



Rule-based vs parametric approaches for developing climate-sensitive site index models: a case study for Scots pine stands in northwestern Spain

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Abstract

- **Key message** Parametric indirect models derived from stem analysis of dominant trees were more robust than rule-based machine learning techniques for predicting Site Index of Scots pine stands as a function of climate.
- **Context** The uncertainties derived from climate change make it necessary to develop new methods for representing the relationships between site conditions and forest growth.
- **Aims** To compare parametric vs nonparametric approaches for modeling site index (*SI*) of Scots pine stands using bioclimatic variables.
- **Methods** We used Random Forest, Boosted Trees, and Cubist techniques for directly predicting the *SI* of 41 research plots of Scots pine stands, and six parametric models for indirectly predicting *SI* using stem analysis data. As predictors, we used raster maps of 19 bioclimatic variables.
- **Results** The fitted models explained up to ~80% of the *SI* variability, using from five to nine bioclimatic predictors. Though the apparent performance of the parametric models was lower than the rule-based, their bootstrap validation statistics were noticeably higher.
- **Conclusion** Parametric indirect models seemed to be the most robust modeling alternative.

Keywords *Pinus sylvestris* L. · Stand growth modeling · Machine learning · Climate–growth relationships

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1 Introduction

Climate change is presumed to cause a significant impact on forest ecosystems during the XXI century (Kirilenko and Sedjo 2007; Lindner et al. 2008). In recent years, the uncertainties derived from forest growth prediction under climate change have given rise to an intense scientific production. In this regard, the development of growth–environment relationships is a preferred standpoint for adapting traditional empirical growth indicators to a changing climate (Fontes et al. 2010). As site index (*SI*) is the most popular growth indicator for even-aged forest management (Skovsgaard and Vanclay 2008), the development of site index–environment models has become a general research goal (Wang et al. 2004; Seynave et al. 2005; Monserud et al. 2006).

The models developed for this purpose are usually based on the “direct” prediction of *SI* as a function of climatic, edaphic and/or physiographic predictors by means of a certain regression technique. Admittedly, these models have

been increasingly relying on machine learning approaches, which are becoming an attractive modeling alternative since: (1) they provide methods for automatic variable selection, (2) they usually allow for automatically capture nonlinear response–predictor relationships, and (3) some of them allow for automatically model interactions between predictors (González-Rodríguez and Diéguez-Aranda 2020). Reasons (2) and (3) become especially notable when we consider nonparametric learning techniques, such as the “rule-based” approaches, which have become a frequent resource for *SI*-environment modeling (Crookston et al. 2010; Barrio-Anta et al. 2020; Watt et al. 2021).

However, as noted by (Sabatia and Burkhart 2014), there is significant controversy regarding the robustness and interpretability of the rule-based models. Concerning robustness, the high amount of parameters and the model complexity implied by the “nonparametric” approach can be relevant sources of overfitting. Additionally, several authors (Weiskittel et al. 2011; Sabatia and Burkhart 2014) found a significant trend to the observational mean in the predicted values resulting from rule-based *SI*-environment models. These results could be denoting a low extrapolability power for these approaches, which may be a concerning drawback for studies that aim at producing cartographic outputs of forest productivity at regional scales. Concerning interpretability, the model complexity of rule-based approaches may make response–predictor relationships hard to interpret (Aertsen et al. 2010). In this context, using these models for prediction without an adequate interpretation may lead to ecological inconsistencies regarding the theoretical basis of tree growth. Because of these potential disadvantages of rule-based models, parametric approaches that provide similar modeling benefits (automatic variable selection, nonlinear response–predictor relationships and interactions between predictors) have become an attractive line of research in growth–environment relationships modeling (Watt et al. 2015, 2016; Zhu et al. 2019).

Moreover, the observed underperformance of many *SI*-environment models, including rule-based approaches, might not be entirely due to shortcomings in the chosen regression techniques but also to potential inconsistencies between *SI* and the environmental predictors used (as suggested by Bontemps and Bouriaud 2014). These potential inconsistencies might be revealing that the “direct” modeling of *SI* is not really the optimal approach for linking biophysical site attributes with the underlying ecophysiological processes of tree growth. The reason for this might be that the traditional primacy of *SI* as productivity indicator in even-aged forestry responds exclusively to practical reasons (Skovsgaard and Vanclay 2008), as it lacks any direct ecological meaning. For overcoming the uncertainties of predicting *SI*, some studies have successfully modeled it in an “indirect” way, usually relying on other growth indicators or parameters

that have a more sounding ecological background. For instance, Swenson et al. (2005) mapped the *SI* of Douglas-fir forests in the USA as a function of the 3-PG process-based model outputs. In this regard, it is important to note that traditional height growth equations (Hossfeld 1822; Gompertz 1825; Richards 1959) already provide nonlinear parametric forms for describing growth processes over time, which are ecologically meaningful as they rely on theoretical assumptions regarding population dynamics and metabolic ecology. As these nonlinear functions are mainly driven by a certain set of growth parameters, it is reasonable to think that these parameters are significantly correlated with the environmental factors that determine tree growth. Considering that *SI* is an immediate corollary of any age-dependent height growth equation, analyzing the relationships between climate and these growth parameters might be a consistent approach for “indirect” *SI*-environment modeling.

Our primary objective in this study was to test whether *SI* could be effectively predicted using parametric approaches that relate ecologically meaningful parameters from growth equations with climatic factors. For testing this, we compared two different ways of predicting *SI* of Scots pine stands in the northwest of Spain. On the one hand, we performed a direct *SI* prediction using rule-based models, in a similar way to previous studies (Weiskittel et al. 2011; Sabatia and Burkhart 2014; Barrio-Anta et al. 2020). On the other hand, we proposed a new method for developing *SI*-environment models by combining simple parametric models with the nonlinear assumptions behind the Hossfeld growth equation.

2 Materials and methods

2.1 Stand height data

The source of height growth data was a network of permanent research plots established by the Sustainable Forest Management Unit (UXFS) of the University of Santiago de Compostela, Spain. Overall, these plots correspond to pure, even-aged stands of Scots pine (*Pinus sylvestris* L.) located in the provinces of Lugo and Ourense, in the region of Galicia, and consisted of plantations in communal forests mainly located in mountainous sites (Fig. 1). For this study, we used only the first measurements of the network, carried out in 1996–1997, in which stem analyses of dominant trees was carried out for a set 41 of the plots (González-Rodríguez and Diéguez-Aranda 2021).

Diameter at breast height (*dbh*) of all trees and total height were measured in each plot. Core samples were also bored in order to count the growth rings. The stand age (*t*), the number of stems in a hectare (*N*, trees/ha), the basal area (*G*, m²/ha) and the dominant height (*H*, m;

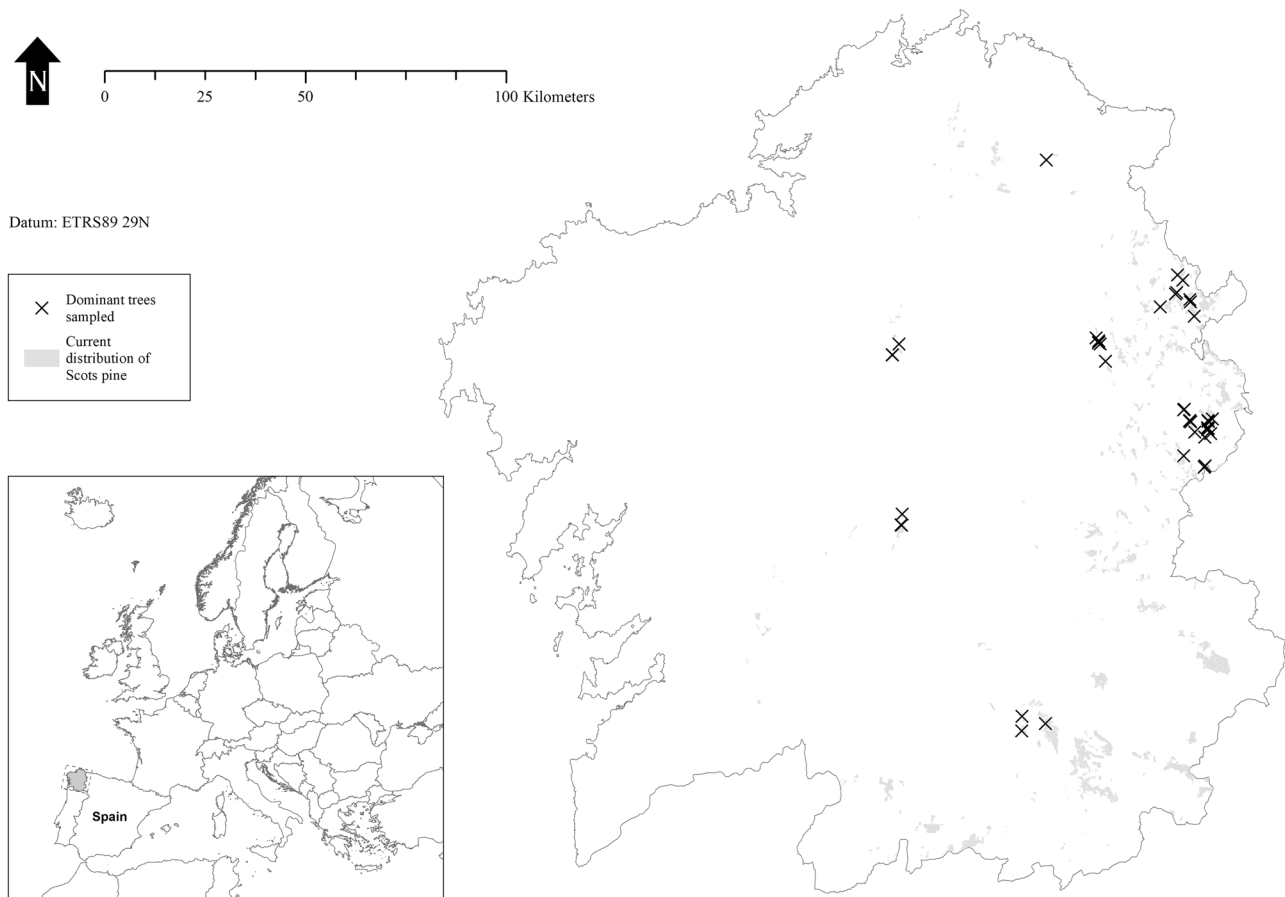


Fig. 1 Geographic extent and locations of the 41 Scots pine inventory plots where dominant trees were sampled

mean height of the 100 largest-*dbh* trees per hectare) were calculated from the previous measurements. A summary of the stand variables of the 41 plots considered in this study is shown in Table 1.

For each plot, the *SI* was estimated using the algebraic difference equation developed by Dieguez-Aranda et al. (2006) for this region, which is based on the Hossfeld growth function (Hossfeld 1822). This was done by projecting the observed dominant height (*H*) at the measurement age (*t*) to the reference age of the species ($t_{ref} = 40$ years):

$$H_2 = \frac{51.39}{1 - \left(1 - \frac{51.39}{H_1}\right) \left(\frac{t_1}{t_2}\right)^{1.277}}, \quad (1)$$

being H_2 the site index when $t_2 = t_{ref}$, $H_1 = H$ and $t_1 = t$.

Stem analyses were carried out following the same procedure described by Dieguez-Aranda et al. (2005a, b). In each of these plots, a subset of two dominant trees per plot (i.e., a total of 82 trees), with heights and diameters differing, respectively, less than 5% to *H* and *D* (dominant diameter of the stand), were destructively sampled. Then, five to ten stem slices per tree were extracted along the trees' height in order to count the growth rings. This allowed for relating tree heights (*h*) with ages (*t*), which were corrected using the method proposed by Carmean (1972) and modified by Newberry (1991). From the *h-t* dataset obtained through stem analysis, we fitted the Hossfeld growth equation for each plot:

$$h(t) = \frac{a}{1 + bt^{-c}}, \quad (2)$$

being *a*, *b* and *c* the growth parameters for each plot.

Table 1 Summary of stand variables for the 41 plot measurements

Variable	Mean	St. dev.	Min.	Max.
<i>t</i> (years)	33	6	19	43
<i>N</i> (trees/ha)	1338	314	720	1984
<i>G</i> (m ² /ha)	34.2	14.6	3.09	74.2
<i>H</i> (m)	12.3	4.11	4.22	21.4
<i>SI</i> (m)	14.7	3.43	8.3	21.4

t stand age, *N* number of stems per hectare, *G* basal area, *H* dominant height and *SI* site index

Once these *basic* parameters were estimated, we calculated another six growth-related derived parameters from Eq. 2: the age, height and growth (t_{ip} , h_{ip} , g_{ip}) at the inflexion point of the $h-t$ curve; and the age, height and growth (t_{mmg} , h_{mmg} , mmg) at the point of maximum mean growth in height. We selected both points in the growth curve because of their potential eco-physiological significance. An example of a fitted growth curve with inflexion and maximum mean growth points represented is shown in Fig. 2. The inflexion point is reached at the age of maximum growth rate, and corresponds to the second derivative of (2). It represents the turning point between “juvenile” growth and “mature” growth. The maximum mean growth occurs at the age when $\frac{d}{dt}\left(\frac{h(t)}{t}\right) = 0$, and represents the moment from which the height/age ratio starts decreasing. The values and the specific methods to calculate each one of the nine alternative growth parameters estimated are summarized in Table 2.

2.2 Climatic data

As a source of climatic data, we used the Worldclim 2 bioclimatic dataset (Fick and Hijmans 2017). This dataset consists of a collection of raster maps with a spatial resolution of 1 km of climatic historical means for the period 1970–2000. The variables included in the maps are 19 bioclimatic indicators often used in species distribution modeling because of its biological significance. Some of them represent annual trends, such as the annual precipitation (*BIO12*), whereas others represent differences between seasons, such as the temperature seasonality (*BIO3*), or extreme climatic events, such as the minimum temperature of the coldest month (*BIO6*). From these raster maps, we extracted the values of the 19 bioclimatic indicators corresponding to the 41 inventory plot locations, so each site was characterized by a *SI* value and a set of potential climatic predictors of forest productivity. A

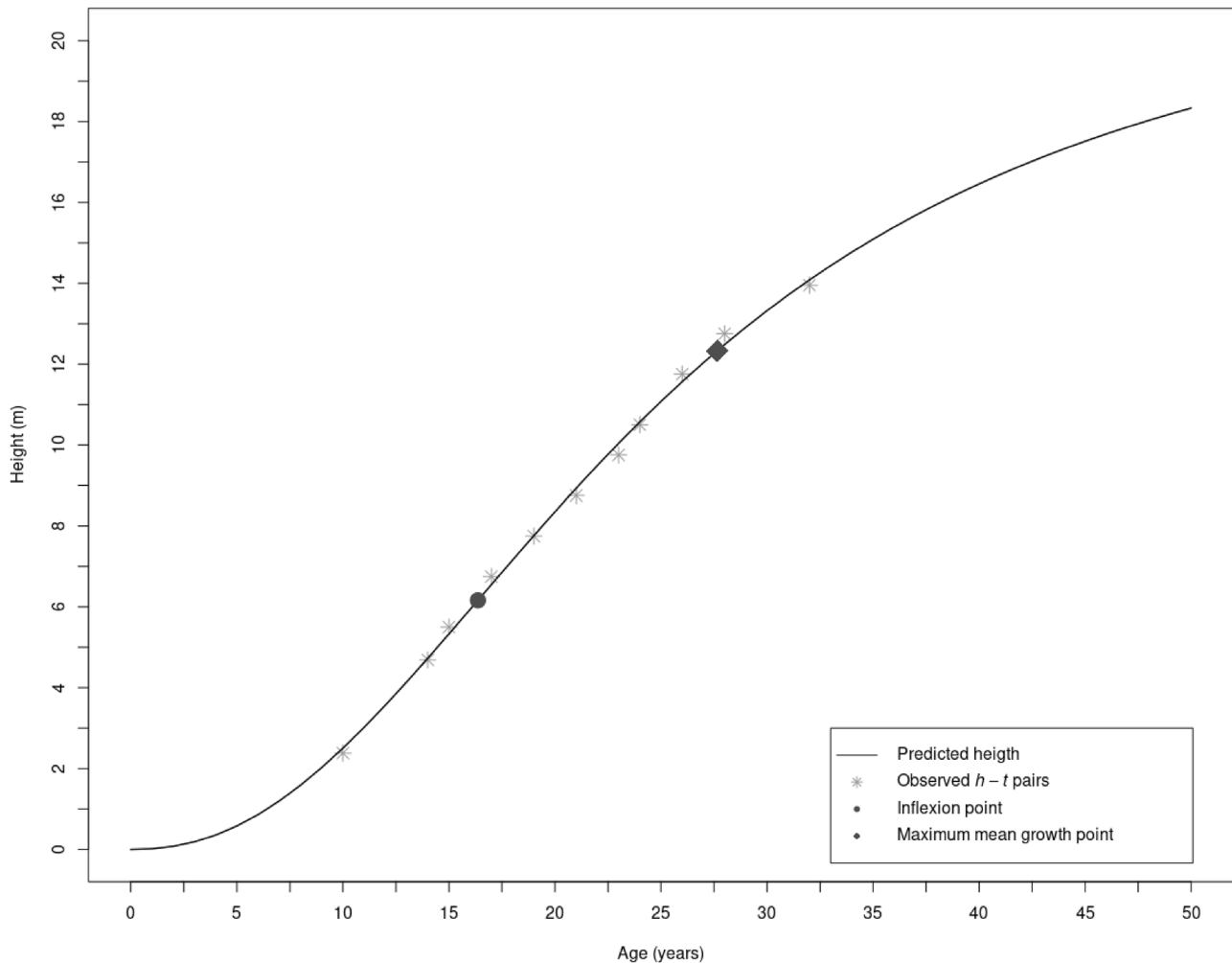


Fig. 2 Scatterplot of observed height vs age for one of the dominant trees included in the stem analysis dataset. The line represents the height predicted by Hossfeld growth equation. Filled markers represent the inflexion and the maximum mean growth points

Table 2 Summary of statistics and calculation methods of the nine growth parameters estimated for the dominant trees of the subset of 41 plots. a , b , and c are the growth parameters from Hossfeld Eq. (2). t_{ip} , h_{ip} and g_{ip} are, respectively, the age, height, and growth rate at the inflexion point in (2) curve. t_{mmg} , h_{mmg} and mmg are the age, height, and growth rate at the maximum mean growth point in (2) curve, respectively

Variable	Calculation method	Mean	St. dev.	Min.	Max.
a	least squares estimate	26.9	8.11	8.39	39.77
b	least squares estimate	473	201	127	798
c	least squares estimate	1.69	0.168	1.32	2.03
t_{ip} (years)	$\left(\frac{2bc}{c+1} - b\right)^{\frac{1}{c}}$	16.03	3.94	8.25	25.003
h_{ip} (m)	$\frac{a}{1+bt_{ip}^{-c}}$	5.26	1.52	2.02	7.97
g_{ip} (m/years)	$\frac{abct_{ip}^{c-1}}{(b+t_{ip}^c)^2}$	0.447	0.108	0.241	0.736
t_{mmg} (years)	$(b(c-1))^{\frac{1}{c}}$	28.8	7.05	14.9	45.4
h_{mmg} (m)	$\frac{a}{1+bt_{mmg}^{-c}}$	10.5	3.04	4.03	15.9
mmg (m/years)	$\frac{a}{t_{mmg}(1+bt_{mmg}^{-c})}$	0.371	0.0915	0.196	0.603

summary of the 19 bioclimatic variables proposed as potential predictors of SI is shown in Table 3.

2.3 SI direct prediction

We used three different rule-based learning techniques for directly relating SI to the bioclimatic predictors: Random

Forest, Boosted Trees and Cubist. The first and second approaches have been successfully used for SI prediction in other studies (Aertsen et al. 2010; Weiskittel et al. 2011; Sabatia and Burkhardt 2014). In contrast, to our knowledge, the Cubist algorithm has never been used before in forest growth modeling. In order to provide a methodological background, we present hereunder a description of the basics and used procedures for fitting these techniques in the current study.

2.3.1 Random forest regression

Random Forest (Breiman 2001) is a rule-based ensemble technique that performs a bagging procedure for developing an unbiased collection of regression trees. At each split of each regression tree, a randomly selected subset of the predictors is used for defining the node, thus granting a unique structure to each tree and avoiding between-tree correlation. This technique has been previously used for SI -environment modeling in other studies (Weiskittel et al. 2011; Sabatia and Burkhardt 2014; Barrio-Anta et al. 2020).

In this work, a Random Forest model was fitted using the R package *randomForest* (Liaw and Wiener 2002). For calibrating the number of trees, we fitted models with trees ranging from 100 to 10000 until we determined that 1000 trees were enough for the model results to be roughly stable, independently on the random seed. We calibrated the predictors' subset size at each split, $mtry$, by trying different values ranging from 1/2 to 1/6

Table 3 Summary of the Worldclim 2 bioclimatic variables corresponding to the 41 Scots pine plot locations considered in this study. $BIO2$ is calculated as the monthly mean of $t_{max} - t_{min}$, being t_{max} and t_{min} respectively the maximum and minimum monthly temperatures. $BIO3$ is calculated as $100 \frac{BIO2}{BIO7}$. $BIO4$ is $100sd_t$, being sd_t the standard deviation of the annual distribution of daily temperatures. $BIO7$ is calculated as $BIO5 - BIO6$. $BIO4$ is the standard deviation of the annual distribution of daily precipitation

Var.	Description	Mean	St. dev.	Min	Max
$BIO1$	Annual Mean Temperature	9.88	0.914	8.14	11.4
$BIO2$	Mean Diurnal Range	8.04	0.393	7.18	8.89
$BIO3$	Isothermality	38.3	1.97	34.2	41.7
$BIO4$	Temperature Seasonality	478	30.3	415	538
$BIO5$	Max. Temperature of Warmest Month	20.2	0.675	18.9	21.8
$BIO6$	Min. Temperature of Coldest Month	-0.842	1.19	-2.77	1.94
$BIO7$	Temperature Annual Range	21.03	0.878	18.6	22.5
$BIO8$	Mean Temperature of Wettest Quarter	5.25	1.21	3.15	7.39
$BIO9$	Mean Temperature of Driest Quarter	15.9	0.636	14.7	17.5
$BIO10$	Mean Temperature of Warmest Quarter	16.11	0.626	14.9	17.5
$BIO11$	Mean Temperature of Coldest Quarter	4.504	1.24	2.34	6.67
$BIO12$	Annual Precipitation	1402	116	1296	1686
$BIO13$	Precipitation of Wettest Month	182	19.3	166	228
$BIO14$	Precipitation of Driest Month	41.5	2.98	31.1	46.5
$BIO15$	Precipitation Seasonality	41.1	2.303	37.3	47.6
$BIO16$	Precipitation of Wettest Quarter	519	49.5	479	638
$BIO17$	Precipitation of Driest Quarter	153	8.27	130	167
$BIO18$	Precipitation of Warmest Quarter	174	11.2	148	198
$BIO19$	Precipitation of Coldest Quarter	492	60.06	442	632

of the total amount of predictors. In order to enhance the stability of these fittings, we performed a repeated tenfold cross-validation. For selecting the least amount of necessary predictors, we carried out a recursive variable elimination (RVE) procedure similar to the one applied by Weiskittel et al. (2011). At each step of this procedure, the least important predictor (measured by the decrease in accuracy due to its removal from the model) was dropped off from the set. Then, a new model with the remaining predictors was fitted. This was repeated until there were only two predictors left. The best alternative along the RVE path was considered to be the one that provided a reasonably high predictive performance, subjected to have the least amount of predictors. The criteria we used for this purpose was to look for the model previous to a significant decrease in R^2 (square of the Pearson's correlation between observed and predicted SI) due to the removal of a certain predictor. Specifically, we selected the model for which dropping off one predictor produced a decrease in R^2 higher than the 90th percentile of all the decreases distribution in the RVE path.

2.3.2 Boosted trees regression

Similarly to Random Forest, Boosted Trees (Valiant 1984) is a rule-based ensemble technique that combines multiple weak learners (regression trees) to enhance performance in the final prediction. Unlike Random Forest, Boosted Trees ensemble is hierarchized, being each additional tree a regressor of predictive residuals of previous trees.

In this study, we fitted a Boosted Trees model using the R package *gbm* (Greenwell et al. 2019). Firstly, we set the optimum values of the calibration constants through a 10 times repeated tenfold cross validation (maximising R^2). These constants were: number of iterations (i.e., number of trees), interaction depth (maximum number of levels of nested nodes in each tree), and shrinkage (penalization applied to each tree's residual prediction). Once the calibration constants were defined, we performed an RVE identical to the one applied to Random Forest for selecting the minimum necessary number of predictors.

2.3.3 Cubist regression

Cubist (Quinlan 1992) is a rule-based technique that performs a boosting-like procedure for enhancing the predictive performance by nestedly re-predicting the residuals throughout a defined number of iterations usually known as "committees". The significant difference with Boosted Trees is that in Cubist the

fitted models for re-predicting residuals are not proper regression trees but a tree-like hierarchized ensemble of linear models. At each tree split, a linear model (which may not include the node predictor) is fitted for predicting the response. As the linear models at the branch ends of trees can make predictions outside the response observed range, a correction factor usually called *extrapolation correction* can be applied for controlling the coherency of the predicted values. For allowing this approach to be comparable to the Random Forest and Boosted Trees fitted models, we set the *extrapolation correction* as a fixed value of 100, which means that the predicted values will be strictly forced to be inside the observational range. Cubist algorithm also includes a nearest-neighbor parameter that allows for correcting each prediction based on similarity to observations used in the training set.

We fitted a Cubist model using the R package *Cubist* (Kuhn and Quinlan 2018). Firstly, we calibrated the number of committees and the number of neighbors for correction through a 10-times repeated 10-fold cross validation (based on R^2 maximization). After this, we performed an RVE procedure similar to the ones applied to Random Forest and Boosted Trees. The importance of each predictor was measured by the usage rate, which indicates the frequency of each predictor as node-ruler or as linear explainer throughout the committees.

The RVE path of the three rule-based models fitted is shown in Fig. 3.

2.4 SI indirect prediction

We proposed an alternative indirect methodology for SI prediction based on multivariate linear models. This methodology consisted of two stages: (1) predicting the nine growth parameters we previously estimated (a , b , c , h_{ip} , t_{ip} , g_{ip} , h_{mmg} , t_{mmg} , mmg) as a function of the WorldClim 2 bioclimatic variables, and (2) to estimate SI as a function of the new climate-sensitive predictions of growth parameters (\hat{a} , \hat{b} , \hat{c} , \hat{h}_{ip} , \hat{t}_{ip} , \hat{g}_{ip} , \hat{h}_{mmg} , \hat{t}_{mmg} , $m\hat{m}g$).

For the first stage, we used stepwise regression technique using the R language package *stats* (R Core Team 2018) for carrying out a generalized least squares coefficients estimation (generalized linear model, GLM) and automatic variable selection. This technique has been recurrently used in forestry, and specifically for SI -environment modeling (Codilan et al. 2015; Tange and Ge 2020). For attaining model parsimony, we used Akaike's information criterion (AIC), so the fitting procedure involved the minimization of the following loss function:

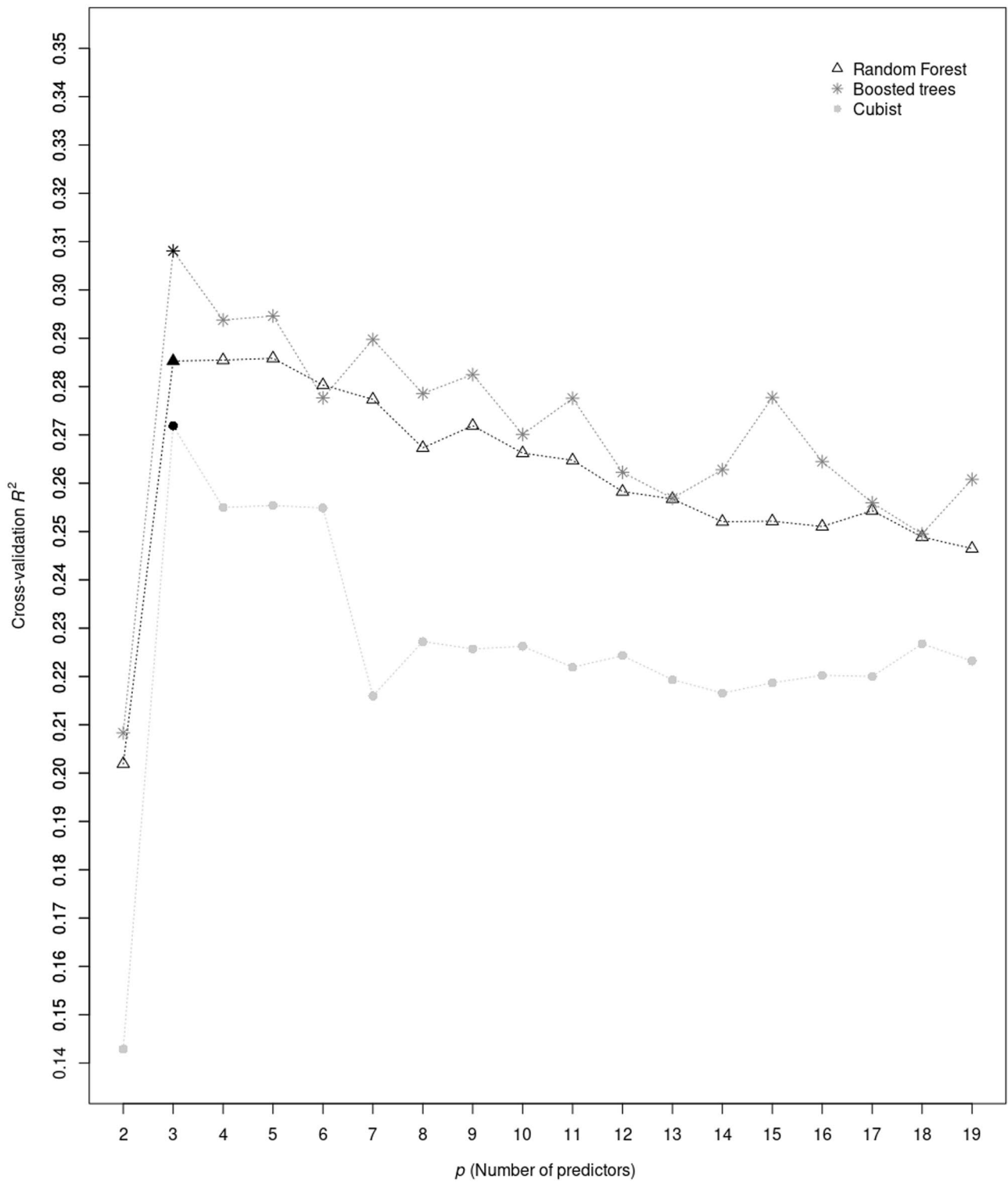


Fig. 3 Recursive variable elimination paths for the three rule-based models fitted

$$AIC = k \cdot p + N \log MSE, \tag{3}$$

being k a penalty p the number of parameters in the model, N the number of observations, and MSE the mean square error. For calibrating k , we used a tenfold cross-validation procedure. Within this procedure, we chose the best k for each case that maximized the R^2 , submitted to provide significant coefficients at a minimum confidence level of 90%.

Regarding the second stage of indirect SI modeling, we developed different transformations derived from Eq. (2) for extracting SI out of the predicted values of the nine alternative growth parameters. From Eq. (2), we can estimate the site index as:

$$SI = \frac{a}{1 + bt_{ref}^{-c}}, \tag{4}$$

being a , b and c the previously fitted parameters for each plot. Considering this, we could also perform an indirect climate-sensitive SI prediction (SI_{abc}) as follows:

$$SI_{abc} = \frac{\hat{a}}{1 + \hat{b}t_{ref}^{-\hat{c}}}, \tag{5}$$

being \hat{a} , \hat{b} and \hat{c} the growth parameters predicted as a function of the bioclimatic explainers.

Combining Eq. (4) with the calculation methods summarized in Table 2 allowed us for predicting SI from different sets of three growth parameters. We accomplished this by isolating a and b parameters from equations in Table 2 and substituting in Eq. (4). As a result, we developed six different methods for estimating SI from the

nine alternative growth parameters predicted, which are summarized in Table 4.

As a “control” method for allowing a reliable comparison between direct rule-based and indirect parametric models, we also fitted a direct stepwise regression (GLM) for predicting SI as a function of the 19 WorldClim predictors using the same procedure described in this section for predicting the nine growth parameters.

2.5 Model evaluation

For testing the robustness of the fitted models we performed a bootstrap validation procedure based on the 632+ rule (Efron and Tibshirani 1997), which we already tested in a previous study (González-Rodríguez and Diéguez-Aranda 2020). We calculated the bootstrap error of each model fitted through a resampling set of 100 realizations per model using the R package boot (Canty and Ripley 2017). Then, we estimated the overall predictive error of each model by doing a weighted mean of statistics between apparent and bootstrap performance:

$$MSE_{632+} = (1 - w)MSE_{training} + wMSE_{bootstrap}, \tag{6}$$

where $MSE_{training}$ is the apparent mean square error (MSE), $MSE_{bootstrap}$ is the mean bootstrap MSE, MSE_{632+} is the corrected MSE, and w is the weight parameter that accounts for the observed relative overfitting and the no information rate (i.e., the potential error if observed and predicted values were completely uncorrelated).

Once we carried out the bootstrap validation, we examined the plots of residuals to detect possible patterns of heteroscedasticity or regression to the mean in the fitted models. In addition, we assessed the role of each predictor within the SI model with the best validation performance in order to evaluate its ecological coherence. Considering the potential difficulty of directly understanding the behaviour of the fitted models, we based our interpretation on the visualization of standardized predictors against predicted SI values. To facilitate this task, we preferred to focus on LOESS fitted curves rather than directly analysing the point clouds. This interpretation method gave us an overview of the role of each predictor throughout the different site conditions that exist in the training dataset.

Table 4 Summary of the equations used for indirectly predicting SI as a function of the ten growth parameters

Model label	Equation	Variables
ABC	$SI_{abc} = \frac{\hat{a}}{1 + \hat{b}t_{ref}^{-\hat{c}}}$	$\hat{a}, \hat{b}, \hat{c}$
IP1	$SI_{ip1} = \hat{h}_{ip} \frac{1 + \frac{1}{2\hat{c}/(\hat{c}+1)-1}}{\frac{\hat{c}^2 t_{ref}^{-\hat{c}}}{1 + \frac{\hat{c}^2 t_{ref}^{-\hat{c}}}{2\hat{c}/(\hat{c}+1)-1}}}$	$\hat{h}_{ip}, \hat{t}_{ip}, \hat{c}$
IP2	$SI_{ip2} = \hat{g}_{ip} \hat{t}_{ip}^{2\hat{c}} \frac{(1 + \frac{1}{2\hat{c}/(\hat{c}+1)-1})^2}{1 + \frac{\hat{c}^2 t_{ref}^{-\hat{c}}}{2\hat{c}/(\hat{c}+1)-1}} \frac{\hat{c}^{2\hat{c}+1}}{2\hat{c}/(\hat{c}+1)-1}$	$\hat{g}_{ip}, \hat{t}_{ip}, \hat{c}$
MMG1	$SI_{mmg1} = \hat{h}_{mmg} \frac{1 + \frac{1}{\hat{c}-1}}{1 + \frac{\hat{c}^2 t_{ref}^{-\hat{c}}}{\hat{c}-1}}$	$\hat{h}_{mmg}, \hat{t}_{mmg}, \hat{c}$
MMG2	$SI_{mmg2} = m\hat{m}g \hat{t}_{mmg} \frac{1 + \frac{1}{\hat{c}-1}}{1 + \frac{\hat{c}^2 t_{ref}^{-\hat{c}}}{\hat{c}-1}}$	$m\hat{m}g, \hat{t}_{mmg}, \hat{c}$
MMG3	$SI_{mmg3} = \hat{h}_{mmg} \frac{1 + \frac{1}{\hat{c}-1}}{1 + \frac{(\hat{h}_{mmg}/m\hat{m}g)^2 t_{ref}^{-\hat{c}}}{\hat{c}-1}}$	$m\hat{m}g, \hat{h}_{mmg}, \hat{c}$

3 Results

A summary of goodness-of-fit statistics for the SI models fitted is shown in Table 5. Regarding model calibration, Random Forest had an optimum mtry value of 2/3 and Boosted Trees had optimum values of 20 for the number

Table 5 Summary of the number predictors and parameters, calibration constants and goodness-of-fit statistics of the models fitted. p is the number of predictors included in the model and R is the relative overfitting rate

Model	R^2	p	Predictors	NRMSE_{632+}	R^2_{632+}	R
GLM	0.414	3	<i>BIO7, BIO8, BIO9</i>	0.259	0.136	0.804
Random Forest	0.802	3	<i>BIO1, BIO2, BIO3</i>	0.216	0.265	0.724
Boosted Trees	0.657	3	<i>BIO1, BIO2, BIO3</i>	0.212	0.268	0.671
Cubist	0.539	3	<i>BIO1, BIO2, BIO3</i>	0.206	0.285	0.535
ABC	0.339	6	<i>BIO4, BIO5, BIO6, BIO7, BIO8, BIO9</i>	0.235	0.203	0.512
IP1	0.372	9	<i>BIO3, BIO4, BIO9, BIO2, BIO7, BIO12, BIO14, BIO18, BIO19</i>	0.205	0.292	0.332
IP2	0.272	9	<i>BIO7, BIO8, BIO9, BIO2, BIO4, BIO12, BIO14, BIO18, BIO19</i>	0.215	0.192	0.311
MMG1	0.384	5	<i>BIO3, BIO4, BIO9, BIO2, BIO7</i>	0.204	0.298	0.313
MMG2	0.351	5	<i>BIO7, BIO8, BIO9, BIO2, BIO4</i>	0.223	0.187	0.581
MMG3	0.375	5	<i>BIO7, BIO8, BIO9, BIO3, BIO4</i>	0.218	0.219	0.529

of iterations (trees), one for the interaction depth and 0.1 for the shrinkage penalization. The optimum constants for the Cubist model where 20 committees and nine neighbors for correction. The parameter estimates and p values of the stepwise models fitted for predicting the nine growth parameters are presented in the Appendix (Table 6). All the slope parameters estimated for these models were significant at least at 95% level of confidence. The average amount of predictors per models was three, having a maximum of seven for the t_{ip} model and a minimum of zero for the c model, which resulted a null model.

Concerning model performance, the rule-based approaches provided the highest apparent values of R^2 , having the Random Forest model the best performance ($R^2=0.802$), followed by Boosted Trees and Cubist. In contrast, the indirect parametric models had significantly smaller values of apparent R^2 , with a maximum value of 0.384 for the case of MMG1. The direct GLM had apparent performance slightly higher than MMG1 ($R^2=0.414$), but much lower than the rule-based approaches. Overall, the models fitted had a number of predictors ranging from five (MMG1, MMG2, MMG and Boosted Trees models) to nine (IP1, IP2 models). Considering our variable selection criterion, the three rule-based models fitted reached the maximum cross-validated performance using three predictors, which were, in all cases, *BIO1*, *BIO2* and *BIO3*. The AIC-based variable selection for the direct GLM also produced an optimum number of predictors equal to three, which were *BIO7*, *BIO8*, *BIO9*.

Concerning bootstrap validation, rule-based models presented a very high relative overfitting rate, ranging from 54% to 72%. Among these models, Cubist resulted in the model with the best performance both in NRMSE_{632+} (0.206) and R^2_{632+} (0.285) and also with the

lowest relative overfitting rate (54%). The direct GLM seemed extremely prone to overfitting, with a very low validation performance ($R^2_{632+} = 0.136$) and a relative overfitting rate reaching 80%. In comparison, the fitted indirect parametric models produced more variable bootstrap performances, with R^2_{632+} values ranging from 0.187 to 0.298, and relative overfitting rates (R) ranging from 0.311 to 0.581. Models ABC, MMG2, and MMG3 produced low performances but also had very high overfitting rates. Model IP2 had a poor apparent performance but also showed a low relative overfitting rate. Models MMG1 and IP1 were the ones with the best overall bootstrap performance, presenting a high R^2_{632+} , a low NRMSE_{632+} and a moderate relative overfitting rate. Considering that the performance estimates of MMG1 were slightly higher than IP2, we selected this model as the best parametric alternative for subsequent analyses. The final form of MMG1 model, after combining the corresponding equation in Table 4 with the linear models fitted was as follows:

$$SI = \frac{a_0 + a_1 \text{BIO3} + a_2 \text{BIO4} + a_3 \text{BIO9}}{1 + a_4(a_5 \text{BIO2} + a_6 \text{BIO4} + a_7 \text{BIO7})^{a_8}}, \quad (7)$$

where $a_0=-117.677$, $a_1= 5.132701$, $a_2=0.159120$, $a_3=-8.09051$, $a_4= 0.00283399$, $a_5=46.4528$, $a_6=1.34853$, $a_7=-47.092005$, and $a_8= 1.69057$.

Plots of observed SI vs predicted SI and predicted SI vs residuals for Cubist and MMG1 models are shown in Fig. 4. After analyzing the model residuals of both approaches, we did not find any significant trace of heteroscedasticity. In order to support model interpretation, a plot of LOESS curves that represent predicted SI vs. standardized predictors for MMG1 model is presented in Fig 5.

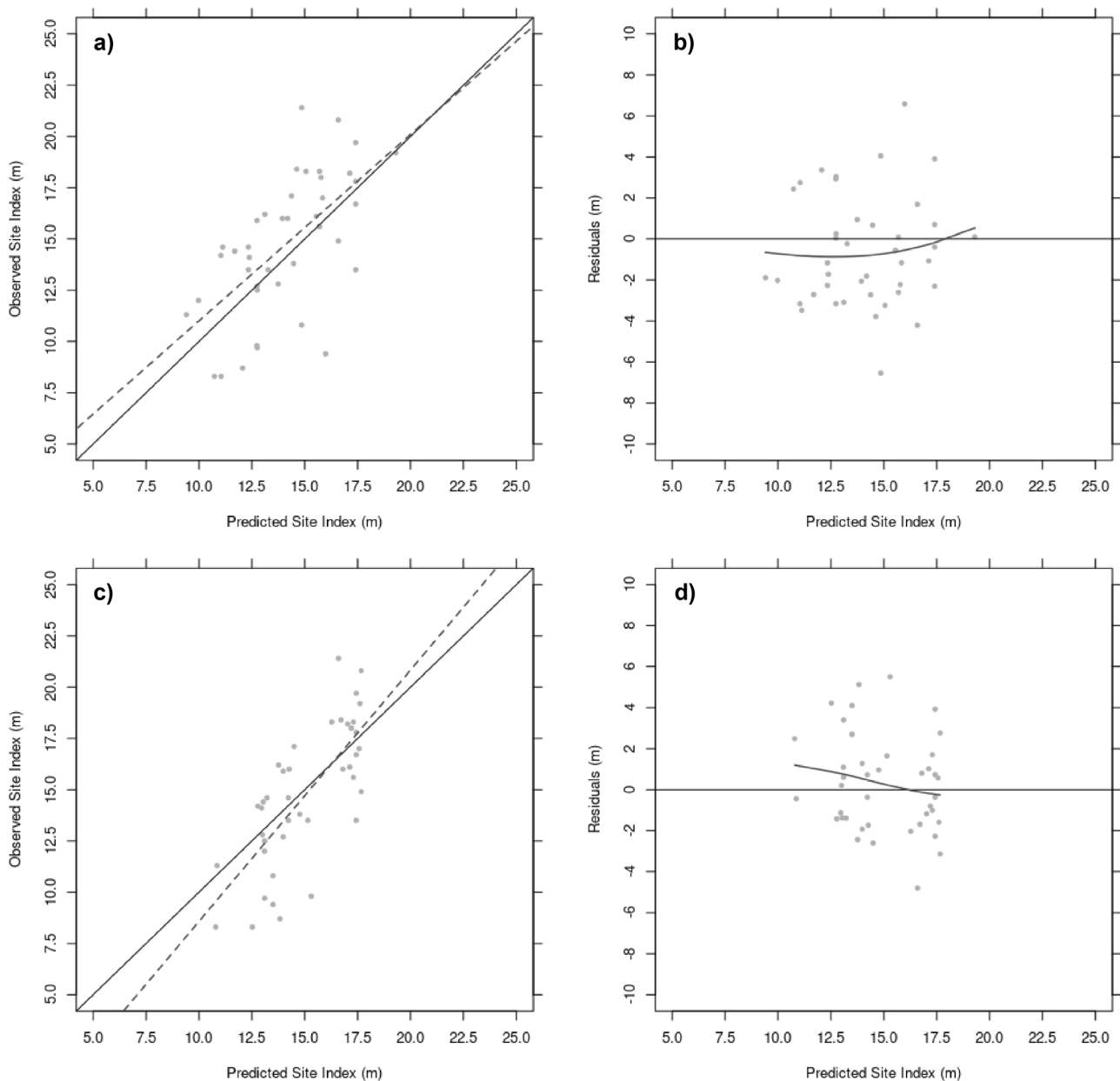


Fig. 4 Plots of: **a** observed *SI* vs predicted *SI* for MMG1; **b** predicted *SI* vs residuals for MMG1; **c** observed *SI* vs predicted *SI* for Cubist; and **d** predicted *SI* vs residuals for Cubist. The dashed line in plots

a and **c** represents the linear trend of observed vs predicted *SI*, while the solid line in plots **b** and **d** represents the LOESS-smoothed trend of residuals vs predicted *SI*

4 Discussion

The fitted models explained from 10% to 80% of the *SI* variability. The apparent performance range of the rule-based models fitted is similar to the observed in other studies for Random Forest ($R^2=0.68$, Weiskittel et al. 2011; $R^2=0.59$, Barrio-Anta et al. 2020) and Boosted Trees (R^2 from 0.44 to 0.64, Aertsens et al. 2010).

Similarly, the performance of the parametric models fitted ($R^2 \sim 0.27$ -0.38) was on average near the spectrum that can be found in literature (24%-27%, Monsrud et al. 2006, 31%-52%, Aertsens et al. 2010, 34%-42%, Sabatia and Burkhardt 2014 of explained variability).

Among the rule-based approaches, Random Forest showed the best apparent R^2 . However, its bootstrap validation performance was very similar to Boosted

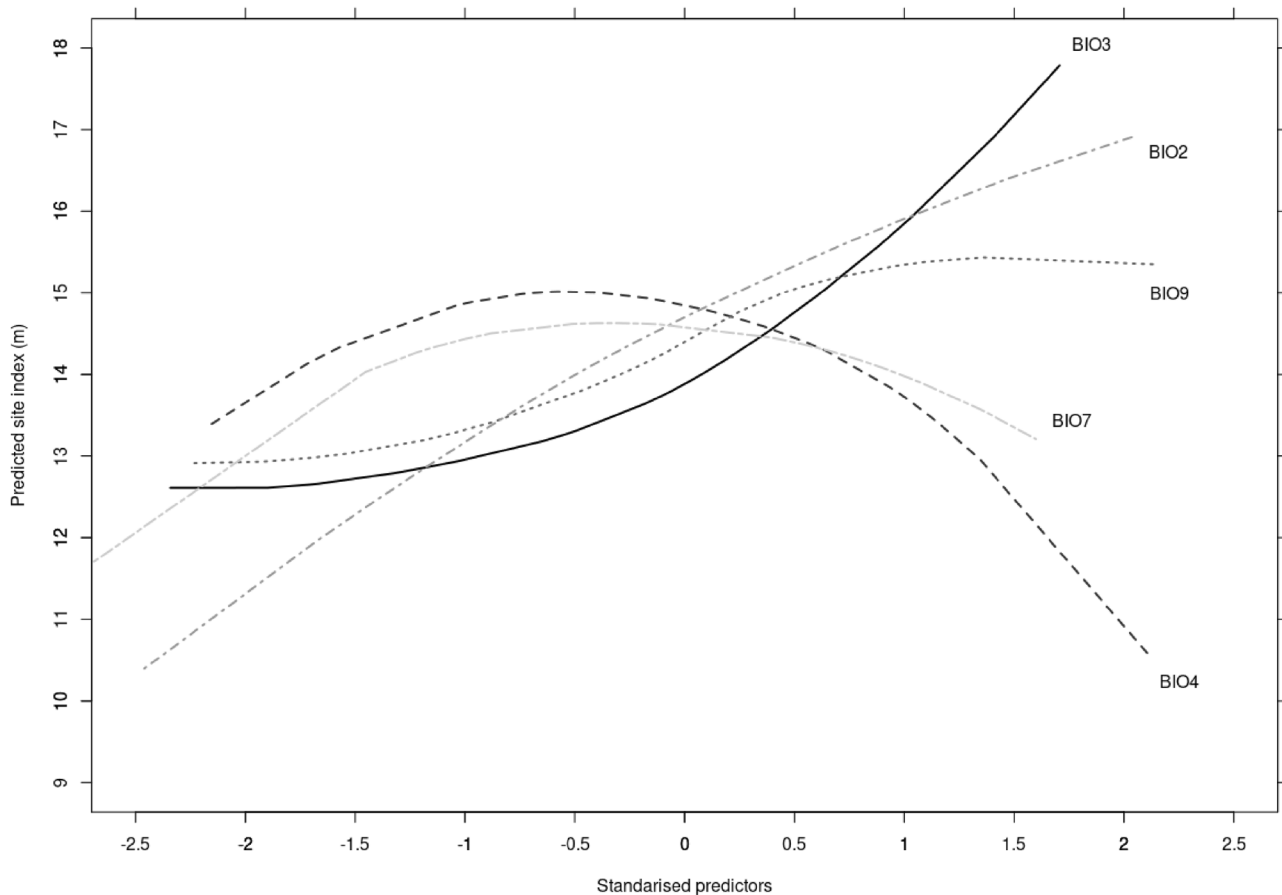


Fig. 5 LOESS curves of predicted *SI* vs standardized predictors for MMG1 model. For ease of visualization lines are represented in different styles (dark grey + dash-dot line: *BIO2*, black + solid line:

BIO3, black + dashed line: *BIO4*, grey + dotted line: *BIO9*, and light grey + dash-dot line: *BIO7*)

Trees and slightly lower than Cubist, which, despite being the model with the lowest apparent performance of the three, resulted in the most robust alternative. Though the differences in R^2_{632+} between the three tested techniques might be too slight to undoubtedly conclude that Cubist is the most suitable rule-based technique for *SI*-environment modeling, its lesser tendency to overfitting should be considered an important advantage. However, even considering the better robusticity shown by Cubist, the relative overfitting rates found for rule-based techniques are still very high in comparison with the ones provided by some indirect parametric models. We think that this could be an important concern for using these rule-based models for predicting *SI* out of the frame of this study. Using a complementary dataset for validation would be a necessary line of action for addressing this uncertainty in further research.

Regarding indirect parametric models, we observed that models based on the combination of growth + age (IP2 and MMG2 models) had lower performance. In contrast, combinations of height + age (IP1 and MMG1) had the highest performance. The fact that MMG1 outperformed the rest of the parametric models, both in apparent and validation statistics, may suggest that h_{mmg} and t_{mmg} are more effective than the rest of growth parameters for representing growth–climate relationships. In this context, using h_{mmg} and t_{mmg} directly for dominant height projection—as t_1 and H_1 inside Eq. 1—would be a reasonable modeling alternative to explore in further research.

Despite the higher apparent performance of the Random Forest model, the observed robustness of MMG1 may make this parametric approach a better alternative for *SI* prediction. This finding runs parallel to the results found

by Sabatia and Burkhart (2014), where a parametric model outperformed Random Forest, in terms of robustness and reliability. After checking the observed vs predicted *SI* values (Fig. 4), we found a moderate regression to the mean in both models. Besides, the range of predicted values was slightly narrower for Random Forest than for the parametric approach. This regression to the mean was also found in previous studies (Hamel et al. 2004; Weiskittel et al. 2011), and it has been suggested to be a common characteristic of the *SI*-environment models (Sabatia and Burkhart 2014).

The comparison between performance statistics of the direct GLM and MMG1 revealed that the indirect approach was more robust, being less prone to overfitting than the direct model. We think this finding might imply that, indeed, the indirect methods could be more effective at capturing the existing relationships between tree growth and climate and, hence, more ecologically consistent than direct *SI* modeling approaches. However, the proposed indirect method has got also some potential drawbacks. Regarding data acquisition, stem analysis is much more expensive and technically complex than a simple forest inventory of temporal research plots. We think that this is a crucial aspect to consider for practical applications of indirect *SI* modeling.

Concerning the ecological interpretation of MMG1 model, assessing the role of each predictor in Eq. 7 is not a straightforward task, as some predictors appear both in the numerator and in the denominator of the model form, apparently with a similar behaviour. The analysis of LOESS curves in Fig. 5 revealed that, overall, BIO2 and BIO3 had a strong positive influence on *SI*. As these variables are proportional to thermal diurnal ranges, and therefore potential indicators of altitude and continentality (Oliver 2005), we propose two possible reasons for their impact on *SI*: (1) altitude can imply cooler winter and night temperatures, which is positive for satisfying the *chilling* needs of the species, and (2) continentality may imply the absence of salty sea winds, potentially harmful for Scots pine (Øyen et al. 2006; Savill 2013). A special comment about the *chilling* effect is needed. Admittedly, certain conifer species, especially those naturally distributed in cold regions, such as Scots pine (Øyen et al. 2006), might suffer from a certain stress on carbon balance due to high respiration rates during mild winters (Pâques 2013; Smith et al. 1995). We already found this to be an important restriction for growth of radiata pine in the same region in a previous study (González-Rodríguez and Diéguez-Aranda 2020). We think this may be a particular feature of the studied region, characterized by a very humid and temperate-warm oceanic climate (predominantly Csb climate with

Cfa and Cfb local variations, according to the Köppen-Geiger classification, updated by Kottek et al. 2006).

The predictor BIO9 showed, overall, a very slight positive influence on *SI*, occurring mostly on the second half of its range. We hypothesize that this slight trend may represent the positive influence of temperatures for growth during the growing season, specially for coldest sites at higher altitudes (corresponding to Cfb local variants). Thought this predictor should also capture the negative effect of summer drought stress on growth, the high precipitation registered in the set of sampled sites—with a minimum of 1246 mm—may make the latter a not significant constraint for growth. BIO4 and BIO7 showed a similar influence on predicted *SI*, having a maximum at the middle of their ranges, showing, respectively, a positive and negative contribution on growth towards the extremes. In the case of BIO7, low values of this predictor may have a negative influence on *SI* because of the same reason explained for BIO2 and BIO3. High values of BIO7 may contribute negatively to *SI* representing the effect of frost stress factors in very contrasted temperature regimes. Finally, concerning BIO4, the positive effect on *SI* of its left tail may be also related to the influence of frost stress in sites with very regular precipitation regimes, associated with high altitudes (Cfb climates).

5 Conclusion

We fitted a set of rule-based and indirect parametric models for predicting site index (*SI*) of Scots pine stands as a function of bioclimatic variables. The models fitted explained from ~10% to ~80% of the response's variability. The rule-based approaches tested showed very high apparent performance statistics, being Random Forest the one with the highest R^2 . However, the bootstrap validation procedure carried out revealed that these techniques were also very prone to overfitting, and besides their actual differences in performance were little. In contrast, indirect parametric models showed a much lower overfitting rate. Two of these models, MMG1 and IP1, had better bootstrap error estimates than the rule-based approaches. Specifically, MMG1, a parametric model derived from height and age at the maximum mean growth point, showed the highest validation R^2 among the set of fitted models, explaining up to 38% of the *SI* variability. According to this model, *SI* was mainly conditioned by different measures of continentality, but also by heat and rainfall variables. We concluded that, for the specific scope of our study, the use of an indirect approach based on easily interpretable parametric models was a better modeling alternative than the direct prediction of *SI* using rule-based techniques.

Appendix

Table 6 Summary of parameter estimates and p values for the ten stepwise models fitted

Model	Variable	Estimate	P value	Significance	
a	Intercept	-346.374	0.0247899	*	
	BIO4	2.46477	0.0115361	*	
	BIO5	-4241178	0.0279334	*	
	BIO6	4241207	0.0279328	*	
	BIO7	4241218	0.0279323	*	
	BIO8	112.622	0.0075643002	**	
	BIO9	-139.704	0.00228569	**	
	b	Intercept	-1026.50	0.0288415	*
BIO4		3.13169	0.00194989	**	
c	Intercept	1.69057	$< 2 \cdot 10^{-16}$	***	
h_{ip}	Intercept	-24.0346	0.0695317	.	
	BIO3	1.04831	0.00174623	**	
	BIO4	0.0324989	0.0222145	*	
	BIO9	-1.65242	0.0175229	*	
t_{ip}	Intercept	126.053	0.083082	.	
	BIO2	46.0774	0.00547604	**	
	BIO4	0.833430	0.0159734	*	
	BIO7	-39.1731	0.00772911	**	
	BIO1	-0.256227	0.0468519	*	
	BIO1	7.18568	0.0222929	*	
	BIO1	-2.05499	0.0326695	*	
	BIO1	0.740449	0.0269895	*	
	g_{ip}	BIO7	0.289329	0.000100529	***
		BIO8	0.386769	0.0000697722	***
	BIO9	-0.480405	0.000293752	***	
h_{mmg}	Intercept	-48.0693	0.0695317	.	
	BIO3	2.09663	0.00174623	**	
	BIO4	0.0649979	0.0222145	*	
	BIO9	-3.30484	0.0175229	*	
t_{mmg}	BIO2	46.4528	0.0351728	*	
	BIO4	1.34853	0.0243512	*	
	BIO7	-47.092005	0.0309513	*	
mmg	BIO7	0.221143	0.000442736	***	
	BIO8	0.301835	0.000241219	***	
	BIO9	-0.3674004	0.000600666	***	

. significant at 90%; * significant at 95%; ** significant at 99%; *** significant at 99.9%

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Data availability The datasets analysed during the current study are available in the Zenodo repository, <https://doi.org/10.5281/zenodo.4535243>.

Declarations

Conflicts of interest The authors declare that they have no conflict of interest.

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