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Artificial neural networks in modeling of environmental time series for yerba-mate growth dynamics

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Highlights: The artificial neural networks (ANN) are a solution to model the nonlinear systems. The monthly mean values of environmental and morphological data were used to build time series related to yerba-mate growth. Time series and data relative to rhythmic growth were used for ANN training. The final results of this FSPM are yerba-mate mock-ups, related to two particular environmental conditions.

Keywords: backpropagation algorithm, multilayer perceptron, shoot elongation, temperature

INTRODUCTION

InterpolMateS1 software allows the 3D reconstructions during a biennial yerba-mate growth (Matsunaga et al. 2012) considering male (MA) and female (FE) individuals in two distinct light environments - forest understory (FUS) and cultivation under open area - in monoculture (MO). The growth flushes and pauses of yerba-mate rhythmic growth are controlled endogenously and modified by environment (Rakocevic and Martim, 2011). The representations of leaf and shoot dynamics are the central components of this specific yerba-mate FSPM, based on cubic splines interpolation, which considers a biennial period between two subsequent prunings coupled with VPlants for 3D reconstructions.

Many mathematical and computational modeling principles were performed in modeling of plant growth dynamics related to environmental conditions. The multiple regression models can be used for this purpose, but their performance could be low, especially when the nonlinear relationships were established, which is very common in ecology (Lek et al. 1996). The uses of differential equations (Zhang et al. 2007), or predefined equations (Laaboudi et al. 2012), give better performance and accuracy, but require a larger number of not always available ecological parameters.

Methodologically advanced solution in nonlinear system modeling is the use of artificial neural networks (ANN). ANN requires only some input parameters, even when some are unknown. Han and Fan (2006) used ANN and principle component analysis to solve multivariate time series prediction problems. Bayesian generalized associative functional networks were applied to model the dynamical plant growth process of greenhouse crops and predict their dry matter production (Qu and Hu, 2009).

Our actual interest in yerba-mate FSPM development is focused on the inclusion of the environmental impacts on yerba-mate growth responses and synchronization of growth variables. Time series analysis permitted the emphasizing of growth degree days and night/day length as principal environmental factors affecting yerba-mate shoot elongation and the number of green leaves (Rakocevic and Martim, 2011) in two light environments. It was hypothesized that correlations between environmental and growth time series could be recognized by ANN. The aim of this work was to improve the InterpolMateS1 software using the ANN training for: 1/correlation between the environmental impacts relative to two particular growth environments and the morphological responses of yerba-mate males and females, and 2/ synchronization of morphological responses.

APPLICATION OF ANN TO MODEL TIME SERIES IN YERBA-MATE GROWTH AND STRUCTURE

Data sets for yerba-mate (*Ilex paraguariensis*) growth were built from measurements differencing plant growth environment (MO and FUS) and gender (MA and FE). The plant architecture (Rakocevic et al. 2011) and growth were reconstructed from morphological parameters followed on 90 branches of thirty plants, considering: rate of shoot elongation, metamer number increase, leaf number increase, leaf shed and leaf area increase per shoot. The morphogenetic parameters were followed monthly at three branches for each individual, during a biennial period (June 2003 – June 2005), resulting in 25 observations. Those responses represent the intrinsic plant program modified by environmental conditions, where the average minimum (minT) and maximum temperatures (maxT), sum of growing degree days (GDD), average rainfalls (RF) and night length (NL) were observed. The monthly mean values of morphological and environmental data were applied to build plant growth and environmental time series. Those time series, information about periods of rhythmic growth and respective growth pauses, were used for ANN training.

The perceptron multilayer ANN was chosen to model time series in yerba-mate growth because of its facilities of interpretation and ability to solve non-linear problems (Jantzen, 1998). It generates a mathematical-computational model of morphological responses to input variables (environmental inputs and yerba-mate growth cycle definition). The developed ANN for yerba-mate growth uses the supervised machine learning, which consists of: 1/ backpropagation algorithm and 2/ rules for morphological parameters synchronization within ANN training. The backpropagation algorithm extends the analysis that underpins the delta rule to neural nets with hidden nodes formulae. The delta rule algorithm always makes a change in weights of connections, and is based on activation of nodes opposed to output (Hecht-Nielsen, 1989). The synchronization is performed by logical functions, centralizing the rate of metamer appearance and defining its interrelations with other parameters during the periods of growth flushes and pauses.

The architecture of yerba-mate ANN (Fig. 1) consists of three layers: 1/ an input layer containing six nodes to receive input variables, 2/ a hidden layer with $2n+1$ nodes (Hecht-Nielsen, 1989), where n is the number of input variables and 3/ an output layer that computes the simulated data and back-propagates the errors to the hidden layer. The training phase of the ANN consists on the feed-forward phase and the back-propagation phase. During the feed-forward phase, the nodes compute the outputs using an activation sigmoid function in the hidden layer, and pass the results of the function to the nodes in the output layer.

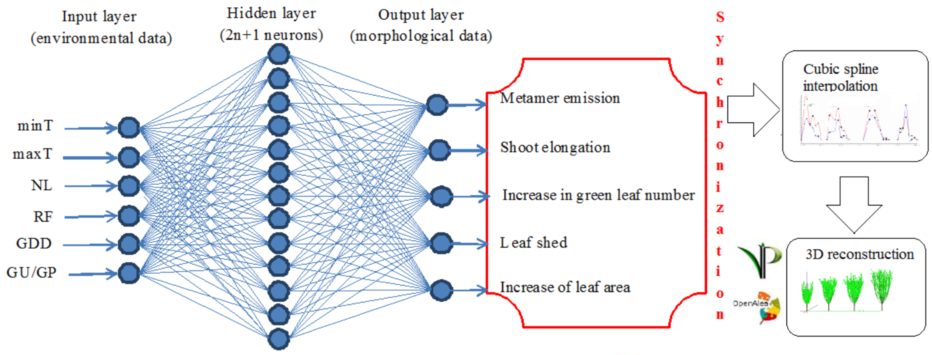

Fig. 1. Schema of ANN used for modeling the yerba-mate time series, and growth parameter synchronization. The network input variables are average minimum and maximum temperatures (minT and maxT), night length (NL), rainfalls (RF), growth degree days (GDD), and periods of growth flushes and pauses (GU/GP). The output consists of morphological responses that are synchronized by logical functions. Cubic splines interpolation helps the 3D reconstruction in VPlants.

After the synchronization of the morphological outputs, those values are interpolated using the cubic splines interpolation method (Matsunaga *et al.*, 2012), permitting the daily-step reconstructions of yerba-mate structure in 3D (Fig. 1, right side).

RESULTS AND DISCUSSION

ANN training was able to detect the correlations between yerba-mate growth and environmental variables in two growth environments. The empirical tests of yerba-mate ANN were resulted in 10^5 as the maximum iterations for a stable network functioning. The root mean square error (RMSE, fitted to 1), and bias were used for ANN validation (Tab. 1). The correlations between yerba-mate environmental and growth variables in FUS were less recognized by ANN than those in MO. The leaf area increase was the response with the lowest adjustments for both genders, when time series were modeled for yerba-mate growth under a forest shade. In a future work, it is possible to improve those outputs by adding momentum constant on delta rule in ANN (Jantzen, 1998).

Tab. 1. Bias and RMSE calculated for artificial neural network outputs obtained after 100,000 iterations, and adjusted to measured shoot parameters for yerba-mate male and female plants grown in two contrasted light environments (open areas and forest understory).

Growth parameters	**Females**				**Males**			
Environment	Monoculture		Forest understory		Open area		Forest understory	
	RMSE	bias	RMSE	bias	RMSE	bias	RMSE	bias
Shoot elongation	1	**-0.005**	0.480	**0.177**	1	**-0.241**	1.860	**-0.119**
Metamer emission	1	**-0.005**	0.819	**-0.177**	1	**0.116**	0.706	**-0.006**
Leaf number increase	1	**-0.058**	0.037	**0.039**	1	**0.040**	1.067	**-0.028**
Leaf shed	1	**-0.280**	1	**0.027**	1	**-0.030**	1	**0.053**
Increase of leaf area	1	**-1.641**	0.631	**0.910**	1	**0.519**	7.628	**-0.848**

The ANN training performed more precise 3D reconstruction outputs (Fig. 2), due to accurate definition relative to periods of growth flushes and variable synchronization (Fig. 1). The metamer emission, branching and leaf shed respected the environmental conditions and logical rules (Fig. 2A *versus* Fig. 2B), permitting the leaf area distribution according to the most probable occurrence.

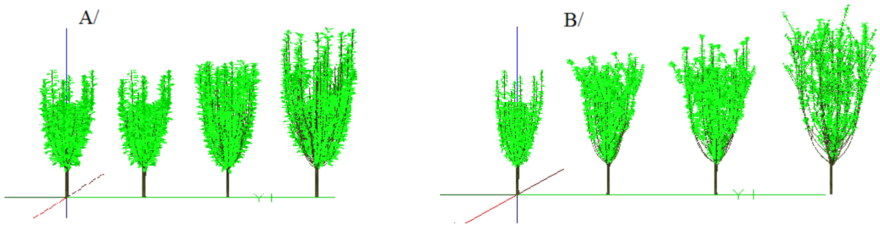

Fig. 2. Reconstructions of one female cultivated in monoculture relative to four growth unit formations A/ before and B/ after the ANN training.

ANNs use the supervised learning and are precise only for established conditions according to known and expected outputs (Zhang et al. 2007). This modeling approach could permit the accuracy for simulations using different environmental conditions and variety of morphological definitions for yerba-mate shoot architecture, but would require the additional training.

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