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Original Research

A comparison of empirical and mechanistic models for wheat yield prediction at field level in Moroccan rainfed areas

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Abstract. In the context of climate change, in-season and longer-term yield predictions are needed to anticipate local and regional food crises and propose adaptations to farmers' practices. Mechanistic models and machine learning are two modelling options to consider from this perspective. In this study, multiple regression (MR) and random forest (RF) models were calibrated for wheat yield prediction in Morocco, using data collected from 125 farmers' wheat fields. Additionally, MR and RF models were calibrated both with or without remotely sensed leaf area index (LAI), while considering all farmers' fields, or specifically to agroecological zoning in Morocco. The same farmers' fields were simulated using a mechanistic model (APSIM-wheat). We compared the predictive performances of the empirical models and APSIM-wheat. Results showed that both MR and RF showed rather good predictive quality (normalized root mean square errors (NRMSEs) below 35 %), but were always outperformed by the APSIM model. Both RF and MR selected remotely sensed LAI at heading, climate variables (maximal temperatures at emergence and tillering), and fertilization practices (amount of nitrogen applied at heading) as major yield predictors. Integration of remotely sensed LAI in the calibration process reduced NRMSE by 4.5 % and 1.8 % on average for MR and RF models, respectively. Calibration of region-specific models did not significantly improve the predictive. These findings lead to the conclusion that mechanistic models are better at capturing the impacts of in-season climate variability and would be preferred to support short-term tactical adjustments to farmers' practices, while machine learning models are easier to use in the perspective of mid-term regional prediction.

KEYWORDS: APSIM-wheat; empirical model; machine learning; model comparison; Morocco; yield prediction.

1. INTRODUCTION

Ongoing climate change has reinforced the need to deliver crop yield predictions over short or longer time horizons (Crane-Droesch 2018; Hasegawa *et al.* 2022). As extreme climatic events are more frequent and unpredictable (Savin *et al.* 2022), farmers need to take tactical decisions in-season to adapt their practices according to the expected production levels and production costs. Over several years, cropping practices may also require adaptation to cope with the local evolution of mean temperatures and rainfall distribution. In the rainfed areas of Morocco, farmers are particularly vulnerable to climate change. Recurrent droughts, aggravated by limited access to fertilizer, are responsible for highly variable crop yields and large yield gaps (Henaou and Baanan 1999; Roy *et al.* 2003; Bregaglio *et al.* 2015). Rainfed

cereal production represents 80 % of the total cereal production of the country (Shroyer *et al.* 1990), putting the food and economic balances of the country at risk.

Model-assisted decision-making in agriculture can reduce farmers' vulnerability to climatic risks and support adaptation to fluctuations in market inputs, the allocation of subsidies and the recommendation of efficient and sustainable management practices for farmers (De Wit *et al.* 2013; Wang *et al.* 2014; Kasampalis *et al.* 2018; Asseng *et al.* 2019). National or regional crop yield prediction systems have been developed to support farmers and other stakeholders of the food chain, using numerical models. Two types of modelling approaches have been reported in the literature on yield prediction: (i) process-based approaches (i.e. mechanistic models) that represent the processes involved in crop development,

growth, resource allocation and the interactions between these through equations (Graeff et al. 2012; Basso et al. 2013; Jones et al. 2017). For example, the Global Yield Gap Atlas maps potential yield for major food crops in a large number of countries across the world, using processed-based crop model simulations (www.yieldgap.org). (ii) Empirical approaches that relate grain yield to agronomic and environmental factors (i.e. climate, soil, crop management information, etc.) including simple statistical relations (e.g. multiple regression (MR) analysis) (Thompson 1969; Palm 1994) or complex statistical algorithms (e.g. machine learning algorithms) (Marques Ramos et al. 2020; Droutsas et al. 2022; Son et al. 2022). For example, in Morocco, the national prediction system CGMS-MAROC, coordinated by the National Institute of Agriculture (INRA) produces maps of expected wheat production across Morocco, every year, using empirical models (<http://www.cgms-maroc.ma/>). It is worthy to note that in this second category, the degree of empiricism varies between model-based statistical approach in which predictors or distributions can be set based on biological assumptions to purely algorithmic.

Crop simulation models are valuable tools to predict yield in variable soil and climatic contexts and to support the adaptation of cropping practices. They can provide a better understanding of the interactions between the major processes of the soil-plant-climate continuum and its global functioning at a daily time step. However, they often require a large number of input parameters (Cavalari et al. 2021), which makes their deployment at large geographic scales over a variety of agroecosystems costly due to the logistics and financial resources needed to acquire parameter values (Makowski et al. 2006; Varella et al. 2010).

Conversely, empirical models estimate yield at a cropping season time step and can be easily used in research studies that target broad geographic ranges. The statistical approach provides a simple qualitative understanding of the links between grain yield measurements and environmental variables through regression and correlation analyses (Oteng-Darko et al. 2013), mainly represented in past studies by climate variables and remotely sensed vegetation indices or biophysical variables (e.g. leaf area index—LAI, normalized difference vegetation index—NDVI, etc.) (Andarzian et al. 2008; Bolton and Friedl 2013; Son et al. 2022).

High throughput data gathering methods employing remote sensing and satellite images have reshaped yield modelling over the past 10 years and diminished the divide between empirical and crop simulation models. The number of spectral indicators linked to crop state that may be integrated into empirical models has significantly increased as a result of recent technology advancements (Launay and Guerif 2005; de Wit and van Diepen 2007; Huang et al. 2019). Likewise, the integration of remotely obtained vegetation indexes into crop modelling pipelines has made it possible to reduce the degree of uncertainty in predictions of national yields (Luo et al. 2023).

Overall, empirical models are simpler to use, with a reduced number of parameters and possibly shorter calculation time requirements compared to crop models (Sultan et al. 2010). However, agronomic recommendations can be difficult to infer from these types of models that bypass the relations between climate, practices and soil on one hand and crop functioning on the other (Jones et al. 2001; Heil et al. 2018). This difficulty is increased by the possibility of identifying different sets of predictors for yield with equivalent performance using machine

learning approaches. This is particularly the case with multivariate regression models, and results from the collinearity among variables used in the model (Lischeid et al. 2022). Additionally, the vast majority of simple or complex statistical models used worldwide for yield prediction are non-spatial (Qu et al. 2022). They provide unique sets of selected environmental predictors of yield for an entire region; whilst—from an agronomic perspective—climatic, paedological and management determinants of yield are known to vary across these large geographic regions. Simple customization of empirical models could outperform this limitation if zoning of the region of interest into sub-regions with homogenous climate conditions, soil status or practices exists so that different sets of predictors could be independently selected for each sub-region. In Morocco, zoning of the wheat production area was delimited by the FAO, within the framework of Strategy for the Conservation and Restoration of Agricultural Land (ISCRA), which divides the Moroccan rainfed wheat production areas into four main climatic areas mainly defined by annual rainfall (i.e. favourable, unfavourable, intermediate and mountain rainfed areas) (Ait el Mekki 2006; MAPMDREF 2008; Harbouz et al. 2019).

The objective of the present study is to compare the predictive capacity of empirical models (MR and random forests (RF) models) and a process-based model (APSIM-wheat model) for wheat yield across the rainfed areas of Morocco and discuss their suitability for different modelling objectives. The precision of the different prediction methods and sets of selected predictors will be compared, and the effect of recent advances in remote sensing technologies on the prediction gap between the empirical and process-based approaches will be assessed by integrating (i) the effect of incorporating a satellite-based vegetation index (LAI) in MR and RF models, (ii) the effect of stratifying the dataset into different climatic sub-regions of Morocco for calibration of sub-region-specific empirical models. The performances of both improved and original empirical models as well as the mechanistic model will be discussed in the light of the time horizon targeted for prediction and support to farmers' decision-making.

2. MATERIALS AND METHODS

2.1 Study area

Morocco covers about 710,850 km², and most of the country (93%) is characterized by an arid to semi-arid climate (Dahan et al. 2012). The agricultural production zones in Morocco are located between the mountains (Rif and Atlas), the Atlantic Ocean and the Mediterranean Sea. In the present study, 125 farmers' wheat fields were selected randomly across the main Moroccan rainfed areas based on the FAO's ISCRA zoning (i.e. favourable (with precipitation > 400 mm), intermediate (300–400 mm) and unfavourable rainfed areas (<300 mm) (Fig. 1), and monitored during three cropping seasons (from 2018 to 2021). The selected farmers' fields represent a diversity of conditions (i.e. soil, management practices and climatic conditions) (Fig. 1) under the Moroccan rainfed areas, to ensure robust calibration and evaluation processes of both empirical and mechanistic models. The datasets were assembled from fieldwork conducted in the framework of the 'SoilPhorLife' project and 'Al Moutmir' program led by the Office Chérifien des Phosphates (OCP group).

2.2 Datasets

2.2.1 Phenological stages observations and grain yield measurement

During the three growing seasons, the main wheat phenological stages were monitored in the farmers' wheat fields based on Zadoks scale (Zadoks *et al.* 1974). To achieve an accurate scoring of each field as a whole, Zadoks scale scores were identified at 10 locations in each field, selected along a zigzag pattern.

Actual grain yield (Table 1) was measured at harvest in each farmer's field by harvesting five samples of 1 m² selected randomly across the field based on Bell and Fisher's methodology (Bell and Fischer 1994).

2.2.2 Meteorological data

Daily maximum and minimum temperatures and daily rainfall were extracted from three sources. Weather station-based data were provided by the Office Régional de Mise en Valeur Agricole and from a public website (www.tutiempo.net) (Tutiempo Network, S.L. 2021) that offers data from airport weather

stations. Since daily solar radiation was not available at most of these weather stations, data were completed with daily global radiation extracted from the satellite-based platform of NASA's Prediction of Worldwide Energy Resources (POWER) Project (<https://power.larc.nasa.gov/data-access-viewer/>) with a resolution of 0.5° × 0.5° (i.e. about 50 × 50 km) (Zhang *et al.* 2008; Sparks 2018). For each field, the closest weather station was chosen to represent the field's meteorological conditions. Using 15 different weather stations allowed to keep the distance between a field and the corresponding weather station below 50 km.

For each field, climatic variable variables were calculated by aggregating daily weather data over the main develop phase of wheat as recorded in the field (see Section 2.2.1): (i) emergence (Z0 to Z20), (ii) tillering (Z20 to Z30), (iii) elongation (Z30 to Z50), (iv) heading and anthesis, (Z50 to Z70), and (v) grain filling and maturity (Z70 to Z90). Cumulative rainfall (R1 to R5), means of maximum daily temperatures (T_{max1} to T_{max5}), minimum daily temperatures (T_{min1} to T_{min5}) and the cumulative growing degree days (GDD1 to GDD5) were calculated for each development phase and each field (Table 2). Moreover, the total

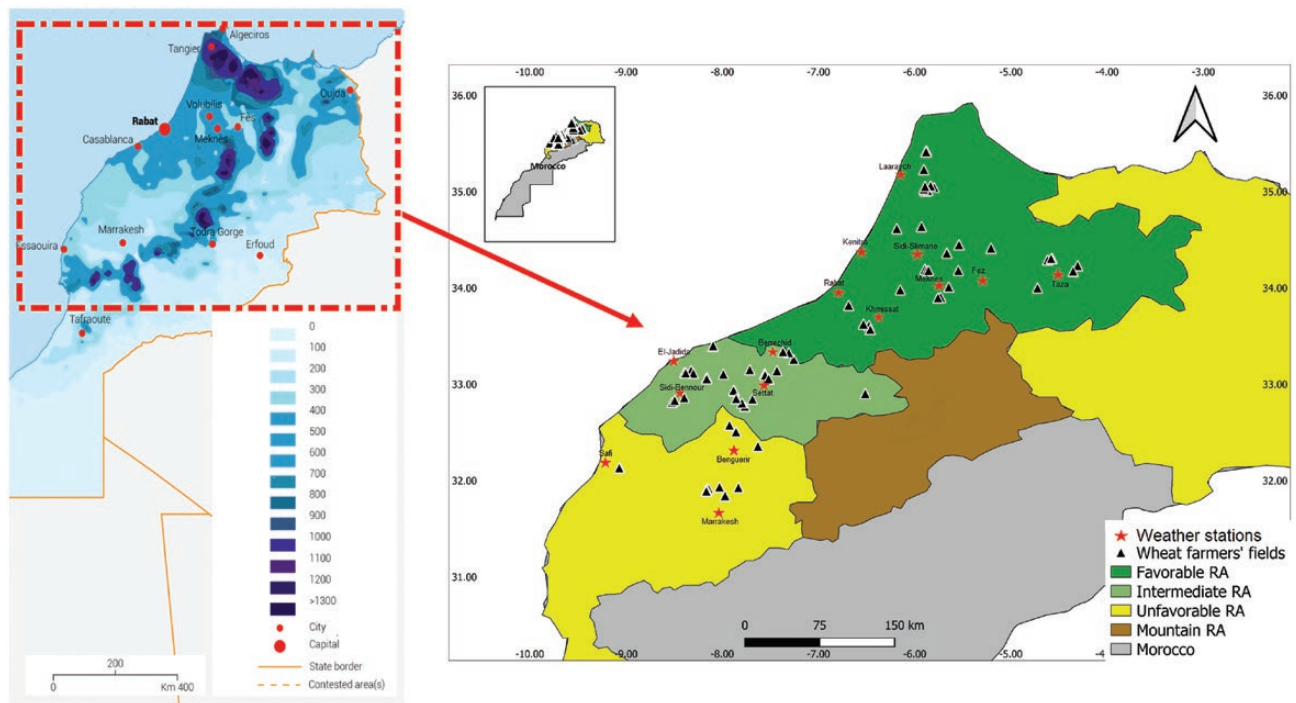


Figure 1. Location of the 125 monitored farmers' fields across agroecological zones in Morocco. (A) Distribution of cumulative annual rainfall across Morocco (Wala *et al.* 2019), (B) field locations and limits of the four agroclimatic zones in northern Morocco (favourable, intermediate, unfavourable and mountain rainfed areas) (Gommes *et al.* 2009). RA, rainfed area.

Table 1. Descriptive statistics for wheat yield in Moroccan rainfed areas. Figures in brackets indicate the number of fields in each zone.

	Wheat yield (Mg·ha ⁻¹)			
	Favourable rainfed areas (61)	Intermediate rainfed areas (44)	Unfavourable rainfed areas (20)	Overall
Mean	3.74	1.81	0.67	2.57
Median	3.80	1.85	0.60	2.20
Maximum	7.10	3.80	1.40	7.10
Minimum	0.50	0.20	0.20	0.20
SD	1.70	1.04	0.40	1.82

Table 2. Variables used to calibrate the empirical models of yield prediction in Moroccan rainfed areas. R1 to R5: Cumulative rainfall, T_{max1} to T_{max5} : means of maximum daily temperatures, T_{min1} to T_{min5} : means of minimum daily temperatures and GDD1 to GDD5: cumulative growing degree days, respectively at (i) emergence (Z0 to Z20), (ii) tillering (Z20 to Z30), (iii) elongation (Z30 to Z50), (iv) heading and anthesis, (Z50 to Z70) and (s) grain filling and maturity (Z70 to Z90). Z0, Z30, Z50, Z70, Z90: developmental stages on Zadock's scale.

Data type	Variable	Symbol	Unit	Description
Climate	Cumulative rainfall	R1 to R5, R_{tot}	mm	See Section 2.2.1
	Minimum temperature	T_{max1} to T_{max5} , T_{min}	°C	
	Maximum temperature	T_{min1} to T_{min5} , T_{max}	°C	
Soil fertility	Organic matter	OM	%	See Section 2.2.2
	Available phosphorus	P	ppm	
	Exchangeable potassium	K	ppm	
Crop management practices	pH	pH	-	
	Cultivar	VAR	-	See Section 2.2.3
	Sowing dates	SD	Julian days	
	Nitrogen fertilization	N_0 , N_1 , N_2 , N_d , N_{tot}	kg·ha ⁻¹	
	Phosphorus fertilization	P_2O_5	kg·ha ⁻¹	
Duration of phenological stages	Potassium fertilization	K_2O	kg·ha ⁻¹	See Sections 2.2.1 2.2.4
	Growing degree days	GDD1 to GDD5, GDDtot	C°·day ⁻¹	
Satellite-based metrics related to wheat growth	Leaf area index	LAI Z30, LAI Z50	m ² ·m ⁻²	See Section 2.2.5

cumulative precipitation (R_{tot}), the means of maximum (T_{max}) and minimum (T_{min}) daily temperature and the total cumulative growing degree days (GDD_{tot}) were calculated for the entire crop cycle (i.e. from sowing date to harvesting date) (Table 2). The purpose of calculating these auxiliary variables was to capture yield potential as determined by wheat variety and local climate through GDD variables, as well as the effect of the main abiotic stresses (water stress, heat stress and cold stress) for each development phase estimated through $T_{\text{min}1}$ to $T_{\text{min}5}$, $T_{\text{max}1}$ to $T_{\text{max}5}$, and R1 to R5 variables. Cumulative incident radiation available during each phenological stage was not considered due to the uncertainty of this climatic variable (estimated from a satellite-based meteorological dataset) and the presence of a high collinearity effect between global radiation and maximum temperatures.

2.2.3 Soil data

Soil samples were collected in each field before the sowing date, at two depths (maximum depth depending on soil development, and, in most cases, less than 60 cm). Variables related to soil chemical properties (available-P (P), exchangeable-K (K), organic matter (OM) and pH) were determined by standard procedures. Data were averaged over the two soil layers, using soil layer thickness as weights for each field and each variable (Table 2).

2.2.4 Crop management data

The main crop management input variables, used during the calibration of empirical models and to parameterize the APSIM-wheat crop model, describe farmers' fertilization practices as recommended by experts. Crop management variables include the wheat cultivar and sowing date, the amount of nitrogen-, phosphorus- and potassium-based deep fertilizers applied at the sowing date (respectively, N_0 , P_2O_5 and K_2O), and the amount of nitrogen top-dressing fertilizer applied at tillering stage (N_1) and at the heading stage (N_2). Total applied nitrogen ($N_{\text{tot}} = N_0 + N_1 + N_2$) and the total top-dressing nitrogen ($N_d = N_1 + N_2$) were calculated and also used to calibrate empirical models.

2.2.5 Wheat growth satellite-based parameters

Sentinel-2 satellite images covering the monitored farmers' wheat fields during the three crop seasons (from 2018 to 2021) were downloaded from the Copernicus platform (<https://scihub.copernicus.eu/dhus/>) (European Space Agency 2021a). Sentinel-2 optical imagery provides a series of products with high temporal (5 days), spatial (10 to 60 m) and spectral (13 bands) resolution adapted for field-scale monitoring (Mohamed Sallah *et al.* 2019; Zhao *et al.* 2020).

Due to the large number of monitored fields, we extracted satellite images for two specific dates that represent determinant phenological stages, framing the period of maximum vegetative growth: at Z30 (end of tillering/start of elongation) and Z50 (end of elongation/start of heading). Only images with cloud cover lower or equal to 15 % were considered. Due to the 5-day time resolution of Sentinel, the temporal uncertainties for variables extracted from satellite images were equal to 3 days. Unfavourable cloud cover (>15 %) can occasionally increase this uncertainty, forcing us to skip overcast images and use images

with low cloud cast on close dates. The downloaded images were preprocessed using the Sentinel Application Platform (SNAP) software (version 8.0.0) (<https://step.esa.int/main/toolboxes/snap/>) (European Space Agency 2021b), freely provided by Sentinel. Images underwent sequential pre-processing steps: resampling and creating subsets. Then, a SNAP algorithm was applied to compute and extract a leaf area index (LAI) raster map from each image. LAI was calculated based on spectral bands with a spatial resolution ranging between 10 and 20 m. Finally, field polygons were delimited, excluding borders and LAI was averaged over the pixel of each field polygon.

2.3 Calibration of empirical models

2.3.1 Modelling strategies for calibration of MR and RF models

Data collected in the field and derived from the soil and weather dataset for each field were compiled into a database (Table 1).

To test the possibility of integrating the spatial and temporal variation of the main determinants of wheat yield, two different modelling strategies were tested to split the dataset into a calibration and an evaluation subset:

- Extraction of one generic model covering the whole range of monitored farmers' fields across the rainfed wheat-growing area in Morocco (S1). The generic model was obtained by stratifying the available field data set: crop seasons (2019, 2020 and 2021) represent the strata and 70 % of the data from each of the three strata were used to calibrate models while 30 % was used to evaluate the models.
- Extraction of three region-specific models for each of the rainfed agroclimatic areas (S2) (i.e. favourable, intermediate and unfavourable). Region-specific (or agroclimate-specific) models were extracted using 70 % of the observations while 30 % of the dataset was used to evaluate those specific models.

To ensure the robustness of the comparisons between MR and RF models, both types of models were built on the same calibration and evaluation datasets described by the two strategies (S1 and S2). Modelling strategy (S1) was considered as the baseline for empirical models, compared to (S2) and models incorporating satellite-based LAI variables (Section 2.3.4).

2.3.2 MR models

Regression models with one predicted variable and more than one independent predictive variable are known as multivariate linear regression analysis (MR). The corresponding model is formulated as follows:

$$Y = b_0 + b_1 \cdot X_1 + \dots + b_i \cdot X_i + \dots + b_n \cdot X_n$$

where Y is the predicted variable, X_i represents n distinct independent variables (predictors), and b_i is the estimated regression coefficients.

Simple stepwise linear regression analyses were conducted using IBM-SPSS Statistics software (v 25.0) (SPSS Inc.) to examine whether independent quantitative variables (Table 1) were successful in predicting the dependent variable (wheat yield) and to assess the quality of contributions of each predictive

variable. Assumptions of linearity, normal distribution and multicollinearity of the predictor variables were verified. The model that minimized the minimum standard in the absence of multicollinearity was selected by the stepwise algorithm as the most appropriate to predict yield. The variance inflation factor 'VIF' was calculated to interpret the multicollinearity and VIF values under 2.5 were considered to represent an acceptable level of collinearity based on the literature (Fomby et al. 1984). Finally, relative standardized estimators (β_i) were used to evaluate the contributions of individual predictors to the variation of yield. Relative standardized estimators of effects in the MR models were obtained by calculating the ratio between estimators for each predictor and the maximum of all estimators (\hat{b}_i) in the selected model. Overall, the use of β values to estimate the predictors' relative importance is conditioned by the hypothesis of the absence of multicollinearity (Cosnefroy and Sabatier 2011), which was our second rule of MR model selection during the calibration process.

2.3.3 RFs model

A set of RFs models was designed in R (version 4.1.2) (<https://cran.r-project.org/>), using the same variables as the MR model. Similarly, two modelling strategies were tested (see Section 2.3.3). The 'caret' package (version 6.0-90) (Kuhn 2021) was used throughout the procedure.

In a RFs model, a set of trees—in our case 500—is built in a training phase and the outcome of the model is obtained by averaging the output of all the trees (Breiman 2001). This operation was realized on the calibration samples described in Section 2.3.1. The principle behind the RFs procedure is to increase the performance of the model by combining the outputs of a large number of different, average-performing models (Breiman 1996). The variety in the models (trees) is obtained through two elements containing a random component. First, each tree is built on a randomly selected fraction (two-thirds) of the training dataset (calibration sample) by bootstrap aggregating (bagging) while the remaining part of the dataset (out-of-bag sample) is used to assess the prediction error of the tree (Breiman 2001). Metrics describing the performance of the model in the training phase are reported here as 'calibration results'. A second random effect is introduced at each node when the best split is determined among the variables. In the case of the RFs algorithm, only a randomly selected sample of the independent variables is used at each node. In the models, the number of variables, controlled by the parameter 'mtry', was set as equal to the square root of the number of independent variables (Strobl et al. 2009), rounded to the nearest integer, in our case 6.

RFs models feature the computation of a variable called permutation feature importance, a metric used to evaluate the impact of a variable on the model's performance. Permutation importance is based on the principle that if a variable is not important in the model, randomly permutating its values will not affect the model's performance, while it will if the variable is important. The metric, therefore, represents the difference in model accuracy before and after permutation and grows larger as variables are more important (Breiman 2001). In this study, the 'cforest' method, from the R package party version 1.3-9 (Hothorn et al. 2006; Strobl et al. 2007, 2008) was used. This

algorithm was designed to improve the estimation of importance in the presence of correlated predictors (Hothorn et al. 2006; Strobl et al. 2007, 2008). Finally, the performance of the final model (i.e. the average of the 500 trees) was assessed using the evaluation samples described in Section 2.3.1 and by computing the metrics defined in Section 2.5.

2.3.4 Integration of satellite-based wheat LAI dataset into empirical models

To assess the impact of integrating the satellite-based wheat LAI on the statistical models' structure (choice and weight of the selected predictors) and performance for grain yield estimation, the calibration and evaluation of both MR and RF models was repeated including (with) or excluding (without) satellite-based LAI determinations at Z30 (LAI-Z30) and at Z50 (LAI-Z50) as input variables, in addition to variables related to climate, soil and fertilizing practices. The comparison of the two approaches allowed us to quantify the degree of improvement in the models' potential for yield prediction through the incorporation of satellite-based information. Satellite-based LAI was preferred to NDVI or other remote sensing vegetation indices based on previous unpublished commercial exploration work conducted for an insurance company in Morocco. This choice was also supported by Abi Saab et al. (2021) who compared, under Mediterranean conditions, the correlation between winter wheat biomass as measured in the field and five remotely sensed vegetation indexes derived from Sentinel 2. They found that LAI was notably more correlated to biomass compared to NDVI.

2.4 Mechanistic model: APSIM-wheat

APSIM 'Agricultural Production Systems Simulator' (Keating et al. 2003) is a crop growth model that integrates, at a daily time step, the effect of soil, climate, crop cultivar and crop management on interconnected processes (development, growth, resource allocation and effect of abiotic stresses) involved in the elaboration of final yield (Keating et al. 2003; Ahmed et al. 2016). It has been employed to simulate a wide range of crops with a focus on addressing global challenges such as climate change and food and energy security, as it expresses the response of crops to meteorological, soil and biological factors (Mohanty et al. 2012; Zhao et al. 2014; He et al. 2017). Moreover, it has been widely used in ex-ante studies to explore the effect of crop management strategies such as fertilization, irrigation, weed management and control, land planning or crop rotation. The detailed development history of APSIM was reported by Gaydon (2014).

Mamassi et al. (2022) previously conducted calibration and evaluation of the APSIM-wheat model in the Moroccan context, using the same dataset as in the present study. The same parameterization procedure was applied in the present study: plant parameters and soil parameters were inferred from on-site measurements for each of the 125 farmers' fields that were simulated, and complemented by data from the literature, and open-access databases. Plant parameters were estimated separately for the five cultivars planted in the whole sample of farmer fields then calibrated according to a three-step procedure: (i) exploring influential and non-influential crop cultivars parameters to identify the parameters that required calibration, (ii) using an Australian cultivar (also cultivated in Mediterranean conditions to set

default values for unknown plant coefficients, (iii) using the trial-and-errors simplified approach to adjust the plant parameters values. Calibration process was done by adjusting successively crop phenology, leaf area development and yield, as per Boote's systematic approach (Boote 1999; Li *et al.* 2018), and (iv) daily climate data (temperatures and precipitations) originated from the closest weather station of each field with a maximum distance of 50 km between the field and the weather station. Daily global radiation was extracted from NASA's Prediction Of Worldwide Energy Resources (NASA's POWER project) (<https://power.larc.nasa.gov/data-access-viewer/>). The detailed procedure used for APSIM-wheat model calibration and evaluation was reported in Mamassi *et al.* (2022).

2.5 Evaluation metrics

Statistical metrics were computed to evaluate the uncertainty of both empirical (RF and MR, generic or region-specific) and mechanistic (APSIM-wheat) models after calibration and validation phases: the root mean square error (RMSE) and the normalized root mean square error (NRMSE) as indicators of model precision, as well as the coefficient of determination (R^2) as an indicator of accuracy as per Equations (1), (2) and (3), respectively.

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n [x_{s_i} - x_{m_i}]^2} \quad (1)$$

$$\text{NRMSE} = \frac{\sqrt{1/n \sum_{i=1}^n [x_{s_i} - x_{m_i}]^2}}{\bar{x}_m} \times 100 \quad (2)$$

$$R^2 = 1 - \frac{\sum_{i=1}^n [x_{s_i} - (\hat{a}x_{m_i} + \hat{b})]^2}{\sum_{i=1}^n [x_{m_i} - \bar{x}_m]^2} \quad (3)$$

where x_{m_i} is the measured values, x_{s_i} is the simulated values, \bar{x}_m is the mean of the observed value, n is the number of observations (i.e. fields), and \hat{a} and \hat{b} are the estimators of the simple linear regression between models simulated values and observed or measured values in the real field.

RMSE and NRMSE were calculated in R (R Core Team 2020), while R^2 of MR models were obtained using IBM-SPSS Statistics software (v 25.0) (SPSS Inc.). For evaluating the benefit of incorporating satellite-based data as an input in MR and RF models, RMSE, NRMSE and R^2 , were computed for each case.

3. RESULTS

3.1 Comparison between empirical and mechanistic models

The indicators of predictive capacity of the calibrated and evaluated APSIM-wheat model for wheat yield in Moroccan rainfed areas are depicted in Fig. 2; further details are available in Mamassi *et al.* (2022). The overall comparison between the empirical and mechanistic models showed that APSIM-wheat outperformed the baseline empirical models (S1, i.e. RF and MR generic models that were calibrated over the whole

rainfed wheat-growing region without LAI variables), and the region-specific models in favourable areas (S2-Fav). However, in the intermediate and unfavourable rainfed areas of Morocco, the best predictive performances were achieved by region-specific MR models when integrating the satellite-based variables (i.e. S2-with-Int/Unfav), with RMSEs equal to 0.47 and 0.17 t·ha⁻¹, respectively.

3.2 Structure and predictive quality of generic empirical models (S1) without LAI variables (baseline models)

'Baseline models' (S1) refers to RF and MR generic models that were calibrated over the whole rainfed wheat-growing region in Morocco, and included only variables measured on the ground (without LAI variables) as possible predictors (Figs. 2B and 3B). Quality metrics calculated on the calibration dataset showed good to acceptable predictive quality for both MR and RF baseline models. The lowest NRMSE value was obtained for the MR model (NRMSE = 24.9%). High R^2 values generally exceeding 0.7 (Fig. 2B) were obtained for both MR and RF models, indicating good model accuracy.

After the model calibration process, the validation of models using independent datasets aimed to verify their potential for predicting wheat yield in Moroccan rainfed areas (Fig. 3). RF and MR baseline models showed almost identical wheat yield estimation performances with RMSEs ranging between 0.8 and 0.9 t·ha⁻¹ (Fig. 3B) corresponding to NRMSE below 35 %, while R^2 exceeded 0.8 in both cases. The values of RMSE, NRMSE and R^2 obtained in the model evaluation step confirmed that both MR and RF-calibrated baseline models had rather good predictive capacities for yield across the rainfed wheat production area in Morocco (Fig. 2B).

Analysis of the models' structure (Fig. 4 and Supporting Information—Fig. S1) indicates that the RF and MR calibration process selected the same predictors, and the best predictor variables for wheat yield, by decreasing order of importance, were: (i) nitrogen fertilization, represented mainly by (N_{tot}) and (N_{d}) and (ii) meteorological variables, mainly maximal temperature variables ($T_{\text{max}1}$, $T_{\text{max}2}$ and $T_{\text{max}4}$) and cumulative rainfall variables (R_{tot} and $R5$).

Among the soil fertility and fertilization practice-related variables, only soil OM and soil pH (pH) were selected as predictors in models, with a secondary relative importance (Fig. 4). Similarly, these variables were among those with the lowest relative and absolute importance in the RF baseline model (Supporting Information—Table S1). Moreover, bivariate correlations between yield and predictive variables confirmed the weak contribution of K_2O and to a lesser extent of P_2O_5 to the explanation of yield variations (Supporting Information—Fig. S2).

3.3 Effect of calibrating separate region-specific (or agroclimate-specific) models

Separately calibrating region-specific models for each agroclimatic zone (S2) did not significantly improve models' predictive power according to R^2 , RMSE and NRMSE values as calculated after calibration (Figs. 2 and 3). Region-specific models, obtained with the MR algorithm with or without satellite-based variables, had a better predictive quality than

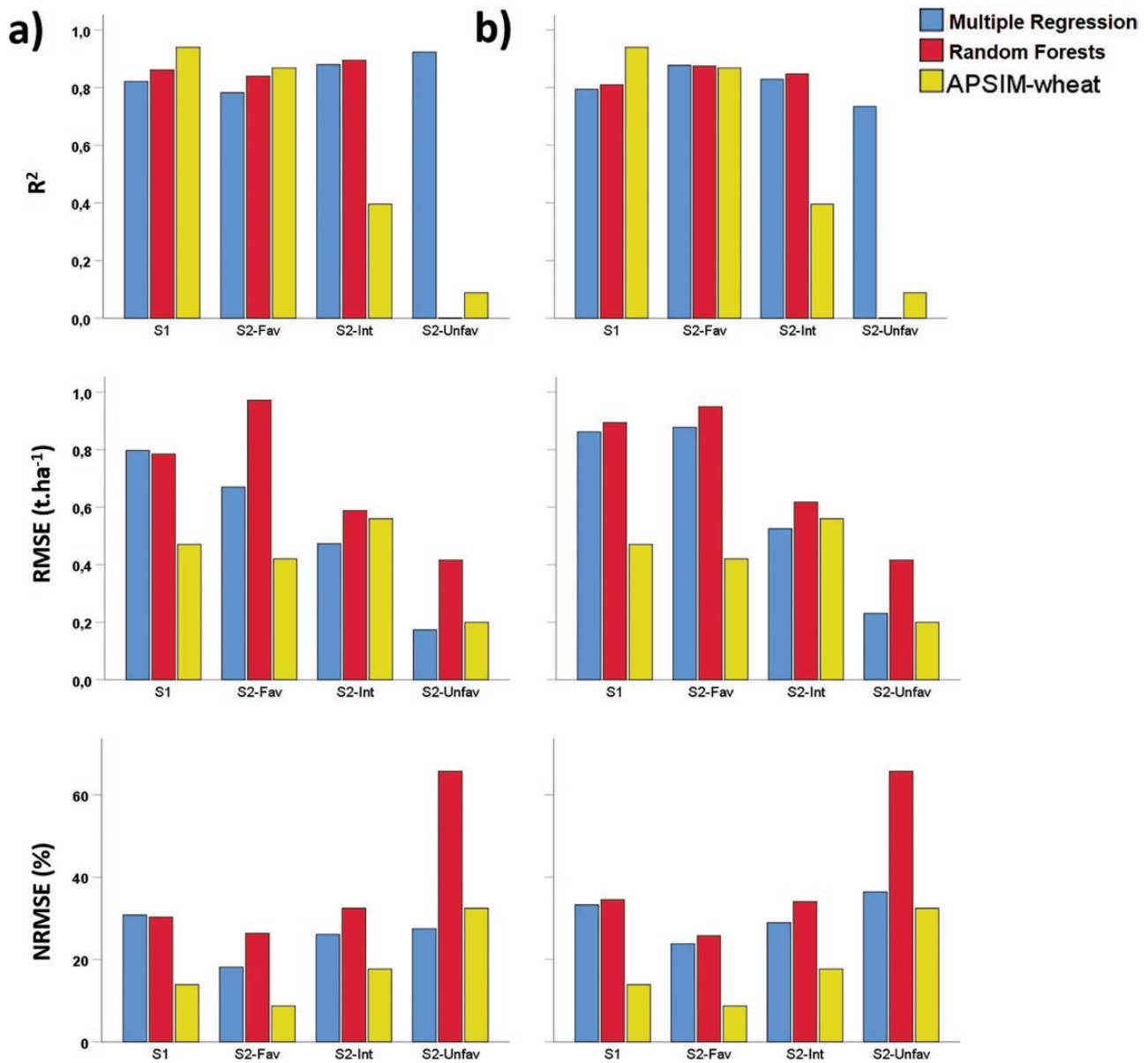


Figure 2. Comparison of MR, RF and APSIM-wheat models' predictive performances calculated on the evaluation-independent dataset. Coefficient of determination (R^2), RMSE and NRMSE is the statistical indices used to evaluate and compare models' precision and accuracy, (A) with and (B) without integrating satellite-based variables. S1 refers to generic models while S2-Fav: favourable, S2-Int: Intermediate, and S2-Unfav: Unfavourable rainfed areas, refer to agroclimate-specific models, respectively for favourable, intermediate and unfavourable agroclimatic areas.

RF region-specific models, overall. Moreover, the RF algorithm failed to extract a model for the unfavourable rainfed areas (S2-Unfav). This was due to the limited number of fields in this region (nine fields only), which was inferior to the minimum number of observations needed by the algorithm to perform a split (parameter 'minsplit' with a default value of 20). Although the algorithm allows setting one's own value for the parameter 'minsplit', we decided not to alter the default value as designing an RF model based on such a limited sample would seriously limit its interpretability. As a result, the best fit proposed by the algorithm in this case was a constant value equal to the average yield (which prevented the computation of R^2 and variable importance).

During the evaluation phase (Fig. 2), nearly identical model predictive performances were obtained when applying the RF method for the two sampling strategies (S1 and S2), with NRMSE ranging between 26 % and 34 %, and R^2 exceeding 0.8 (except for the S2-Unfav model that could not be calibrated with the RF approach). Conversely to what was observed after calibration, region-specific MR models outperformed the baseline models' (S1) precision in the case of favourable and intermediate rainfed areas (S2-Fav/Int), with NRMSE values ranging between 18 % and 29 % against NRMSE above 30 % for (S1) models. R^2 values remained above 0.7 for both MR and RF agroclimate-specific models (S2), except for the failure of the RF model in the unfavourable zone.

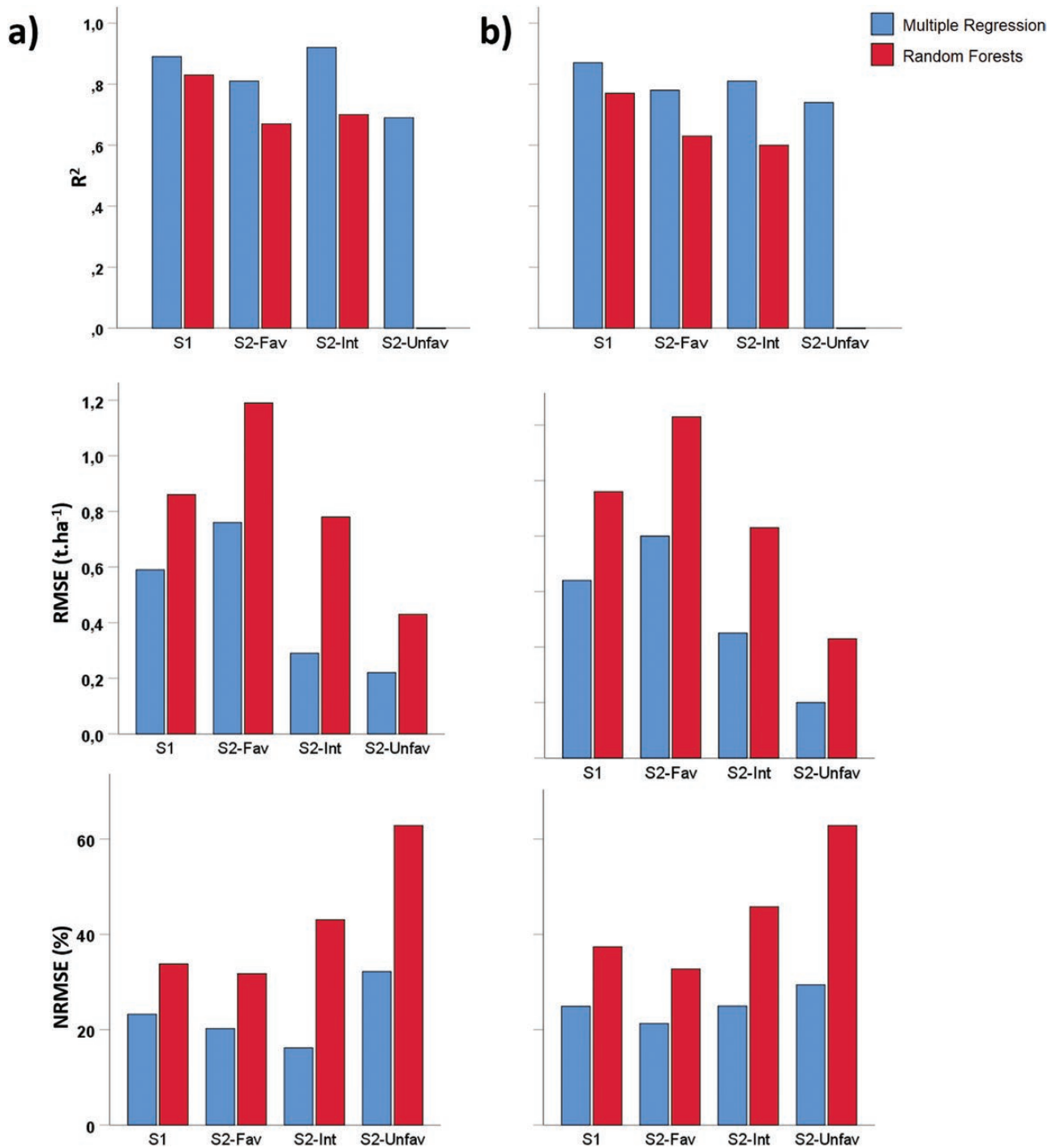


Figure 3. Coefficient of determination (R^2), RMSE and NRMSE of MR and RF models calculated on the calibration dataset. S1: generic model. S2: region-specific models with fav: favourable (>4000 mm per year), Int: intermediate (300–400 mm) and Unfav: unfavourable (<300 mm) rainfed areas. (A) With and (B) without integrating satellite-based variables during the calibration process.

4. EFFECT OF INTEGRATING SATELLITE-BASED DATA ON MODEL PREDICTIVE QUALITY

Calibration of generic and region-specific models with the MR and RF approaches was repeated when integrating LAI-Z30 and LAI-Z50 among the possible predictors of yield. Using remotely sensed variables allowed us to minimize the NRMSE of models calculated on the evaluation dataset by 4.9 % on average for MR models and 1.8 % for RF models (Fig. 2A). LAI-Z50 was selected

as the most influential predictor variable for yield in most RF and MR models (generic or region specific). On the contrary, LAI-Z30 parameter was not selected as a major predictor for any type of model (Fig. 3A and Supporting Information—Fig. S2). The inclusion of LAI-Z50 in yield RF models mainly resulted in changing the order of importance of predictors: maximum temperatures, total cumulated rainfall and N fertilization remained the main predictors together with LAI_Z50. The inclusion of LAI-Z50 in MR models was more disruptive of their structure,

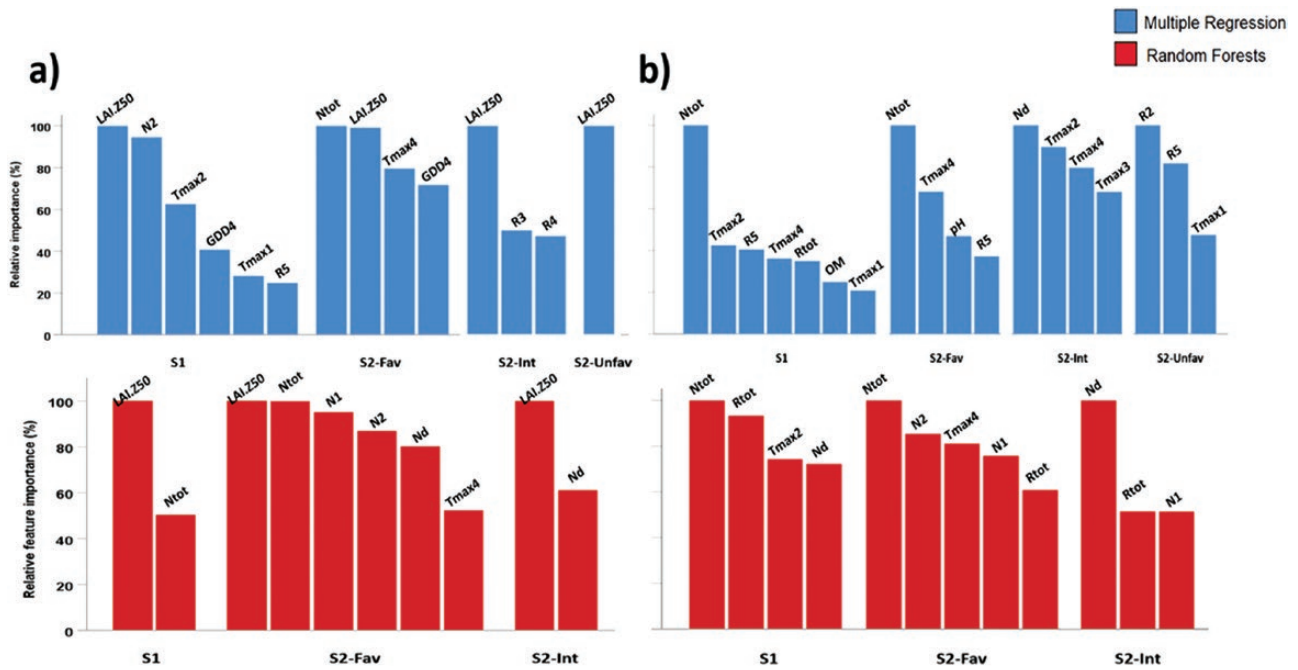


Figure 4. Relative importance of the main predictors of wheat yield in MR and RF models when calibrated as S1: generic models and S2: region-specific models with fav: for favourable, Int: for intermediate and Unfav: for unfavourable rainfed areas. (A) With and (B) without integrating satellite-based variables.

especially for region-specific models: Incorporation of LAI-Z50 in MR models was compensated by the exclusion of soil fertility variables (OM, pH) and the reduction of the number of variables derived from maximum temperatures while cumulated rainfall in different phases appeared amongst the main predictors (Fig. 3).

5. DISCUSSION

5.1 Main environmental determinants of wheat yield in rainfed areas of Morocco

The MR and RF models were fairly consistent in selecting climate, soil and practice-related predictors for yield, even when creating models specific to different regions or agroclimates. Both generic models obtained using the S1 strategy and models specific to intermediate or unfavorable areas identified metrics derived from local rainfall and maximum temperatures as the primary determinant predictors of yield. This finding aligns with the understanding that water is the main limiting factor for cereal production in rainfed agricultural areas of Mediterranean countries, especially in regions where cumulative annual rainfall peaks at 400 mm (Wani et al. 2009; Perniola et al. 2015).

The significance of maximum temperature in predicting final yield can be interpreted through two pathways. Firstly, high temperatures can indicate the occurrence and severity of heat stress, which decreases yield. However, maximum temperature (T_{max}) is also correlated with mean daily temperatures (T_{mean}) and daily incoming radiation, indicating its role in determining the duration of the crop cycle and the amount of radiation available to the crop. Due to these contrasting relationships between T_{max} and final yield, its role as a primary predictor in RF and MR models is not immediately intuitive.

The MR and RF models also identified specific periods in the crop cycle when rainfall and maximum daily temperatures have a greater impact on the final yield. T_{max2} (tillering phase) and T_{max4} (heading to flowering phase) were the temperature-related metrics most frequently selected as predictors in both types of models. These two metrics were consistently chosen in every RF model. T_{max1} (emergence to tillering) and T_{max3} (tillering to booting) were occasionally selected as secondary predictors in MR models. Thus, tillering and pre-flowering phases can be identified as the two phenological phases in wheat development that are more likely to be subject to and sensitive to heat stress. The observation of maximum temperature dynamics throughout the crop cycle in rainfed areas in Morocco further supports these results, showing that maximum daily temperatures exceed 26 °C on average from the start of February, which coincides with the full tillering phase and the beginning of elongation in wheat crops. Furthermore, several studies have demonstrated that heat stress during the vegetative growth phase of wheat reduces photosynthesis and dry matter accumulation, affecting the first yield components such as tiller and spike number per plant. Heat stress events during the pre-anthesis stages also increase pollen sterility, leading to a decrease in grain number (Porter and Gawith 1999; Farooq et al. 2011).

In terms of rainfall, the RF model selected in-season total cumulative rainfall (R_{tot}) as an important predictor of wheat yield, rather than stage-specific cumulative rainfall. This could be due to variations in soil water storage capacity across different fields, which can blur the relationship between the timing of rainfall and the effective timing of water stress, and its impact on yield. On the other hand, the MR models identified cumulative rainfall at specific stages, particularly R5 (cumulative rainfall during the grain filling period), as a significant predictor variable for wheat yield. This discrepancy between the RF and

predictors. In this study, the baseline MR and RF models, which incorporate satellite-based variables, identified LAI-Z50 as the primary yield predictor, followed by $T_{\max 2}$ and N_{tot} . These predictor values could be acquired in time to predict wheat yield a few days after the Z50 stage, occurring approximately 2 months before harvest in Morocco. RF agroclimate-specific models also allowed reasonably accurate yield prediction one to 2 months before harvest. However, the selection of R_{tot} and RS as yield predictors in other models hindered their use for yield prediction before the grain-filling stage. Overall, empirical models can appear more manageable for advising and supporting farmers compared to crop models. As a result, empirical models have been integrated into various tools and national operational systems for yield prediction in various countries (Fritz et al. 2019).

However, the machine learning approach cannot be considered a complete surrogate for a decision support tool as they struggle to determine the effects of practice changes. For example, beyond fertilization amounts, which are important predictors in RF and MR models in this study, farmers may modify the type of applied N-fertilizers or add other minerals to the crop. The RF and MR models cannot anticipate the effects of such decisions, requiring a recalibration of the models to understand the impact of tactical adaptations on yield. In contrast, crop models like APSIM-wheat are designed to represent the key processes that determine crop production, considering interactions with soil, climate and farming practices (Asseng et al. 2013) that confers more robustness to models and the capacity to simulate a larger range of cropping practices. The primary challenge preventing crop models from being widely used as decision support tools lies in the extensive data requirements for field-specific parameterization, including access to local daily weather data from sowing to harvest that hinders the possibility of running the model during the cropping season. To address this challenge, an ensemble of possible (generated or historic) climatic series can be utilized to complete the climate file in season. This approach has been employed in the development of commercial decision support tools like the Yield Prophet (Hunt et al. 2006) (<https://www.yieldprophet.com.au/yp/Home.aspx>), which advises farmers in-season based on APSIM-wheat simulations. Another potential strategy involves integrating remote sensing data, such as satellite images, into crop modelling tools to improve model calibration and correct dynamical model outputs in season (Huang et al. 2019).

4.3.3 Conservation of predictive capacity in the long term

In the long-term perspective, mechanistic crop models such as APSIM may be more efficient in predicting yield despite the introduction of improved cultivars in cropping systems. Crop model algorithms may be refined as new processes are integrated or revised into additional or improved modules but the core structure and principles of the model are not meant to be questioned by changes in the cropping environment or practices. Conversely, empirical models may require re-calibration and new predictors may be selected under changing environmental conditions, especially climate change, since climatic variables are major predictors for these models. Similarly, changes in fertilization practices, influenced by factors such as fertilizer and crop market prices or public policies, can impact the utility of some

predictors, such as N_2 or N_{tot} in the models assessed in this study. This, in turn, may increase model uncertainty if recalibration is not performed.

An open question arises regarding whether advancements in remote sensing technologies, automated data analysis pipelines and computational capabilities will alleviate the need for frequent recalibration of empirical models. Such recalibration would otherwise be necessary every few years or across different regions, in order to accommodate contextual changes.

Several recent studies in the literature have suggested that hybridization of process-based models together with empirical models would result in improved predictive capacity both in the long and short term (Shahhosseini et al. 2021; Maestrini et al. 2022; Zhang et al. 2023). While empirical models could support parameter estimation for crop models, crop output variables from crop models such as APSIM may be adequate predictors to statistical models and improve their predictive capacity.

6. CONCLUSION

While this work has not demonstrated a clear superiority of empirical models over a mechanistic model to predict crop yield in the case of wheat produced in the rainfed areas of Morocco, it evidenced the capacity of machine learning approaches to consistently identify the major yield determinants among a set of possible predictors, including when considering various algorithms. All the empirical models tested selected nitrogen fertilization and climatic variables as major yield predictors, before soil and crop management-related variables: in Morocco, rainfall and high temperatures are definitely the main determinants of yield, while soil and plant mineral status only explain marginal variation. Integrating recent advances in remote sensing, allowing the use of satellite-based vegetation indices such as LAI, into these models resulted in the incorporation of such variables as major predictors, before climatic predictors—but only slightly increased the models' predictive capacity. The attempt to make empirical models more site-specific to capture variation of yield determinants from one region to another was not conclusive. It is difficult to conclude if this is due to climatic determinants being actually the same all over the production area or due to a lack of sensitivity of empirical algorithms. However, this attempt revealed that resource-limited situations were equally difficult to model and predict for empirical and mechanistic models. Rather than clearly supporting the superiority of one type of model over another (empirical vs. mechanistic), the result of this work advocated a complementary use of one or another approach depending on data availability but also on the targeted time horizon for yield simulations (one-year vs. decades) and the modelling objectives (in-season guidance for tactical adaptation of crop management vs. ex-ante or ex-post assessment of practices).

SUPPORTING INFORMATION

The following additional information is available in the online version of this article –

Table S1. Relative importance of predictors in RF models.

Figure S1. Frequency of appearance of wheat yield predictors in the MR and RF models' structure; (A) with and (B) without integrating the satellite-based variables. For each type of model,

the frequency can vary from 0 to 4, as one generic and three region-specific models have been calibrated in each case.

Figure S2. Pearson correlation coefficients among wheat yield, meteorological variables, satellite-based biophysical variables, soil variables and fertilization variables.

<https://github.com/Achraf-UM6P/Scripts-and-fields-dataset-ML-and-APSIM-for-yield-prediction/blob/fd67ef5444157a2a1abea699215bb6041778313c/Script%20and%20dataset.rar>

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CONTRIBUTIONS BY THE AUTHORS

A.M.: Conceptualization, methodology, data analysis, data curation, data visualization, writing—original draft, writing—review & editing. **M.L.:** Methodology, data analysis, data curation, writing—original draft, data visualization. **H.M.:** Conceptualization, methodology, writing—original draft, writing—review & editing, supervision. **M.L.:** Methodology, supervision. **J.W.:** Methodology, supervision. **M.E.G.:** Funding acquisition. **B.T.:** Conceptualization, methodology, writing—review & editing, supervision, project administration, funding acquisition.

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CONFLICT OF INTEREST

None declared.

DATA AVAILABILITY

The datasets generated and/or analysed during the current study are available from the corresponding author on reasonable request. All data have been deposited on a github repository (link below) to which users may request access from the authors.

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