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Modeling *Avena fatua* seedling emergence dynamics: An artificial neural network approach

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ABSTRACT

Avena fatua is an invasive weed of the semiarid region of Argentina. Seedling emergence patterns are very irregular along the season showing a great year-to-year variability mainly due to a highly unpredictable precipitation regime. Non-linear regression techniques are usually unable to accurately predict field emergence under such environmental conditions. Artificial Neural Networks (ANNs) are known for their capacity to describe highly non-linear relationships among variables thus showing a high potential applicability in ecological systems. The objectives of the present work were to develop different ANN models for *A. fatua* seedling emergence prediction and to compare their predictive capability against non-linear regression techniques. Classical hydrothermal-time indices were used as input variable for the development of univariate models, while thermal-time and hydro-time were used as independent input variables for developing bivariate models. The accumulated proportion of seedling emergence was the output variable in all cases. A total of 528 input/output data pairs corresponding to 11 years of data collection were used in this study. Obtained results indicate a higher accuracy and generalization performance of the optimal ANN model in comparison to non-linear regression approaches. It is also demonstrated that the use of thermal-time and hydro-time as independent explanatory variables in ANN models yields better prediction than using combined hydrothermal-time indices in classical NLR models. The best obtained ANN model outperformed in 43.3% the best NLR model in terms of RMSE of the test set. Moreover, the best obtained ANN predicted accumulated emergence within the first 50% of total emergence 48.3% better in average than the best developed NLR model. These outcomes suggest the potential applicability of the proposed modeling approach in weed management decision support systems design.

1. Introduction

Field emergence predictive models are essential tools for the development of weed management support systems aimed to design sustainable weed control programs while optimizing crop yield. Such models should be able to minimize the degree of uncertainty on the estimation of the time and magnitude of seedling emergence (Forcella et al., 2000).

Empirical models have been based on the effect of soil temperature and soil water potential to predict weed seedling emergence in agronomical systems. Soil microclimate derived indices such as hydrothermal-time or thermal-time are commonly used for model development to quantify the effect of the above mentioned environmental variables. They assume that emergence rates are proportional to the amount by which soil temperature and soil water potential exceed a given threshold value for such environmental factors (Bradford, 2002). Based on these indices, non-linear regression (NLR) sigmoid shaped models (Weibull, Gompertz, Logistic, etc.) have been extensively adopted for weed emergence prediction in the field (Forcella, 1998; Roman et al., 2000; Leguizamón et al., 2005; Schutte et al., 2008; Hadi and González-Andújar, 2009; Royo-Esnal et al., 2010). Such models provide adequate representation for regular, single cohort, emergence patterns, typical of temperate environments where precipitations are not seasonally restricted. However, they are not expected to represent well complex weed emergence patterns, as those observed in regions of highly variable soil environmental conditions. One of the limitations of the classical models for weed emergence prediction is that they are univariate. Therefore, they require the use of only one explanatory variable. If it is desired to investigate several independent explanatory variables to estimate emergence, some alternative modeling approach is required. Another limitation with classical emergence models is that the underlying non-linearity is

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fixed. As pointed out in Cao et al. (2011) "*parametric models are sometimes not flexible enough to capture complex features in the hydrothermal time distribution, such as abrupt jumps or heavy tails*". If more flexible structures are required, other approaches should be adopted.

Avena fatua L. is a noxious weed species distributed worldwide which produces severe yield and quality losses in cereal and oil seed crops (Holm et al., 1977; Sharma and Van den Born, 1978). Several empirical NLR models were developed specifically for *A. fatua* field emergence prediction (Page, 2004; Page et al., 2006; Martinson et al., 2007). These models adequately described typical S-shaped cumulative emergence curves as a function of hydrothermal-time showing a good correlation between observed and predicted emergence data. Conversely, in the semiarid region of Argentina, *A. fatua* shows an irregular seedling emergence behavior along the season and a great variability among years mainly due to a highly unpredictable precipitation regime, also influenced by a fluctuating thermal environment and seed dormancy level variations within the population. For this system, Moschini et al. (2009, 2011) observed a limited capability to predict field emergence dynamics at the onset of the germination time-window using a hydrothermal-time based Weibull model. Therefore, alternative modeling approaches are required to study such a complex system.

Artificial Neural Networks (ANNs) are machines with complex functional relations learnable with a limited amount of training data emulating data processing functions of the brain (Çakmak and Yıldız, 2011). ANNs are known for their capacity to describe highly non-linear relationships among variables thus showing a high potential applicability in ecological systems (Lek and Guégan, 1999). Among the most attractive features of ANNs for empirical modeling are the possibility of using any number of input (explanatory) variables and a flexible modeling framework, non-dependant on specific underlying non-linear structures.

As reviewed by Huang et al. (2010), most ANNs based works in agricultural and biological engineering have been accomplished using a multilayer feed-forward ANN. The feed-forward network with a single hidden layer that contains a finite number of neurons implementing an arbitrary activation function was proven to be a universal approximator for solving non-linear mapping problems of high complexity level (Cybenko, 1989; Hornick et al., 1989; Huang et al., 2010).

In the last decade, ANNs have been systematically adopted to model many agronomical systems (Park et al., 2005; Saberali et al., 2007; Alvarez, 2009; Fortin et al., 2010; Dai et al., 2011). However, to the best of our knowledge, no applications of ANNs for modeling weed emergence have been reported in the open literature. Only recently, preliminary ANNs emergence models were developed for *A. fatua*, based on meteorological data (Chantre et al., 2011a) and soil microclimate derived indices (Chantre et al., 2011b).

The objectives of the present work were to: (i) develop different ANN models for *A. fatua* emergence prediction based on soil microclimate derived indices for the semiarid region of Argentina; (ii) obtain an optimal ANN model to predict field emergence patterns; (iii) compare the predictive accuracy of non-linear regression models with the ANN approach.

2. Materials and methods

2.1. Field experimental data

A. fatua emergence data was collected at weekly intervals from 2000 to 2010 at the experimental field of EEA INTA Bordenave (37°50′S; 63°01′W), located in Buenos Aires province, Argentina. The experiment was conducted on an undisturbed field with a high natural population density of *A. fatua* without crop presence. Seedling counting was performed on three quadrats (1 m^2 each) randomly distributed on the field.

2.2. Estimation of soil temperature and soil water potential

The Soil Temperature and Moisture Model (STM^2) developed by USDA-ARS (http://www.ars.usda.gov/services/software/software.htm) was used to estimate soil microclimate conditions (Spokas and Forcella, 2009). STM^2 is a user-friendly software for soil temperature and moisture modeling which requires very limited user input data.

STM^2 is general in purpose and calculates soil moisture and temperature based on soil composition and daily minimum and maximum air temperature and precipitation. The model was tested for many global sites in Spokas and Forcella (2009). Specifically for the Bordenave region (Argentina), STM^2 predictions were validated against experimental data showing satisfactory agreement (Damiano et al., 2010).

The model was calibrated using soil site-specific parameters: soil texture (sandy loam = 53% sand, 31% silt, 16% clay), organic matter content (3.1%) and bulk density (1.2 Mg/m^3). Daily mean soil temperature (T) and water potential (Ψ) at 1 cm burial depth were estimated using weather data registered at a meteorological station located in the experimental field.

Evidence suggests that seeds of *A. fatua* might be located within the 0–5 cm of the soil layer depending on the tillage degree (Damiano et al., 2010). In this work, 1 cm was considered to be a representative seed burial depth of an undisturbed soil condition emulating a non-tillage field scenario. However, the choice of the optimal depth for soil microclimate calculation is an open issue, since large differences in hydrothermal-time can exist between different soil layers, as demonstrated in Cao et al. (2011).

2.3. Input variables for emergence models

Recent models for weed emergence prediction adopt hydrothermal-time as explanatory variable since both, temperature and moisture have proven to be critical variables for seedling emergence. Therefore, an index that combines both magnitudes is necessary for the development of univariate models. In Martinson et al. (2007) it was demonstrated that a hydrothermal-time based Weibull model predicted far more accurately than its thermal-time counterpart in years with dry periods occurrence. Similar evidence has been also reported by Leguizamón et al. (2005) and McGiffen et al. (2008). For the specific case of the Bordenave region, it has been reported that NLR hydrothermal-time based models outperform thermal-time based ones (Moschini et al., 2009, 2011). Based on these arguments and on the fact that the region under study is characterized by severe soil moisture limitations, a hydrothermal-time index was adopted in this contribution for the univariate modeling approach.

The following indices were used as input variables for model development: hydrothermal-time (θ_{HT}) for univariate models, thermal-time (θ_T) and hydro-time (θ_H) for bivariate models.

2.3.1. Thermal time

Thermal-time (θ_T) accumulation for seedling emergence was calculated according to Hammer et al. (1993):

$$\theta_T = \sum_{i=1,n} (T - T_b) \quad \text{if } T_b < T < T_o \tag{1a}$$

$$\theta_T = \sum_{i=1,n} (T_o - T_b)\left(1 - \frac{T - T_b}{T_m - T_b}\right) \quad \text{if } T_o < T < T_m \tag{1b}$$

$$\theta_T = 0 \quad \text{otherwise} \tag{1c}$$

Eqs. (1a) and (1b) are defined for the sub-optimal and supra-optimal thermal ranges, respectively. T is the estimated mean daily soil temperature, T_b, T_o and T_m are the base, optimal and maximum temperatures for *A. fatua* seedling emergence, respectively. The following cardinal temperatures values were used: T_b = 1 °C (Cousens et al., 1992), T_o = 15 °C and T_m = 35 °C (estimated from Sharma et al., 1976).

2.3.2. Hydro-time (I)

Hydro-time (θ_H^I) was calculated as (Gummerson, 1986; Bradford, 1990):

$$\theta_H^I = \sum_{i=1,n} (\Psi - \Psi_b) \quad \text{if } \Psi > \Psi_b \tag{2a}$$

$$\theta_H^I = 0 \quad \text{otherwise} \tag{2b}$$

where Ψ is the estimated mean daily soil water potential and Ψ_b is the base water potential for emergence. A figure of Ψ_b = −1.2 MPa was adopted from Page (2004).

2.3.3. Hydro-time (II)

The following alternative definition of hydro-time was also adopted (Leguizamón et al., 2005; Martinson et al., 2007):

$$\theta_H^{II} = 1 \quad \text{when } \Psi > \Psi_b \tag{3a}$$

$$\theta_H^{II} = 0 \quad \text{when } \Psi < \Psi_b \tag{3b}$$

2.3.4. Hydrothermal-time

Two alternative approaches for the hydrothermal-time (θ_{HT}) calculation were considered:

$$\theta_{HT}^I = \theta_T \theta_H^I \tag{4}$$

and

$$\theta_{HT}^{II} = \theta_T \theta_H^{II} \tag{5}$$

where θ_H^I and θ_{HT}^{II} are defined according to (2) and (3), respectively.

It should be noticed that the definitions of thermal-time and hydro-time are functions of the cardinal parameters (T_b, T_o, T_m and Ψ_b). For the purposes of this contribution, such parameters were chosen following the work of other authors but there is evidence that their values affect the prediction results (Moschini et al., 2011). In this sense, many other explanatory variables could be obtained by modifying the values of the cardinal parameters in the definition of the thermal-time index (Eq. (1)). Moreover, by appropriately choosing the value of Ψ_b in Eqs. (3a) and (3b), θ_{HT}^{II} reduces to the actual thermal-time (θ_T), meaning that θ_T might be thought as a particular case of hydrothermal-time. There also exist alternative definitions of θ_T different than that of Eq. (1) (Leguizamón et al., 2005; Martinson et al., 2007).

2.4. ANN modeling

ANNs are modeling tools that provide a practical and flexible framework for input–output data correlation. For a thorough introduction to ANNs see Fausett (1994). In Fig. 1, a three layer feed-forward ANN is depicted. The network has two inputs (x_1, x_2), one output (y) and eight neurons in the hidden layer.

Each of the two input layer's neurons receive one input (x_1, x_2) and broadcasts such signal to each one of the hidden layer's neurons. Each hidden neuron computes its activation function and sends its result ($z_1, \ldots, z_8$) to the output layer's neuron which finally produces the response of the network (y). The output signal of each hidden neuron (z_j) is calculated as:

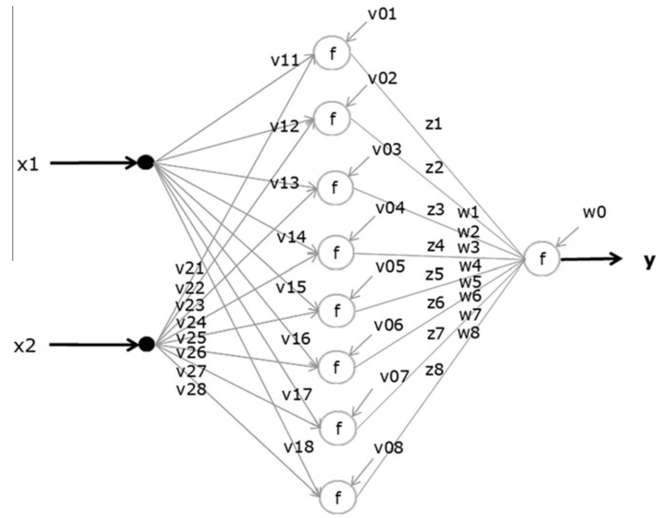

Fig. 1. ANN architecture with three layers, two inputs and one output.

$$z_j = f\left(\sum_{i=1,2} v_{ij} x_i + v_{0j}\right) \quad j = 1, \ldots, 8 \tag{6}$$

while the output of the network is given by:

$$y = f\left(\sum_{j=1,8} w_j z_j + w_0\right) \tag{7}$$

In Eqs. (6) and (7) $f(\cdot)$ is the activation function of the network, v_{ij} are the weights of the connections between the input and hidden neurons and v_{0j} is the bias on hidden neuron j. Similarly, w_j represent the weights of the connections between the hidden and output neuron and w_0 is the bias on the output neuron.

Hyperbolic tangent sigmoid transfer functions (Eq. (8)) were used, both in the hidden and the output layer's neurons.

$$Y = \frac{2}{1 + \exp(-2X)} - 1 \tag{8}$$

In this contribution, a feed-forward neural network structure with three layers was adopted (Fig. 1). Several ANNs with different number of neurons in the hidden layer were investigated. Input/output data was normalized to fall in the range [−1, 1] to improve the network performance (Maier and Dandy, 2001). The Neural Network Toolbox of Matlab (Beale et al., 2011) was used for programming the ANNs. The Bayesian Regularization algorithm was selected for training purposes because it produces networks with better generalization capabilities than other training options. It updates the weights and biases values according to Levenberg–Marquardt optimization, seeking to minimize a linear combination of the squared errors and of the parameters' magnitudes. Keeping the network parameters small, the network response is ensured to be smooth. The Bayesian Regularization method (Foresee and Hagan, 1997) consists on the minimization of the following performance function:

$$F(\mathbf{y}, \mathbf{W}) = \varphi E_S + \xi E_W \tag{9}$$

where

$$E_S = \frac{1}{N} \sum_{i=1,N} (y_i^t - y_i^0)^2 \tag{10}$$

and

$$E_W = \frac{1}{N} \sum_{j=1,n} W_j^2 \tag{11}$$

E_s is the mean sum of squares of the network errors. $\mathbf{y}^t$ and $\mathbf{y}^0$ represent the target values and outputs of the network respectively. E_w is the mean sum of squares of the network weights and biases represented by vector $\mathbf{W}$. N is the size of the training data set. Parameters φ and ξ are dynamically estimated as the network training proceeds, together with the so called *effective number of parameters* (η), a measure of how many of the weights and biases of the network are effectively used in reducing the error function (Foresee and Hagan, 1997).

2.5. NLR models

Weibull and logistic models (12), (13) were also developed to model emergence data for comparison purposes.

$$y = 1 - \exp\left(-\ln(2)\left(\frac{x}{\alpha}\right)^{\beta}\right) \quad (12)$$

$$y = \frac{\gamma}{1+\exp(-\delta(x-\lambda))} \quad (13)$$

In (12) and (13) y is the accumulated emergence (in proportion), x is the applied hydrothermal-time index ($\theta^{\mathrm{I}}_{\mathrm{HT}}$ or $\theta^{\mathrm{II}}_{\mathrm{HT}}$), α, β, γ, δ and λ are model parameters. A non-linear regression fitting routine was applied for parameters estimation using the Levenverg–Marquardt algorithm.

2.6. Models analysis

In all cases goodness-of-fit measures were based on Akaike's information criterion (AIC) and root mean square error (RMSE) of the training set. The predictive capability of the developed models was based on the RMSE of the test set.

The general definition of AIC provided in Qi and Zhang (2001) was adopted (Eq. (14)), where m is the number of parameters of the model, N is the number of observations and d is a user defined constant, which allows the tuning of the penalty term.

$$\mathrm{AIC}_d = \log(\mathrm{RMSE}^2) + \frac{2m^{\mathrm{d}}}{N} \quad (14)$$

It should be noticed however that quantitative analysis of ANNs is open since many classical model selection criteria do not seem to be straightforwardly applicable to this modeling approach. On one side there is evidence that penalty-based in-sample criteria are not adequate measures for ANNs comparison as reported by Qi and Zhang (2001). In particular, AIC and BIC methods tend to over-penalize ANN model complexity making the model under-fit the data. Moreover, the different alternatives of AIC and BIC may lead to different "best" models making the analysis subjective. Additionally, as also stated in Qi and Zhang (2001), model selection based on in-sample data either by penalty-based criteria or no-penalty-related performance measures (MAE, RMSE, MAPE, etc.) is not always consistent with the best performances in out-sample data (test sets).

2.7. Training and test sets

A total of 528 input/output data pairs corresponding to 11 years of data collection were divided into training (82%) and test (18%) subsets. Although the meteorological conditions of the different years were quite diverse, 9 of 11 years of the data pool were characterized by moderate to severe soil water availability limitations for seedling emergence, regarding the period where $\Psi < \Psi_b$. Thus, the training set was chosen such that a wide spectrum of precipitation scenarios was included. In order to expose the performance of the derived models, years 2006 and 2008 were selected as test subsets representing extreme and intermediate drought conditions, respectively.

3. Results

3.1. Models developed

Several univariate models were tuned with the available data set. In all cases, accumulated emergence (AcEm) was adopted as output variable and calculated as a function of the previously described indices: $\theta^{\mathrm{I}}_{\mathrm{HT}}$, $\theta^{\mathrm{II}}_{\mathrm{HT}}$. Specifically, the following models were developed: AcEm = Weibull(θ_{HT}), AcEm = Logistic(θ_{HT}) and AcEm = $\mathrm{ANN}_{\mathrm{hn}=1,5}(\theta_{\mathrm{HT}})$, where hn represent the number of neurons in the hidden layer.

In Tables 1 and 2, the results corresponding to hydrothermal-time based models are reported. The number of parameters of each model (m) is shown together with statistical measures. For the ANNs, the number of effective parameters (η), meaning the number of model parameters which effectively reduce the error function, are also provided. In Table 3, the parameters corresponding to the NLR models are presented.

Alternatively, a bivariate modeling approach based on ANNs using thermal-time and hydro-time as two independent variables was proposed. Specifically the following networks were studied: AcEm = $\mathrm{ANN}_{\mathrm{hn}}(\theta_{\mathrm{T}}, \theta^{\mathrm{I}}_{\mathrm{H}})$, where hn = 1, 2, 3, 5, 6, 7. In Table 4, the statistical results for the different networks are presented.

Table 1
Results for univariate models based on $\theta^{\mathrm{I}}_{\mathrm{HT}}$. m = total number of model parameters, η = number of effective parameters, AIC_d = Akaike's Information Criterion with different weight on the penalty term, RMSE = root mean square error.

Model	m	η	AIC_d		RMSE	
			1	0.5	Train	Test
AcEm = Weibull($\theta^{\mathrm{I}}_{\mathrm{HT}}$)	2	–	−1.29	−1.29	0.224	0.204
AcEm = Logistic($\theta^{\mathrm{I}}_{\mathrm{HT}}$)	3	–	−1.26	−1.26	0.232	0.191
AcEm = $\mathrm{ANN}_1(\theta^{\mathrm{I}}_{\mathrm{HT}})$	4	3.1	−1.21	−1.22	0.243	0.186
AcEm = $\mathrm{ANN}_2(\theta^{\mathrm{I}}_{\mathrm{HT}})$	7	4.7	−1.23	−1.25	0.235	0.200
AcEm = $\mathrm{ANN}_3(\theta^{\mathrm{I}}_{\mathrm{HT}})$	10	4.7	−1.22	−1.25	0.235	0.198
AcEm = $\mathrm{ANN}_5(\theta^{\mathrm{I}}_{\mathrm{HT}})$	16	7.8	−1.20	−1.25	0.233	0.194

Table 2
Results for univariate models based on $\theta^{\mathrm{II}}_{\mathrm{HT}}$. m = total number of model parameters, η = number of effective parameters, AIC_d = Akaike's Information Criterion with different weight on the penalty term, RMSE = root mean square error.

Model	m	η	AIC_d		RMSE	
			1	0.5	Train	Test
AcEm = Weibull($\theta^{\mathrm{II}}_{\mathrm{HT}}$)	2	–	−1.33	−1.33	0.215	0.187
AcEm = Logistic($\theta^{\mathrm{II}}_{\mathrm{HT}}$)	3	–	−1.29	−1.30	0.222	0.177
AcEm = $\mathrm{ANN}_1(\theta^{\mathrm{II}}_{\mathrm{HT}})$	4	3.1	−1.30	−1.31	0.220	0.168
AcEm = $\mathrm{ANN}_2(\theta^{\mathrm{II}}_{\mathrm{HT}})$	7	4.9	−1.31	−1.32	0.215	0.180
AcEm = $\mathrm{ANN}_3(\theta^{\mathrm{II}}_{\mathrm{HT}})$	10	4.9	−1.29	−1.32	0.215	0.180
AcEm = $\mathrm{ANN}_5(\theta^{\mathrm{II}}_{\mathrm{HT}})$	16	7.7	−1.27	−1.32	0.214	0.178

Table 3
Parameters of the NLR models.

Parameters		α	β	γ	δ	λ
$\theta^{\mathrm{I}}_{\mathrm{HT}}$	Weibull	964.8	1.161	–	–	–
	Logistic	–	–	0.920	0.0022	952.5
$\theta^{\mathrm{II}}_{\mathrm{HT}}$	Weibull	764.2	1.281	–	–	–
	Logistic	–	–	0.962	0.0027	801.2

Table 4
Results for bivariate ANNs based on θ_T and θ_H^I. m = total number of model parameters, η = number of effective parameters, AIC_d = Akaike's Information Criterion with different weight on the penalty term, RMSE = root mean square error.

Model	m	η	AIC_d		RMSE	
			1.0	0.5	Train	Test
AcEm = $ANN_1(\theta_T, \theta_H^I)$	5	4.1	−1.98	−1.99	0.100	0.122
AcEm = $ANN_2(\theta_T, \theta_H^I)$	9	7.6	−2.00	−2.03	0.096	0.120
AcEm = $ANN_3(\theta_T, \theta_H^I)$	13	10.2	−1.99	−2.03	0.095	0.120
AcEm = $ANN_5(\theta_T, \theta_H^I)$	21	15.5	−1.97	−2.04	0.093	0.108
AcEm = $ANN_6(\theta_T, \theta_H^I)$	25	20.1	−1.97	−2.05	0.092	0.106
AcEm = $ANN_7(\theta_T, \theta_H^I)$	29	26.1	−1.98	−2.08	0.089	0.089

3.2. Models performance

Obtained results for models with θ_{HT}^I (Table 1) showed that the Weibull model outperformed all other models based on AIC and RMSE measures of the training set. However, ANN_1 predictions outperformed NLR and all other ANN models, as indicated by RMSE values of the test set (Table 1). Similarly, for θ_{HT}^{II} based models, AIC selected the model with the lowest number of parameters (Table 2) as the best modeling alternative (Weibull). Conversely, the model with the best predictive performance was ANN_1, as indicated by the lowest RMSE value of all tested models.

According to the AIC method, the best single-input variable modeling alternative would be the NLR-Weibull (θ_{HT}^{II}) model (Table 2). However, the $ANN_1(\theta_{HT}^{II})$ model showed the best predictive performance based on the test RMSE.

Predicted cumulative emergence curves for both NLR-Weibull (θ_{HT}^{II}) and $ANN_1(\theta_{HT}^{II})$ models vs. observed data are presented for two test years of different precipitation regimes (Fig. 2).

It can be seen that both models have a low predictive performance. Under severe drought conditions, the accumulated emergence was significantly overestimated in a large proportion during the first part of year 2006 and underestimated during the remaining period (Fig. 2A). Such notorious overestimation was registered since the onset of the emergence time-window (March 2006) till August 2006 in coincidence with a 136 day-period of precipitation deficit ($\Psi < \Psi_b$).

For a year of intermediate soil water availability (Fig. 2B), the models provide an acceptable prediction for the first emergent cohort but significantly underestimate the second. The biphasic emergence pattern observed in the field was partially due to a 44 day-period of precipitation deficit concentrated between April and May 2008. Although, such drought period did not affect model predictions for the first cohort, the second cohort was greatly underestimated indicating the inability of such models to adequately predict the remaining of the seedling emergence after soil water replenishment by precipitation.

For bivariate ANNs, a higher predictive capacity was observed as the number of hidden neurons and therefore the number of effective parameters (η) increased (Table 4). Model selection based on AIC was clearly affected by the penalty term. For $d = 1.0$, ANN_2 outperformed all other ANNs, while for $d = 0.5$, ANN_7 seemed the best modeling alternative. RMSE measures on both training and test sets also indicate ANN_7 as the best modeling option (Table 4).

By comparing Tables 2 and 4, it should be noticed that the bivariate ANN_2 model showed an improved prediction capacity ($RMSE_{test} = 0.120$) compared to the best univariate ANN ($RMSE_{test} = 0.168$). However, $ANN_2(\theta_T, \theta_H^I)$ offered a poor representation along the whole season, together with the inability to properly identify the zones of extreme accumulated emergence (Fig. 3).

ANN_7 allowed for the closest representation of the observed emergence data along the whole season for both test years (Fig. 4). However, such an improvement was obtained at the expense of an unrealistic behavior, a reduction of the accumulated emergence, several times along both seasons. Such a behavior suggests that ANN_7 is a model with an excessive number of parameters (Table 4) which produces data over-fitting and yields a (locally) reduced generalization capability.

In order to overcome ANN_7 unrealistic predictions while minimizing the prediction error, the ANN_6 predictive outcome was studied.

ANN_6 (Fig. 5) showed a smooth prediction with excellent representation at low and high accumulated emergences (beginning and end of the season, respectively). However, for year 2006, ANN_6 overestimated emergence from June till October while for 2008 both emergence cohorts were somewhat underestimated.

From these results, ANN_6 model was selected as the best bivariate modeling alternative based on both test error based measure ($RMSE_{test} = 0.106$) and a satisfactory qualitative representation of *A. fatua* cumulative emergence curves.

Prediction errors of the best univariate and bivariate modeling alternatives, NLR-Weibull (θ_{HT}^{II}) model (AIC selected) and ANN_6 (θ_T, θ_H^I) model (quantitatively and qualitatively selected) are

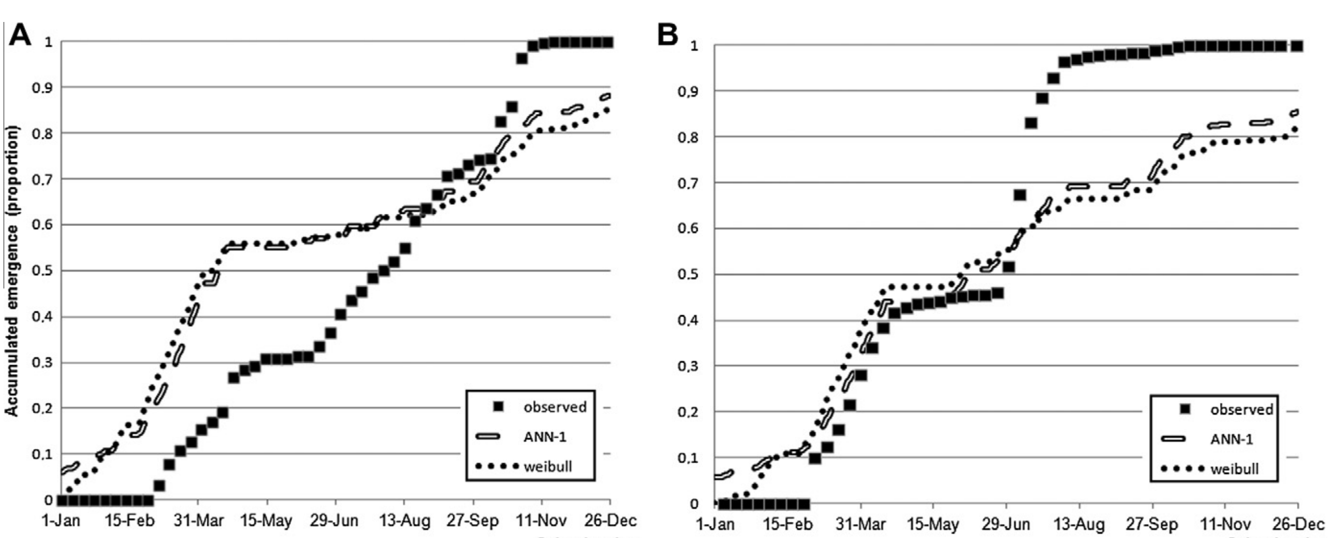

Fig. 2. Observed vs. predicted *A. fatua* cumulative emergence curves for Weibull(θ_{HT}^{II}) and $ANN_1(\theta_{HT}^{II})$ models for the test set: 2006 (A) and 2008 (B).

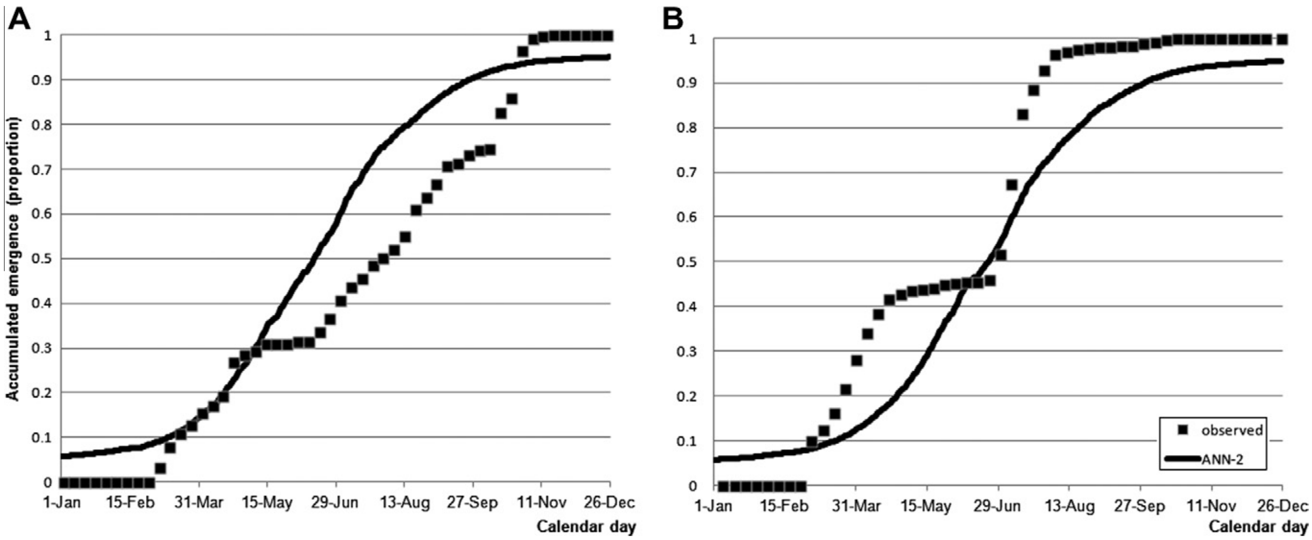

Fig. 3. Observed vs. predicted *A. fatua* cumulative emergence curves for $ANN_2(\theta_T, \theta_H^I)$ model for the test set: 2006 (A) and 2008 (B).

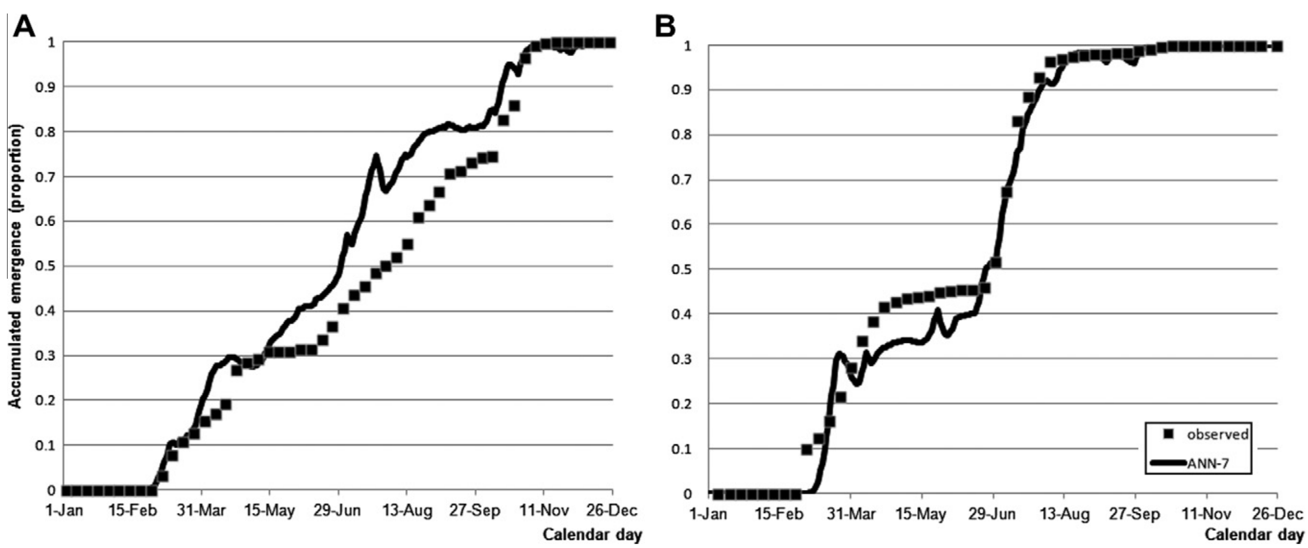

Fig. 4. Observed vs. predicted *A. fatua* cumulative emergence curves for $ANN_7(\theta_T, \theta_H^I)$ model for the test set: 2006 (A) and 2008 (B).

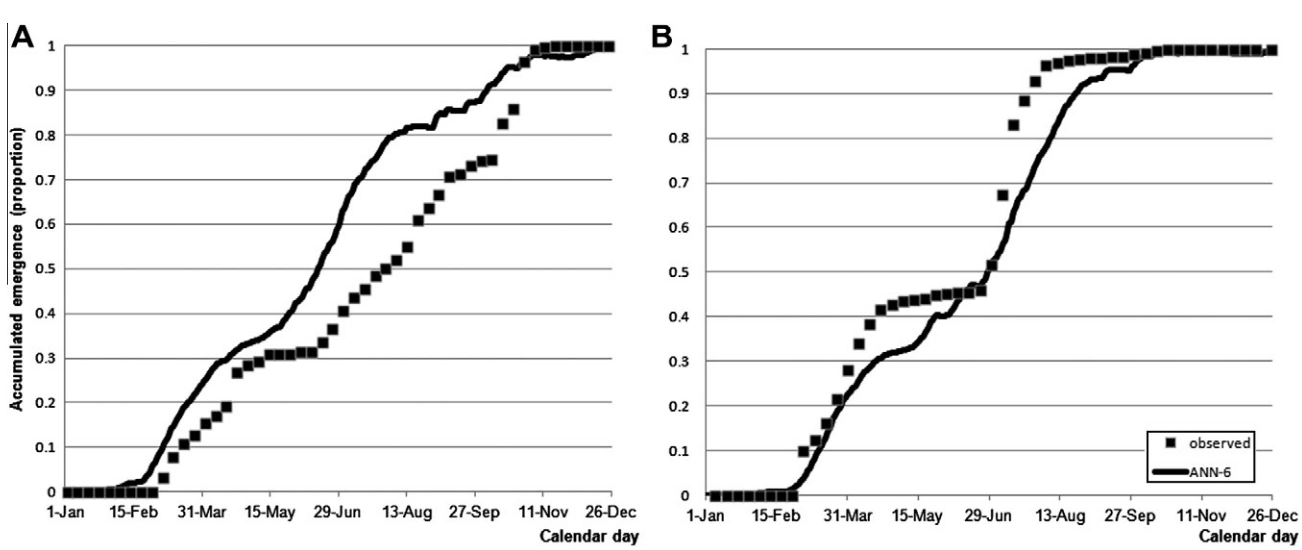

Fig. 5. Observed vs. predicted *A. fatua* cumulative emergence curves for $ANN_6(\theta_T, \theta_H^I)$ model for the test set: 2006 (A) and 2008 (B).

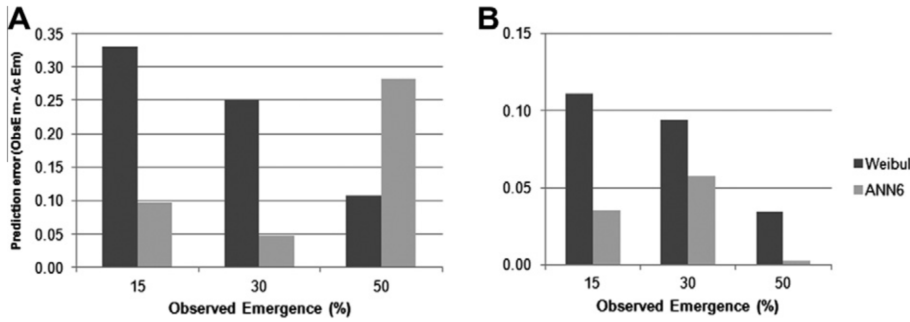

Fig. 6. Prediction errors of Weibull(θ^{II}_{HT}) and ANN$_6$(θ_T, θ^{I}_{H}) models for the test set: 2006 (A) and 2008 (B) as a function of different *A. fatua* cumulative emergence percentages.

reported for the test set at specific cumulative emergences (Fig. 6). An average improvement of 69.5%, 60.0% and 15.5% was obtained with the ANN-6 compared to the NLR-Weibull model at 15, 30 and 50% of *A. fatua* observed cumulative emergence, respectively.

4. Discussion and agronomic insight

From the analysis of the previous sections, the following leading conclusions can be drawn:

i. For the system under study, hydrothermal-time index based models are poor predictors of *A. fatua* field emergence patterns, no matter the modeling framework (NLR or ANNs).
ii. ANNs with thermal-time and hydro-time as independent input variables provide better predictions than univariate hydrothermal-time approaches.
iii. In the bivariate ANN modeling approach, as the number of neurons (parameters) increase, goodness of fit (RMSE$_{train}$) and prediction (RMSE$_{test}$) measures were improved.
iv. If parsimony is heavily weighted in the AIC evaluation (d = 1.0), ANNs with a small number of parameters (neurons) are preferred.
v. If parsimony is less weighted in the AIC evaluation (d = 0.5), ANNs with a large number of parameters (neurons) are preferred.
vi. ANNs with a large number of parameters predicts unrealistic reductions in accumulated emergence (i.e. ANN$_7$).

None of the statistical measures used for evaluating models performance (AIC and RMSE) allowed determining the optimum number of parameters of the network, since a compromise between error minimization and parsimony could be obtained only by graphical inspection of the predictions against the observed data. Thus, our results agree with Qi and Zhang (2001), in the sense that neither penalty-based in-sample (training set) criteria nor no-penalty-related performance measures seem to be adequate tools for ANNs assessment. In addition, as stated by Qi and Zhang (2001), such measures are not always consistent with the best performances in out-sample data (test sets).

In our study, bivariate ANN$_6$ (thermal-time and hydro-time based) model was considered the best modeling alternative since it provides the closest representation of the data while verifying the actual, ever increasing behavior of the accumulated emergence.

Our results confirmed the limited capability of hydrothermal-time based Weibull models to accurately predict the onset of *A. fatua* emergence "time-window" under semiarid conditions (Moschini et al., 2009, 2011). As stated by Martinson et al. (2007), models that significantly under-predict seedling emergence will produce delayed control leading to prolonged competition, additional herbicide applications and reduced crop yields. On the other hand, over-prediction would induce early control interventions allowing late emergence cohorts to prosper leading to competition and seed bank replenishment.

From an agronomic point of view, an accurate prediction of weed emergence flushes is vital in the design of effective control tactics. The proposed model would help to improve decision-making regarding sustainable weed management practices in semiarid regions. Finally, it should be mentioned, that better results could be obtained if the data sets were classified according, for example, to low, medium and high precipitation regimes and a specific model adjusted for each case. This way the decision maker would have a more specific predictive tool adapted for a year of particular weather features. Moreover, a more accurate prediction of the onset of *A. fatua* emergence "time-window" could be obtained by using training data belonging, for example, to the first 50% of cumulative emergence. However, such approaches were not adopted here since the objective was to investigate the performance of the different ANNs for the whole emergence spectrum.

5. Conclusions

ANNs for empirical modeling allow the use of any number of input variables and provides a flexible modeling framework non-dependant on specific underlying non-linear structures. These features redounded in improved prediction capability compared to the commonly used univariate non-linear regression approaches.

From a practical agronomical perspective, these results suggest that the development of ANN models offer an enormous potential to be implemented as emergence predictors within weed management decision support tools currently under development (Lodovichi et al., 2012).

Additional studies, including the use of alternative explanatory variables and seed burial depths would be of interest. Moreover, complementary analysis aimed to quantify the contribution of each input variable to the ANNs outcome would serve to improve the understanding of the underlying ecological and biological processes, which are difficult to unravel within a network (Olden and Jackson, 2002).

Finally, it should be stressed that despite the acceptable predictive outcome of the developed ANN models obtained in this work, the approach remains a "black box". Process-based deterministic models, as those used for crop growth calculation (Brisson et al., 2008) might be conceived in order to represent the underlying biological processes of weeds physiology. Further studies should focus on the development of seed dormancy and germination models in order to address the estimation of emergence from a more mechanistic approach.

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