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Nonlinear Modeling with Sandwich Estimator Approach to Analyze Soil Carbon Profile

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Introduction

Since the 1970s, the city of Paragominas has experienced several changes in land use and become part of the deforestation belt. However, since 2009, integrated production systems have been gaining popularity, grain production has increased, and deforestation has decreased, which makes the city a reference in agriculture and livestock production and awarded it the green city seal in the Amazon. Studying the effects caused by changes in soil use in the Amazon is very important since, in recent years, this region has been an intense agricultural frontier. The implementation of pastures and annual crops led to a significant increase in the removal of natural soil cover as well as high CO_2 emissions in the Amazon region (BRASIL, 2002).

Soil carbon (C) content distribution can be modeled based on measurements over time that assess the chemical kinetics of released carbon. The description of the mineralization process takes into account the simple exponential model with two parameters, namely $\beta 1$ the initial carbon content and $\beta 0$ the mineralization rate (Martines et al., 2006).

In soil carbon mineralization trials, the characteristics inherent to the process may cause issues in data analysis such as non-normal error, variance heterogeneity, and autocorrelation between soil contents along the soil profile. According to Ritz and Streiberg (2008), these issues may be dealt with in two ways. One is based on the use of nonlinear mixed-effects models, which are quite flexible by allowing the variance and covariance matrix structure to be changed. The other approach is based on robust standard error estimates, i.e., sandwich estimators (Zeileis, 2006).

This study aimed to *i*) apply the basis of the nonlinear models theory with least squares method using sandwich estimators to a dataset formed by the C content along the soil profile in the Crop-Livestock-Forest Integration system (ILPF); *ii*) use bootstrap resampling to enhance the precision of the estimates and carbon dynamics along the soil profile.

Material and Methods

The research was carried out at Vitória Farm, located in the city of Paragominas, southeast Pará, Brazil, at the geographic coordinates 2°59′58.37″ SE 47°21′21.29″ W. This study approaches the agrosilvopastoral system established in 2009 with *Khaya ivorensis* A. Chev. and rotation with *Brachiaria ruziziensis* R. Germ Evrard with *Zea mays* L. (corn). Annual crop rotation remained until 2012, after which the area was managed only with pasture and the forest species. Soil was collected in 2013 by opening five trenches (I, II, III, IV, and V) in the study site, in which samples were collected from three walls in the layers 0-10, 10-20, 20-30, 30-40, 40-60, 60-80, and 80-100 cm deep.

The exponential nonlinear model was used to describe the mean behavior of the carbon content responses in the ILPF system. Overall, the C content in the i^{th} sample (subject) at the j^{th} depth of the u^{th} system can be represented by $y_{iju} = \beta_{0u} x_{ij}^{-\beta_{1u}} + \varepsilon_{iju}$, where x_{ij} is the depth of the i^{th} sample (i = 1,..., N) at the j^{th} depth (j = 1, ..., n_i). The poor specification of distribution assumptions (spatial correlation and variance heterogeneity) led to the estimation of the robust variance and covariance matrices called sandwich estimator, implemented in the sandwich package (Zeileis, 2006).

Results and Conclusions

The estimates of the model with and without the sandwich estimator are presented, respectively, in Tables 1 and 2. The corresponding standard errors and p-value significance differ between the approaches presented. For instance, the parameter β_1 (initial carbon content) for the third trench was not statistically significant with the use of the sandwich estimator, whereas this parameter was significant when that estimator was not used. Modeling with no validity of the assumptions lead to inadequate standard errors, Student's t-distribution, p-value, and confidence intervals and, consequently, cause mistaken inferences and decision-making (Table 1).

Table 1. Estimate using the nonlinear model with least squares method with no sandwich estimator.

		Least squares method with no sandwich estimator			
Trench	Parameters	Estimate	Std. Error	Student's t-distribution	*p*-value
I	β_1	-1.1254	0.0555	-20.28	$<2\times10^{-16}$ ***
	β_0	35.9524	1.1466	31.36	$<2\times10^{-16}$ ***
II	β_1	-0.8069	0.0723	-11.17	$<2\times10^{-16}$ ***
	β_0	19.7100	1.1216	17.57	$<2\times10^{-16}$ ***
III	β_1	-0.8886	0.0767	-11.58	$<2\times10^{-16}$ ***
	β_0	20.1946	1.1294	17.88	$<2\times10^{-16}$ ***
IV	β_1	-0.7875	0.0608	-12.95	$<2\times10^{-16}$ ***
	β_0	22.9507	1.1196	20.50	$<2\times10^{-16}$ ***
V	β_1	-1.2150	0.0629	-19.33	$<2\times10^{-16}$ ***
	β_0	34.9525	1.1514	30.36	$<2\times10^{-16}$ ***

Table 2. Estimate using the nonlinear model with least squares method with sandwich estimator.

		Least squares method with sandwich estimator			
Trench	Parameters	Estimate	Std. Error	Student' s t-distribution	*p*-value
I	β_1	-1.1254	0.0794	-14.1790	1.475×10^{-11} ***
	β_0	35.9524	3.2059	11.2140	8.059×10^{-10} ***
II	β_1	-0.8069	0.0485	-16.6220	8.927×10^{-13} ***
	β_0	19.7100	0.6594	29.8890	$< 2.2\times10^{-16}$ ***
III	β_1	-0.8886	0.0558	-15.9350	1.89×10^{-12}
	β_0	20.1946	0.4660	43.3360	$< 2.2\times10^{-16}$ ***
IV	β_1	-0.7875	0.0520	-15.1170	4.802×10^{-12} ***
	β_0	22.9507	0.7697	29.8160	$< 2.2\times10^{-16}$ ***
V	β_1	-1.2150	0.0487	-24.9300	5.609×10^{-16} ***
	β_0	34.9525	0.5486	63.7050	$< 2.2\times10^{-16}$ ***

Bootstrap methods were used to obtain the confidence intervals, using the exponential model with sandwich estimators, and significantly improved the precision and accuracy of the inferences with significantly lower amplitude of the intervals (Table 3). Figure 1 shows the fit of the model's curves to the carbon content observed for each sample.

Table 3. Percentile bootstrap using sandwich estimator.

					IC
Trench	Parameters	Estimate	Std. Error	Median	(LI; LS)
I	β_1	-1.1259	0.0618	-1.1228	(-1.2564; -1.0083)
	β_0	36.0112	1.2476	36.0819	(33.1501; 38.3087)
II	β_1	-0.8099	0.0539	-0.8092	(-0.9198; -0.7066)
	β_0	19.7195	0.8209	19.6945	(18.1812; 21.3417)
III	β_1	-0.8913	0.0620	-0.8895	(-1.0202; -0.7708)
	β_0	20.1946	0.9067	20.3205	(18.1152; 21.6851)
IV	β_1	-0.7903	0.0733	-0.7889	(-0.9303; -0.6475)
	β_0	22.9541	1.3135	22.9725	(20.2676; 25.5094)
V	β_1	-1.2162	0.0513	-1.2135	(-1.3220; -1.1207)
	β_0	34.9470	0.9071	35.1552	(32.9121; 36.2438)

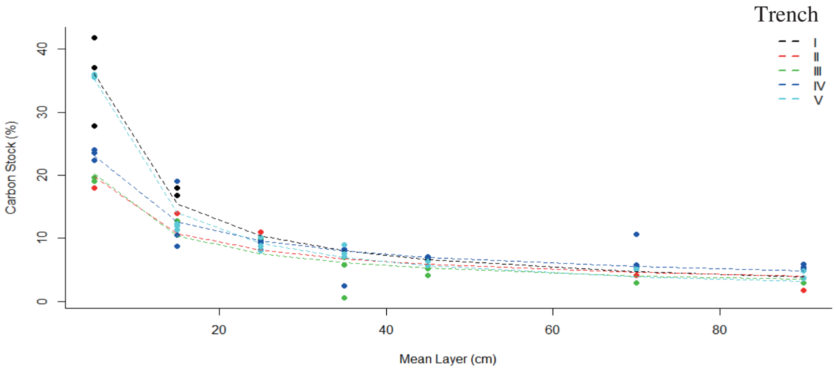

Figure 1. Fit of the nonlinear mixed-effects model using sandwich estimator per trench.

Using bootstrap resamplings in the exponential nonlinear model with the use of sandwich estimators is a viable, more precise and accurate way of spatially estimating soil C content and fits situations such as small samples. Soil organic matter enables high variability in chemical element content in the soil, which impacts the modeling along the profile. Robust methods such as the sandwich estimator have great potential to be applied in this type of study.

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