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Carbon stock and biomass estimate by additive models applied to *Ilex paraguariensis*[1]

Ernandes Macedo da Cunha Neto[2], Gabriel Mendes Santana[2], Emmanoella Costa Guaraná Araujo[3], Hudson Franklin Pessoa Veras[2], Douglas Prado Marcos[4], Flaviana Friedrich[5], Carlos Roberto Sanquetta[2]

ABSTRACT

Ilex paraguariensis is an important non-timber forest product in southern Brazil, where it is cultivated in association with native species, given its demand for shading, which contributes to the conservation and carbon fixation in its biomass. However, determining this biomass is difficult, since the estimates do not guarantee additivity between the compartments and the total aboveground biomass. This study aimed to evaluate additive (seemingly unrelated regression - SUR) and non-additive (ordinary least squares - OLS) biomass models in an *Ilex paraguariensis* stand and comparing its carbon stock with other land use types, consolidating its potential in the face of climate change. A total of 30 trees were cut, compartmentalized and weighed on a digital scale, and four biomass models were adjusted. The carbon stocks were compared with values found in the literature. The bias in the SUR model was less than 2 %, except for the leaves, while the bias in the OLS model varied between 1 and 14 %. The error ranged between 23 and 49 % for SUR, and between 31 and 50 % for OLS. The models adjusted by SUR ensured the accuracy and additivity of the compartments. The *Ilex paraguariensis* stand stored more carbon than agriculture and pasture areas, removing more CO_2, evidencing the sustainability of this system and favoring the climate stability.

KEYWORDS: Yerba mate, greenhouse effect, climate change, non-timber forest products.

RESUMO

Estoque de carbono e modelos aditivos na estimativa da biomassa de *Ilex paraguariensis*

A erva-mate é um produto florestal não-madeireiro importante no Sul do Brasil, sendo cultivada junto com espécies nativas devido à sua necessidade de sombreamento, o que contribui para a conservação e fixação do carbono na sua biomassa. Contudo, a determinação da biomassa é difícil, pois as estimativas não garantem a aditividade entre os compartimentos e a biomassa total acima do solo. Objetivou-se avaliar modelo aditivo (seemingly unrelated regression - SUR) e não aditivo (ordinary least squares - OLS) de biomassa para um povoamento de erva-mate, além de comparar seu estoque de carbono com outros tipos de uso do solo, consolidando o seu potencial frente às mudanças climáticas. Um total de 30 árvores foram cortadas, compartimentadas e pesadas em balança digital, a fim de ajustar quatro modelos de biomassa. Os estoques de carbono foram comparados com valores encontrados na literatura. O viés do modelo SUR foi inferior a 2 %, exceto para as folhas, enquanto, no modelo OLS, variou entre 1 e 14 %. O erro variou entre 23 e 49 % para o SUR e entre 31 e 50 % para o OLS. Os modelos ajustados por SUR garantiram acurácia e aditividade dos compartimentos. O plantio de *Ilex paraguariensis* estocou mais carbono que áreas de agricultura e pasto, removendo mais gás CO_2, evidenciando a sustentabilidade desse sistema e favorecendo a estabilidade climática.

PALAVRAS-CHAVE: Erva-mate, efeito estufa, mudanças climáticas, produtos florestais não-madeireiros.

INTRODUCTION

Ilex paraguariensis is a species popularly known as "yerba mate", native to South America and present in southern Brazil, northeast of Paraguay and Argentina. This plant is widely consumed in the form of non-alcoholic, medicinal, cosmetic and food beverages, conquering market space in more than 130 countries (Cardozo Júnior & Morand 2016). Its production chain moves R$ 2 billion year^{-1}, in Brazil, occupying an area of over 72,000 ha and generating income for more than 30,000 families (IBGE 2017). Thus, *I. paraguariensis* is the second most produced extractive product in Brazil, with revenue only being

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[2] Universidade Federal do Paraná, Departamento de Ciências Florestais, Curitiba, PR, Brasil.
E-mail/ORCID: netomacedo878@gmail.com/0000-0001-6775-0365; gsantanaflorestal@gmail.com/0000-0002-0447-4559; hudsonveras@gmail.com/0000-0002-0203-1914; carlossanquetta@gmail.com/0000-0001-6277-6371.
[3] Universidade Federal de Rondônia, Departamento de Ciências Florestais, Rolim de Moura, RO, Brasil.
E-mail/ORCID: manuguarana@gmail.com/0000-0002-4493-904X.
[4] Administrador de Empresas, Curitiba, PR, Brasil. *E-mail/ORCID*: douglasmarco@gmail.com/0000-0002-8177-3077.
[5] Engenheira Florestal, Curitiba, PR, Brasil. *E-mail/ORCID*: flaviana.friedrich@gmail.com/0000-0002-4509-2880.

surpassed by açaí, but ahead of Brazil nut, pine nut, pequi and palm heart (Alfosin 2021).

The species develops better in the shade, requiring management to be carried out in combination with native tree species, what contributes to the conservation of native forests (Schuhli et al. 2019). Plants can store carbon in biomass and soils, and residues return to the soil, collaborating with the nutrient cycling. Thus, it is important to know the biomass stock of this species, since its contribution to maintain Atlantic Forest fragments and economic value added to the drink derived from leaves are of great importance, especially in the southern region of the country.

Given the cultivation associated with native species, *I. paraguariensis* stands can mitigate climate change, since there is no native forest deforestation for the implementation of the crop and, consequently, no burning, reducing the emission of greenhouse gases. In addition, the *I. paraguariensis* cycle removes CO_2 from the atmosphere, reducing climate change risks.

Determining biomass may be performed by two methods. In the direct or destructive method, trees are cut and their compartments separated and weighed. In the indirect or non-destructive method, allometric equations present in the literature are used, being generated from the data obtained by the direct method (Balbinot et al. 2017). However, there is still no consensus on the best methodology to estimate biomass in native forests, since the calculations still generate controversy and variable estimates (Gatto et al. 2011). Depending on the method used, the same database may generate significantly different results.

Thus, regardless of the method (direct or indirect), the existence of allometric equations is essential, in such a way that they are obtained by regression models that use dendrometric variables collected in the tree measuring process. The models fitting to estimate the biomass is generally carried out independently when modeling the total biomass and the compartments, with one being performed for each compartment of the tree or forest, which generates non-additivity, culminating in different results between the total biomass and compartments. However, there is a growing demand for studies which aim to obtain the additivity of the biomass compartments, in such a way that the sum of these is equal to the total aboveground biomass (Behling et al. 2018, Behling et al. 2019, Behling et al. 2020, Sanquetta et al. 2015).

It is necessary that equations for the different compartments are estimated together to obtain the additivity. As proposed by Zellner (1962), using seemingly unrelated regression (SUR), the simultaneous fitting technique guarantees the additivity of mathematical models (Kozak 1970, Reed & Green 1985). The methodology provides a statistically correlated system of equations, guaranteeing the models' additivity and imposing restrictions on the parameters (Parresol 1999).

It is also necessary that fitted models are mathematically consistent, robust in composing the system of equations and accurate to obtain a set of precise equations (Genet et al. 2011). Generalized additive regression models differ from generalized linear models with regard to the incorporation of non-parametric compartments (Lizzi & Garrido 2020).

Thus, the hypothesis of this study is that the models fitted by seemingly unrelated regression are biologically consistent, thus ensuring the model additivity and providing a greater accuracy in determining the *I. paraguariensis* biomass, which is necessary to quantify the biomass stocks present in the forest. Therefore, it aimed to evaluate the performance of biomass additive and non-additive allometric models in an *I. paraguariensis* stand, as well as to compare the carbon stocks of the stand with other soil use classes (e.g., agriculture and pasture), in order to consolidate its cultivation potential in the face of climate change.

MATERIAL AND METHODS

The study was carried out in an *Ilex paraguariensis* St. Hill. stand of 19 years old, in an area of 16.73 ha, in Canoinhas, Santa Catarina state, Brazil (26º15'26.17"S and 50º33'34.37"W), in October 2020. The climate of the municipality is Cfb (according to the Köppen classification), with average annual temperature of 17 ºC and average annual rainfall of 1,550 mm (Alvares et al. 2013). The predominant soils in the region are Cambiossolos, Neossolos Litólicos, Latossolos and Gleissolos (Almeida et al. 2018), or Cambisols, Leptsols, Ferralsols and Gleysols (Santos et al. 2018).

A total of 30 circular plots of 400 m² were installed and measured. Data for diameter at 1.30 m from the ground, canopy diameter and total height were collected. The trees were subsequently separated into five diameter classes: < 7 cm; 7.1-9 cm; 9.1-11 cm; 11.1-13 cm; and > 13 cm. For determining biomass, six trees per diameter class were felled, totaling 30 trees (Sanquetta et al. 2006). It is worth mentioning that the measurements took place one year after harvesting the leaf biomass of the trees for the *I. paraguariensis* production.

After cutting, the trees had their compartments separated into stem, leaves (re-sprouted) and branches. The compartments were weighed separately on a digital scale with precision of 10 g. Samples with an average weight of 350 g were randomly taken from each compartment to quantify the dry mass in the laboratory. The fresh samples were packed in plastic packages and weighed. After this process, they were placed in kraft paper bags, duly identified and kept in a forced ventilation oven until reaching a constant weight.

The dry biomass of the sample was calculated by determining the dry mass of each sample (ABNT 2017). The dry biomass calculation followed the methodology described by Klock & Andrade (2013) and was extrapolated to the total value of each compartment of the trees weighed in the field, thus obtaining the compartments and total dry biomass.

Four biomass estimation models were fitted using the ordinary least squares (OLS) method: Husch ($w = \beta_0 + \beta_1 d$), Kopezky-Gehrhardt ($w = \beta_0 + \beta_1 d^2$), Spurr ($w = \beta_0 + \beta_1 d^2 h$) and Schumacher-Hall ($w = \beta_0 + \beta_1 ln_d + \beta_2 ln_h$), where: w is the biomass, β the model coefficient, d the diameter and h the tree height. Each model was fitted for the biomass (stem, branches and leaves) and total aboveground biomass compartments.

The models were fitted based on the bootstrap procedure, which performs resampling with replication from the database, maintaining the number of replications and allowing the model fitting in the face of various scenarios, in order to ascertain its sensitivity (Figure 1). Bootstrap tuning was performed in the caret package (Kuhn et al. 2019) in the R programming language (R Core Team 2021). In order to fit the models, 1,000 bootstrap resampling were used.

The models were evaluated by statistical metrics: coefficient of determination (R^2), standard estimate error (SEE), root mean square error (RMSE), bias and Akaike information criterion (AIC). The residual graphic analysis was additionally applied, as well as the Shapiro-Wilk and White tests at 1 % of significance, to verify if the residuals follow a normal distribution and if they are homoscedastic. Moreover, the Chi-squared adherence test was carried out at 95 % of probability to verify if the biomasses estimated by the models are statistically similar to the biomass measured in the field.

The models selected for the stem, branch and leaf compartments were fitted by the seemingly unrelated regression method (SUR), which assumes

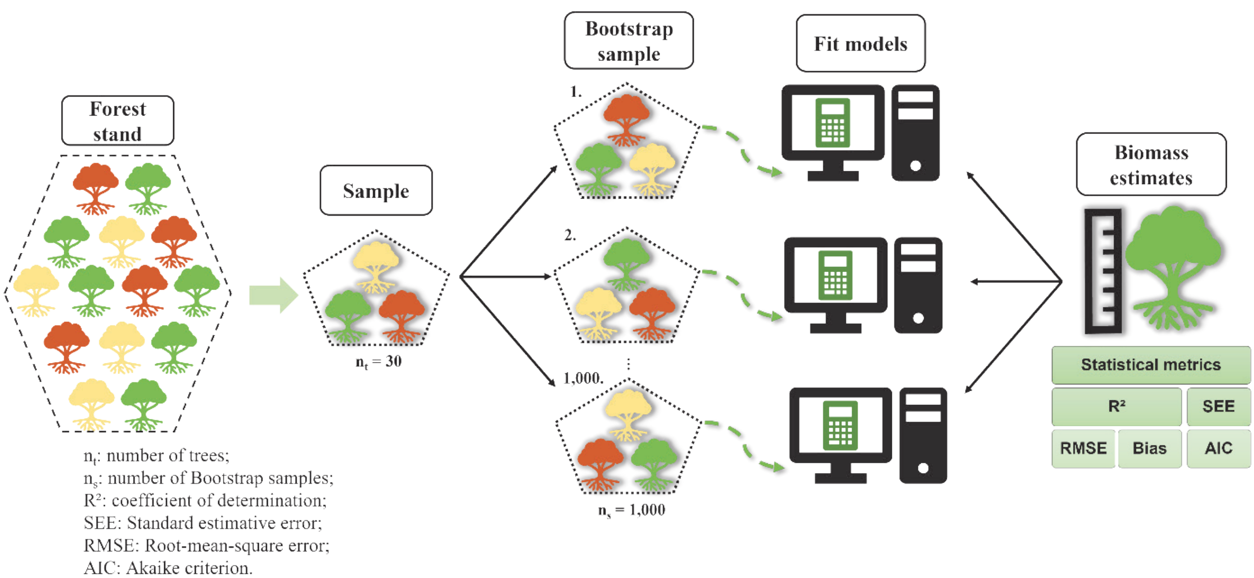

Figure 1. Flowchart of bootstrap samples and fitted models in *Ilex paraguariensis* biomass estimates.

that the estimated total aboveground biomass (AGB) results from the sum of the biomass estimates for each compartment, guaranteeing the additivity of the models and, consequently, their biological consistency. The system of equations was fitted to the systemfit package (Henningsen & Hamann 2007) implemented in the R programming language (R Core Team 2019). As the independent models, the additive model was fitted with 1,000 bootstrap resampling in such a way that the same metrics and statistical tests were applied to evaluate the SUR model.

The *I. paraguariensis* carbon stock was determined as the product of dry mass by the respective carbon content (Marcos et al. 2020). A simulation was performed based on values from the literature for other soil covers (IPCC 2006, Brasil 2010, Albuquerque 2015, Brasil 2016, Brasil 2020). The aboveground biomass was considered for biomass purposes. A 44/12 conversion factor was used to determine the fixed CO_2 equivalent and simulation of the emitted CO_2 equivalent, referring to the ratio between the molecular weight of CO_2 and carbon emissions.

RESULTS AND DISCUSSION

The diameter at breast height, canopy diameter and height showed a low dispersion (standard deviation less than 3) and averages of 9.79 cm (Figure 2a), 1.75 m (Figure 2b) and 3.68 m (Figure 2c), respectively. The stem biomass had an average of 7.66 kg and a standard deviation of 4.36 (Figure 2d), while branches (Figure 2e) and leaves (Figure 2f) had a standard deviation of less than 1.1. The total aboveground biomass (AGB) obtained a standard deviation of 4.12, denoting a high variation (Figure 2g).

A high correlation between crown diameter and branch biomass was observed, while the correlation was inverse between crown diameter and leaves. The crown diameter presented a low correlation with bole and total aboveground biomass (AGB). The diameter at 1.30 m from the ground (diameter at breast height) had a moderate inverse correlation with leaf biomass, low with branch biomass and high with stem biomass and AGB. The height had a low correlation with leaf biomass and low with the other compartments, as well as AGB (Figure 3).

The Spurr model was selected on the independent fitting for stem, branches and AGB. The coefficient of determination (R^2) was higher than 0.60 for the stem, branches and AGB. The dispersion metrics were adequate for the biomass estimate, with a standard estimate error (SEE) of 31.06 % for stem, 36.49 % for branches and 24.76 % for AGB. The model which best fitted the leaf biomass was the Schumacher-Hall (Table 1).

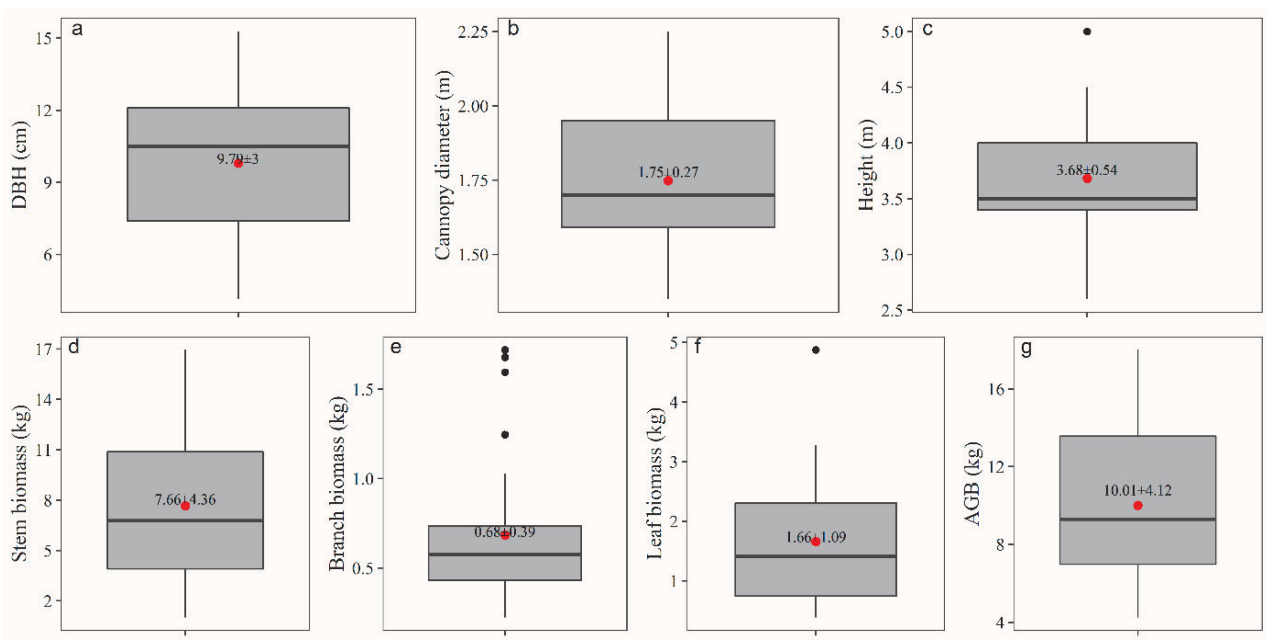

Figure 2. Boxplot of *Ilex paraguariensis* variables and biomass compartments. DBH: diameter at breast height; AGB: aboveground biomass.

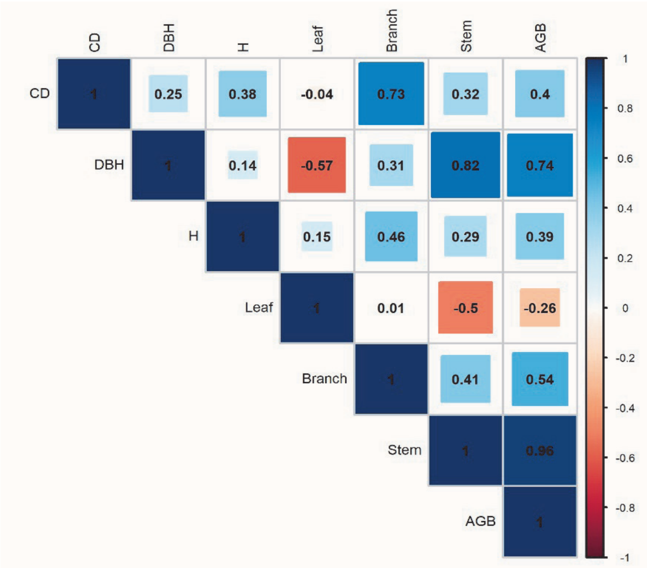

Figure 3. Correlation between *Ilex paraguariensis* variables and biomass compartments. CD: canopy diameter; DBH: diameter at breast height; H: tree height; AGB: aboveground biomass.

The root mean square error (RMSE) obtained similar results to the SEE. The selected models generally tended to underestimate (bias) the observed values (Table 1). The residues from all compartments showed a distribution close to normal at 1 % of significance (Table 1). The residuals of the fitted models showed homoscedasticity according to the White's test at 1 % of significance (Table 1). Statistical similarity was verified between the biomasses estimated by the models and the biomasses measured in the field (Table 1).

The coefficient of determination (R^2) in the SUR method was similar to that of the OLS method. There was a reduction in the SEE and RMSE, in relation to the OLS. The models fitted by the simultaneous fitting methodology obtained slight tendencies to underestimate (bias) the biomass, except for leaves, in which the bias was greater than 10 %. Only the stem biomass and AGB presented similar residual distribution to the normal distribution. The residuals were homoscedastic for all compartments. The total and compartment biomass estimated by the SUR methodology showed no statistical difference with the biomass observed in the field, according to the chi-squared test (Table 2).

The residuals of the independently fitted models (OLS) resulted in dispersion, varying between -3 and 3 deviations for all compartments, resulting in accurate estimates. The dispersion for the model estimated by SUR with homoscedasticity of the residuals obtained better results, which are concentrated close to 0 deviations (Figure 4).

The residuals analysis indicated that the values estimated by SUR are more accurate, in relation to OLS, with dispersion close to the mean line. The stem biomass and AGB showed dispersion close to perfect correlation, evidencing the accuracy of the models. Branches and leaves showed trends in the estimates (Figure 5).

Table 1. Best fit models by the ordinary least squares method to *Ilex paraguariensis* biomass for each compartment.

Compartment	Models	R^2	SEE (%)	RMSE (%)	Bias (%)	AIC	SW	WT	χ^2	β_0	β_1	β_2
Stem	Husch	0.65	33.83	33.63	4.02	144.29	0.080^{ns}	0.894^{ns}	27.11^{ns}	-2.186*	1.804*	-
	Kopezky-Gehrhardt	0.65	33.61	33.61	5.28	143.91	0.614^{ns}	0.003*	27.93^{ns}	1.385*	0.060*	-
	Spurr	0.70	31.06	31.06	1.45	139.17	0.915^{ns}	0.013*	22.93^{ns}	1.336*	0.016*	-
	Schumacher-Hall	0.70	31.02	30.96	3.73	139.09	0.651^{ns}	0.088^{ns}	22.32^{ns}	-3.047*	1.747*	0.764*
Branch	Husch	0.57	37.81	38.60	5.87	6.00	0.023*	0.143^{ns}	2.41^{ns}	-1.815*	2.392*	-
	Kopezky-Gehrhardt	0.57	37.65	37.65	-2.70	5.74	0.310^{ns}	0.060^{ns}	2.56^{ns}	-0.249*	0.298*	-
	Spurr	0.60	36.49	36.49	8.12	3.85	0.397^{ns}	0.015^{ns}	2.37^{ns}	-0.069*	0.064*	-
	Schumacher-Hall	0.60	36.47	37.17	5.37	3.83	0.144^{ns}	0.482^{ns}	2.26^{ns}	-2.673*	2.110*	0.783*
Leaf	Husch	0.34	53.42	55.07	14.30	79.91	0.219^{ns}	0.655^{ns}	22.21^{ns}	2.635*	-1.054*	-
	Kopezky-Gehrhardt	0.33	53.85	53.85	1.14	80.39	0.227^{ns}	0.034^{ns}	23.90^{ns}	2.748*	-0.010*	-
	Spurr	0.25	57.09	57.09	-4.47	83.89	0.154^{ns}	0.085^{ns}	25.54^{ns}	2.553*	-0.002*	-
	Schumacher-Hall	0.41	50.49	52.14	12.99	76.52	0.997^{ns}	0.642^{ns}	19.79^{ns}	1.091*	-1.156*	1.370*
AGB	Husch	0.56	27.21	27.52	3.80	147.23	0.629^{ns}	0.601^{ns}	25.22^{ns}	0.046	0.973	-
	Kopezky-Gehrhardt	0.54	27.95	27.95	-2.37	148.85	0.659^{ns}	0.003*	25.66^{ns}	4.626	0.051	-
	Spurr	0.64	24.76	24.76	1.02	139.60	0.978^{ns}	0.018^{ns}	20.01^{ns}	4.307	0.015	-
	Schumacher-Hall	0.66	23.96	24.28	3.27	141.57	0.380^{ns}	0.238^{ns}	19.74^{ns}	-0.852	0.914	0.796

R^2: coefficient of determination; SEE: standard estimate error; RMSE: root mean square error; AIC: Akaike criterion; SW: p-value of the Shapiro-Wilk test; WT: p-value of the White test; χ^2: chi-square test; β: model's coefficient. * Significant; ^{ns} non-significant.

Table 2. Models fitted by seemingly unrelated regression method to *Ilex paraguariensis* biomass for each compartment.

Compartment	R^2	SEE (%)	RMSE (%)	Bias (%)	SW	WT	χ^2	β_0	β_1	β_2
Stem	0.72	29.82	29.61	0.16	0.101^{ns}	0.039^{ns}	28.14^{ns}	0.907*	0.017*	-
Branch	0.64	34.36	33.71	0.04	0.00004*	0.015^{ns}	1.25^{ns}	0.038*	0.047*	-
Leaf	0.40	49.94	49.83	11.00	0.004*	0.015^{ns}	10.74^{ns}	-0.667*	-1.250*	2.756*
AGB	0.66	23.51	23.34	1.96	0.124^{ns}	0.066^{ns}	19.55^{ns}	-	-	-

R^2: coefficient of determination; SEE: standard estimate error; RMSE: root mean square error; AIC: Akaike criterion; SW: p-value of the Shapiro-Wilk test; WT: p-value of the White test; χ^2: chi-square test; β: model's coefficient; AGB: aboveground biomass. * Significant; ^{ns} non-significant.

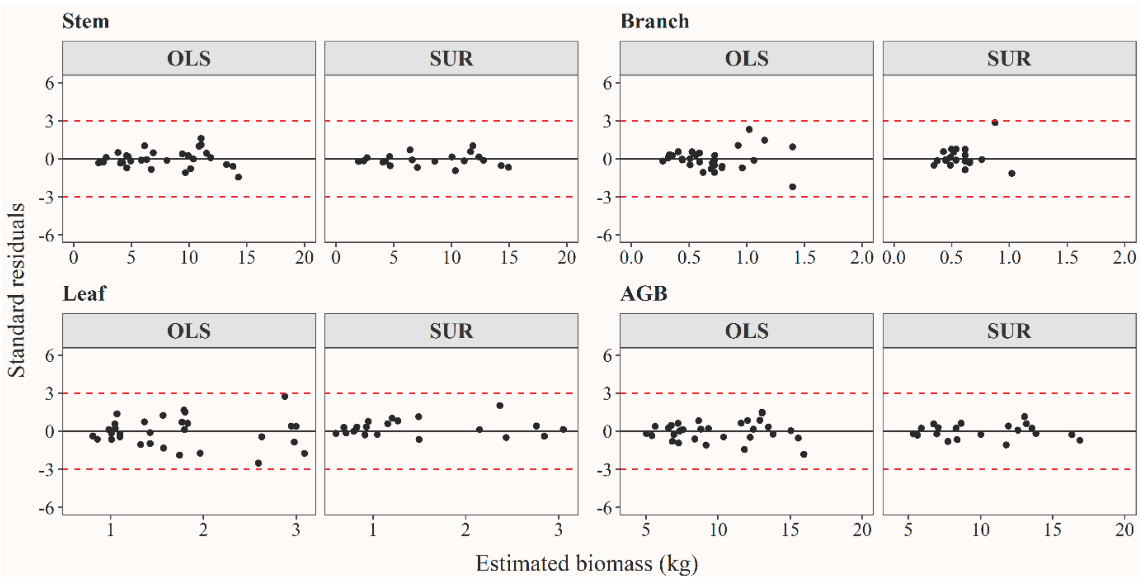

Figure 4. Residuals of the best fitted models in *Ilex paraguariensis* biomass estimates. OLS: ordinary least squares; SUR: seemingly unrelated regression; AGB: aboveground biomass.

The SUR fitted model confirmed additivity in such a way that the sum of all compartments biomass resulted in the total biomass. The independently fitted models using the OLS methodology did not show additivity. The sum of all compartments biomass resulted in differences of up to 2.5 kg with the estimated total aboveground biomass (AGB) (Figure 6).

By comparing the *I. paraguariensis* environment with the forest environment, agriculture and pasture, it was possible to notice that there is CO_2 emission in replacing forest vegetation with *I. paraguariensis* plantations in both the Atlantic Forest and in commercial plantations of forest species in Santa Catarina. However, there is a removal of atmospheric CO_2, when compared to other crops (Table 3).

Despite the low variation in leaf biomass (Figure 1f), this variable obtained a higher SEE for the two estimation methods used in this study, what

Table 3. Carbon stock comparison for different soil uses in the Atlantic Forest and Santa Catarina state, Brazil.

Soil use	t ha^{-1} of C	Stock difference	$CO_{2\,eq}$	$CO_{2\,eq}$ difference	Situation	Source
Ilex paraguariensis stands	18.50	-	67.83	-	-	Marcos et al. 2020
Mixed Ombrophylous Forest	129.63	-111.13	475.31	-407.48	Emission	Brasil 2020
Annual agriculture	3.83	14.67	14.04	53.79	Removing	Brasil 2010
Pasture	2.60	15.90	9.53	58.30	Removing	Albuquerque 2015
Forest stands (Santa Catarina)	64.68	-46.18	237.16	-169.33	Emission	Brasil 2016
Annual agriculture (Santa Catarina)	4.73	13.77	17.34	50.49	Removing	Brasil 2010

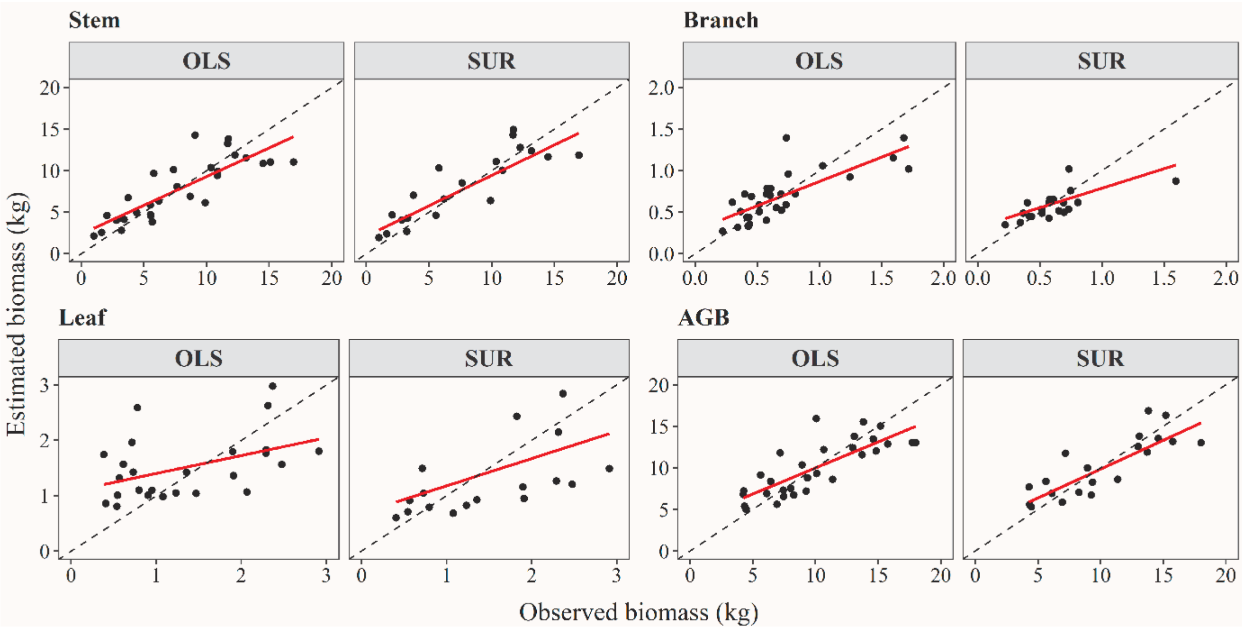

Figure 5. Dispersion of fitted and observed *Ilex paraguariensis* biomass. OLS: ordinary least squares; SUR: seemingly unrelated regression; AGB: aboveground biomass. Red line: dispersion close to the mean line; dashed line: dispersion close to perfect correlation.

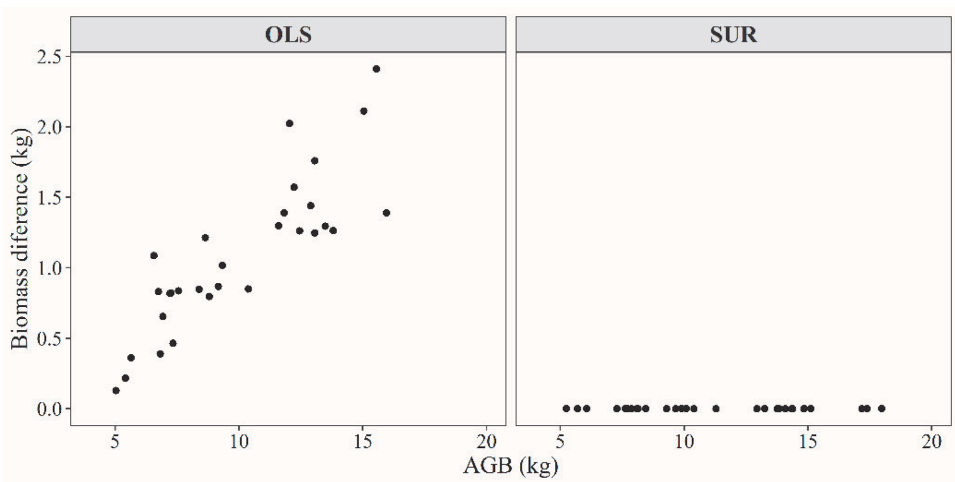

Figure 6. Additive effect in *Ilex paraguariensis* fitted models. OLS: ordinary least squares; SUR: seemingly unrelated regression; AGB: aboveground biomass.

may be related to the low correlation of this variable with the others (Figure 3), as well as the pruning that was applied to this population. According to Poorter et al. (2012), the environmental growth conditions of a plant may directly influence the biomass of the leaf and branch compartments. Thus, *I. paraguariensis* is sensitive to environmental variations, as it is an understory species, directly reflecting on the biomass of the canopy-related compartments.

Comparing the two fitting methods, it is possible to detect that there are no considerable statistical differences between the models. The result infers that the simultaneous fitting method does not have the characteristic of improving the fitting statistics, when compared to the independent fitting method. The exception occurs for the confidence interval statistic, where the simultaneous fitting appears to be more efficient, which, attached to the additivity, provides the method with biological consistency. Similar results were found by Sanquetta et al. (2015) and Behling et al. (2018), working with the NSUR simultaneous fitting method.

The equations fitted by SUR provided consistent biomass estimates for the compartments and total, as well as a smaller confidence interval. Thus, the estimator by the simultaneous method is more efficient, presenting important relevance in the forest area, especially in biomass inventories. This same behavior was observed by Parresol (1999), Carvalho & Parresol (2003) and Sanquetta et al. (2015).

The model statistics obtained a better result for the SUR method, when compared with the OLS methodology (Behling et al. 2018). This is due to the estimator's flexibility in meeting the additivity requirement, ensuring that the sum of the fitted values for the compartments is equal to the estimated value for the total (Reed & Green 1985, Behling et al. 2018, Behling et al. 2019, Behling et al. 2020). The simultaneous fitting is statistically more efficient than the independent fitting, as it produces an estimate with lower variance and considers the interdependence between the compartments' biomass and the AGB (Behling et al. 2018).

Besides, the simultaneous fitting promotes the equations system's biological consistency, since the sum of the compartment biomasses is exactly equal to AGB (Kozak 1970, Chiyenda & Kozak 1984, Parresol 1999, Parresol 2001, Carvalho & Parresol 2003, Sanquetta et al. 2015, Behling et al. 2018). On the other hand, the OLS fitting does not demonstrate biological consistency (Figure 6), what generates inconsistent estimates and changes the forest inventory results, directly inferring the stocks, which will be incorrectly quantified, since there is no biological consistency.

The SUR estimates consider the interdependence of compartments and the allometric relationship among them, favoring the correct quantification of forest biomass stocks. Kozak (1970), Sanquetta et at. (2015) and Behling et al. (2018) emphasize the importance of using additive equations to estimate the compartments and total biomasses.

Despite representing the same type of cultivation, pine and eucalyptus plantations in Santa Catarina represented about 250 % more stocked carbon than the *I. paraguariensis* plantation in this study. This fact may be attributed to the age of the plantations, as well as the species and spacing, what highlights the need for local studies. However, *I. paraguariensis* plantations undergo a constant pruning process, as it is a species cultivated to produce non-timber forest products, in which the main by-product are leaves for tea production.

Additionally, *I. paraguariensis* is not a pure plantation, as it is intercropped with native forest species, and at the time only the *I. paraguariensis* biomass was quantified. This shows the species importance, what contributes to climate resilience in the carbon balance, the sector's productivity and a consequent income of the surrounding population. In addition, it demonstrates the production chain's sustainability, since it maintains native species during its cultivation, being able to mitigate the environmental impacts and climate change in this productive arrangement, when compared to other cultivation types.

CONCLUSIONS

1. The biomass estimates by the seemingly unrelated regression (SUR) method obtained accuracy for determining forest biomass stocks and guarantees the additivity of the compartments (leaves, branches and stem), what did not happen for the ordinary least squares (OLS) method.
2. The *Ilex paraguariensis* stands store more carbon than agriculture and pasture, sequestering more CO_2 than these areas and evidencing the sustainability of this system, and favor the climate stability.

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