this context, geostatistical analyses and methods have been applied successfully to model the spatial behavior of natural phenomena over specific regions of the Earth surface (DEUTSCH; JOURNEL, 1998; GOOVAERTS, 1997; ISAAKS; SRIVASTAVA, 1989). One of the great advantages for the use of geostatistical approaches is that one can determine and consider the spatial autocorrelation of the attribute by semivariogram analyses performed directly in the sample set. Isotropic or anisotropic semivariograms, along with the sample set, are used to estimate local and global uncertainty models of the random variables that represent the spatial attribute in the region of interest. From these uncertainty models it is possible to derive maps representing local statistical properties of the phenomena, such as, mean, variance, quantile and confidence interval values.

This article presents a geostatistical methodology for spatial modeling of CO_2 emissions from a set of samples obtained at the southern Pantanal wetland of Mato Grosso do Sul State (MS), Brazil, in the Negro River basin. Previous inspection of the samples, by surface semivariogram analyses, showed that the behavior of CO_2 emissions is anisotropic inside the region under study.

OBJECTIVE

The objective of this work is to model the spatial distribution of CO_2 emitted from soils in a specific geographical region. A case study was made in the Negro River basin located at the Southern Pantanal Biome, Mato Grosso do Sul State. The CO_2 input dataset is constituted by sample points and the attribute is modeled using the kriging geostatistical approach. Isotropic and anisotropic spatial behavior of the attributes are explored, for comparison purposes. The methodology and the results are presented and the models are analyzed both qualitatively and quantitatively with graphics, maps and table reports.

MATERIAL AND METHODS

CONCEPTUAL ASPECTS

Geostatistical approaches for estimations, and also simulations, are based on previous analyses of the spatial correlation from a set of sample points to represent the spatial variability, of the attribute in a geographical region. This variability in function of the spatial distance is represented by semivariogram models. Empirical, or experimental, semivariogram models, $\gamma^*(\mathbf{h})$, can be estimated, from a set of sample points, according to the Equation:

$$\gamma^*(\mathbf{h}) = \frac{1}{2 \operatorname{N}(\mathbf{h})} \sum_{(i,j)/\mathbf{h}_{ij} \approx \mathbf{h}} (z(\mathbf{u}_i) - z(\mathbf{u}_j))^2$$

where $z(\mathbf{u}_i)$ and $z(\mathbf{u}_j)$ are attribute values observed at spatial locations \mathbf{u}_i and \mathbf{u}_j separated by the distance \mathbf{h} . $N(\mathbf{h})$ is the number of samples found inside a circumference with radius distance approximately equal to \mathbf{h} .

The empirical semivariograms are fitted by theoretical, or mathematical, models in order to be used for the estimation of the attribute variability value between any two spatial locations.

Directional semivariograms must be considered when the spatial variability of the attribute is not omnidirectional. In this case the angle of greater continuity, i.e. of less variability, is detected, directly from the sample set, and considered, along with the perpendicular direction, in order to model the anisotropy of the attribute (CAMARGO et al., 2001). It is very important to model the anisotropy shown by the samples to get more reliable spatial modeling of the attribute considered. The quality of the semivariogram modeling is reflected in the kriging system, which uses this information to estimate values at unsampled locations.

The geostatistical kriging procedure allows to infer statistical parameters, the mean and the variance values, of the attribute from a number $n(\mathbf{u})$ of neighbor samples, $z(\mathbf{u}_{\alpha})$ $\alpha=1,...,n(\mathbf{u})$, of the spatial location \mathbf{u} . The general formulation of kriging for the mean value estimations is:

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$$z^{*}(\mathbf{u}) - \mu(\mathbf{u}) = \sum_{\alpha=1}^{n(\mathbf{u})} \lambda_{\alpha}(\mathbf{u}) \cdot [z(\mathbf{u}_{\alpha}) - \mu(\mathbf{u}_{\alpha})]$$

where $\mu(\mathbf{u}) = m(\mathbf{u})$ is the tendency, or the mean value, of the attribute in the spatial location \mathbf{u} , $\mu(\mathbf{u}_{\alpha})$ is the mean value in each sampled location \mathbf{u}_{α} . The weights $\lambda_{\alpha}(\mathbf{u})$ are estimated considering the correlation structure defined by the modeled semivariograms for the set of sample points considered. These weights are also considered for the estimation of variance values (DEUTSCH; JOURNEL, 1998; ISAAKS; SRIVASTAVA, 1989).

A CASE STUDY

This work uses the software SPRING - Sistema de Processamento de Informações Georeferenciadas - to create a geographic database and to perform the geostatistical analyses from the sample set of CO_2 considered. SPRING is a Geographic Information System (GIS) which is used to input, store, manipulate, analyze and output spatial information, including remote sensing images, in a single integrated computational platform (CAMARA et al., 1996).

The area under study is the Negro River basin in the Pantanal biome, whose coordinates of geographic location and projection information are shown in figure 1. The Pantanal Biome occupies 7% of the southern part of the State Mato Grosso (MT) and 25% of the northwestern part of the State of Mato Grosso do Sul (MS), in Brazil, covering a total area of 150,355 km². Beyond the Brazilian border, it extends through northern Paraguay and eastern Bolivia. It is an alluvial plain influenced by rivers that drain the basin of the Upper Paraguay, where it develops beautiful and abundant fauna and flora.

Data used in this work were provided by FUNCATE - Fundação de Ciência e Tecnologia Espaciais - the Foundation for Space Science and Technology, under the document named "Segunda Comunicação Nacional do Brasil à Convenção-Quadro das Nações Unidas sobre Mudança do Clima" ("Second Brazilian National Communication to the United Nations Framework Convention on Climate Change"), available at: www.mct.gov.br/index.php/content/view/ 326988/Texto_Completo_Publicado.html.

For this study three types of data were used. The first is a polygon representing the outline of the Negro Basin, which was used as a clipping mask for the resulting maps. The second is a set of 4601 sample points, with values associated to the estimated CO₂ emissions (kg/m²) inside each soil class polygon as shown in figure 2. The third is a set of 1,000 sample points used for performing validations on the resulting models. The CO₂ emissions vary according to the soil types of the region.



Figure 1 - Negro basin highlighted from the Pantanal biome



Figure 2 - Soil map with CO₂ emissions in the Negro Basin

METHODOLOGY

The methodology used in this work follows these steps: the original CO₂ sample set and the polygon surrounding the region of interest were stored in a geographical database as data layers in the SPRING GIS. Exploratory data analyses of the sample set was performed in order to know statistical properties of the data. Trends in the CO_2 original data were removed to obtain residual information, resulting in a constant stationary mean over the whole region, to assess the semivariograms. Anisotropy in the residual data was verified by analyses of surface semivariograms. Empirical semivariograms were generated for the isotropic and the anisotropic behavior and were fitted by theoretical models. The resulting mathematical equations were defined for the isotropic case and for the two directions of the anisotropic semivariograms. The CO_2 emissions were modeled by rectangular grids, applying the geostatistical kriging estimator over the original sample set and considering the final mathematical semivariograms. The rectangular grid representations were cut out by the polygon surrounding the region of interest. Numerical validations were performed to compare and to analyze the quality of the final maps of isotropic and anisotropic CO_2 emissions. The flowchart of figure 3 summarizes the methodology of this work.



Figure 3 - Flowchart of the methodology employed in this work

RESULTS AND DISCUSSION

Figure 4 illustrates the spatial distribution of the CO_2 emission samples in the Negro basin region. The red marks are the original samples while the blue ones are the test samples. One observes that the original and test samples are sparse and well distributed in the whole region of interest. No sample clusters or sample empty regions are observed avoiding bias problems with spatial analyses performed in the sample set.



Figure 4 - Spatial distribution of the CO₂ emission samples in the Negro basin

Figure 5 presents the univariate statistics, along with the histogram, of the CO_2 samples. The similar analyses for the residuals are presented at figure 6.



Figure 5 - Univariate statistics and histogram of the CO₂ emission samples

These residuals were obtained after running the function to remove trends of the SPRING software. The residuals of the CO_2 samples present a distribution closer to the normal one, N(-0.16, 7.84), with a constant mean value closer to value 0 and a standard deviation about 7.84.



Figure 6 - Univariate statistics and histogram of the residuals of CO, emissions

Figure 7 presents the anisotropy detection using a surface semivariogram of the residuals. In this semivariogram it was detected that 45 degrees is more continuous direction while the perpendicular direction, 135 degrees, is less continuous direction.



Figure 8 shows the empirical and the theoretical, fitted, unidirectional semivariograms for the omnidirectional and detected anisotropic directions. All directions were modeled with spherical functions and the individual parameters of each fitted curve are reported in table 1.



Figure 8 - Empirical, and fitted theoretical, semivariograms for the Omni (left), 45° (middle) and 135° (right) directions

			tions	
Direction (degrees)	Model	Nugget Effect Co	Sill C	Range a (meters)
Omni	Spherical	14.7	50.9	6695.3
45°	Spherical	17.8	45.8	9746.4
135°	Spherical	10.9	60.1	5513.5

 Table 1 – Semivariogram parameters for isotropic and two anisotropic directions

Considering the values reported in Table 1, the isotropic semivariogram model $\gamma({\bf h})$ can be represented by the following equation:

$$\gamma(\mathbf{h}) = 14.7 + 50.9 * Sph$$
 (|**h**| /6695.3)

where Sph is the mathematical Spherical function and ${\bf h}$ is the distance vector between any two spatial locations ${\bf u}$ and ${\bf u}+{\bf h}$.

Semivariogram models $\gamma_{45}(\mathbf{h})$ and $\gamma_{135}(\mathbf{h})$, in the directions 45° and 135° respectively, can be individually represented by the following equations:

$$\gamma_{AS}(\mathbf{h}) = 17.8 + 45.8 \text{ sph} (|\mathbf{h}|_{AS}/9746.4)$$

$$\gamma_{125}(\mathbf{h}) = 10.9 + 60.1 * Sph (|\mathbf{h}|_{125} / 5513.5)$$

where: $|\mathbf{h}|_{_{45}}$ and $|\mathbf{h}|_{_{135}}$ are the module values of the distance vector projections in the directions 45° and 135° respectively.

The final anisotropic semivariogram model $\gamma(\mathbf{h})$, built from the combination of the two models above, in directions 45° and 135°, is defined by the following equation:

$$y(\mathbf{h}) = 10.9 + 6.9 * Sph (|\mathbf{h}|_{45} / .000001, |\mathbf{h}|_{135} / 5513.5) + 0.00001$$

 $45.8*Sph(|\mathbf{h}|_{45}/9746.4, |\mathbf{h}|_{135}/5513.5) + 7.4*Sph(|\mathbf{h}|_{45}/100000, |\mathbf{h}|_{135}/5513.5)$

Figure 9 shows kriging maps of CO_2 emissions assessed by the proposed methodology. The resulting models are presented in maps of CO_2 emission values, clipped by the boundaries of the Negro basin, which can be used individually or in spatial modeling for future decision-making activities related to this phenomenon in the Pantanal region. The isotropic map considers that the spatial variation is the same for all directions. The anisotropic map reflects the non omnidirectional spatial behavior that has been previously detected by the surface semivariogram in the CO_2 sample analyses. Qualitative analyses, by visual inspection, of the two maps at figure 9, shows that the anisotropic model represents more faithfully the fact that there is a stronger continuity for the CO_2 in the 45° direction.



To evaluate the accuracy of the isotropic and anisotropic models, in table 2 the numerical results of statistical validations applied to the maps of figure 9 are presented. Three types of validations were considered: cross validation considering the 4601 original samples, used in the interpolations; validation with 1000 CO₂ test samples and validation with all 5601 CO₂, including test plus original samples. The results of validation errors are the statistical measures of Mean, Standard Deviation and the difference between Maximum and Minimum values.

Models	Isotropic (kg/m²)			Anisotropic (kg/m²)		
Type of Validation	Mean Value	Standard Deviation	Maximum- Minimum	Mean Value	Standard Deviation	Maximum- Minimum
Cross- validation	0.003	5.38	88.62	0.001	5.32	87.34
With test samples	-0.018	5.48	73.92	-0.042	5.45	72.13
With all samples	0.019	4.68	73.92	0.010	4.56	72.13

Table 2 - Validations	performed in	n the models	presented in	n Figure 9
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Mean values of table 2 are very close to 0 (zero) showing that both representations, isotropic and anisotropic, do not present a modeling bias. Considering the errors based on the Standard Deviation and on the Maximum-Minimum values of table 2, one observes that the anisotropic modeling presents lower error values than the isotropic one. Although the differences of the error values are low, the quantitative results also show that the anisotropic modeling represents better the behavior of the CO_2 emissions in the Negro River Basin region.

Figure 10 shows the kriging variance maps, considered as uncertainty maps, resulting from the isotropic and anisotropic kriging modeling presented in Figure 9.



Figure 10 - Kriging variance maps of CO_2 emissions: (a) isotropic and (b) anisotropic

A qualitative analyses, by visual comparison, between the maps of figure 10 shows that kriging variance information is better represented by the anisotropic map that takes into account the greater variability in the 45° spatial direction.

Table 3 reports some univariate global statistics of the kriging variance maps of figure 10.

of the variance maps				
	Global Statistics			
Kriging Variance Model	Mean (kg/m²)	Standard Deviation (kg/m²)	Variance (kg/m ²) ²	
Isotropic	49.3	14.9	223.0	
Anisotropic	48.4	14.3	205.0	

Table 3 - Univariate Global Statisticsof the variance maps

This table reports that the global mean, along with the variance and the standard deviation values, are smaller for the model that took into account the anisotropy of the

attribute under study. Therefore this quantitative analyses shows that the global uncertainties, measured by global statistics, are smaller for the anisotropic modeling.

CONCLUSIONS AND SUGGESTIONS

One of the great advantages of using geostatistical approaches, compared with deterministic methods, for example, is that one can determine and consider the isotropic and anisotropic spatial autocorrelation of the attributes that are modeled by directional semivariograms obtained directly from the sample set.

This study suggests the use of anisotropic modeling for the CO_2 emissions in the Negro basin firstly because this type of behavior has been previously detected in the surface semivariogram obtained from the sample set. In addition, the qualitative and quantitative analyses of the resulting maps show that the anisotropic modeling represents better the behavior of the CO_2 emissions in the region under consideration.

The geostatistical module of the SPRING GIS was used successfully to model the distribution of CO_2 emissions in the Negro river basin, considering their isotropic and anisotropic behavior. Also the GIS database facilitates the use of the spatial representations, individually or integrated in spatial models, for decision-making activities related to the phenomenon under study.

The results presented in this paper indicate that this methodology can be applied to model other attributes of the Pantanal region, such as temperature, elevations, soil nutrients, etc. It is intended, in the future, to apply variations of geostatistical approaches, as indicators and regression kriging, in the same $\rm CO_2$ sample set to compare the results with those ones obtained in this work.

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