Accommodating heteroscedasticity in allometric biomass models

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13 Abstract

Allometric models are commonly used to predict forest biomass. These models typically take nonlinear power-law forms that predict individual tree aboveground biomass (AGB) as functions of diameter at breast height (D) and/or tree height (H). Because the residual variance is in most cases heteroscedastic, accommodating the heteroscedasticity (i.e., heterogeneity of variance) becomes necessary when estimating model parameters. We tested several weighting procedures and a logarithmic transformation for nonlinear allometric biomass models. We further evaluated the effectiveness of these procedures with emphasis on how they affected estimates of mean AGB per hectare and their standard errors for large forest areas. Our results revealed that some weighting procedures were more effective for accommodating heteroscedasticity than others and that effectiveness was greater for single predictor models but less for models based on both D and H. Failing to effectively accommodate heteroscedasticity produced small to moderate differences in the estimates of mean AGB per hectare and their standard errors. However, these differences were greater between model forms (models based on D and H versus models based on D only), regardless of the weighting approach. Similar consequences were observed with respect to whether model prediction uncertainty was or was not included when estimating mean AGB per hectare and standard errors. When including model prediction uncertainty, the standard errors of the estimated means increased

substantially, by 44-59%. Therefore, to avoid possible negative consequences on large-area biomass estimation, we recommend three steps: (i) testing the effectiveness of a weighting procedure when accommodating heteroscedasticity in allometric biomass models, (ii) incorporating model prediction uncertainty in the total uncertainty estimate and (iii) including H as an additional predictor variable in allometric biomass models.

- Keywords: aboveground biomass, allometric model, weighted regression, error propagation,
- 37 homoscedasticity.

1. Introduction

The accuracy and precision of forest biomass estimates play a critical role for the relevance of forests within the climate change mitigation framework (Bonan, 2008; Canadell and Raupach, 2008; Grassi et al., 2017; Pan et al., 2011). Large area forest biomass estimates typically rely on individual tree allometric models constructed using individual tree measurements of aboveground biomass (AGB, kg), diameter at breast height (D, cm) and tree height (H, m) for a sample of trees, hereafter designated the *calibration sample*. Ideally, these trees should be selected from the same population as the population to which the models will be applied, but in practice they are often at least partially selected from outside the population of interest (McRoberts et al., 2016). The models are applied using measurements of a set of individual tree D and H for all trees on a second sample of plots, hereafter designated the *inventory sample*.

By combining the information from the calibration and the inventory samples, the aim is to develop an estimator of mean biomass per hectare for the population of interest which is then converted to carbon estimates using a biomass to carbon conversion factor. Often, the uncertainty associated with the allometric biomass model predictions is ignored with only the sampling variability (i.e., plot-to-plot variability) associated with the probability-based (design-based) estimator reported. In some circumstances, this practice is justified by the insignificant levels of uncertainty associated with the allometric model predictions relative to the sampling variability (McRoberts et al., 2016, 2015; McRoberts and Westfall, 2014). To incorporate the allometric model prediction uncertainty and/or other sources of uncertainty, a "hybrid inference" approach can be used (Condés and McRoberts, 2017; Corona et al., 2014; McRoberts et al., 2019, 2016; Ståhl et al., 2016) to produce more accurate estimates of uncertainty.

Allometric biomass models are often in the form of nonlinear regression models with the power model being particularly popular:

$$AGB_i = \beta_0 \cdot X_i^{\beta_1} + \varepsilon_i \tag{1}$$

where AGB_i is aboveground biomass of the i^{th} tree, X_i is a biomass predictor and ε_i is a random residual term. Diameter at breast height (D) is commonly used as predictor of tree AGB, being used

frequently as the sole predictor (Chave et al., 2005; Forrester et al., 2017; Luo et al., 2020; Picard et al., 2012; Zianis et al., 2005; Zianis and Mencuccini, 2004), or in combination with tree height (H) (Picard et al., 2015, 2012; Zianis et al., 2005). To explain the effects of interspecific variability, wood density may be added as a third predictor variable, especially for the tropical forests (Chave et al., 2014, 2005; Vieilledent et al., 2012). Compared to simple allometric biomass models that use only D as predictor of AGB, including H has improved the fit of the models (Dutcă, 2019; Rutishauser et al., 2013). Although H can be included in the form of D²H, Dutcă et al. (2019) suggested that using D and H as distinct predictor variables should be preferred.

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To ascertain the biological meaning of the scaling exponent β_1 in Eq. (1), Huxley (1932), introduced logarithmic transformations of both response and predictor variables as a way to express the model. Because the residuals associated with allometric biomass model predictions often exhibit heteroscedasticity (i.e. heterogeneity of variance, showing an increase in residual variances with increases in predicted values), logarithmic transformations have been promoted as a way to stabilize the variance, a technique that is widely used nowadays as the default method for fitting allometric models (Asrat et al., 2020; Dutcă et al., 2020, 2018; Luo et al., 2020). With logarithmic transformation, the objective is to obtain a model that has homoscedastic (or relatively homoscedastic) residuals. An advantageous by-product of the transformation is that the model is often linearized which facilitates fitting the model using simpler linear regression rather than nonlinear regression methods. Yet, achieving homoscedasticity and an accurate linear model on the transformed scale is not guaranteed by a ln-ln transformation, thereby leading to an intense debate as to whether logarithmic transformations should or should not be used as the default fitting method (Kerkhoff and Enquist, 2009; Packard, 2014; Packard and Boardman, 2008; Xiao et al., 2011). Nevertheless, the increase in computational power and the widespread availability of nonlinear regression routines in statistical software packages in the last decades has greatly facilitated fitting the models directly in their original untransformed nonlinear forms, thereby avoiding back-transformation correction factors (Baskerville, 1972; Goldberger, 1968; Sprugel, 1983). On the original untransformed scale, a method for accommodating the commonly encountered heteroscedasticity (Cunia, 1964) should be used. In a recent analysis, using both weighted nonlinear regression and logarithmic transformation, Dutcă et al.

(2019) showed that the differences between parameter estimates for the two methods were minor when appropriate weighting for heteroscedasticity was used. However, they concluded that the weighted nonlinear approach is generally more versatile, being able to more easily address different patterns of heteroscedasticity compared to logarithmic transformations which are limited in that sense.

Although ordinary least squares is assumed to be an unbiased estimator for regression model parameters in the presence of heteroscedasticity, it may be a biased and inconsistent estimator of the parameter variance-covariance matrix (Hayes and Cai, 2007; Parresol, 1993; White, 1980). However, Mascaro et al. (2011) showed that the ignoring the heteroscedasticity in allometric biomass models may cause systematic errors in predictions for small trees, because the small variance of small trees means low leverage, if unweighted for heteroscedasticity. It was also shown that ignoring the heteroscedasticity may result in erroneous confidence intervals of estimates (Saint-André et al., 2005), which may further affect the uncertainty of biomass estimates. Nevertheless, it is not well known how ignoring residual heteroscedasticity associated with allometric model may impact the estimates of biomass over large forest areas.

For models with heteroscedastic residual variance such as the allometric biomass models described in Eq. (1), the variance of ε_i is not constant (i.e., $var(\varepsilon_i) \neq \sigma^2$). Therefore, with weighted least squares $var(\varepsilon_i|X_i) = \sigma^2 w_i$, where $w_i \propto \sigma_i^{-2}$ is a function that describes the weight for the ith observation. The weighting function should produce an estimate of the inverse of the variance for the ith observation ($w_i = \hat{\sigma}_i^{-2}$) and should always be positive. Therefore, weighted nonlinear least squares regression allows residuals to have different variances but requires a function to describe the heteroscedastic residual variance.

Multiple weighting functions have been proposed in the literature for allometric models. For example, Cunia (1964) proposed a generic weighting function where the inverse of the predictor variable to the power of 4, $w_i = D_i^{-4}$ or $w_i = (D_i^2 H_i)^{-2} = D_i^{-4} H_i^{-2}$ was used to compensate for heteroscedasticity associated with tree volume model residuals. Other authors suggested $w_i = D_i^{-1}$ or $w_i = D_i^{-2}$ as weighting functions for use with AGB or belowground allometric biomass models (Kralicek et al., 2017). However, these functions with fixed parameters were shown to be

insufficiently flexible to describe the heteroscedasticity for any specific situation (Meng and Tsai, 1986; Williams and Gregoire, 1993). As a result, Meng and Tsai (1986) proposed a method to specifically adjust the weights for each dataset, $w_i = (D_i^{\lambda})^{-2}$ or $w_i = (D_i^{\lambda} H_i)^{-2}$, where λ is estimated using maximum likelihood techniques. Williams and Gregoire (1993) recommended a more general function $w_i = (D_i^{\lambda_2} H_i^{\lambda_3})^{-\lambda_1}$ which suggests that a function of predicted biomass, $w_i = (\widehat{AGB}_i)^{-\lambda_1}$, can work as well, because the predicted AGB is itself a function of predictor variables D and H. A version of a weighting function based on D, $w_i = (D_i)^{-k}$, is widely used (Balboa-Murias et al., 2006; Huff et al., 2018; Huy et al., 2019; Vonderach et al., 2018) where the parameter k can be estimated in many different ways. One way is to estimate the slope of a linear model on the ln-ln scale, predicting $ln(\varepsilon_t)$ where ε are the residuals from an unweighted model, as a function of ln(D_i), where k is the estimated slope (Harvey, 1976; Park, 1966). Another way is to divide the D_i observations into several classes (or groups, D_g) and then estimate the variance of AGB observations within each class (σ_g^2) ; the parameter k is the slope of a linear model that predicts $\ln(\sigma_g^2)$ as a function of ln(D_g) (Picard et al., 2012). Dutcă et al. (2019) used a similar approach but based on predicted AGB instead of D and on variances of residuals within groups from an unweighted model instead of variance of AGB.

In the light of this wide range of choices, selecting a weighting approach can become a rather difficult decision. In this paper we review multiple weighting approaches for nonlinear allometric biomass models and assess their effectiveness for accommodating heteroscedasticity for multiple biomass datasets. Furthermore, using a calibration dataset consisting of measurements of AGB, D and H, coupled with an inventory dataset consisting of measurements of D and H for all trees on plots, we assess the sensitivity of large area biomass estimates to the effects of the following analytical factors: (i) ignoring or dealing with heteroscedasticity, (ii) ignoring or accommodating allometric model prediction uncertainty, and (iii) use of D versus D and H as model predictor variables.

2. Material and methods

2.1. Data

For testing the effectiveness of the weighting approaches, we used six biomass datasets, whereas for assessing the sensitivity of large area biomass estimates to the effects of the weighting approaches we used a biomass calibration dataset to calibrate the models and an inventory dataset to assess the effects on large area estimates.

2.1.1. Biomass datasets for testing the efficiency of weighting approaches

The five biomass datasets used in this study are from different regions of the world (Fig. 1). Dataset 6 consists of the merger of Datasets 1, 3, 4 and 5. Dataset 2 was not included in the merged dataset because it used a different definition for D. For each dataset we fit allometric biomass models that incorporated weighting to accommodate heteroscedasticity, and then tested the effectiveness of the weighting approaches for accommodating heteroscedasticity. Information such as the sample size and the range of D, H, AGB and latitude for the datasets are presented in Table 1.

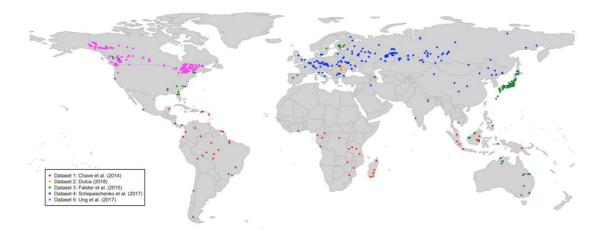


Fig. 1. The distribution of sampling sites by dataset

Table 1 The biomass datasets.

Dataset Species	Latitude range (Deg.)	Sample size	D range (cm)	H range (m)	AGB range (kg)	References
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Dataset 1	Multiple	-24.9, 25.0	4004	5.0-212.0	1.2-70.7	1.2-76063.5	(Chave et al., 2014)
Dataset 2	Norway spruce	45.4, 47.6	240	0.6-10.0*	0.5-5.5	0.1-15.5	(Dutcă, 2018)
Dataset 3	Multiple	-51.6, 62.3	3489	5.0-139.6	1.5-46.5	0.4-16418.4	(Falster et al., 2015)
Dataset 4	Multiple	31.5, 69.9	5144	5.0-72.9	2.3-42.8	0.6-4291.3	(Schepaschenko et al., 2017)
Dataset 5	Multiple	43.9, 64.0	8659	5.0-74.3	2.5-52.2	2.2-2951.4	(Ung et al., 2017)
Dataset 6	Multiple	-51.6, 64.0	21296	5.0-212.0	1.2-70.7	0.4-76 063.5	Datasets 1, 2, 4 and 5

*Dataset 2 (Dutcă, 2018) uses diameter at collar height instead of diameter at breast height.

2.1.2. Data for assessing the sensitivity of large area biomass estimates to the effects of the weighting approaches

To investigate the sensitivity of large area biomass estimates to the effects of methods for accommodating heteroscedasticity, we used a calibration sample to fit the weighted allometric model and then used the resulting model to predict individual tree biomass for trees in the inventory sample.

i) The calibration sample

The calibration sample is a subset of Dataset 4 (Table 1, Schepaschenko et al. 2017), containing data for only Norway spruce trees. The calibration dataset includes measurements of D ranging from 5.0 to 67.6 cm, measurements of H ranging from 4.0 to 42.8 m and measurements of AGB ranging from 4.9 to 3364.2 kg for 503 Norway spruce trees from several European countries.

ii) The inventory sample

The inventory sample consists of measurements of D and H for trees on 243 sample plots from Romania. The inventory dataset was used with the calibration dataset to assess the effects of weighting approaches on large area biomass estimates. The 243 sample plots were selected from the Romanian National Forest Inventory (NFI) and included only Norway spruce trees. Norway spruce is an important species for Romania, often found in pure stands but also in mixtures, covering approximately 1.3 million ha (19% of Romanian forests). Because the Romanian NFI uses a 4 km by 4 km grid-based sampling design in the mountain area where pure Norway spruce grows (Marin et al., 2020), the 243 plots represent 388.8 thousand hectares of forest. The circular sample plots are located at the intersections of the grid lines and have a radius of 12.62 m with an area of 500 m². For each

plot, D and H were measured for all trees with D > 28.5 cm. For a smaller, concentric circular subplot of radius 7.98 m and area of 200 m², D and H were also measured for trees with $5.6 \le D \le 28.5$ cm.

Relationships for datasets with different H-D ratios (H, in m, divided by D, in cm) may require different model forms. Therefore, to ensure a model developed for the calibration dataset is applicable to the inventory data, H-D ratios for the two datasets were compared. Figure 2 shows good agreement between the histogram (i.e., the calibration sample) and the density curve (i.e., the inventory sample).

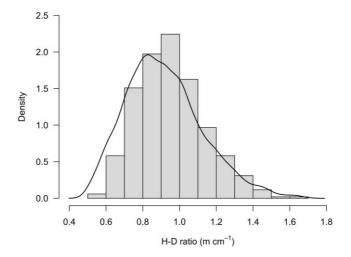


Fig. 2. The distribution of H-D ratio for the calibration sample (histogram) and the inventory sample (density line)

The H-D ratio (in m cm⁻¹) ranged between 0.36 and 2.56 for the calibration sample and between 0.42 and 2.11 for the inventory sample. The ranges of D and H for the inventory and calibration samples were also similar (Table 1 and section 2.1.2), varying between 5.6 to 72.2 cm for D and between 3.1 and 47.5 m for H.

2.2. Statistical analysis

2.2.1. Modelling AGB and heteroscedasticity

We modelled AGB using two allometric biomass model forms:

(a) Using D as the single predictor variable (Asrat et al., 2020):

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$$AGB = \beta_{01} \cdot D^{\beta_{11}} + \varepsilon_1 \tag{2}$$

210 (b) Using both D and H as predictor variables (Dutcă et al., 2019):

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$$AGB = \beta_{02} \cdot D^{\beta_{12}} \cdot H^{\beta_{22}} + \varepsilon_2 \tag{3}$$

where AGB, D, and H are as previously defined; the βs are the model parameters to be estimated; and

 ε_1 and ε_2 are random residual terms. Initially, we fit these models without accommodation for

heteroscedasticity. However, because the residuals for Eq. (2) and Eq. (3) usually exhibit

heteroscedasticity, multiple weighting procedures were considered (Table 2).

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217 Table 2

The weighting procedures tested.

Weighting procedure	Weighting variable	Computation details
For Eqs. (2)	and (3)	
1	$w_i = \frac{1}{D_i}$	The weight of the i^{th} observation (w_i) was calculated as the inverse of diameter (D_i) (Kralicek et al., 2017).
2	$w_i = \frac{1}{{D_i}^2}$	The inverse of $\mathrm{D_{i}}^{2}$ (Kralicek et al., 2017; Meng and Tsai, 1986).
3	$w_i = \frac{1}{{D_i}^4}$	The inverse of D _i ⁴ (Cunia, 1964).
4	$w_i = \frac{1}{D_i^{\lambda}}$	 Prediction of heteroscedastic variance as a function of D. This approach was proposed by (Harvey, 1976; Park, 1966), and consists of multiple steps: (i) fit a nonlinear unweighted model and calculate the squared residual for th ith tree (ê_i²); (ii) ln-ln transform the ê_i² and D_i values; (iii) fit a linear model: ln(ê_i²) = α + λ · ln(D_i) + ε;
		(iv) using the slope λ and D_i to calculate the weight of i^{th} tree.
5	$w_i = \frac{1}{D_i^{\lambda}}$	Prediction of heteroscedastic variance as a function of D, using a grouping approach (Picard et al., 2012): (i) divide the D observations into u classes (u = 5), centred on D _u ; (ii) calculate the variance of AGB for each class (σ_u^2); (iii) ln-ln transform the σ_u^2 and D _u values; (iv) fit a linear model: $\ln(\sigma_u^2) = \alpha + \lambda \cdot \ln(D_u) + \varepsilon$; (v) use the slope λ and D _i to calculate the weight of i th tree.
6	$w_i = \frac{1}{D_i^{\lambda}}$	 Prediction of heteroscedastic variance as a function of D, using a grouping method (McRoberts and Westfall, 2014): (i) fitting an unweighted nonlinear model to data and calculate the heteroscedastic residuals (ê_i); (ii) sort the pairs D_i and ê_i in ascending order with respect to D_i; (iii) group the pairs D_i and ê_i in u groups of size 25; (iv) for each group, calculate the mean of D_i (D̄_u) and the variance of ê_i (σ_u²) (v) In-In transform the σ_u² and D̄_u values; (vi) fit a linear model: ln(σ_u²) = α + λ · ln(D̄_u) + ε; (vii) use the parameter λ and D_i to compute the weight of ith tree.
7	$w_i = \frac{1}{D_i^{\lambda}}$	Prediction of heteroscedastic variance as a function of D, in two stages, and using a grouping method: (i) fit a weighted nonlinear model (using the weights from procedure #6) and calculate the heteroscedastic residuals (ê ₁); (ii) sort the pairs D _i and ê _i in ascending order with respect to D _i ;

- for each group, calculate the mean of D_i ($\overline{D_u}$) and the variance of \hat{e}_i (σ_u^2); (iv)
- (v)
- In-In transform the σ_u^2 and $\overline{D_u}$ values; fit a linear model: $\ln(\sigma_u^2) = \alpha + \lambda \cdot \ln(\overline{D_u}) + \varepsilon$; (vi)
- use the parameter λ and D_i to compute the weight of i^{th} tree.

$$w_i = \frac{1}{\widehat{AGB}_i}^{\lambda}$$

Prediction of heteroscedastic variance as a function of predicted AGB (Dutcă et al., 2019; McRoberts and Westfall, 2014). This is similar to procedure #6, however, predicted AGB is used instead of D as predictor of variance:

- fitting an unweighted nonlinear model to data and calculate the predicted AGB (\widehat{AGB}_i) and the heteroscedastic residuals (\hat{e}_i);
- sort the pairs \widehat{AGB}_i and \widehat{e}_i in ascending order with respect to \widehat{AGB}_i ; (ii)
- group the pairs \widehat{AGB}_i and \hat{e}_i in u groups of size 25; (iii)
- for each group, calculate the mean of \widehat{AGB}_i (\widehat{AGB}_u) and the variance of \hat{e}_i
- In-In transform the σ_u^2 and \overline{AGB}_u values; (v)
- fit a linear model: $\ln(\sigma_u^2) = \alpha + \lambda \cdot \ln(\overline{\widehat{AGB}_u}) + \varepsilon$;
- use the parameter λ and \widehat{AGB}_i (from first step) to compute the weight of ith

$$w_i = \frac{1}{\widehat{AGB}_i^{\lambda}}$$

Prediction of heteroscedastic variance as a function of predicted AGB, in two stages, and using a grouping method:

- fitting a weighted nonlinear model (using the weights from procedure #8) and calculate the predicted AGB (\widehat{AGB}_i) and the heteroscedastic residuals
- (ii) sort the pairs \widehat{AGB}_i and \widehat{e}_i in ascending order with respect to \widehat{AGB}_i ;
- group the pairs \widehat{AGB}_i and \hat{e}_i in u groups of size 25;
- for each group, calculate the mean of \widehat{AGB}_i (\widehat{AGB}_u) and the variance of \hat{e}_i $(\sigma_u^2);$
- In-In transform the σ_u^2 and \widehat{AGB}_u values; (v)
- fit a linear model: $\ln(\sigma_u^2) = \alpha + \lambda \cdot \ln(\overline{\widehat{AGB}_u}) + \varepsilon$;
- use the parameter λ and \widehat{AGB}_i (from first step) to compute the weight of ith

$$10 w_i = \frac{1}{[\exp(\ln(\widehat{AGB})_i)]^2}$$

Using the predicted AGB (from a ln-ln transformed model) as a predictor of heteroscedastic variance:

- fit a linear model on ln-ln transformed data (Eq. 4 or Eq. 5);
- calculate the predicted ln(AGB) of ith tree (i.e. $ln(\widehat{AGB})_i$); (ii)
- calculate the weight of ith tree as the inverse of squared back-transformed AGB. Including the back transformation correction factor (Baskerville, 1972; Goldberger, 1968; Sprugel, 1983) is not necessary since the correction factor is a constant and, therefore, would have a redundant effect.

$$w_i = \frac{1}{{D_i}^4 {H_i}^2}$$

The inverse of squared D²H (Cunia, 1964; Jacobs and Monteith, 1981).

 $w_i = \frac{1}{(D_i^2 H_i)^{\lambda}}$ 12

Prediction of heteroscedastic variance as a function of D²H, using a grouping method:

- fitting an unweighted nonlinear model, $AGB = f(D^2H)$, to data and calculate (i) the heteroscedastic residuals (ê_i);
- sort the pairs D²H_i and \hat{e}_i in ascending order with respect to D²H_i; (ii)
- group the pairs D^2H_i and \hat{e}_i in u groups of size 25;
- (iv) for each group, calculate the mean of $D^2H_i(\overline{D^2H_u})$ and the variance of \hat{e}_i $(\sigma_u^2);$
- fit a nonlinear model: $\ln (\sigma_u^2) = \alpha + \lambda \cdot \overline{D^2 H_u} + \varepsilon;$ (v)
- use the parameter estimate λ to compute the weight of i^{th} tree.

$$w_i = \frac{1}{D_i^{\lambda_1} H_i^{\lambda_2}}$$

Prediction of heteroscedastic variance as a function of D and H, adapted after (Harvey, 1976; Park, 1966):

- fitting an unweighted nonlinear model as in Eq. (3), and calculate the (i) heteroscedastic residuals (ê_i);
- (ii) ln-ln transform ê_i, D and H;

(iii) fit a linear model:
$$\ln(\hat{e}_i^2) = \alpha + \lambda_1 \cdot \ln(D) + \lambda_2 \cdot \ln(H) + \varepsilon$$
;

(iv) use the slopes estimates λ_1 and λ_2 to compute the weight of ith tree.

$$w_i = \frac{1}{D_i^{\lambda_1} H_i^{\lambda_2}}$$

Prediction of heteroscedastic variance as a function of D and H, using a grouping approach:

- (i) fit a linear model to predict ln(AGB) as a function of ln(D) and ln(H);
- (ii) calculate the back transformed predicted AGB using a correction factor: $\widehat{AGB} = \exp(\ln(\widehat{AGB})) \cdot \exp(0.5 \cdot RSE^2)$, where RSE is the residual standard error of the model in ln-ln scale;
- (iii) calculate the heteroscedastic residuals (ê_i) as difference between observed AGB and predicted AGB;
- (iv) sort the triple D_i, H_i and ê_i in ascending order with respect to D_i;
- (v) group the triple D_i , H_i and \hat{e}_i in u groups of size 25;
- (vi) for each group, calculate the mean of D_i $(\overline{D_u})$, mean of H_i $(\overline{H_u})$ and the variance of \hat{e}_i (σ_u^2) ;
- (vii) In-In transform the $\overline{D_u}$, $\overline{H_u}$ and σ_u^2 values;
- (viii) fit a linear model: $\ln(\sigma_u^2) = \alpha + \lambda_1 \cdot \ln(\overline{D_u}) + \lambda_2 \cdot \ln(\overline{H_u}) + \varepsilon$;
- (ix) use the slopes λ_1 and λ_2 to compute the weight of ith tree.

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- In addition to these nonlinear weighting procedures, we also tested the ln-ln transformation as a way
- to accommodate heteroscedasticity. The ln-ln transformed models corresponding to Eq. (2) and (3)
- 222 were:

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$$\ln(AGB) = b_{01} + b_{11} \cdot \ln(D) + \varepsilon_1 \tag{4}$$

$$\ln(AGB) = b_{02} + b_{12} \cdot \ln(D) + b_{22} \cdot \ln(H) + \varepsilon_2 \tag{5}$$

- where ε_1 and ε_2 are random, normally distributed residuals but not the same residuals as for Eq. (2)
- and Eq. (3). When back-transforming Eqs. (4) and (5), the distribution of residuals becomes
- 227 lognormal. Further, back-transforming induces systematic error into predictions on the original scale
- 228 with the result that a correction factor is required. We adopted the correction factor $CF = \exp(0.5 \cdot$
- RSE^2), where RSE is the residual standard error on the ln-ln scale (Baskerville, 1972; Goldberger,
- 230 1968).

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2.2.3. Testing the effectiveness of weighting procedures

- The Breusch-Pagan test is widely used to test for heteroscedasticity in linear models (Breusch and
- Pagan, 1979). We adapted the Breusch-Pagan test for nonlinear weighted models using the following
- 235 steps:
- 236 (i) calculate the weighted residuals, (\widehat{ew}_i) , resulting from the nonlinear model predictions:

$$\widehat{ew}_i = (AGB_i - \widehat{AGB}_i) \cdot \sqrt{w_i} \tag{6}$$

where AGB_i is the observed AGB for the ith tree; \widehat{AGB}_i is the predicted AGB for the ith tree; w_i is the same weight for the ith tree as was used to fit the nonlinear model. For the unweighted model, $\sqrt{w_i} = 1$.

241 (ii) define the auxiliary linear models that predict squared weighted residuals as a function of the predictor variable(s):

$$\widehat{ew}_i^2 = a_1 + b_1 D + \varepsilon \tag{7}$$

$$\widehat{ew}_i^2 = a_2 + b_2 D + c_2 H + \varepsilon \tag{8}$$

245 (iii) retain the R^2 values for these linear models and use them to calculate χ^2 :

$$\chi^2 = n_b \cdot R^2 \tag{9}$$

where, n_b is the sample size of biomass datasets.

(iv) calculate the p-value of the χ^2 statistic, using the right tail of a χ^2 distribution with df = 1 for Eq. 7 and df = 2 for Eq. 8, degrees of freedom. The null hypothesis of homoscedasticity is rejected if p < 0.05.

2.3. Assessing the sensitivity of large area biomass estimates to the effects of the weighting

procedures

To assess the sensitivity of large area biomass estimates to the effects of the weighting procedures we used a probability sample (i.e., the inventory sample) together with a calibration sample (see section 2.1.2). However, because the simple expansion estimator (Cochran, 1977, p.157; Särndal et al., 1992, p.104) is unbiased under the assumption of at most negligible uncertainty in the plot-level AGB values, and because this assumption may or may not be appropriate, depending on the level of uncertainty in the allometric model parameter estimates and residuals, we considered two options when estimating the uncertainty of large area biomass estimates: (i) model prediction uncertainty is ignored (excluded) and (ii) model prediction uncertainty is included.

2.3.1. Ignoring model prediction uncertainty

When the model prediction uncertainty was not included, the AGB of every tree in every plot was predicted based on the parameter estimates of Eq. (2) and Eq. (3), that either included or excluded weighting for heteroscedasticity (Table 2). For the ln-ln transformation approach we used the back transformed prediction from Eq. (4) and Eq. (5). Assuming an equal probability sample, the population mean AGB per hectare ($\hat{\mu}$) and the standard error of the mean (SE($\hat{\mu}$)) were estimated using a simple expansion estimator:

$$\hat{\mu} = \frac{1}{n} \sum_{j=1}^{n} \widehat{AGB}_{j} \tag{10}$$

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$$SE(\hat{\mu}) = \sqrt{\frac{1}{n(n-1)} \sum_{j=1}^{n} (\widehat{AGB}_{j} - \hat{\mu})^{2}}$$
 (11)

where \widehat{AGB}_i is the predicted AGB of the jth plot (j is the plot index); n is the total number of plots.

2.3.2. Assessing the effects of allometric model prediction uncertainty

The simple expansion estimators (Eq. 10 and Eq. 11) were used under the assumption of, at most, negligible uncertainty in the plot-level AGB values. However, because the plot-level AGB values were obtained by summation of within plot individual tree predictions, this assumption may not be reasonable. Therefore, we used a form of "hybrid inference" (Condés and McRoberts, 2017; McRoberts et al., 2019, 2016, 2015; Ståhl et al., 2016) to incorporate both model prediction uncertainty and sampling variability. Because the inventory sample consisted of sample plots for which individual tree biomass was not measured, we used the calibration sample to predict the biomass of the trees inside the plots to obtain plot biomass predictions. However, because the plot biomass was not measured but predicted, we used a Monte-Carlo procedure to propagate uncertainty from model parameter estimates and residuals to large area biomass estimates and their standard errors. Because the variance-covariance matrix for the model parameter estimates is usually based on linear approximations using Taylor series, which may be biased for nonlinear models (McRoberts and Westfall, 2014), we used a bootstrap approach within the Monte Carlo procedure instead of the more commonly used estimated variance-covariance matrix. The following steps describe the Monte-Carlo error propagation procedure:

Step (1) Select a simple random bootstrap resample (using "bootstrap residuals" approach) of trees with replacement from the calibration sample and fit the model using weighted least squares. For the "bootstrap residuals" procedure, we calculated the weighted residuals as in Eq. (6). The vector of weighted residuals was resampled with replacement, to obtain the resampled weighted residuals. The resampled residuals were added to the predicted AGB (obtained from the weighted nonlinear model fitted to the original calibration dataset), to obtain the resampled AGB. The vector of resampled AGB was further merged with the vectors of the two predictor variables, D and H, to form the resampled AGB dataset. A weighted nonlinear model was further fitted to the resampled AGB dataset. For ln-ln transformation (Eqs. 4 and 5), since the transformation is assumed to produce homoscedastic residuals, we resampled the ln-ln transformed dataset and fitted an allometric model (in ln-ln scale) to the resampled dataset.

Step (2) Select a simple random bootstrap resample of plots with replacement from the inventory sample;

Step (3) For every tree on every plot in the inventory sample from step (2):

(3.a) predict the individual tree biomass using the parameters estimated from step (1); (3.b) add a random heteroscedastic residual. A value was randomly selected from a normal distribution N(0, 1), which was truncated to the interval [-3, 3]. The selected random value was further multiplied by the predicted heteroscedastic residual standard deviation. To model the standard deviation of heteroscedastic residuals we used a similar approach to modelling heteroscedasticity (see Table 2).

Step (4) Add the tree-level predictions to obtain plot-level biomass predictions for all plots selected in step (2) and scale the plot-level biomass prediction to a per unit area basis.

Step (5) For the repth repetition, estimate mean AGB per hectare $(\hat{\mu}^{rep})$ and the variance of the mean $(\widehat{\text{var}}(\hat{\mu}^{rep}))$ from the plot-level scaled biomass predictions from step (5):

$$\hat{\mu}^{rep} = \frac{1}{n} \sum_{j=1}^{n} \widehat{AGB}_{j}^{rep}$$
 (12)

where rep is the repetition index, n is the total number of plots (i.e., n = 243), \widehat{AGB}_{j}^{rep} is the predicted AGB of the jth plot scaled to hectare, for repth repetition. The variance of the mean AGB per hectare (i.e., the within simulation variance) was estimated as:

319
$$\widehat{var}(\hat{\mu}^{rep}) = \frac{1}{n(n-1)} \sum_{j=1}^{n} (\widehat{AGB}_{j}^{rep} - \hat{\mu}^{rep})^{2}$$
 (13)

Step (6) Repeat steps (1)-(5) many times ($n_{rep} = 5000$). The population mean AGB per hectare ($\hat{\mu}$), the mean of within simulation variance ($\overline{\widehat{var}(\hat{\mu}^{rep})}$), the between simulation variance ($\widehat{\widehat{var}(\hat{\mu})}$) were calculated as:

323
$$\hat{\mu} = \frac{1}{n_{rep}} \sum_{rep=1}^{n_{rep}} \hat{\mu}^{rep}$$
 (14)

324
$$\overline{\widehat{var}(\hat{\mu}^{rep})} = \frac{1}{n_{rep}} \sum_{rep=1}^{n_{rep}} \widehat{var}(\hat{\mu}^{rep})$$
 (15)

325
$$\widehat{var}(\hat{\mu}) = \left(1 + \frac{1}{n_{rep}}\right) \cdot \frac{1}{n_{rep}-1} \sum_{rep=1}^{n_{rep}} (\hat{\mu}^{rep} - \hat{\mu})^2$$
 (16)

326 Step (7) Replicate steps (1)-(6) until the estimate of mean AGB per hectare (Eq. 14) and the 327 variances presented in Eq. (15) and Eq. (16) stabilize. For each additional replication we calculated the mean of $\hat{\mu}$, mean of $\overline{\widehat{\text{var}}(\hat{\mu}^{\text{rep}})}$ and mean of $\widehat{\text{var}}(\hat{\mu})$ over the executed 328 replications. The replications continued until the largest difference between any two values 329 of means of $\hat{\mathfrak{g}}$, means of $\widehat{\text{var}}(\hat{\mathfrak{g}}^{\text{rep}})$ and respectively means of $\widehat{\text{var}}(\hat{\mathfrak{g}})$, for the last 30% of 330 replications, were less than 5%, however, executing not less than 500 replications. We 331 332 further reported the mean of $\hat{\mu}$ over the stabilization replications (i.e., the stabilized mean) 333 and the standard error of the mean, calculated based on stabilized variances (Eq. 15 and Eq. 334 16):

335
$$SE(\hat{\mu}) = \sqrt{\widehat{var}(\hat{\mu}^{rep}) + \widehat{var}(\hat{\mu})}$$
 (17)

Statistical analysis was performed in R (R Core Team, 2017) with the RStudio interface (RStudio Team, 2016) and using the package 'MASS' (Venables et al., 2002).

3. Results

3.1. Testing weighting procedures

The results of the Breusch-Pagan test for heteroscedasticity are presented in Table 3. When p < 0.05 the null hypothesis of homoscedasticity was rejected, and the residuals were assumed to exhibit heteroscedasticity, whereas when p > 0.05 we assumed homoscedastic residuals. The models that ignored heteroscedasticity (weighting procedure 0, Table 3) produced statistically significant Breusch-Pagan test results for all datasets (and model forms), thereby justifying accommodation for heteroscedasticity.

Table 3
 The Breusch-Pagan test results (p-values of the test), by dataset, model form and weighting procedure.

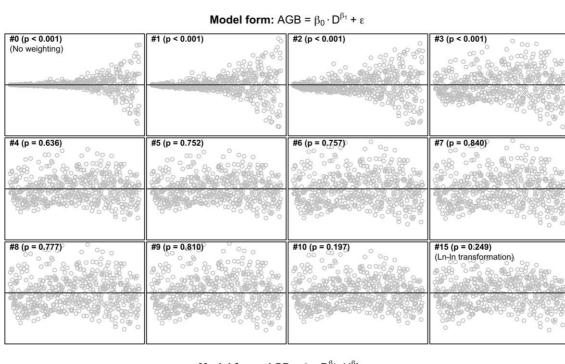
	Weighting	Weighting	Dataset	Dataset	Dataset	Dataset	Dataset	Dataset
Model form	procedure	variable	1	2	3	4	5	6
	O ^a	N.A.	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
	1	D^{-1}	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
	2	D^{-2}	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
	3	D^{-4}	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
	4	$D^{-\lambda}$	< 0.001	< 0.001	< 0.001	0.192	< 0.001	< 0.001
AGB	5	$D^{-\lambda}$	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
$=\beta_0\cdot D^{\beta_1}+\varepsilon$	6	$D^{-\lambda}$	0.151	0.293	< 0.001	0.023	0.602	0.282
	7	$D^{-\lambda}$	0.093	0.412	0.202	0.623	0.519	0.288
	8	$\widehat{AGB}^{-\lambda}$	0.265	0.434	0.720	0.477	0.951	< 0.001
	9	$\widehat{AGB}^{-\lambda}$	0.202	0.649	0.321	0.389	0.970	0.584
	10	$[\exp(\ln(\widehat{AGB}))]^{-2}$	0.014	0.492	0.011	0.029	0.007	< 0.001
	15 ^b	N.A.	< 0.001	0.726	< 0.001	< 0.001	< 0.001	0.681
	Oa	N.A.	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
	1	D^{-1}	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
	2	D^{-2}	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
	3	D^{-4}	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
	4	$D^{-\lambda}$	< 0.001	0.006	< 0.001	< 0.001	< 0.001	< 0.001
	5	$D^{-\lambda}$	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
4.6.0	6	$D^{-\lambda}$	< 0.001	0.010	0.021	0.003	< 0.001	< 0.001
AGB	7	$D^{-\lambda}$	< 0.001	0.126	0.026	0.104	< 0.001	< 0.001
$=\beta_0\cdot D^{\beta_1}\cdot H^{\beta_2}$	8	$\widehat{AGB}^{-\lambda}$	< 0.001	< 0.001	0.034	0.001	< 0.001	< 0.001
+ε	9	$\widehat{AGB}^{-\lambda}$	0.156	0.013	0.001	< 0.001	< 0.001	< 0.001
	10	$[\exp(\ln(\widehat{AGB}))]^{-2}$	< 0.001	0.010	< 0.001	< 0.001	< 0.001	< 0.001
	11	$D^{-4}H^{-2}$	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
	12	$(D^2H)^{-\lambda}$	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
	13	$D^{-\lambda_1}H^{-\lambda_2}$	< 0.001	0.002	< 0.001	< 0.001	< 0.001	< 0.001
	14	$D^{-\lambda_1}H^{-\lambda_2}$	0.376	0.084	0.158	0.141	< 0.001	< 0.001
	15 ^b	N.A.	< 0.001	0.047	< 0.001	< 0.001	< 0.001	< 0.001

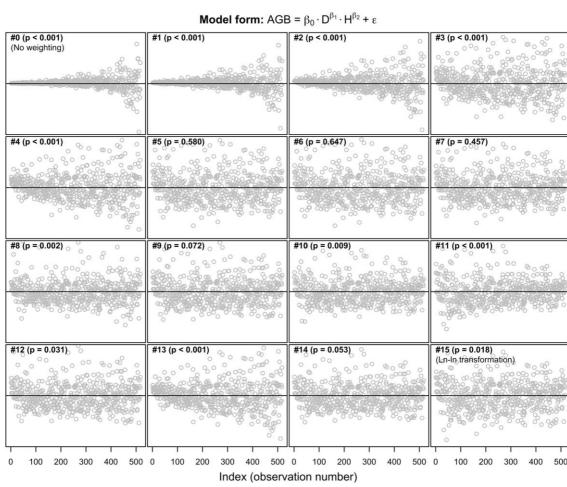
^a No weighting; ^b Ln-ln transformation.

The large number of p-values greater than 0.05 for models based on single predictors (Eq. 2, models based on D only) suggests that the tested weighting procedures are more effective for single predictor models. For the single predictor models, the two weighting procedures that predicted the variance in two stages (procedures 7 and 9), successfully accommodated heteroscedasticity for all datasets. However, for models based on two predictors (Eq. 3), weighting procedure 7 accommodated heteroscedasticity for only three of seven datasets (if including here the calibration dataset, Fig. 3), procedure 9 was effective for only two of seven datasets, whereas procedure 14 that predicts heteroscedastic variance as a function of both D and H was the most effective, accommodating heteroscedasticity for five of seven datasets (Table 3 and Fig. 3).

Logarithmic transformation was not very effective in accommodating heteroscedasticity. For models based on D (Eq. 2), the heteroscedasticity was satisfactorily accommodated for three of seven datasets, whereas for Eq. (3) the ln-ln transformation resulted in statistically significant heteroscedasticity for all datasets (Table 3 and Fig. 3).

For the calibration dataset, the results of the Breusch-Pagan test are presented in Fig. 3, along with the weighted residuals. The residuals were relatively homoscedastic when the p-value was larger than 0.05. It can also be observed that the unweighted residuals (weighting procedure 0, Fig. 3) were heavily heteroscedastic (p < 0.001), with the variance increasing as tree size increased. Moreover, for single predictor models slight systematic lack of fit can be observed but was mostly eliminated by addition of H as a model predictor variable. Logarithmic transformation (i.e., procedure 15, Fig. 3) produced relatively homoscedastic residuals for both model forms, although for models based on both D and H (Eq. 3) the p-value was just below the significance level (p = 0.018) which suggests heteroscedasticity.





Weighted residuals (kg)

Fig. 3. The weighted residuals (expressed in kg) by index of observation for the calibration sample, shown for each model form and each weighting procedure (see Table 2). Note: The labels on y-axis not shown because the range differs by graph.

3.2. The effects of weighting procedures on large area biomass estimates

The large-area biomass estimates were affected by the weighting approach to a moderate degree. For the models of Eq. (2) and Eq. (3), the weighting procedures and the sources of uncertainty considered, the estimates of mean AGB per hectare varied between 177.45 Mg ha⁻¹ and 188.47 Mg ha⁻¹ (Table 4), i.e., with a range of 11.02 Mg ha⁻¹ (i.e., 6.2%). However, this range is less than the 95% confidence interval width estimated using the smallest SE (Table 4) which suggests that these differences are due to random effects rather than any bias in the estimation procedure.

Table 4 Estimates of mean AGB per hectare $(\hat{\mu})$ and the standard error of the estimate of mean $(SE(\hat{\mu}))$, in Mg ha⁻¹, by weighting procedure, excluding, and including model prediction uncertainty, for models based on Eq. (2) and Eq. (3).

	P	redictor varia	ble: D (Eq. 2)		Predictor variables: D and H (Eq. 3)				
Weighting	Excluding	g model	Including model		Excluding model		Including model		
procedure	prediction u	ncertainty	prediction u	ncertainty	prediction uncertainty		prediction uncertainty		
	μ	SE(µ̂)	μ	SE(µ̂)	μ	SE(µ̂)	μ̂	SE(µ̂)	
O ^a	182.13	7.75	183.32	11.23	179.35	8.39	181.50	12.05	
1	183.66	7.76	183.70	11.09	181.17	8.36	183.01	11.93	
2	183.85	7.76	183.33	11.05	182.36	8.28	183.62	11.79	
3	185.38	7.92	185.21	14.99	181.96	8.04	182.24	15.09	
4	187.25	8.04	187.05	11.61	182.41	8.11	182.90	11.58	
5	187.33	8.04	187.11	11.68	180.99	7.94	181.09	11.51	
6	187.64	8.06	187.64	11.69	181.18	7.96	181.29	11.43	
7	187.59	8.06	187.59	11.68	180.88	7.93	180.98	11.41	
8	187.63	8.06	187.63	11.70	180.65	7.90	180.67	11.32	
9	187.60	8.06	187.60	11.69	180.49	7.90	180.52	11.33	
10	188.46	8.11	188.47	12.88	179.76	7.84	179.76	12.25	
11	N.A.	N.A.	N.A.	N.A.	177.45	7.69	177.77	289.32	
12	N.A.	N.A.	N.A.	N.A.	180.39	7.88	180.41	11.31	
13	N.A.	N.A.	N.A.	N.A.	182.41	8.15	183.08	11.66	
14	N.A.	N.A.	N.A.	N.A.	180.21	7.87	180.22	11.31	
15 ^b	188.82	8.13	188.73	11.83	180.08	7.86	179.86	11.28	

^a no weighting, ^b ln-ln transformation

Ignoring heteroscedasticity resulted in estimates of mean AGB per hectare that were slightly different compared to estimates obtained from models calibrated with effective weighting of observations (Table 4). The differences were larger for Eq. (2) (models based on D), as great as 3.7%; therefore, when including H as a predictor variable, the negative effect of ignoring heteroscedasticity on mean AGB per hectare was reduced (differences less than 2.2%). Nevertheless, differences in estimates of mean AGB per hectare between model forms were greater than between weighting

procedures. Models based on D only, regardless of the weighting procedure, produced greater estimates of mean AGB per hectare than did models based on both D and H (Table 4).

The weighting procedures that were effective in accommodating heteroscedasticity (p-values larger than 0.05, Fig. 3) produced more consistent large-area estimates (mean AGB per hectare and SE, Table 4). For example, for models based on D and H to predict AGB, although the largest difference in mean AGB per hectare between any two weighting procedures was 5.6 Mg ha⁻¹ (i.e., weighting procedures 11 and 13, Table 4), the largest difference between any two effective weighting procedures (p > 0.05, see Fig. 3) was 1.1 Mg ha⁻¹ (i.e., procedures 6 and 14, Table 4). Similar results were observed for models based on D only (Table 4).

The estimates of uncertainty were also affected by the weighting procedure. For models based on D only, ignoring heteroscedasticity resulted in a slight underestimation of SEs (compared to uncertainty estimates from models that used weighting procedures effective in accommodating heteroscedasticity), whereas for models based on both D and H, we observed an opposite effect, a slight overestimation of uncertainty (Table 4). There were two weighting procedures (procedures 3 and 11, Table 2) that produced substantially overestimated uncertainty, suggesting that due care is necessary when using fixed-parameter functions to model the standard deviation of heteroscedastic residuals within the Monte Carlo error propagation procedure (see step 3b, section 2.3.2).

3.3. The effects of allometric biomass model prediction uncertainty

We compared the estimates of mean biomass per hectare and of uncertainty when both including and excluding model prediction uncertainty for purposes of assessing the effects of this source of uncertainty. As expected, the estimates of mean AGB per hectare were similar, especially for weighting procedures that were effective in accommodating heteroscedasticity. Differences as great as 1.2% were observed for models ignoring heteroscedasticity or using an ineffective weighting procedure, and as great as 0.1% for models that used effective weighting procedures (Table 4).

Relative to the uncertainty that was due to sampling variability alone (SE, Eq. 11), incorporating the model prediction uncertainty (SE, Eq. 17) resulted in substantial increase of SEs.

For the most effective weighting procedures (p > 0.05, see Fig. 3), when model prediction uncertainty was included, the SE increased by 44.4% to 58.7% for models based on D-only and by 43.6% to 44.9% for models based on both D and H (Table 4). Therefore, the effects of allometric model prediction uncertainty were less when both D and H were used to predict the AGB, because addition of H as predictor variable resulted in a reduction of residual standard error of the model. Nevertheless, for weighting procedures 3 and 11, the differences were substantial (as great as 3661%), given the large overestimation of uncertainty shown earlier.

4. Discussion

We examined weighting approaches for power-law nonlinear allometric biomass models whose prediction residuals exhibit heteroscedasticity. The results showed that some weighting procedures were more effective in accommodating heteroscedasticity than others. In general, the weighting procedures based on fixed parameter functions such as D^{-1} , D^{-2} , D^{-4} or $(D^2H)^{-2}$ were less effective compared to specifically tailored functions (e.g., $D^{-\lambda}$, $\overline{AGB}^{-\lambda}$). In fact, these fixed parameter functions did not produce any p-value larger than 0.05 which, under the Breusch-Pagan test, means effective compensation for heteroscedasticity (see Table 3) for any of the datasets. In addition, some of the fixed parameter functions (e.g., D^{-4} and $(D^2H)^{-2}$) produced serious overestimation of uncertainty. Therefore, we recommend avoiding using fixed parameter functions for weighting the observations in allometric biomass models.

Because heteroscedasticity is evaluated against all predictor variables used in the model, it was expected that for single predictor models the heteroscedasticity will be accommodated more easily compared to models that have two or more predictor variables. For example, in our analysis, given the number of datasets and number of weighting procedures, for models based on D only, heteroscedasticity was adequately accommodated for 33 of 77 cases (Table 3 and Fig. 3), which represents a ratio of 43%. By comparison, for models based on D and H, the heteroscedasticity was adequately accommodated for only 12 out of 105 cases (Table 3 and Fig. 3), which indicates a much smaller rate of just 11%. Modelling heteroscedasticity is challenging because variance can hardly be approximated at the level of individual observations directly, without a grouping of the residuals first. The data are recommended to be first ordered with respect to the model predictor variable in case of a model with only a single predictor variable (which often was D or \widehat{AGB}). The procedure is more complex when two predictor variables are used concomitantly to predict the heteroscedastic variance. We used, however, four procedures that involved both D and H to predict the heteroscedastic variance, of which only one approach was effective. Weighting procedure 14 was effective in five of seven datasets, which is substantial, given the more complex nature of heteroscedasticity in models with two predictors. Nevertheless, because using two or more predictor variables increases the

complexity of the heteroscedasticity models, using just the most significant predictor variable (e.g., D or \widehat{AGB} as predictors of heteroscedasticity) should be preferred.

Both D and \widehat{AGB} can be used as predictors of heteroscedastic variance. Weighting procedures 6 and 8 are similar to procedures 7 and 9, respectively, except procedures 6 and 7 use D to predict heteroscedastic variance, whereas procedures 8 and 9 use \widehat{AGB} . Comparable effectiveness of weighting functions based on D and \widehat{AGB} in compensating for heteroscedasticity was observed with the functions based on D being effective in 16 of 28 cases and functions based on \widehat{AGB} in 15 of 28 cases (Table 3 and Fig. 3). Therefore, either D or \widehat{AGB} can be used as predictor of heteroscedastic variance with good results.

Modelling heteroscedasticity in two stages (modelling the heteroscedasticity resulted from a weighted nonlinear model, as in procedures 7 and 9) produced weights that were more effective in compensating for heteroscedasticity. Procedures 7 and 9 that used two modelling stages were 100% effective for single predictor models (Table 3). The reason two stage modelling was more effective was because the residuals that are modelled should be as similar as possible to those of the weighted model. The residuals resulting from an unweighted nonlinear model can be sometimes slightly different than those resulted from a weighted nonlinear model and, therefore, the group variance is affected, thereby further affecting the parameter estimates for the heteroscedasticity model. Therefore, we recommend using two modelling stages of heteroscedasticity, whenever a single stage modelling is ineffective. Furthermore, it has been shown that weighted power-law nonlinear regression and logarithmic transformation produce similar estimates of model parameters (Dutcă et al., 2019). As a result, logarithmic transformation can be used as a first stage approximation, as it was used in procedure 14, which had the greatest effectiveness (i.e., accommodating heteroscedasticity for five of seven datasets, see Table 3 and Fig. 3) among models based on Eq. (3).

Logarithmic transformation has long been promoted as the standard way to fit allometric models (Chave et al., 2014; Huxley, 1932; Kerkhoff and Enquist, 2009). Ln-ln transformation, besides linearization of the power-law nonlinear model can also possibly serve as a way to accommodate heteroscedasticity. In our application, the residuals became homoscedastic for three of

seven datasets in the case of single predictor models, whereas none of the models based on D and H showed homoscedastic residuals as a result of transformation. However, the logarithmic transformation, although failing to effectively accommodate heteroscedasticity (Fig. 3, procedure 15), produced AGB estimates and SEs that were very similar to those resulting from weighting procedures that satisfactorily accommodated heteroscedasticity (Table 4). As a result, ln-ln transformation can be preferred to other ineffective weighting procedures (Table 3). Nevertheless, we recommend testing the heteroscedasticity of residuals on ln-ln scale before selecting the ln-ln transformation as the method to fit the models.

For weighting procedures that used grouping, the size of the groups when modelling the heteroscedastic variance was an important parameter. We set up the group size to 25, because it was a good compromise: it was large enough so that the group variances can be calculated in good conditions, and small enough to catch most irregularities within the pattern of heteroscedastic variance across the predictor range. However, the group size can be modified by the user to find an accurate pattern of heteroscedasticity for each biomass model. Another important point is that when sample size is small the grouping approach becomes challenging, to the point that if the group sample size is very small, the grouping approach becomes irrelevant. In these conditions logarithmic transformation remains a good compromise that can be used to fit the models.

The model form used to predict the heteroscedastic variance is also important. Our results confirmed that, in general, heteroscedastic variance was well approximated by a power function of the predictor variable (e.g., D or \widehat{AGB}). For some of the weighting procedures we employed the ln-ln transformation instead of nonlinear fitting (see step (vi) of procedures 6-9, Table 2) for two reasons: first, the user can easily check the linear fit by graphing the variables, and second, ln-ln transformation may deal with potential presence of heteroscedasticity within the heteroscedasticity model. Nevertheless, for weighting procedures 6-9 (Table 2) we performed a parallel analysis, using nonlinear models instead of ln-ln transformation approach. When using ln-ln transformation, the mean AGB per hectare varied between 180.49 Mg ha⁻¹ and 181.29 Mg ha⁻¹ (for weighting procedures 6-9, Table 4). Using the nonlinear approach instead of ln-ln transformation, the estimates of mean AGB per hectare were between 175.38 Mg ha⁻¹ and 181.71 Mg ha⁻¹. The estimates of uncertainty were less

affected. Therefore, using ln-ln transformation to model heteroscedasticity gives more consistent estimates, this being the reason we recommend using the ln-ln transformation approach.

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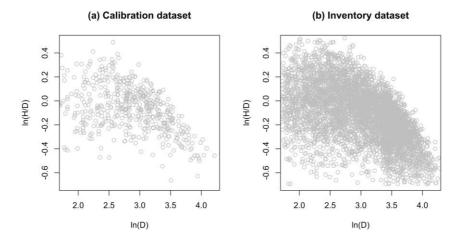
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This general pattern of heteroscedasticity that is often described by a power function explains why logarithmic transformation sometimes produces homoscedastic residuals in allometric models. However, for weighting procedures that used two predictor variables to predict the heteroscedastic variance (e.g., procedure 14) we observed for some datasets a nonlinear relationship on ln-ln scale, between H and the group variance. Consequently, the relationship between heteroscedastic variance and the predictor variables D and H was not well described by a power function. This was observed for Datasets 6 and 7, for which procedure 14 was not effective in accommodating heteroscedasticity. In such cases, more complex functions for predicting heteroscedastic variance may be investigated.

Our results showed a larger difference in estimates of mean AGB per hectare between model forms (Eq. 2 vs. Eq. 3) than between weighting approaches within each model form. This difference could be attributed to two different causes: (i) the effect of including H in allometric models, being shown that addition of H in allometric models would improve the accuracy of AGB prediction, compared to models based on D only (Dutcă, 2019; Dutcă et al., 2020) and (ii) model misspecification as shown in Fig. (3). The models based on D only showed a nonlinear trend in the weighted residuals that disappeared once H was added as predictor variable. This nonlinear trend in the weighted residuals for models based on D only was likely caused by the relationship between D and H, which is reflected by the H-D ratio. Small trees, usually growing in denser stands, with stronger tree competition, exhibit a larger H-D ratio, compared to large trees (Vospernik et al., 2010). However, some of the small trees (i.e., small D) within our calibration dataset showed a comparable H-D ratio to that of large trees (Fig. 4, a). Moreover, it is to be expected that for trees of similar D, a smaller H-D ratio will result in a smaller observed AGB. Therefore, the nonlinear trend in the residuals of models based on D (Fig. 3) was likely caused by a smaller-than-expected H for small trees, reflected in the nonlinear trend of relationship between D and H-D ratio (presented in ln-ln scale, see Fig. 4, a). A similar nonlinear trend was observed for the inventory dataset (Fig. 4, b), confirming the good agreement between the calibration dataset and inventory dataset.



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Fig. 4. The relationship between D and H-D ratio, in ln-ln scale, for the calibration dataset (a) and the inventory dataset (b).

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The differences in estimates of mean AGB per hectare between different weighting approaches were generally small to moderate. For example, using both D and H to predict tree AGB (Eq. 3), the estimates of mean AGB per hectare were 181.50 Mg ha⁻¹ when ignoring heteroscedasticity (approach 0, Table 4) and 181.29 Mg ha⁻¹ for weighting approach 6 which, according to the p-value presented in Fig. 3, can be considered the most effective weighting approach when using Eq. 3. These results suggest a confirmation that ordinary least squares estimators of model parameters are unbiased in the presence of heteroscedasticity (Hayes and Cai, 2007; White, 1980). However, Mascaro et al. (2011) showed that ignoring heteroscedasticity may result in systematic errors in AGB predictions for small trees and, consequently, for plots containing small trees. To investigate this premise, for every tree in the inventory sample (section 2.1.2) we calculated the individual tree prediction differences between the unweighted nonlinear model and model using the weighting approach 6. These differences were then divided by the means of individual tree predictions (two predictions for each tree), to obtain the relative differences of individual tree predictions, as in Bland-Altman plots (Bland and Altman, 1986). In Fig. 5 can be observed that, for small trees, ignoring the heteroscedasticity resulted in underestimation of individual tree predictions as great as 71%, confirming the results of Mascaro et al. (2011). Nevertheless, despite these large relative differences for small trees, the estimates of mean AGB per hectare were barely different (i.e., 181.50 vs. 181.29 Mg ha⁻¹). We suspect that was because the differences in small trees, although

important when judged as relative differences, are negligible in terms of absolute values when compared to estimates of the large trees.

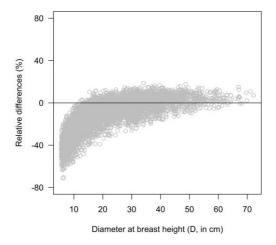


Fig. 5. The relative differences in individual tree predictions when ignoring heteroscedasticity. Note: The relative differences were calculated for each individual tree in the inventory dataset as: $(\widehat{AGB0}_i - \widehat{AGB1}_i)/(\frac{\widehat{AGB0}_i + \widehat{AGB1}_i}{2}) \cdot 100$, where $\widehat{AGB0}_i$ is the predicted AGB of ith tree in the inventory dataset based on unweighted nonlinear model (Eq. 3); $\widehat{AGB1}_i$ is the predicted AGB of ith tree in the inventory dataset, based on Eq. (3) with the weighting approach 6.

For models based on D and H, the coefficient of variation (i.e., SE relative to estimated mean AGB per hectare) was approximately 6.3% when including model prediction uncertainty and approximately 4.4% when ignoring model prediction uncertainty for models that used an effective weighting procedure. Smaller ratios, of approximately 2.6% and 1.9% were reported by McRoberts and Westfall (2014) and McRoberts et al. (2015), but involving a much larger number of plots compared to our study (1074 and respectively 2178 plots, compared to 243 plots used in this study). A comparable ratio of 5.0% was reported by Duncanson et al. (2017) based on 179 sample plots. The uncertainty due to allometric model prediction was not negligible, as has been reported for some studies (Breidenbach et al., 2014; McRoberts et al., 2016, 2015). For this study, this component of uncertainty contributed to an approximate 45% increase in SEs and, therefore, we recommend that it should at least be considered whenever using allometric biomass models.

5. Conclusions

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The conclusions of this study can be summarized as follows:

- 584 (i) We tested several procedures for weighting of observations to accommodate
 585 heteroscedasticity in allometric biomass models. Some weighting procedures were more
 586 effective than others in accommodating heteroscedasticity. For single predictor models,
 587 heteroscedasticity was more effectively accommodated than for models based on D and H.
 588 For models based on D only, weighting procedures 7 and 9 were 100% effective in
 589 accommodating heteroscedasticity; for models based on D and H, procedure 14 was the most
 590 effective.
- 591 (ii) Failing to effectively accommodate heteroscedasticity resulted in small-to-moderate 592 differences of estimates of mean AGB per hectare and of standard errors.
- 593 (iii) Including H as predictor variable in allometric biomass models greatly improved the AGB
 594 prediction. The estimates of mean AGB per hectare and of standard errors were more
 595 seriously affected by omitting H as a predictor of AGB (models based on D and H versus
 596 models based on D only), than by the weighting approach. Therefore, we highly recommend
 597 including H as predictor variable in allometric biomass models.
 - (iv) The standard errors of the estimated mean AGB per hectare increased by 44-59% when model prediction uncertainty was included, therefore, we recommend incorporating model prediction uncertainty in the total uncertainty estimate.
 - (v) We highly recommend testing the efficiency of the weighting procedure by using the adapted Breusch-Pagan test proposed here.

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CRediT author statement:

Ioan Dutcă: Conceptualization, Methodology, Formal analysis, Writing – original draft; Ronald E.

McRoberts: Conceptualization, Methodology, Writing – reviewing and editing; Erik Næsset: Writing

- reviewing and editing; Viorel N.B. Blujdea: Writing – reviewing and editing.

Abbreviations: AGB – aboveground biomass; D – diameter at breast height (1.3 m from the ground); H – tree height; SE – standard error. Funding: This work was supported by a grant of the Romanian Ministry of Education and Research, CNCS—UEFISCDI, within PNCDI III [project number PN-III-P1-1.1-TE-2019-1744, BIOPREDICT]; and by ERA-NET FACCE ERA-GAS and with national support from Romanian National Authority for Scientific Research and Innovation, CCCDI – UEFISCDI [grant number 82/2017, FORCLIMIT project]. FACCE ERA-GAS has received funding from the European Union's Horizon 2020 research and innovation programme [grant agreement 696356].

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