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2	A Stacked Machine Learning Algorithm for Multi-Step Ahead Prediction of Soil Moisture
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### 33 Abstract

A trustworthy assessment of soil moisture content plays a significant role in irrigation planning 34 and in controlling various natural disasters such as floods, landslides, and droughts. Various Machine 35 Learning Models (MLMs) have been used to increase the accuracy of soil moisture content prediction. 36 The present investigation aims to apply MLMs with novel structures for the estimation of daily 37 volumetric soil water content, based on the stacking of the Multilayer Perceptron (MLP), Random 38 Forest (RF), and Support Vector Regression (SVR). Two groups of input variables were considered: 39 the first (Model A) consisted of various meteorological variables (i.e., daily precipitation, air 40 temperature, humidity, and wind speed), and the second (Model B) included only daily precipitation. 41 The Stacked Model (SM) had the best performance ( $R^2 = 0.962$ ) in the prediction of daily volumetric 42 soil water content for both categories of input variables when compared with the MLP ( $R^2 = 0.957$ ), 43 RF ( $R^2 = 0.956$ ), and SVR ( $R^2 = 0.951$ ) models. Overall, the SM, which in general allows the 44 weaknesses of the individual basic algorithms to be overcome while still maintaining a limited 45 number of parameters and short calculation times, can enhance the precision level of water moisture 46 47 content more than other well-known MLMs.

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49 Keywords: Machine learning models; Soil moisture content; Stacked Model; Statistical measures.

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### 51 **1. Introduction**

Soil moisture is a variable that substantially affects the interactions between the earth's surface 52 53 and the atmosphere, both in meteorological and climatic aspects (Seneviratne et al. 2010). It plays a fundamental role in rainfall-runoff processes (Sit and Demir, 2019), influencing the division of 54 precipitation into surface runoff, subsurface flow, and infiltration. It also affects the transformation 55 56 of incoming radiation fluxes to the soil into latent and sensible heat fluxes from the soil to the atmosphere. Soil moisture also strongly impacts the interaction between climate and vegetation in its 57 multiple aspects, primarily the phenomenon of evapotranspiration. Moreover, soil moisture is a major 58 discriminating factor in the type and condition of vegetation in a region. Variations in soil moisture 59 can therefore have a massive impact on agriculture, forestry, and ecosystems. 60

Soil moisture measurement can be conducted by using in-situ probes (Walker et al. 2004, Demir et al. 2015) or by remote sensing methods (Mohanty et al. 2017). The significant impact on infiltration and runoff phenomena gives soil moisture prediction a key role in flood risk management (Yildirim & Demir 2022) and landslide risk monitoring (Brocca et al. 2017). Furthermore, predicting soil moisture and its changes is essential for predicting the onset of drought and planning irrigation (Soulis et al. 2015), as soil moisture is a critical limiting factor for crop growth.

Traditional soil moisture prediction techniques include empirical formulas, models based on soil water balance, models based on soil water dynamics, and autoregressive moving average models (ARMA). Compared to these traditional methodologies, higher prediction accuracy can be achieved by models based on Artificial Intelligence algorithms, which have found increasingly widespread use in the prediction of hydrological quantities over the past two decades (Kisi 2007, Nourani et al. 2011, Di Nunno & Granata 2020, Xiang & Demir 2020, Granata & Di Nunno 2021, Granata et al. 2022a). A large number of studies on soil moisture estimation were carried out using various machine

<sup>74</sup> learning algorithms: Support Vector Regression (SVR), Artificial Neural Networks (ANNs), Model

75 Tree (MT), Multivariate Adaptive Regression Spline (MARS), and Adaptive Neurofuzzy Inference

76 System (ANFIS) (Elshorbagy & Parasuraman 2008, Si et al. 2015, Zanetti et al. 2015, Cui et al. 2016,

Prasad et al. 2018a, Prasad et al. 2018b, Prasad et al. 2019, Maroufpoor et al. 2019, Achieng 2019,
Wenn et al. 2020, He dawn 2021)

78 Yuan et al. 2020, Heddam 2021).

79 Elshorbagy & Parasuraman (2008) employed two types of ANNs, i.e., Multilayer Perceptron (MLP) and the Higher-Order (HO-NN) types, to estimate soil moisture by accumulating field data at 80 three subwatersheds soil covers. They considered precipitation, air temperature, net solar radiation, 81 and soil temperature at various depths for feeding MLP and HO-NN models. They found that HO-82 NN model had better performance than MLP. Liu et al. (2008) proposed a hybrid ANN - SVR 83 architecture to estimate water content at a study site located in Chongqing, China. The authors noted 84 85 that the hybrid model clearly outperformed the individual models. Additionally, Ahmad et al. (2010) used SVR to assess soil moisture at 10 sites in the Lower Colorado River Basin. SVR models were 86 trained using 5 years of data. The best results obtained were characterized by correlation coefficients 87 between 0.34 and 0.77, with a root mean square error (RMSE) of less than 2%. Furthermore, the 88 89 authors made a comparison with the results obtained from models based on ANN and Multiple Linear Regressions (MLR), showing that they were outperformed by SVR. 90

Si et al. (2015) employed ANFIS, MLP, and the Bayesian Regularization Neural Network 91 (BRNN) in order to estimate soil moisture content at two various depths: 40 and 60 cm. They applied 92 93 900 data sets from field measurement in order to develop the AI models. From their results, it was 94 found that ANFIS provided more accurate prediction soil moisture than the BRNN and the MLP models. In addition, Zanetti et al. (2015) employed MLP model to assess soil moisture content while 95 considering various properties of five types of soils such as the apparent dielectric constant, clay and 96 organic matter contents, bulk density and sand, and the silt content. They found that the MLP model 97 98 with various combinations of input variables, such as organic matter combined with apparent dielectric constant, was particularly effective. Karandish & Simunek (2016) evaluated superiority of 99 ANFIS and SVR with HYDRUS-2D for predicting time dependent-soil moisture content obtained by 100 a physical model under various water stress circumstances over the maize growing time-period of 101 2010 and 2011. Later, Cui et al. (2016) utilized successfully the MLP-NN using a good many MODIS 102 optical products for soil moisture retrieval and found permissible level of precision. In another study, 103 Prasad et al. (2018b) developed an ensemble Committee Machine (CoM) learning model based on 104 ANN (ANN-CoM) and utilized it to predict monthly soil moisture at upper and lower layer of soil. 105 From their study, statistical results indicated outperformance of the ANN-CoM model in comparison 106 with those yielded by the ELM, RF, and M5Tree. 107

Moreover, Prasad et al. (2019) found superiority of ELM with ensemble empirical mode 108 decomposition and the Boruta wrapper algorithm (EEMD-Boruta-ELM) over standalone MARS, 109 110 ELM, and the EEMD-Boruta-MARS models for estimating weekly values of soil moisture content. Cai et al. (2019) found that the Deep Learning NN (DLNN) provided a more accurate prediction of 111 daily soil moisture based on various meteorological factors (e.g., daily precipitation, daily mean 112 surface temperature, average wind speed, average relative humidity, average air pressure, and average 113 temperature) than the MLP model at depths of 10 and 20 cm. Achieng (2019) used successfully SVR 114 model by Gaussian kernel to simulate soil moisture content when compared with SVR models 115 developed by polynomial and linear kernels, MLP, and the DLNN models. In recent years, Yuan et 116 al. (2020) reported permissible level of accuracy when the Generalized Regression NN (GR-NN) was 117 employed in order to estimate the regional surface soil moisture by means of satellite observations as 118

input factors. Adab et al. (2020) used RF, SVR, ANN and Elastic Network (EN) regression to estimate
soil moisture from data obtained from Landsat 8 optical and thermal sensors, and knowledge of land
use in a semi-arid region of Iran. The best results, characterised by a Nash-Sutcliffe efficiency value
of 0.73, were obtained with the RF algorithm. In Heddam's (2021) study, four MLMs (i.e., MT, RF,
MARS, and MLP-NN) have been successfully employed to estimate soil moisture content while
considering only hourly soil temperature as input variable (obtained from two USGS stations) and
compared with Multivariate Linear Regression (MLR) technique.

- Therefore, in the current literature, various MLMs indicated promising performance in the estimation 126 of soil moisture content for various conditions of soil physical properties. However, there is a shortage 127 of models for predicting future soil water content (SWC), even in the short term, that are both simple, 128 129 based on a few easily measurable input variables, and highly accurate. The main objective of this study is to propose a novel ensemble daily SWC prediction model obtained by stacking (Granata et 130 al. 2022b) three individual Machine Learning algorithms; MLP, RF, and SVR. These three standalone 131 algorithms were chosen both because individually they showed good predictive capabilities, and 132 133 because they have different structures and thus their combination can overcome the weaknesses of each algorithm. Furthermore, these three algorithms, compared with more complex algorithms such 134 as Deep Learning, have the advantage that they depend on few parameters, facilitating training and 135 optimisation operations, and are characterised by significantly shorter calculation times. To the best 136 of the authors' knowledge, there are no applications of stacked algorithms for short-term prediction 137 of SWC in the literature so far. The performance of the stacked model is compared with that of the 138 individual algorithms considering two different scenarios of input variables. The proposed model is 139 trained and tested with data obtained from a measurement site in East Anglia, UK. In addition, 140 141 changes in model accuracy are statistically analysed as the prediction horizon increases, while remaining within the scope of short-term forecasts. 142
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#### 144 **2. Materials and Methods**

### 145 2.1. Standalone Machine Learning Algorithms

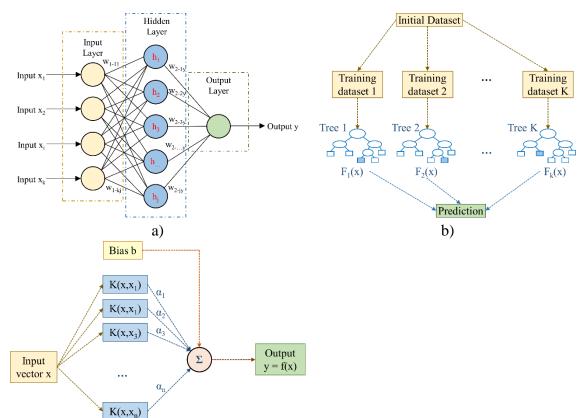
In this research, MLP, RF, and SVR algorithms were used both individually and combined through 146 stacking. An MLP is a simple feedforward (Rosenblatt 1961, Murtagh 1991) ANN that can 147 approximate any continuous function. An MLP consists of at least three layers of nodes: an input 148 layer, at least one hidden layer, and an output layer. The input layer includes the nodes that acquire 149 the input data. Each node of the hidden layer processes the values of the previous layer using a 150 weighted linear sum, followed by a non-linear activation function. The output layer receives the 151 processed data from the last hidden layer and transforms it into the resulting values. The training of 152 153 the algorithm is performed using the back-propagation technique. The neural networks employed in this study had only one hidden layer. 154

RF (Breiman 2001) is an ensemble prediction algorithm obtained by combining a set of individual regression trees in order to predict a single value of the target variable. In each individual regression tree (Breiman et al. 2017) it is possible to identify a root node, which comprises the training dataset, a number of internal nodes, which define the conditions on the input variables, and leaves, which represent the actual values assigned to the target variables. A tree regression model is developed by recursively dividing the input dataset into subsets, conducted in such a way as to minimise the internal node variance. A multivariable linear regression model provides predictions for each subset. Each tree grows from a different bootstrap of the training dataset. In addition, at each node, only a portion of the variables are randomly chosen with respect to which to split. The number of these variables is kept constant during the growth of the forest. A pruning process significantly reduces the risk of overfitting.

166 The idea behind the SVR algorithm (Cortes & Vapnik 1995) is to provide an approximation of the true value with a function that is as flat as possible, and that brings the error within a certain 167 threshold, defined by an ε-value. A simple way to understand the SVR algorithm is to imagine a 168 "tube" with an estimated function (hyperplane) as the centre line and boundaries on both sides defined 169 by ε. The goal of the algorithm is to minimise the error by identifying a function that places as many 170 points of the training dataset as possible within the tube, while reducing the "slack". The concept of 171 slack variables is simple: for any value that falls outside  $\varepsilon$ , its deviation from the margin is denoted 172 as  $\xi$ . When these deviations are to be tolerated, the algorithm tends to minimise them as well. 173 Therefore, the deviations  $\xi$  are added to the objective function to be minimised in the constrained 174 optimisation problem into which the regression problem turns. The need to ensure a balance between 175 the flatness of the regression function and the tolerated slacks is met by tuning a regularisation 176 parameter C. In SVR, regression is performed in a higher dimension. For this purpose, a function is 177 required that maps the data points in a higher dimension. This function is defined as kernel. In this 178 179 study, the radial basis function (RBF) was chosen as the kernel  $K(x_i, x_i)$ :

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$$K(x_i, x_j) = \exp\left(-\gamma \left\|x_i - x_j\right\|^2\right), \ \gamma > 0 \tag{1}$$

- 182 where  $x_i$ ,  $x_j$  are two input vectors.
- 183 Fig. 1 shows a schematic representation of the architectures of the algorithms introduced above.



c)

Figure 1. Architecture of individual algorithms considered in the study: a) Multilayer Perceptron, b)
 Random Forest, c) Support Vector Regression

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# 187 2.2. Evaluation Criteria

Four different evaluation criteria were employed to assess the accuracy of the prediction models: coefficient of determination ( $R^2$ ), Root Mean Square Error (RMSE), Mean Absolute Error (MAE), and Mean Absolute Percentage Error (MAPE). The  $R^2$  coefficient is an estimation of goodness of fit, taking values in the range [0, 1]. The more accurate a model's predictions are, the closer its  $R^2$  will be to 1. It is defined as:

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$$R^{2} = \left[1 - \frac{\sum_{t} (f_{t} - y_{t})}{\sum_{t} (y_{a} - y_{t})^{2}}\right]$$
(2)

 $\left( \sum_{i=1}^{n} \left( c_{i}^{2} \right)^{2} \right)$ 

where  $f_t$  is the predicted value at time t,  $y_t$  is the measured value at time t, and  $y_a$  is the averaged value of the measured data.

196 The RMSE is the standard deviation of the prediction errors, the so-called residuals, which measure

the distance of the experimental points from the regression line. In practice, the RMSE quantifies thedispersion of the data around the line of best fit. It is evaluated as:

in which *N* is the total number of predicted values in the time series.

The MAE estimates the average size of errors in the forecasts as a whole, without taking their direction into account:

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$$MAE = \frac{\sum_{t} |f_t - y_t|}{N}$$
(4)

The mean absolute percentage error (MAPE) evaluates the average of the absolute percentage errors of the prediction model. For the purpose of calculating MAPE, percentage errors are considered without taking the sign into account:

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$$MAPE = \frac{100}{N} \sum_{i} \left| \frac{y_{i} - f_{i}}{y_{i}} \right|$$
(5)

#### 208 2.3. Stacked Model Development

Stacking is an ensemble machine learning procedure that combines a number of classification or regression models through a metaclassifier. Stacking can exploit the capabilities of several wellperforming models on a regression task in order to outperform standalone models in achieving predictions. The individual regression models are developed on the basis of the entire training data set, then a metaclassifier is applied on the basis of the outputs (meta-features) of the individual models. The Elastic Net (EN) algorithm was selected as the meta-classifier to develop the stacked prediction models. EN algorithm (Zou & Hastie 2005) is a combination of the two most commonly used regularised variants of linear regression: the Least Absolute Shrinkage and Selection Operator
(LASSO) method and the Ridge method. The LASSO method selects the most explanatory variables
by introducing an absolute penalty in the ordinary least squares (OLS) regression. Ridge
regularisation also introduces a penalty in the OLS formulation by penalising square weights instead
of absolute weights. Thus, large weights are penalised significantly, and many small weights are
distributed over the feature spectrum.

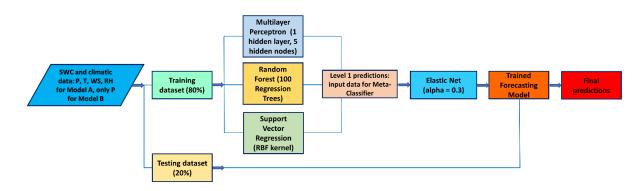




Figure 2. Flowchart of the Stacked model implementation

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Two prediction models, differing in input variables, were developed in this study. Each model was developed in four variants, each based on one of the different ML algorithms introduced before, namely MLP, RF, SVR and the combination by stacking of the previous ones. Model A includes the following exogenous input variables: cumulative daily precipitation (P), average daily air temperature T, average daily wind speed (WS), and average daily relative humidity (RH). On the other hand, Model B only includes cumulative daily precipitation P as an exogenous input. In addition, both models include lagged values of SWC as input variables.

The optimal number of lagged values of SWC, as well as the optimal values of the hyperparameters of the individual ML algorithms, were chosen by means of a grid search optimisation procedure aimed at minimising the RMSE of individual forecasting algorithms. It was found that in the case study investigated, the optimal number of lagged values of SWC to be considered as input is 7. In addition, the main hyper-parameters of the forecast models are shown in Table 1. Therefore, based on the optimisation process, the following input and output values can be indicated for the two forecast models:

- Model A input: SWCt-6, SWCt-5, ..., SWCt, Pt, Tt, WSt, RHt; output: SWCt+1, SWCt+2, SWCt+3
  - Model B input: SWC<sub>t-6</sub>, SWC<sub>t-5</sub>, ..., SWC<sub>t</sub>, P<sub>t</sub>; output: SWC<sub>t+1</sub>, SWC<sub>t+2</sub>, SWC<sub>t+3</sub>

where subscripts indicate the number of the day. The generic variable was normalized according tothe equation:

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$$x_{Ni} = \frac{x_i - x_{\min}}{x_{\max} - x_{\min}} \tag{6}$$

The training of each model was carried out using 80% of the time series data, while testing was conducted on the remaining 20%. This division allowed the most accurate results to be obtained.

Algorithm	Hyperparameter	Value
	Number of hidden layers	1
MLP	Number of hidden neurons	5
	Activation function	Sigmoid
RF	Number of trees	100
	Kernel function	RBF
SVR	С	2
	ε	0.01
EN	α	0.3

Table 1. Main hyperparameters of the forecasting algorithms.

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## 250 **2.4.** Case Study

The data used in this study were provided by the COSMOS-UK network of the UK Centre for 251 Ecology & Hydrology. Specifically, data were obtained from the COSMOS-UK site in Fincham 252 253 (https://cosmos.ceh.ac.uk/data), East England (Fig. 3). The Fincham site is located in a large flat field planted with winter wheat, oilseed rape and sugar beet in a 6-year rotation. The soil type is a chalky 254 loam, a calcareous mineral soil. Like the other sites in the network, the Fincham site is equipped with 255 an instrument that uses cosmic rays to measure soil moisture. More details on the measurement 256 257 technique can be found in Zreda et al. (2008), Desilets et al. (2010), and Andreasen et al. (2016). Experimental data are related to volumetric SWC (%) = (volume of water/volume of soil)  $\times$  100. The 258 time series of daily hydrological variables of interest analysed (soil water content, cumulative rainfall, 259 average air temperature, average wind speed, average relative air humidity) include data collected 260 from 22/06/2017 to 31/12/2019. Figure 4 shows the time series of cumulative daily rainfall and SWC 261 262 during the period under investigation, while Table 2 shows the essential statistical parameters of the 263 SWC time series and climate variables of interest, excluding rainfall.

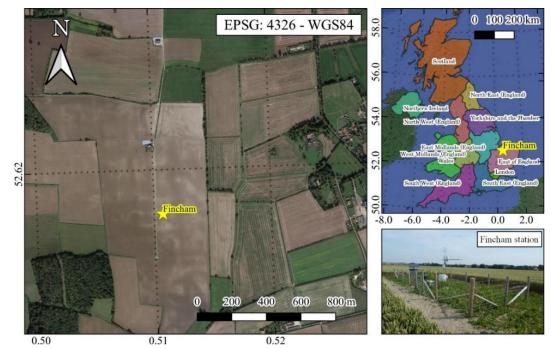


Figure 3. Case study location at the Fincham measurement site

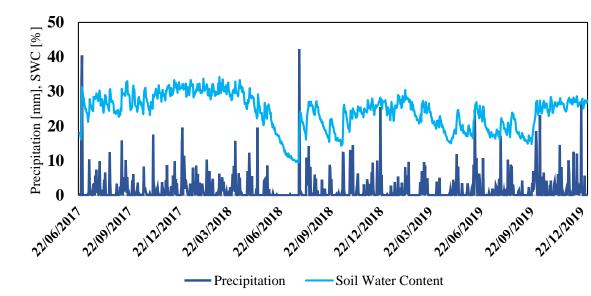


Figure 4. Time series of cumulative daily rainfall and SWC during the period under investigation



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Table 2. Essential time series characteristics of measured SWC and other climatic variables

	SWC [%]	Air Temp. [°C]	Wind Speed [m/s]	<b>Rel. Hum. [%]</b>
Mean	24.18	11.06	3.28	80.12
Median	25.00	11.12	3.03	81.43
Max	34.20	27.36	8.52	99.62
Min	9.40	-4.82	0.67	53.36
St. Deviation	5.16	5.54	1.42	9.50
CV	0.21	0.50	0.43	0.12
1st Quartile	20.55	6.79	2.20	73.00
<b>3rd Quartile</b>	27.90	15.50	4.14	87.82
Skewness	-0.57	0.00	0.88	-0.31

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# 274 **3. Results**

Table 3 shows the values of the evaluation metrics for the prediction model A with reference to the 1
day-ahead, 2 days-ahead and 3 days-ahead SWC. The table shows the metrics for both the training
and testing phase, for each of the individual algorithms and for the SM.

With reference to the 1-day ahead forecast, in the testing phase the three standalone algorithms showed roughly equivalent accuracies, with  $R^2$  varying between 0.957 (MLP) and 0.951 (SVR), while MAPE varies between 3.35% (SVR) and 3.62% (RF). The SM outperformed all other forecasting algorithms, being characterised by a higher  $R^2$  of 0.961 and smaller errors, with MAPE of 3.05%. It should be noted that the metrics values for the testing phase were absolutely comparable to those for the training phase. The only algorithm for which there was a perceptible difference between the two phases was RF.

Table 3. Model A evaluation metrics

			MLP	RF	SVR	Stacked Model
		<b>R</b> <sup>2</sup>	0.957	0.992	0.942	0.968
	1 day-	RMSE	1.092	0.49	1.267	0.937
	ahead	MAE	0.816	0.356	0.911	0.694
		MAPE	3.36%	1.49%	3.73%	2.85%
		<b>R</b> <sup>2</sup>	0.940	0.985	0.912	0.953
Model A	2 days-	RMSE	1.285	0.663	1.569	1.137
(Training)	ahead	MAE	1.009	0.469	1.139	0.861
		MAPE	4.22%	1.94%	4.68%	3.56%
		<b>R</b> <sup>2</sup>	0.928	0.977	0.891	0.941
	3 days-	RMSE	1.406	0.829	1.752	1.276
	ahead	MAE	1.101	0.571	1.266	0.959
		MAPE	4.66%	2.36%	5.24%	3.99%
		<b>R</b> <sup>2</sup>	0.957	0.956	0.951	0.962
	1 day- ahead	RMSE	0.924	0.985	0.996	0.877
		MAE	0.741	0.787	0.744	0.673
		MAPE	3.41%	3.62%	3.35%	3.05%
		<b>R</b> <sup>2</sup>	0.940	0.938	0.927	0.946
Model A	2 days-	RMSE	1.146	1.217	1.264	1.053
(Testing)	ahead	MAE	0.942	0.990	0.945	0.821
		MAPE	4.40%	4.59%	4.27%	3.74%
	3 days-	<b>R</b> <sup>2</sup>	0.921	0.929	0.911	0.935
		RMSE	1.355	1.360	1.442	1.169
	ahead	MAE	1.105	1.113	1.069	0.921
		MAPE	5.25%	5.22%	4.83%	4.22%

Figure 5 shows the scatter plots of the predicted SWC values versus the measured values. The 288 plots show the excellent performance of all forecast models, with the points lying along the line of 289 perfect agreement. With reference to the Stacked model for the 1-day-ahead forecast, Fig. 6a shows 290 the time series of the predicted and measured SWC, while Fig. 6b shows the relative error in the same 291 time series. The relative error is defined as the absolute error in the forecast divided by the actual 292 value of the SWC. The SM could accurately reproduce both SWC peak values and value fluctuations. 293 294 Moreover, the relative error was almost always in the range -5%, +5%, and in a few cases approached ±10%. 295

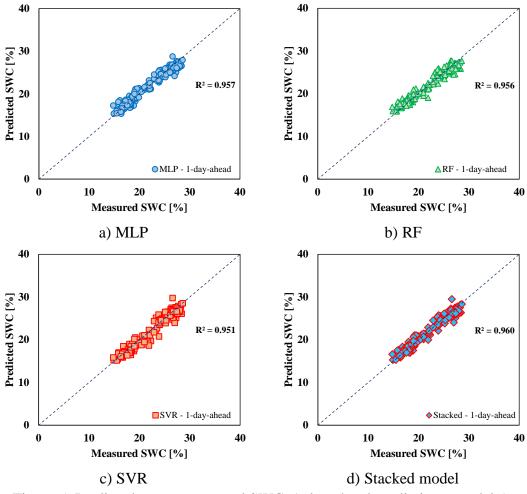
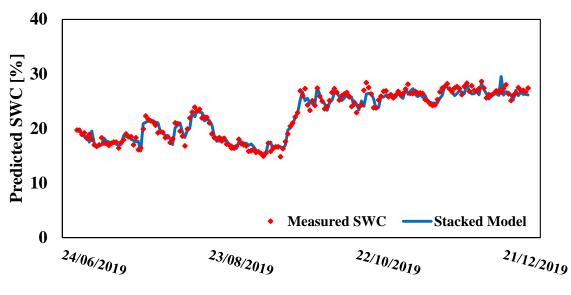
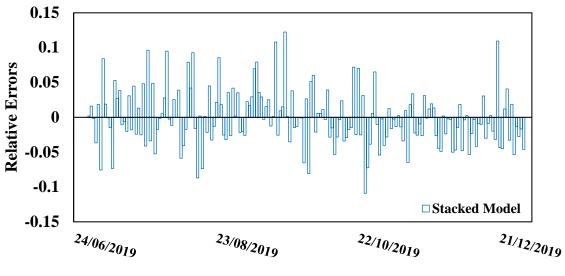


Figure 5. Predicted versus measured SWC, 1-day-ahead predictions, model A.





b)

Figure 6. a) stacked model time series (Model A), b) relative errors for each point in the time series

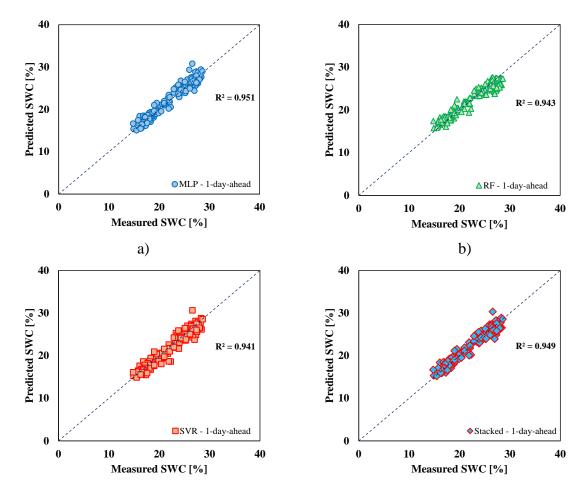
			MLP	RF	SVR	Stacked Model
		$\mathbb{R}^2$	0.946	0.990	0.934	0.965
	1 day-	RMSE	1.222	0.533	1.365	0.989
	ahead	MAE	0.914	0.394	0.979	0.737
		MAPE	3.72%	1.62%	3.94%	3.02%
		$\mathbb{R}^2$	0.919	0.976	0.892	0.943
Model B	2 days-	RMSE	1.495	0.835	1.749	1.258
(Training)	ahead	MAE	1.161	0.586	1.274	0.964
		MAPE	4.77%	2.38%	5.13%	3.98%
		$\mathbb{R}^2$	0.900	0.960	0.863	0.925
	3 days-	RMSE	1.658	1.073	1.989	1.441
	ahead	MAE	1.286	0.745	1.479	1.109
		MAPE	5.32%	3.01%	5.98%	4.62%
		$\mathbb{R}^2$	0.951	0.943	0.941	0.949
	1 day- ahead	RMSE	0.982	1.145	1.069	0.976
		MAE	0.745	0.937	0.810	0.751
		MAPE	3.42%	4.28%	3.64%	3.39%
		$\mathbb{R}^2$	0.928	0.916	0.907	0.924
Model B	2 days-	RMSE	1.249	1.456	1.381	1.224
(Testing)	ahead	MAE	0.964	1.198	1.028	0.973
		MAPE	4.48%	5.53%	4.59%	4.45%
	3 days- ahead	R <sup>2</sup>	0.903	0.896	0.880	0.902
		RMSE	1.513	1.667	1.606	1.411
		MAE	1.185	1.381	1.193	1.144
		MAPE	5.56%	6.43%	5.32%	5.29%

Considering the 2-day-ahead forecasts, it can be seen that all variants of Model A underwent a very slight reduction in accuracy, but the forecasts were still very good. With regard to the SM metrics, for example, it can be observed that R<sup>2</sup> decreased from 0.962 to 0.946, RMSE increased from 0.877 to 1.053, MAE increased from 0.673 to 0.821, and MAPE increased from 3.05% to 3.74%. Again, the Stacked model outperformed the standalone models.

Even with regard to 3-day-ahead forecasts, all variants of Model A showed a further slight decrease in accuracy. Again, the three individual algorithms led to comparable results, while the SM outperformed them all, as proved by the higher R<sup>2</sup> value and lower RMSE, MAE, and MAPE values. Table 4 shows the values of the metrics for the forecast model B with reference to the 1 day-ahead, 2 days-ahead and 3 days-ahead SWC. Again, the table shows the metrics for the training and testing phase, for each of the individual algorithms and for the Stacked model.

With regard to 1-day-ahead forecasts, MLP ( $R^2 = 0.951$ , RMSE = 0.982, MAE = 0.745, and MAPE = 3.42%) led to better results in the testing phase than RF and SVR. The SM ( $R^2 = 0.949$ , RMSE = 0.976, MAE = 0.751, MAPE = 3.39%) led to results practically equivalent to those obtained with MLP. The ensemble model in this case did not lead to better results than the most accurate standalone algorithm. Furthermore, the predictions provided by model B were slightly less accurate than the corresponding ones provided by model A, with the exception of the MLP algorithm, for which negligible differences were observed.

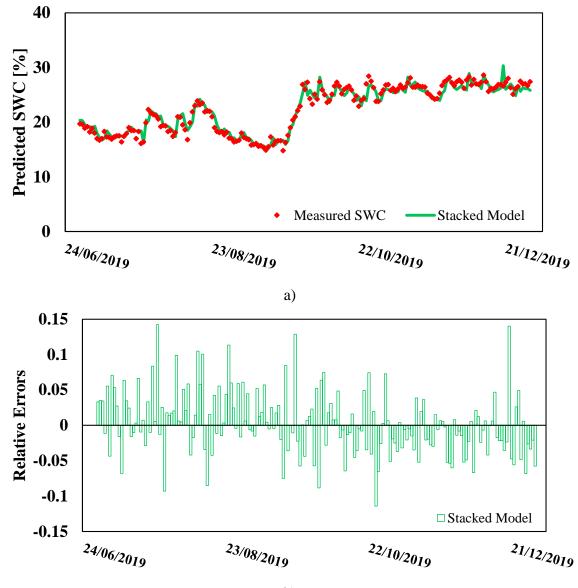
Figure 7 shows the scatter plots of the predicted SWC values compared to the measured values for model B. Again, the regular arrangement of the points along the line of perfect agreement can be seen, with small deviations.



c) d) Figure 7. Predicted versus measured SWC, 1-day-ahead predictions, model B.

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Referring to the SM for the 1-day-ahead prediction, Fig. 8a shows the time series of the predicted and measured SWC, while Figure 8b shows the relative error in the same time series, in the case of model B. Again, the SM was able to accurately reproduce both the peak values of the SWC and the value fluctuations. Moreover, the relative error, although again almost always in the range of -5%, +5%, in some cases exceeded  $\pm 10\%$ , even approaching 15%.



b)

Figure 8. a) Stacked model time series (Model B), b) relative errors for each point in the time series

Focusing on the 2-day-ahead forecasts, it can be seen that, even for model B, all variants suffered a reduction in accuracy. Furthermore, all variants underperformed the corresponding variants of model A. However, the forecasts were still satisfactory. MLP ( $R^2 = 0.928$ , RMSE = 1.249, MAE = 0.964, MAPE = 4.48%) and the SM ( $R^2 = 0.924$ , RMSE = 1.224, MAE = 0.973, MAPE = 4.45%) again led to the best results. Finally, 3-day-ahead forecasts showed a further reduction in accuracy. The SM provided the best results, and its metrics took the following values:  $R^2 = 0.902$ , RMSE = 1.411, MAE = 1.144, MAPE = 5.29%. The forecasts were still very good, even though all model B
variants underperformed the corresponding model A variants.

337

# 338 **4. Discussion**

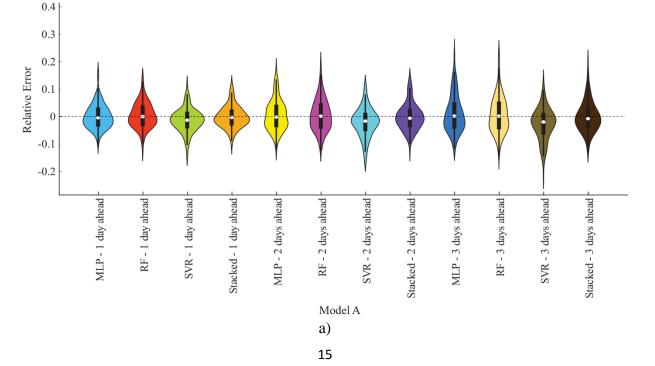
The results shown above demonstrated that both model A and model B are able to provide satisfactory predictions of short-term SWC. Model A proved to be more accurate. The presence of air temperature, relative humidity and wind speed among the input data allows for the consideration of evapotranspiration, which depends on the aforementioned climatic variables and in most cases is the main outflow of moisture from the soil. However, even the availability of daily cumulative rainfall data as the only exogenous variable allowed for accurate short-term SWC forecasts.

The SM generally outperformed the standalone models. In some cases, for model B, it provided comparable performance to the most accurate individual algorithm. It seems that the SM performs significantly better than the individual models from which it is combined if the number of input variables is increased. This statement, however, needs further investigation.

Further insight into the accuracy of the different prediction models can be pursued by analyzing the violin plots in Figure 9, which show the relative error distributions of all variants of model A and model B, for the three forecast horizons considered. The same violin plots also include the corresponding box plots. The following insights can be deduced from these plots:

- a) In the case of model A, only the SVR-based variant was characterised by an appreciable bias,
   whereas in the case of model B, an appreciable bias could be found in both the MLP- and
   SVR-based variants.
- b) The distribution of the relative error in both models was asymmetrical in many cases.
- 357 c) The error distribution tended to become flatter as the forecast horizon increased, and the IQR
   358 of the relative error expanded as the forecast horizon increased.
  - d) The number of outliers resulting from forecasting models was very low.
- 359 360

This additional information provided by the violin plots enhanced the understanding of the results described above in terms of metrics.



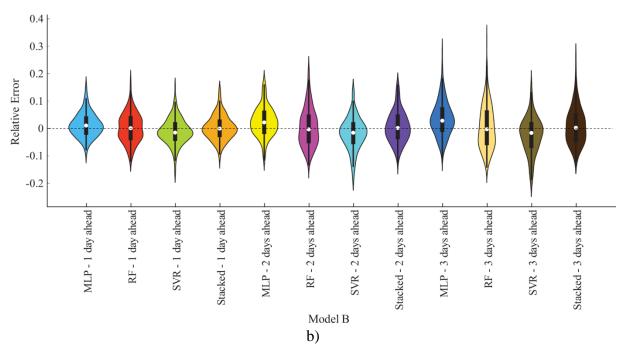




Figure 9. Violin plots of relative errors in a) Model A, b) Model B

The lack of benchmark datasets (Demir et al. 2022) and closely comparable studies prevents direct 364 comparisons of the results. There are also very few studies focused on soil moisture that use stacking 365 algorithms for purposes other than forecasting. A recent study by Das et al. (2022) aimed to map soil 366 surface moisture with a spatial resolution of 30 m in a semi-arid region using optical, thermal, and 367 microwave remote sensing data, and applying machine learning techniques such as bagging, boosting, 368 and stacking. The authors found that the stacking of the cubist, gradient boosting machine (GBM), 369 and RF algorithms led to better results than the individual algorithms, in agreement with the findings 370 of this study. 371

Other recent studies on SWC forecasting are based on the use of hybrid models. In terms of 372 quantitative comparisons, the statistical measures provided by Models A and B showed that an 373 improved MLM (i.e., the Stacked Model) outperformed MLP. This finding was evident in the 374 comparison with Ahmad et al. (2010) (R<sup>2</sup>=0.2601 and 0.1764 for SVM and ANN, respectively). In 375 the investigation by Ahmad et al. (2010), the main limitations were that the input variables were 376 obtained through satellite images, producing a high degree of uncertainty in the angle of incidence 377 378 from the Tropical Rainfall Measuring Mission (TRMM), and in the Normalized Difference Vegetation Index (NDVI) from the Advanced Very High-Resolution Radiometer (AVHRR). 379

The performance of the ML models considered in this study is slightly better than that seen in Si 380 et al. (2015), who used ANN-Bayesian Regularization (R<sup>2</sup>=0.929) and ANN-Levenberg-Marquardt 381 [ANN-LM] ( $R^2$ =0.932). It can be noted that the general structures of some ML models used here (i.e., 382 RF, SVM, and Stacked Model) are more complex than those applied in the research of Si et al. (2015). 383 Prasad et al. (2018a) developed Extreme Learning Machine (ELM)-based models for the prediction 384 of monthly soil moisture, hybridized with the complete ensemble empirical mode decomposition with 385 adaptive noise (CEEMDAN) and the empirical ensemble mode decomposition (EEMD) algorithm, 386 to address the problems associated with non-stationarity in the data. Also, in the study by Prasad et 387 al. (2018a), hybrid models showed very high accuracy and outperformed standalone algorithms, in 388 this case ELM and RF, as in the present study. Additionally, Prasad et al. (2019) developed the ELM 389 (R<sup>2</sup>=0.702), EEMD-Boruta (R<sup>2</sup>=0.785) and MARS (R<sup>2</sup>=0.712) models that have had rather lower 390

accuracy than the present research due to a large number of field measurements with high uncertainty

in the input variables (e.g., weekly values of temperature, runoff volume, evaporation, and heat flux). 392 Moreover, Cie et al. (2019) provided soil moisture content predictions by Deep Neural Network 393 Regression (DNNR) with satisfying a degree of accuracy ( $R^2=0.98$ ) as well as in the present research. 394 Their success in the evaluation of soil moisture was due to considering a variety of input variables, 395 396 such as average temperature, average pressure, relative humidity, wind speed, land temperature, daily 397 precipitation, and initial soil moisture. Maroufpoor et al. (2019) proposed a hybrid model based on the adaptive neurofuzzy inference system (ANFIS) and grey wolf optimization (GWO) algorithms, 398 which was then compared with ANN, SVR, and standalone ANFIS. The input parameters of the 399 model were the dielectric constant, bulk soil density, clay content, and organic matter of 1155 soil 400 samples. The ANFIS-GWO model proved to be the most accurate, followed by the standalone ANFIS 401 and SVR models, while the worst accuracy was found in the ANN model, in contrast to what was 402 observed in the present research, where MLP outperformed SVR. The different choice of input 403 variables justifies this result, as this aspect is fundamental to the performance of forecasting models. 404

405 Furthermore, the performance of the present ML models was slightly better than that obtained by Heddam's (2021) investigation (R<sup>2</sup>=0.925, 0.929, and 0.931 for M5MTree, MARS, and RF, 406 respectively). In addition, the MLP-based model by Heddam (2021) had rather lower accuracy results 407 (R<sup>2</sup>=0.885) than those reported in the present research for both Model A and Model B. Heddam 408 409 (2021) did not refer to the climatic variables that were considered in the present research. In fact, he used the soil temperature, the year number, the month number, and the day number in order to 410 estimate the soil moisture content. His study indicated that climatic variables play a key role in 411 improving the accuracy levels of ML models. 412

The main limitation of this study is that it considers only one case study. Therefore, the possible 413 414 influence of different climatic conditions on the forecast models is not taken into account here. It will be interesting, in future developments of this study, to address the prediction problem under climatic 415 conditions characterized by intense evapotranspiration and periods of widely varying rainfall (e.g., 416 tropical climates). It will also be interesting to compare the results provided by the stacked model 417 with those provided by models based on deep learning algorithms, which are known to perform very 418 well in predicting time series (Sit et al. 2020). Finally, the most ambitious goals will be pursued, such 419 as developing models with a more distant forecasting horizon and models dependent only on 420 exogenous climate variables. 421

### 422 5. Conclusions

This study introduced a novel forecast algorithm of daily volumetric soil water content, based on the stacking of the Multilayer Perceptron, Random Forest, and Support Vector algorithms. Two different input variable scenarios were considered, in order to develop two forecast models: model A, which included daily precipitation, air temperature and humidity, and wind speed as exogenous variables, and model B, which instead included only daily precipitation as an exogenous variable.

Both models provided very accurate predictions, with the coefficient of determination R<sup>2</sup> greater than 0.9 and MAPE not exceeding 5% in almost all cases, and with model A generally outperforming model B. In addition, for both models, the Stacked algorithm-based variant generally outperformed the standalone algorithms. Both models experienced a modest reduction in accuracy as the forecast horizon increased, remaining within the range of short-term forecasts. In any case, even a model that only requires precipitation as an exogenous input variable is capable of providing adequatepredictions for practical applications.

The proposed stacked model is simple, based on a few parameters, very accurate, and has a very limited computational time. In the context of current research, which shows a marked tendency towards increasingly complex models, the proposed model can be considered an effective tool for facilitating the planning of irrigation activities and supporting flood risk management (Yildirim & Demir 2021).

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