

Article

Patterns, Risks, and Forecasting of Irrigation Water Quality Under Drought Conditions in Mediterranean Regions

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Abstract: The seasonal and interannual irregularity of temperature and precipitation is a feature of the Mediterranean climate that is intensified by climate change and constitutes a relevant driver of water and soil degradation. This study was developed during three years in a hydro-agricultural area of the Alqueva irrigation system (Portugal) with Mediterranean climate conditions. The sampling campaigns included collecting water samples from eight irrigation hydrants, analyzed four times yearly. The analysis incorporated meteorological data and indices (precipitation, temperature, and drought conditions) alongside chemical parameters, using multivariate statistics (factor analysis and cluster analysis) to identify key water quality drivers. Additionally, machine learning models (Random Forest regression and Gradient Boosting machine) were employed to predict electrical conductivity (EC_w), sodium adsorption ratio (SAR), and pH based on chemical and climatic variables. Water quality evaluation showed a prevalence of a slight to moderate soil sodification risk. The factor analysis outcome was a three-factor model related to salinity, sodicity, and climate. The cluster analysis revealed a grouping pattern led by year and followed by stage, pointing to the influence of inter-annual climate irregularity. Variations in water quality from the reservoirs to the distribution network were not substantial. The Random Forest algorithm showed superior predictive accuracy, particularly for EC_w and SAR, confirming its potential for the reliable forecasting of irrigation water quality. This research emphasizes the importance of integrating time-sensitive monitoring with data-driven predictions of water quality to support sustainable water resources management in agriculture. This integrated approach offers a promising framework for early warning and informed decision-making in the context of increasing drought vulnerability across Mediterranean agro-environments.

Keywords: climate variability; hydro-agricultural areas; machine learning; multivariate statistics; salinity; sodicity



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1. Introduction

Droughts are becoming more common in Mediterranean regions, with increasingly unpredictable rainfall patterns [1,2]. This variability, heightened by global climate change,

poses a serious threat to food security. Traditional farming schedules are disrupted and water scarcity during key crop-growing periods threatens crop yields [1,2].

Besides the impacts of droughts on water quantity, the quality of water for agricultural and other uses is also compromised [3,4]. The effects of erratic precipitation distribution and interannual climate variability on the deterioration of surface and groundwater quality have been widely reported and are expected to worsen with global climate change [5–11]. Extreme precipitation events can increase runoff, which subsequently causes soil erosion but also transports organic pollutants like pesticides into water bodies, thus resulting in a degradation of water quality [12,13]. Higher temperatures contribute to rising evaporative rates, concentrating dissolved salts and nutrients in water bodies [14]. Extended periods of drought reduce water flows, causing the concentration of contaminants and decreasing the dilution of pollutants [15,16].

The expansion of irrigation systems in drought-prone areas has raised concerns about soil degradation, particularly salinization and the overall loss of soil health [17,18]. In fact, soil salinization is one of the critical physical–chemical degradation processes in drought-prone regions where irrigation is adopted [19,20]. Salt-affected soils occupy more than 20% of the global irrigated area and, in some countries, they occur in more than half of the irrigated land [21]. In the Mediterranean region, 25% of the irrigated cropland is affected by moderate-to-high salinization [22].

Hillel (2000) and Hillel et al. (2008) [19,23] highlighted the importance of having early warning systems to detect salinity and sodicity in irrigated agroecosystems. Besides the routine water monitoring programs in surface or groundwater bodies that supply irrigation perimeters, the diversification of spatial and temporal monitoring could predict the onset of salinization processes, especially when usual patterns of humid and dry periods are disturbed by drought occurrence [24]. Recently, data-driven approaches such as machine learning (ML) have emerged as tools to support environmental monitoring and forecasting. Several studies have highlighted the use of ML to predict water quality based on algorithms like Artificial Neural Networks, Random Forest, Multiple Linear Regression, Gradient Boosting, Support Vector Machines, or K-Nearest Neighbors, among others [25–28]. A prediction of stream water quality based on both chemical and meteorological data was performed by [29] using the RF and Boosted regression tree (BRT) models. Some recent studies have specifically focused on modeling irrigation water quality, typically relying on datasets of physicochemical parameters to predict indices or key target variables [30–32]. Machine learning algorithms can handle complex, nonlinear relationships between large sets of variables, allowing for the prediction of key salinity indicators, the identification of the most influential parameters contributing to water degradation in irrigated systems, and the modernization of irrigation water quality management [33]. While these studies have explored the use of predictive models for irrigation water quality, to the best of our knowledge, none have integrated meteorological variables that describe cumulative dryness during drier years. In this context, the use of ML in irrigation water quality monitoring under climate uncertainty can enhance early detection of salinization risks and support more adaptive water management strategies.

This study aims to evaluate irrigation water quality at the hydrant level under drought conditions and to explore the potential of ML models in predicting key irrigation water quality parameters. Specifically, the objectives are (i) to evaluate the suitability of irrigation water for agricultural use during dry periods, (ii) to evaluate the contribution of hydrant-level water quality assessment to improve spatial monitoring, (iii) to identify the most influential factors affecting water quality variability under drought conditions, and (iv) to compare the performance of two ML algorithms, Random Forest and Gradient Boosting, in predicting salinity-related parameters from chemical and meteorological variables.

2. Materials and Methods

2.1. Study Area

This study was conducted in eight hydrants (H5, H6, H7, H16, H21, H22, H23, and H33, as identified by the water supplier company) distributing water to ten farm fields with a land use of drip-irrigated vineyards and olive orchards and sprinkler-irrigated annual field crops, forages, and pastures (Table 1), totaling 88 ha. All farm fields were located in the Brinches-Enxoé hydro-agricultural area with an equipped area of 5061 ha, part of the Alqueva irrigation system, in the Alentejo region, South Portugal (Figure 1). The conveyance networks of the Brinches-Enxoé hydro-agricultural area originate in the Laje (pressurized) and the Montinhos (gravity) reservoirs, respectively. The former is the upstream reservoir of all the studied hydrants, except for H16, supplied by Montinhos.

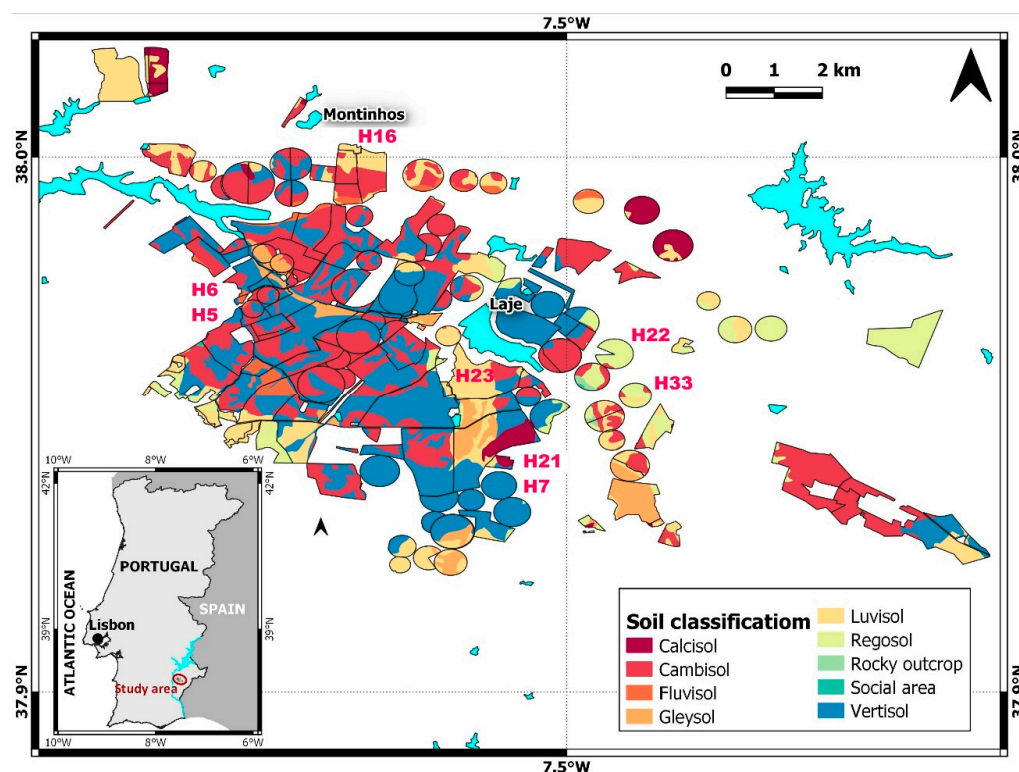


Figure 1. Location of the irrigation hydrants, Montinhos and Laje reservoirs, and predominant soil distribution in the hydro-agricultural area of Brinches-Enxoé, adapted from [20].

The predominant soil types are medium to fine-textured calcaric cambisols, chromic vertisols, and chromic luvisols [34], represented in Figure 1.

The climate in the region is temperate with a hot and dry summer (Mediterranean) with an annual precipitation and average mean monthly temperature of, respectively, 558 mm and 16.9 °C (1981–2010 climatological normal; [35]).

Table 1. Crops in the farm plots supplied by the hydrants (coordinates between brackets), integrated with the Brinches-Enxoé hydro-agricultural area, during the period of study (2018–2020).

Year	H5 (37°58'12.74" N; 7°33'18.17" W)	H6 (37°58'22.99" N; 7°33'26.61" W)	H7 (37°56'1.01" N; 7°31'25.40" W)	H16 (37°59'53.28" N; 7°32'21.02" W)	H21 (37°56'48.39" N; 7°30'17.74" W)	H22 (37°57'12.65" N; 7°29'21.08" W)	H23 (37°57'22.32" N; 7°30'36.72" W)	H33 (37°57'36.03" N; 7°29'18.35" W)
2018	Grapevine (<i>Vitis vinifera</i> L. Cv. 'Aragonez')	Maize (<i>Zea mays</i> L.)	Sunflower (<i>Helianthus annuus</i> L.)	Grapevine (<i>Vitis vinifera</i> L. Cv. 'Antão Vaz') Olive (<i>Olea europaea</i> L. Cv. 'Cordovil')	Olive (<i>Olea europaea</i> L. Cv. 'Cobrançosa')	Permanent Pasture ((grasses (70%), legumes (18%) and others (12%))	Grapevine (<i>Vitis vinifera</i> L. Cv. 'Antão Vaz') Sunflower (<i>Helianthus annuus</i> L.)	Alfalfa (<i>Medicago sativa</i> L.)
2019	Grapevine (<i>Vitis vinifera</i> L. Cv. 'Aragonez')	Sunflower (<i>Helianthus annuus</i> L.)	Arrowleaf clover (<i>Trifolium vesiculosum</i> Savi)	Grapevine (<i>Vitis vinifera</i> L. Cv. 'Antão Vaz') Olive (<i>Olea europaea</i> L. Cv. 'Cordovil')	Olive (<i>Olea europaea</i> L. Cv. 'Cobrançosa')	Permanent Pasture ((grasses (70%), legumes (18%))	Grapevine (<i>Vitis vinifera</i> L. Cv. 'Antão Vaz') Garlic (<i>Allium sativum</i> L.) + Maize (<i>Zea mays</i> L.)	Alfalfa (<i>Medicago sativa</i> L.)
2020	Grapevine (<i>Vitis vinifera</i> L. Cv. 'Aragonez')	Maize (<i>Zea mays</i> L.)	Onion (<i>Allium cepa</i> L.)	Grapevine (<i>Vitis vinifera</i> L. Cv. 'Antão Vaz') Olive (<i>Olea europaea</i> L. Cv. 'Cordovil')	Olive (<i>Olea europaea</i> L. Cv. 'Cobrançosa')	Not sown	Grapevine (<i>Vitis vinifera</i> L. Cv. 'Antão Vaz') Sunflower (<i>Helianthus annuus</i> L.)	Not sown

2.2. Meteorological Data and Drought Characterization

Meteorological data were recorded in an automatic meteorological station of the Irrigation Operating and Technology Center (Centro Operativo e de Tecnologia do Regadio—COTR) located in the area (37.97 N; 7.55 W) [36]. To characterize the meteorological trends during the study period, the monthly Standard Precipitation Index (SPI) was calculated [37]. The SPI is a statistical index that measures precipitation anomalies in a given region and time compared to historical patterns. It was obtained by fitting the long-term monthly precipitation records of the period 1981–2010 [38] to a Gamma probability distribution, which was then transformed into a normal distribution. Droughts can be classified as mild, for $-1.0 < \text{SPI} < 0$; moderate, if $-1.5 < \text{SPI} \leq -1.0$; severe, for $-2.0 < \text{SPI} \leq -1.5$; and extreme, if $\text{SPI} \leq -2.0$.

The occurrence of drought was identified according to [37] as a period in which the SPI is continuously negative and reaches a value ≤ -1.0 , beginning when the SPI first falls below zero and ending with a positive value of the SPI following a value ≤ -1.0 . The duration (number of months), magnitude ($\sum |\text{SPI}|$ during drought), and intensity (magnitude/duration) of droughts were also evaluated.

The values of accumulated precipitation (P_{cum}) and accumulated reference evapotranspiration ($ET0_{\text{cum}}$) until each sampling date were computed to obtain variables in the dataset that could be descriptive of the meteorological conditions when applying the multivariate statistical methods and the ML model.

2.3. Sampling Strategy

This study covered 12 water sampling campaigns, with four campaigns each year, performed in April–May, June–July, September–October, and November, corresponding to the following assigned stages of crop development/irrigation season, respectively: Initial (I); Middle (M); Late (L); and Post-cycle (P). For the assessment, 2 L water samples were collected in polyethylene bottles from the irrigation hydrants. The samples were transported to the laboratory in a cooler at 4 °C and stored, following the requisites for water conservation for each parameter [39].

Water pH was determined by potentiometry with a pH probe, and EC_W was determined by conductometry with a conductivity meter. The concentrations of ions of calcium (Ca), magnesium (Mg), sodium (Na), chloride (Cl), boron (B), and nitrate (NO_3) were determined by the ionic chromatography methodology [39].

2.4. Irrigation Water Quality Assessment

The assessment of water quality for irrigation was performed using the consensual guidelines of the Food and Agriculture Organization of the United Nations (FAO) (Table S1), which consider four types of “potential problems” that can arise from the use of poor quality irrigation water, namely (i) salinity, which can affect soil water availability; (ii) infiltration rate of water into the soil; (iii) specific ion toxicity in sensitive crops; (iv) and miscellaneous effects on susceptible crops [40].

2.5. Exploratory Statistical Analyses

Matrices of Spearman’s correlation coefficients were computed for preliminary examination of the relationships between variables. Factor and cluster analyses were performed to explore data structure and case similarity using the methodology described in Tomaz et al. [41,42]. Analyses were performed with Statistica 7 [43].

2.6. Machine Learning Models

Random Forest (RF) and Gradient Boosting (GB) models were tested to forecast three key indicators of irrigation water quality (target variables), EC_W , SAR, and pH, using a dataset of the average values of continuous physicochemical and meteorological predictors: P_{cum} , $ET0_{cum}$, B, Ca, Mg, Na, Cl, and NO_3 .

RF is a supervised ensemble ML model based on a collection of decision trees (estimators) [44]. Because it is an ensemble technique, it uses the best outcome given by the many decision trees, mitigating and limiting generalization mistakes as the volume of the tree architecture in the forest grows. In addition, it shows the ability to capture nonlinear relationships [28,30].

GB is also a supervised ensemble ML model that uses decision trees as base learners, but builds them sequentially, with each new tree focusing on correcting the prediction errors made by the previous ones. This boosting approach enables the model to gradually improve its accuracy by minimizing a loss function at each step [45].

Both models were developed in Visual Studio Code (version 1.100.1 Python 3.10) using Python libraries, such as scikit-learn, pandas, and matplotlib. For each target variable, the RF models were trained with 100 decision trees, which is the default configuration recommended in the library as a balance between predictive performance and computational efficiency. Similarly, the GB models were also trained using the default hyperparameters, including 100 decision trees and a learning rate of 0.1, which controls how much each new tree influences the final model. Model evaluation was performed using an 80–20% train–test split of the dataset, meaning that the RF algorithm built an input–output relationship with 80% of the dataset and subsequently generalized or predicted outputs for the 20% of unseen inputs [28,46]. For each algorithm and model, the following performance metrics were calculated: coefficient of determination (R^2), root mean square error (RMSE), mean absolute error (MAE), and relative bias (RBIAS). The final model was selected based on cross-validated performance metrics (R^2 , RMSE, MAE, etc.). In addition, the mean decrease in impurity (MDI), or Gini importance, was used to rank the feature importance (of each predictor) in the RF model [47]. Measured and predicted values of each parameter were represented in scatter plots to evaluate the accuracy and goodness of fit for both models.

3. Results and Discussion

3.1. Meteorological Trends and Drought Characterization

The annual precipitation was 603 mm, 343 mm, and 615 mm in 2018, 2019, and 2020, respectively, while the mean annual temperature was 16.7 °C, 17.3 °C, and 17.8 °C. The mean temperature during the growing/irrigation season of the different crops in the study area (March to October) each year was 19.8 °C, 20.2 °C, and 20.5 °C, respectively. The year 2018 was characterized by high precipitation in the spring (March and April) and autumn (October and November); 2019 was a very dry year, characterized by high temperatures and very low precipitation; 2020 registered higher mean monthly temperatures, and despite presenting higher annual precipitation than the two previous years, rain was mostly concentrated in April and the autumn months (October and November) (Figure 2).

Calculations of the monthly SPI were made to better understand the climate's interannual and seasonal variability during the period of the study and the occurrence of drought (Figure 2).

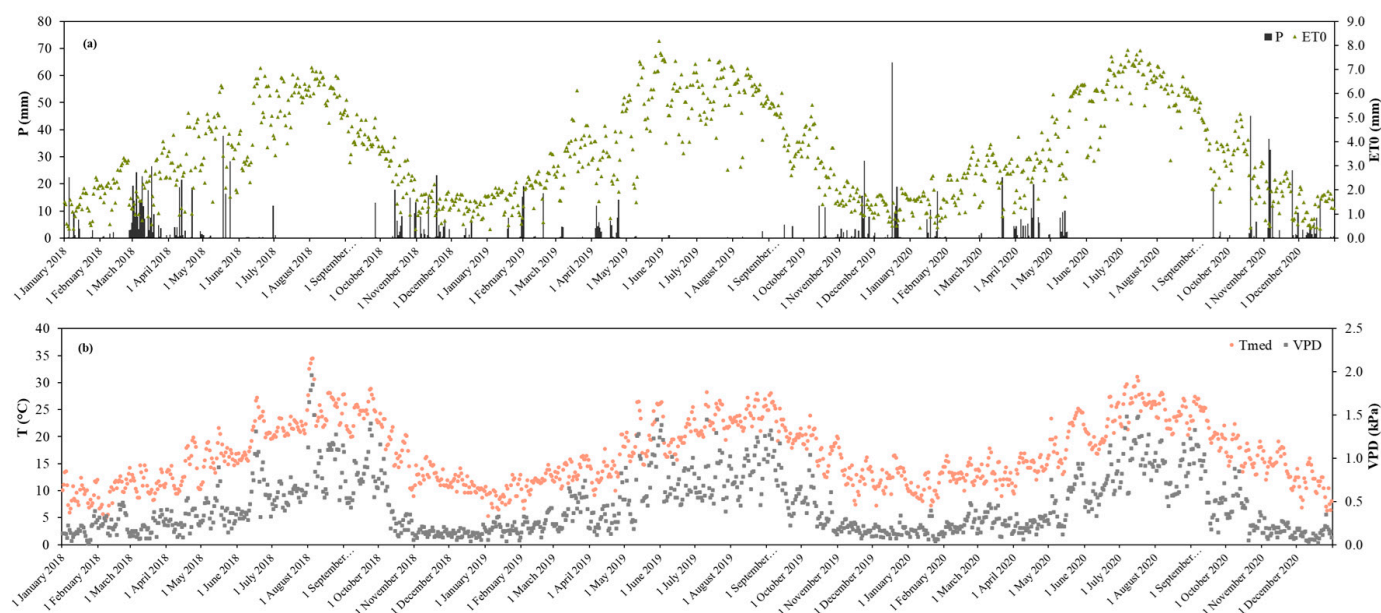


Figure 2. Daily variation of (a) precipitation (P) and reference evapotranspiration (ET0), and (b) mean temperature and vapor pressure deficit (VPD).

A continuing trend of dry conditions started from the end of 2018 through the end of 2019 and the initial months of 2020, with the occurrence of four almost consecutive droughts (Figure 3). The longest drought lasted 5 months (1 December 2018 to 1 April 2019), but the highest drought magnitude occurred from 1 May 2019 to 1 August 2019, when the minimum SPI reached -2.73 , signaling extreme dry weather. These dry conditions continued until the end of 2019 (November). The drought persisted until 1 March 2020. During 2019, precipitation values were consistently lower than the climatological normal (except in April and December), which, along with the high temperatures, contributed to the year's severe dry conditions. In 2020, there was a recovery in precipitation levels, especially in March–April and October–November, but temperatures remained higher than historical records [48].

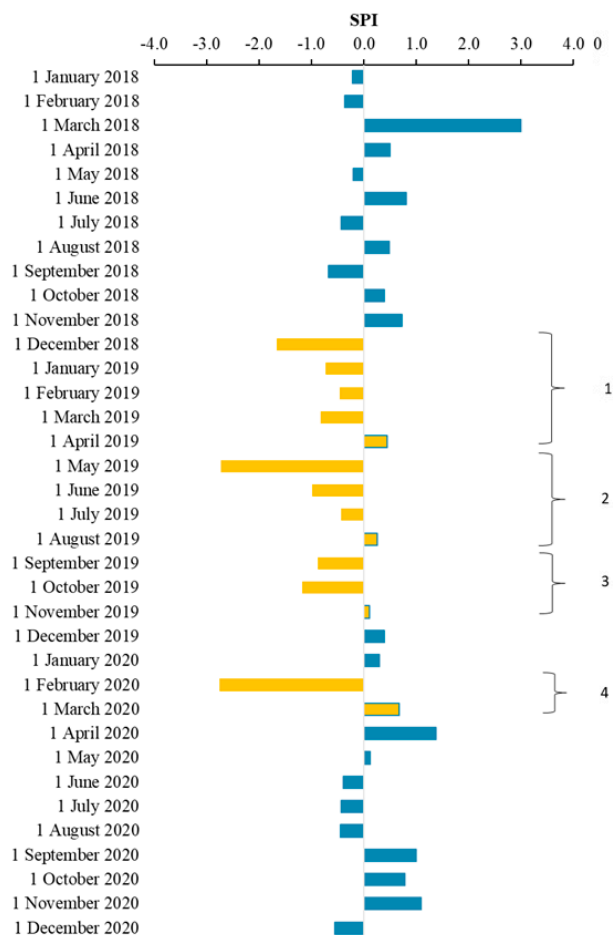
3.2. Irrigation Water Quality

The temporal and spatial variation of water physical–chemical parameters and ions was characterized by their mean and standard deviation (Figures 4 and 5).

The highest ECW value was registered in H5, at the end of 2020. In general, there was a slight increase in ECW during the study period, more evident in 2019, which can be related to the drought conditions observed that year, as was confirmed by the Spearman negative correlation between this parameter and cumulative precipitation ($R = -0.330$; $p < 0.05$) (Table 2). The highest pH values occurred in H16 during the summer period of 2018 and 2019; the lowest value was registered in H5, at the end of 2020. The results highlighted that the increase in pH is negatively correlated with precipitation ($R = -0.371$; $p < 0.05$), indicating that higher frequency of dry periods may be negatively influencing some irrigation water quality parameters, such as pH and ECW.

The dominant ion in most samples was Cl, followed by Na. Overall, the order of cation abundance was $\text{Na} > \text{Ca} > \text{Mg} > \text{B}$. Regarding nitrate, in general, all concentrations quantified in the hydrant system were within the values stipulated for good water quality for irrigation. Exceptionally high nitrate concentrations were observed in October 2019 in H23 (15.7 mg L^{-1}) and in June 2020 in H6 (26.7 mg L^{-1}), classifying the water as having mild to moderate use restrictions, according to the FAO guidelines. As these values did not occur in the Lage reservoir in the same sampling period, as reported by [49], where

maximum NO₃ concentrations were <5 mg L⁻¹, the concentrations may be correlated with contamination with some liquid formulation of nitrogen fertilizer (a common practice in the area), which could have occurred in the conveyance system. Despite the common origin of water, localized phenomena, like contamination or degradation within the pipeline infrastructure, may occasionally lead to deviations in water quality at the hydrant level. As reported in drinking water distribution systems, chemicals may be released from materials and equipment either by leaching due to contact with water or through corrosion in deteriorating pipes [50,51].



Drought	Beggining	End	Duration	SPI min	Magnitude	Average intensity
1	1 December 2018	1 April 2019	5	-1.67	4.14	0.83
2	1 May 2019	1 August 2019	4	-2.73	4.40	1.10
3	1 September 2019	1 November 2019	3	-1.18	2.17	0.72
4	1 February 2020	1 March 2020	2	-2.76	3.43	1.71

Figure 3. Monthly Standard Precipitation Index (SPI) during the study period. Droughts are identified with full yellow bars (yellow bars outlined in blue represent the end of a drought; blue bars represent monthly SPI with no drought). The table below the graph characterizes each drought for duration (months), minimum SPI value, magnitude, and intensity, according to [37].

According to the FAO guidelines, no potential salinity problem was detected, as EC_W values were persistently lower than 0.7 dS m⁻¹ (Tables S2–S4). A slight to moderate risk of soil sodification prevailed, which should be carefully monitored, especially since the predominant soils in the study area are fine-textured and sprinkler-irrigated crops occupy a large area, potentially leading to adverse impacts on soil structure due to adsorbed Na [52]. This mild to moderate risk has already been observed at both the Alqueva and the Lage

reservoirs [24,49], suggesting that the irrigation conveyance network does not significantly alter these parameters, namely, potential salinity issues and the risk of soil sodification.

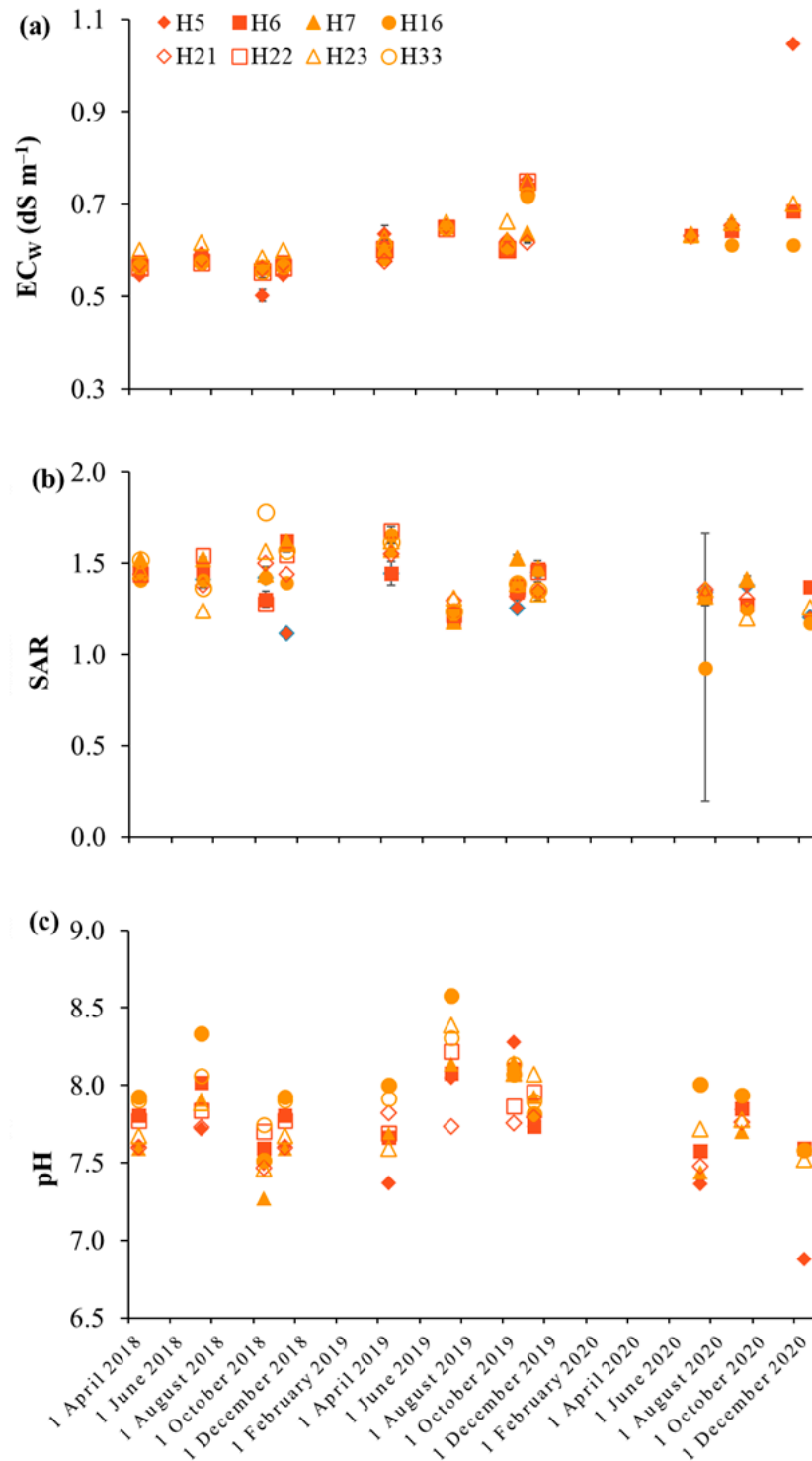


Figure 4. Temporal variation of water (a) EC_w, (b) SAR, and (c) pH during the period of study (12 sampling campaigns), for each hydrant. Markers represent the mean and whiskers represent the standard deviation for three repetitions.

Except for H16 (supplied by the Montinhos reservoir) in mid-season 2019, pH values remained within the normal range. In the study by [49], pH values measured in the Lage reservoir during 2019, the driest year, exceeded the upper limit (pH > 8.4). However, no

similar trend was observed in the hydrant network; in other words, no spatial decline in pH was detected. This represents the most significant difference between the reservoirs and the hydrant system in terms of irrigation water quality assessment.

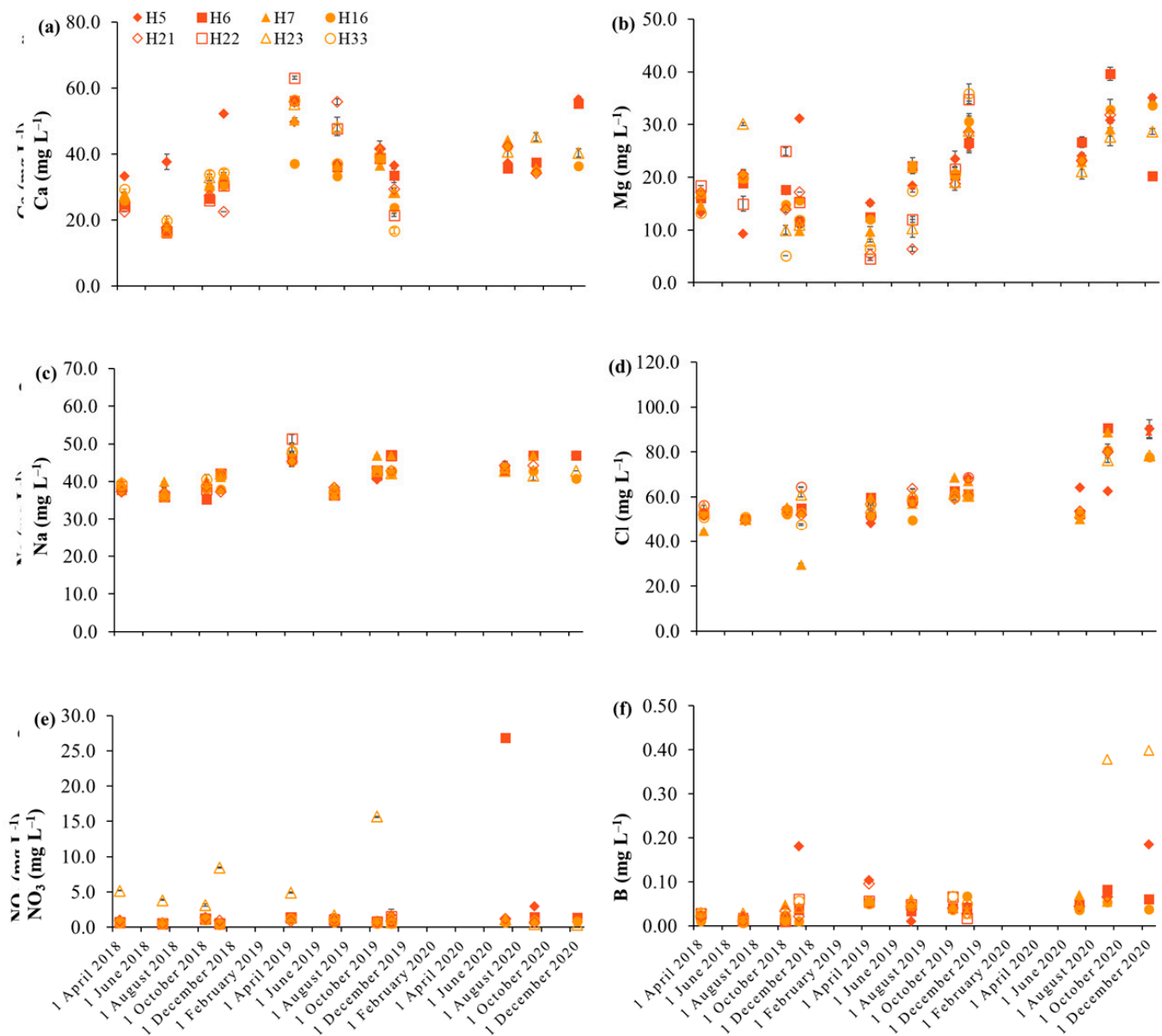


Figure 5. Temporal variation of water ion concentrations ((a) Ca, (b) Mg, (c) Na, (d) Cl, (e) NO₃, and (f) B) during the period of study (12 sampling campaigns), for each hydrant. Markers represent the mean and whiskers represent the standard deviation for three repetitions. (a) Ca, (b) Mg, (c) Na, (d) Cl, (e) NO₃, and (f) B.

3.3. Correlation, Factor Analysis, and Cluster Analysis

To better understand the interactions between chemical parameters and meteorological conditions, exploratory analyses using multivariate statistical methods were conducted. The Spearman correlation coefficient of 11 variables, including water physical-chemical parameters (EC_w, SAR, and pH), ions concentrations (Ca, Mg, Na, Cl, NO₃, and B), as well as cumulative precipitation (P_{cum}) and cumulative reference evapotranspiration (ET_{0cum}) until each sampling date, can be observed in Table 2.

Table 2. Spearman correlation matrix and heat map of water physical–chemical parameters and climate variables. Bold values are significant at $p < 0.05$.

P_{cum}	$ET0_{cum}$	pH	EC_w	B	Ca	Mg	Na	Cl	NO_3	SAR	
1.000	0.294	−0.371	−0.330	−0.168	−0.387	0.105	−0.258	−0.076	−0.111	0.010	P_{cum}
	1.000	0.115	0.401	0.220	−0.040	0.492	0.205	0.615	−0.040	−0.278	$ET0_{cum}$
		1.000	0.193	−0.069	−0.112	0.137	−0.175	0.071	−0.183	−0.171	pH
	<0.200		1.000	0.493	0.393	0.529	0.426	0.576	0.250	−0.454	EC_w
	0.200–0.400			1.000	0.622	0.190	0.581	0.444	0.126	−0.186	B
	0.400–0.600				1.000	−0.073	0.485	0.251	0.139	−0.238	Ca
	>0.600					1.000	0.239	0.429	−0.084	−0.624	Mg
	<−0.600						1.000	0.425	0.228	0.220	Na
	−0.600–−0.400							1.000	0.222	−0.282	Cl
	−0.400–−0.200								1.000	0.106	NO_3
	>−0.200									1.000	SAR

The higher significant correlation coefficients ($> |0.6|$) occurred between [Ca] and [B], [Cl] and $ET0_{cum}$, and SAR and [Mg], highlighting the influence of low Mg concentrations on SAR values. Other highly significant correlation coefficients (>0.5) could be found between [Mg] and EC_w , between [Na] and [B], and [Cl] and EC_w . Regarding correlations between meteorological variables and water physical-chemical parameters, $ET0_{cum}$ was significantly and positively correlated with EC_w , [B], [Mg], [Na], and [Cl], pointing to an influence of high evaporative demand conditions on water salinity, and negatively correlated with SAR; P_{cum} was significantly and positively correlated with $ET0_{cum}$, and negatively correlated with pH, EC_w , [Ca], and [Na], thereby indicating that lower precipitation induced by drought is related to a decline in water quality, as highlighted by other studies on drought impacts on agricultural water quality [24,53,54]. Furthermore, the absence of strong correlations between metals, as is the case of Mg and Na (0.239) and Mg and Ca (−0.073), suggests that these chemicals may have different sources, such as anthropogenic activities (mineral fertilizers) and geologic origins through the natural weathering of carbonate and silicate rocks [55,56].

The relationships observed among variables translated into a three-factor model accounting for around 61% of the total variance in the dataset (Table 3). Factor 1 explained 29% of the variance and presented high positive loadings of $ET0_{cum}$ (0.691), EC_w (0.703), [Cl] (0.751), and [Mg] (0.879), while a moderate positive loading was observed in [B] (0.356).

A high negative loading in Factor 1 belonged to SAR (−0.574). Therefore, Factor 1 was influenced by salinity, given the high weights of EC_w , [Cl], and [Mg]. Factor 2 was responsible for explaining approximately 19% of the total variance and represented a sodicity factor as it was mainly related to [Na] (0.759) and SAR (0.666). Factor 3 represented 14% of the total variance and was positively influenced by P_{cum} (0.887) and $ET0_{cum}$ (0.318) and negatively correlated with pH (−0.693); thus, it can be considered as a climate factor.

When analyzing the score plot of cases of the first two factors, patterns of case gatherings that were year-controlled (Figure 6a) and crop irrigation stage-controlled (Figure 6b) can be recognized. The same did not apply to the grouping of cases by location (hydrants) (Figure 6c).

Table 3. Factor loadings, eigenvalues, and percentage of total variance in a three-factor model of 11 observed variables. Bold values correspond to the higher absolute factor loadings of the variables in each factor.

	Factor 1	Factor 2	Factor 3
P _{cum}	0.099	−0.142	0.887
ET0 _{cum}	0.691	0.090	0.318
pH	0.076	−0.289	− 0.693
EC _w	0.703	0.156	−0.102
B	0.356	−0.135	0.229
Ca	−0.052	0.203	− 0.206
Mg	0.879	−0.128	0.024
Na	0.215	0.759	−0.096
Cl	0.751	0.140	0.065
NO ₃	0.133	0.511	−0.117
SAR	− 0.574	0.666	0.144
Eigenvalues	3.160	2.057	1.485
% Total variance	28.73	18.70	13.50

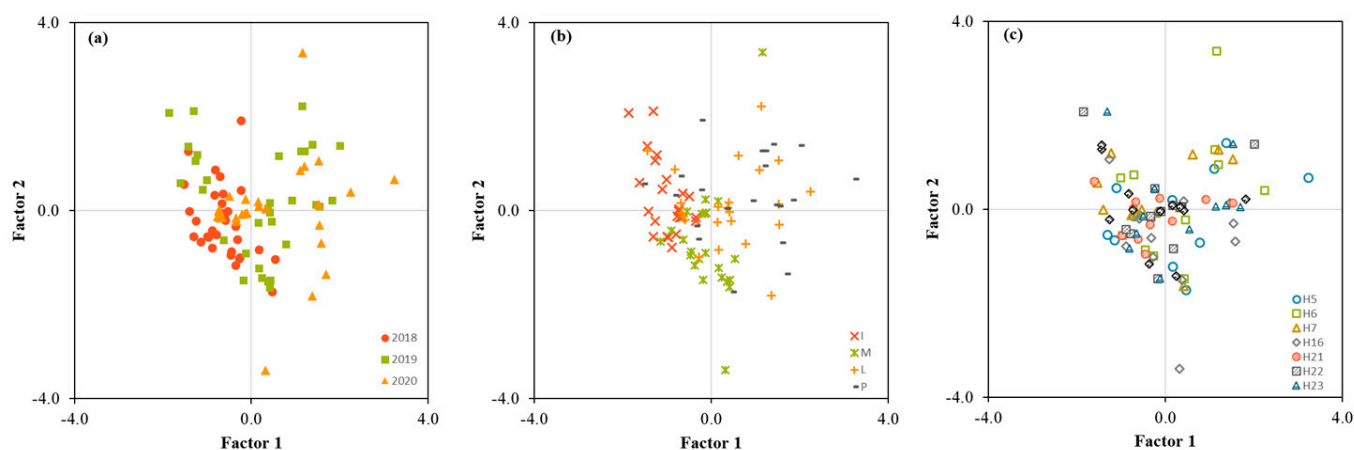


Figure 6. Score plots of cases of the first two factors. Different shapes and colors in each graphic differentiate the year (a), stage of irrigation season: I—Initial; M—Middle; L—Late; and P—Post-cycle (b), and hydrant (c).

To clarify these groupings of cases, a CA was performed, yielding the following cluster structure (Figure 7):

- Cluster 1, positively related to salinity (Factor 1) and sodicity (Factor 2), was composed of 16 cases, with no samples in 2018, eight cases in 2019, and eight cases in 2020; cases were mostly of the Post-cycle (P) stage (10 samples). This structure suggests a degradation of water quality following the peak water demand by crops in Mediterranean regions, that is, a pattern of salt accumulation in water sources resulting from high evapotranspiration during summer and limited water recharge due to drought occurrence and expansion of irrigation areas [57,58].
- Cluster 2, in the second quadrant, thus positively related to salinity, grouped 32 cases, mainly in 2019 (14 samples), with the remaining equally distributed between 2018 and 2020 cases; no samples belonged to the initial period, being mostly of the Middle (M) (13) and Late (L) (11) stages. This result reinforces the idea of the cumulative effects of evaporation and decreased freshwater recharge as the season progresses. A similar trend was reported by [59] in an irrigation district in southern Portugal, where the risk of salinity build-up was high to very high during very dry years in most fields.

In wetlands located in arid/semi-arid zones, periods of higher salinity can occur as a consequence of the highly evaporative conditions and water resources' depletion [60].

- Cluster 3, negatively related to both salinity and sodicity, presented 32 samples, largely of 2018 (18) and 2020 (13), from the I (16) and M (9) stages of the irrigation season.
- Cluster 4, in the 4th quadrant, grouped 13 samples of 2018 (5) and 2019 (8), the majority being of the I (8) period. Together with Cluster 4, this structure reflects the dilution effect of winter rainfall, which improves water quality at the start of the spring–summer crop cycle.

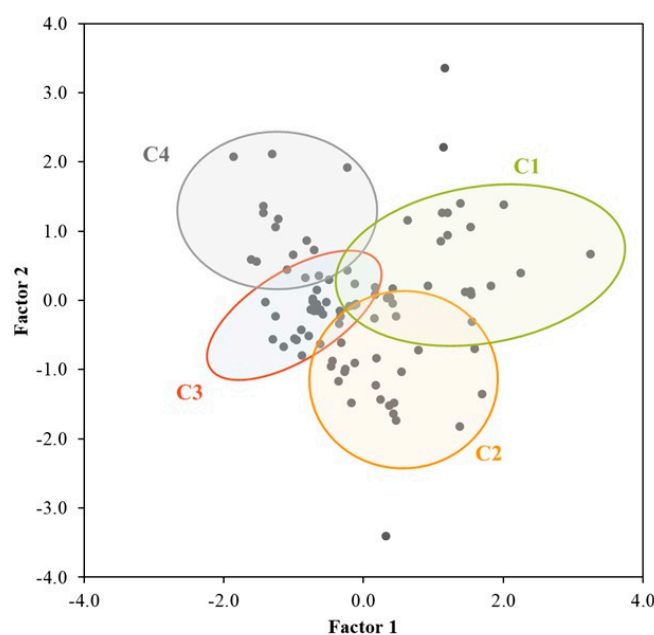


Figure 7. Score plot of cases of the first two factors with ellipses representing significant clusters with $dlink/dmax * 100 < 40\%$.

All in all, this cluster composition reveals two key effects: a drought-induced impact that intensifies salinity and sodicity levels and a seasonal influence associated with different stages of the irrigation calendar and crop cycles. Therefore, the groupings obtained confirmed the trends identified in the FA results, providing further support for the temporal patterns observed in irrigation water quality. In a study on the spatial and temporal variability of irrigation water quality in a large reservoir during a drought year, ref. [24] reported similar results, with a more time- than space-controlled pattern of sample clustering.

3.4. Random Forest and Gradient Boosting Models

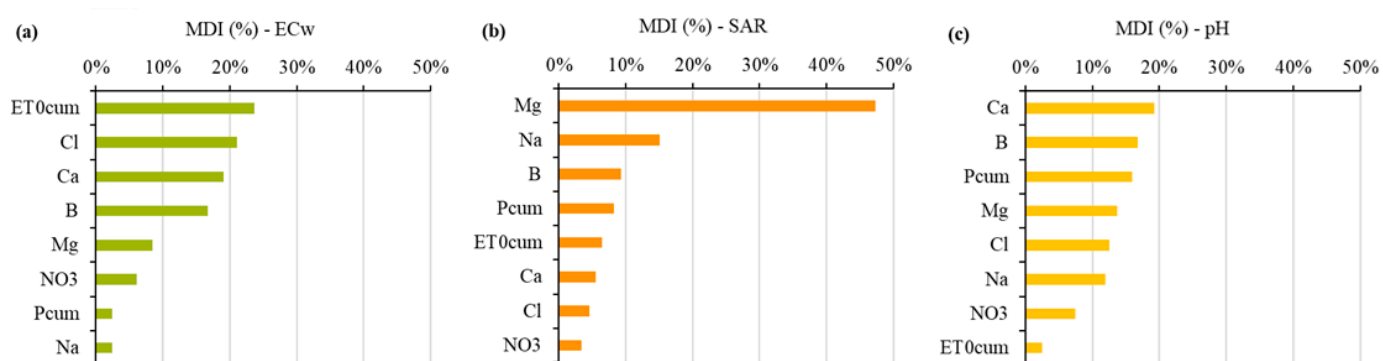
All three RF models demonstrated satisfactory predictive performance, with particularly better results for SAR and EC_W (Table 4). The model predicting SAR achieved an R^2 of 0.622, a root mean square error (RMSE) of 0.106, and a mean absolute error (MAE) of 0.064, indicating a good predictive accuracy and low residual error. Similarly, the EC_W model reached an R^2 of 0.605, an RMSE of 0.021, and an MAE of 0.015, which supports its applicability for forecasting. The pH model presented lower predictive capacity, with $R^2 = 0.485$, MAE = 0.146, and RMSE = 0.175, suggesting a more complex relationship between predictors and pH dynamics. All RF models exhibited low relative bias (RBIAS); namely, +1.27% for EC_W , +1.46% for SAR, and +0.63% for pH, demonstrating that the predictions were not affected by systematic over- or underestimation.

Table 4. Performance statistics of the Random Forest (RF) and Gradient Boosting (GB) models for the prediction of EC_w, SAR, and pH.

Variable	Model	R ²	RMSE	MAE	RBIAS (%)
EC _w	RF	0.605	0.021	0.015	1.266
	GB	0.362	0.001	0.017	2.116
SAR	RF	0.622	0.106	0.064	1.462
	GB	0.670	0.099	0.058	1.306
pH	RF	0.485	0.175	0.146	0.626
	GB	0.256	0.044	0.161	0.733

In the case of GB, the model performance for predicting SAR was slightly better than in the RF regression ($R^2 = 0.670$, $RMSE = 0.099$; $MAE = 0.058$, and $RBIAS = 1.306\%$) but presented a lower predictive capacity both for EC_w and pH. The RBIAS remained low but was generally higher than in the RF regression. Overall, the performance metrics showed that the RF was a better model to predict water quality parameters from chemical and meteorological data. These results follow [30,31], which found RF as one of the models with higher accuracy in the prediction of irrigation water quality indices like SAR, exchangeable sodium percentage (ESP), or total dissolved solids (TDS), making it a good model to be used in water quality forecasting in general but also, as our results show, under drier conditions by using different combinations of chemical and meteorological variables.

The feature importance in RF was assessed using the MDI. Results showed distinct variable contributions across the target variables (Figure 8). For EC_w, the most relevant predictors were ET_{0cum} (23.6%), Cl (21.1%), and Ca (19.1%), pointing out the influence of evapotranspiration and ion concentrations, especially chloride and calcium, on salinity levels (Figure 8a). The SAR model was largely determined by Mg (47.3%) and Na (15.1%), which was expected given their central role in SAR calculation. P_{cum} was one of the contributors, although having a lower weight (Figure 8b).

**Figure 8.** Feature importance of the predictor variables in the RF models, measured by the mean decrease in impurity (MDI). (a) EC_w; (b) SAR; and (c) pH.

In the pH model, the most influential variables were Ca (19.2%), B (16.7%), and P_{cum} (16.0%), followed by Mg and Cl. This result suggests that the acid–base balance in irrigation water is influenced by both precipitation-related dilution and the presence of alkaline earth metals (Figure 8c).

Scatterplots of observed versus predicted values confirmed the quantitative performance of the RF models (Figure 9). Both EC_w and SAR showed high correlations of 0.812 and 0.881, respectively. The pH predictions, while slightly more dispersed, are still well associated with the observed data, with a correlation of 0.772, validating the model structure for exploratory or decision support purposes.

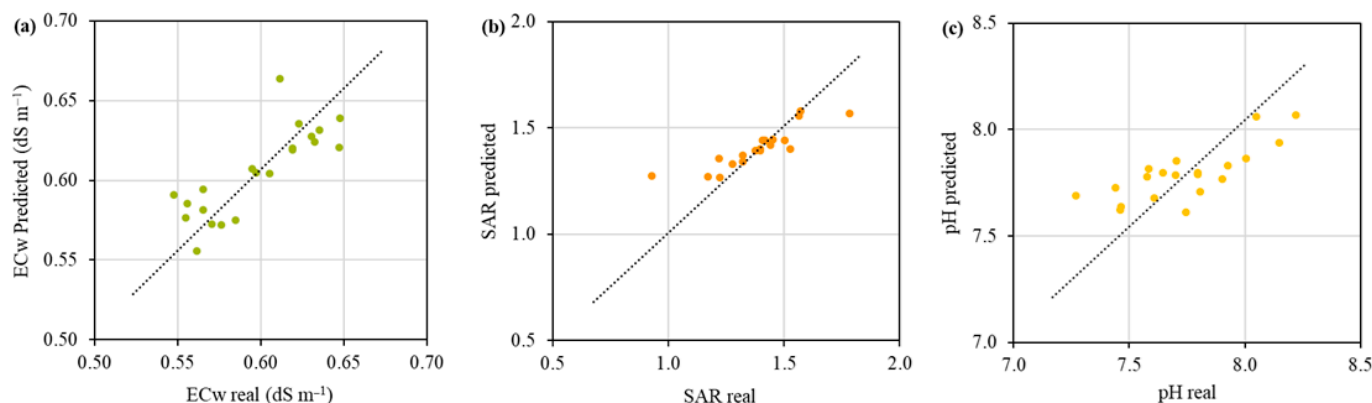


Figure 9. Scatterplots of real versus predicted values of (a) ECw ($r = 0.812$), (b) SAR ($r = 0.881$), and (c) pH ($r = 0.772$), obtained by the RF model.

These results indicate that the models may serve as early warning systems, allowing water management authorities and farmers to anticipate potential water quality deterioration, decline in crop productivity, and long-term degradation of soils due to salt accumulation [24].

To achieve a salt equilibrium in the soil, the influx of salt must be compensated for by salt removal, hence ensuring long-term salt sustainability in irrigated areas [61]. Therefore, the ability to predict irrigation water quality makes it easier to suggest suitable agricultural water management practices to mitigate negative effects, such as the following:

- Preventive irrigation practices, such as the application of leaching fractions and suitably designed subsurface drainage systems [62,63];

- Optimized irrigation timing to maintain favorable soil moisture levels [64,65];

- Management of fertilizers to prevent excessive nutrient application rates, which contribute to soluble salt accumulation [66];

- Selection of salt-tolerant crops [67];

- Precision irrigation technologies, such as variable rate irrigation (VRI) to increase irrigation uniformity and efficiency [68];

- Application of soil chemical amendments, e. g., gypsum, for sodicity control, facilitating the removal of Na ions and their replacement with Ca in the soil exchange complex [61,67].

4. Conclusions

The results in this study indicate that in small-scale hydro-agricultural irrigation systems, changes in irrigation water quality parameters within the conveyance network are not substantial and the water quality monitoring scheme can be focused on the reservoir, although safeguarding temporal scales that attend to the occurrence of extreme meteorological events and disruption of the regular trends typical of Mediterranean climate.

The dynamics of water quality for irrigation are linked to climate patterns. Dry weather during the crop growth cycle, corresponding to the irrigation campaigns, can exacerbate salinity and sodicity problems.

The RF and GB models show good predictive capability of water quality based on ion concentrations and meteorological data, with the RF model presenting, globally, better performance metrics in our study.

In agricultural water management under drought conditions, the application of ML algorithms to predict irrigation water quality based on chemical and meteorological variables can be a significant advancement, particularly in the implementation of early warning systems and the adoption of preventive measures to maintain soil health and crop yields.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/w17121783/s1> (containing Tables S1, S2, S3, and S4). Table S1. FAO guidelines for interpretation of water quality for irrigation (Ayers and Westcot 1985 [40]); Table S2. Irrigation water quality evaluation according to the FAO Guidelines—2018; Table S3. Irrigation water quality evaluation according to the FAO Guidelines—2019; Table S4. Irrigation water quality evaluation according to the FAO Guidelines—2020.

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