Prediction of the daily spatial variation of stem water potential in cherry orchards using weather and Sentinel-2 data

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15 Abstract

16 The common practice for irrigation management is to apply the water lost by evapotranspiration. 17 However, we could manage the irrigation by monitoring the plant's water status by measuring the 18 stem water potential (Ψ s), which is currently costly and time-consuming. The primary goal of this 19 work is to predict the daily spatial variation of Ψ s using machine learning models. We measured Ψ s 20 in two orchards planted with sweet cherry tree variety Regina, and we monitored 30 trees weekly 21 and biweekly in the central part of Chile, during two seasons, 2022-2023 and 2023-2024, and 22 between October and April. To predict the Ψ s, we used the random forest (RF), extreme gradient 23 boosting (XGBoost), and support vector machine (SVM) models. We selected vapor pressure deficit 24 (VPD), reference evapotranspiration (ETO), relative humidity, and temperature as weather 25 predictors. Also, we used as predictors spectral vegetation indices (VIs) and biophysical parameters 26 derived from Sentinel-2. We compared two schemes, one for estimation and another for prediction. 27 We discovered that XGboost and RF worked best for both. The estimation had an R2 of 0.76 and an 28 RMSE of 0.24 MPa. The prediction, on the other hand, had an R2 of 0.59 and an RMSE of 0.36 MPa. 29 The analysis of importance variables reveals that weather predictors, such as VPD, ETO, and 30 temperature, have a higher weight in the model. These are followed by VIs that use short-wave 31 infrared regions, which highlight the moisture stress index (MSI) and the disease and water stress 32 index (DWSI).

33

34 1. Introduction

35 Climate change is increasingly recognized as a major driver of global water scarcity, exacerbating 36 drought conditions and challenging water resources worldwide (Masson-Delmotte et al., 2021). This 37 phenomenon has heightened concerns about agricultural sustainability and food security (Molotoks 38 et al., 2021), as the agricultural sector is particularly vulnerable to changes in precipitation patterns 39 and rising temperatures (Fernández et al., 2023; Zambrano et al., 2016). In recent years, the central 40 and northern regions of Chile have experienced severe reductions in water availability (Garreaud et 41 al., 2017; Zambrano et al., 2024), with profound implications for agricultural productivity 42 (Zambrano, 2023). The ongoing drought in Chile has intensified the need for efficient water use in 43 agriculture (Zúñiga et al., 2021), particularly in fruit orchards, which are highly dependent on 44 consistent and adequate irrigation to maintain productivity and quality (Liu et al., 2023; 45 Vicente-Serrano et al., 2020). Efficient water management is thus crucial not only for reducing water 46 consumption, but also for optimizing plant health and maximizing yields under water-limited 47 conditions (D'Odorico et al., 2020). This, in turn, aids in our adaptation to a changing climate where 48 water resources are limited in certain areas.

49 To ensure efficient irrigation, the plant must replenish both the water lost through transpiration and 50 the moisture removed from the soil by weather conditions, a process known as evapotranspiration 51 (ET) (Allen et al., 1998). However, calculating ET in the field can be challenging. Two of the most 52 precise methods are eddy covariance stations or water balances (Denager et al., 2020), which are 53 costly and thus not used by the average farmer. In consequence, the ET is generally estimated by 54 calculating the reference evapotranspiration (ETO), also known as atmospheric evaporative demand 55 (Shirmohammadi-Aliakbarkhani and Saberali, 2020). ETO can be roughly estimated from pan 56 evaporation measuring the water loss, but the most common methods rely on meteorological data. 57 The Food And Agriculture Organization (FAO) Penman-Monteith method is recommended as the 58 standard for calculating ETO when sufficient weather data is available (Allen et al., 1998). When only 59 temperature data is accessible, the Hargreaves-Samani method (Hargreaves and Samani, 1985) has 60 shown good performance compared to the FAO Penman-Monteith method (Vicente-Serrano et al., 61 2007). Once the ETO is calculated, it must be adjusted to ET by multiplying it by the crop coefficient 62 (K_c), which varies depending on the crop type, growth stage, and condition, with tabulated values 63 available (Allen et al., 1998). Despite their widespread use, these methods often lack spatial 64 precision and may not account for variations in soil and plant water status across different orchard 65 blocks, potentially leading to over- or under-irrigation (Jones, 2004). Furthermore, relying on 66 generalized crop coefficients might not adequately capture the dynamic water needs of trees under 67 varying environmental conditions, underscoring the need for more site-specific irrigation strategies.

68 To optimize irrigation, some studies have used regulated deficit irrigation (RDI), which consists of 69 subjecting the plant to levels of water stress in different phenological stages (Yang et al., 2022). We 70 can accomplish this by recovering by irrigation a portion of the ET that the plant has lost. To ensure 71 good production and quality, irrigation typically recovers 100% of ET. Using RDI, we assess how the 72 plan reacts physiologically and in terms of production and quality during specific phenological stages 73 (Vélez-Sánchez et al., 2021). Alternatively, we could apply RDI and manage the irrigation based on 74 the plant's response. For this, we can measure the plant's water potential (Corell et al., 2020). The 75 water potential has been widely recognized as a reliable indicator of plant water status and a 76 valuable tool for guiding irrigation decisions (Moriana et al., 2012; Naor, 2000). The solute 77 concentration and water pressure in the leaf or stem directly show the water tension inside the 78 plant, which is also called water potential. The water potential reflects the impact of soil water 79 content, atmospheric water demand, and the plant's physiological responses (García-Tejera et al., 80 2021). Typically, we measure the water potential on the leaf, known as the leaf water potential, and 81 on the stem, known as the stem water potential. In the latter case, the leaf is put into a plastic bag 82 and sealed with the aim that the leaf potential equilibrates with the water potential of the stem 83 (Levin, 2019). The water potential usually is taken at different times during the day; when the 84 measure is made around 12:00-14:00, it corresponds to midday stem water potential (Ψ_s). This 85 range time corresponds to the maximum evaporative demand; thus, the Ψ_s tried to capture the 86 water status of the plant at the highest stress time. This measurement has demonstrated 87 consistency and reliability across various species (Carrasco-Benavides et al., 2022; Garofalo et al., 88 2023; Moriana et al., 2012). The Ψ_s vary during the season according to environmental factors and 89 the irrigation applied, which reflects the plant water status. The major drawback of measuring Ψ_s , is 90 that traditional methods, such as using a pressure chamber (Scholander et al., 1964), are 91 labor-intensive, time-consuming, and not suitable for continuous monitoring or large-scale 92 application (Jones, 2004).

93 New developments in remote sensing and modeling have made it possible to indirectly estimate Ψ_s 94 by combining spectral and weather data with machine learning methods. This provides a scalable 95 solution for managing irrigation in real time (Carrasco-Benavides et al., 2022; Garofalo et al., 2023; 96 Savchik et al., 2024). Savchik et al. (2024) predicted Ψ_s in almond orchards, using ET, soil moisture, 97 and spectral reflectance from unmanned aerial vehicles (UAV). They used the machine learning 98 algorithms of random forests and neural networks. They reached R² values ranging from 0.33 to 0.73 99 and a root mean square error (RMSE) between 3.31 and 2.5 bars. In Italy, in an orchard of olives, 100 Garofalo et al. (2023) used random forests to estimate $\Psi_{\rm s}$ based on vegetation indices derived from 101 spectral data from PlanetScope imagery, reaching an R^2 of 0.78. However, when used to predict in an 102 independent year, the results decreased significantly. Carrasco-Benavides et al. (2022) used infrared 103 thermal imagery from UAV and derived the crop water stress index (CWSI). They used artificial 104 neural networks to estimate Ψ_s in cherry-tree variety Regina. The test data produced a Pearson 105 correlation value of 0.83, but the absence of independent selection may have inflated the values. 106 These technologies provide the potential to enhance decision-making processes by enabling more 107 precise and timely irrigation interventions based on the actual water needs of the crop. Remote 108 sensing technologies have emerged as powerful tools for enhancing irrigation management by 109 providing spatially detailed information on crop water status and variability across large areas 110 (Zarco-Tejada et al., 2003). Sentinel-2 (S2), with its high spatial resolution and frequent revisit times, 111 offers the ability to monitor vegetation by spectral indices, canopy cover, and thermal status, which 112 are proxies of plant water stress (Addabbo et al., 2016; Jamshidi et al., 2021; Zhang et al., 2017). 113 These indices, derived from multispectral imagery, can be used to assess crop water needs and 114 optimize irrigation schedules more accurately than traditional methods. By integrating remote 115 sensing data with weather and soil moisture measurements, it is possible to develop advanced 116 irrigation management systems that respond dynamically to the actual water status of the crop, 117 improving water use efficiency and crop performance (Baluja et al., 2012).

118 In this study, we aim to investigate the potential of using S2 and weather data to predict the daily 119 spatial variation of Ψ_s in cherry orchards. To achieve this, we define three specific goals: i) to derive 120 daily spatial predictors from S2 and weather stations; ii) to train and evaluate three machine 121 learning models; and iii) to evaluate the spatio-temporal variation of estimated Ψ_s for monitoring 122 irrigation. For this, we use satellite S2 (A/B) and weather data to derive multiple predictors. 123 Following, we evaluate three machine learning algorithms: random forest (RF), extreme gradient 124 boosting (XGBoost), and support vector machines (SVM). We use two splitting strategies, 125 considering time and space, to obtain training and testing datasets. On the training dataset, we tune 126 the model's parameters, evaluate the models using resampling, and subsequently, we run them on 127 the testing dataset. Finally, we use the best-performing model to estimate and evaluate the daily 128 spatial variation of Ψ_s .

129 2. Materials and Methods

130 2.1. Study Area



132 Figure 1. Study Area. The map on the left shows the orchards' location in Chile's central region. The maps on the right **133** display the orchards in (a) Rio Claro and (b) La Esperanza, and (c) and (d) represent the irrigation treatments (T0, T1, T2, T3, **134** T4). The red and blue dots represent the experimental trees selected for the 2022-2023 and 2023-2024 seasons, **135** respectively, while the yellow dots indicate the trees selected for both seasons.

136 We conducted the study in two commercial orchards of sweet cherry trees (*Prunus avium* L., variety 137 Regina) from the company Garces Fruit (www.garcesfruit.com) in the O'Higgins region of central 138 Chile. The orchards are *Rio Claro*, having 60 ha and 9 year-olds, and *La Esperanza*, with 40 ha and 6 139 year-olds (Fig. 1a and 1b). The study took place during the irrigation seasons 2022–2023 and 140 2023–2024, which run from October to April. In *Rio Claro*, the soil has a sandy loam texture with low 141 moisture retention, whereas in La Esperanza, the field is located on clayey soil with high moisture 142 retention. For the two orchards in both seasons, full bloom occurred in October. The harvest in *Rio* 143 *Claro* was on December 23rd, 2022, and January 3rd, 2024, and in *La Esperanza* on December 12th, 144 for both seasons.

145 The climate of the region is mediterranean (Csb) (Beck et al., 2018) with moderate rainfall and an 146 annual precipitation ranging from 200 to 500 mm year⁻¹ in the past 10 years, concentrated in winter, 147 with a prolonged dry season of 7 to 8 months (DMC, 2024). Each orchard has a private weather 148 station nearby, located 0.6 km from the center in Rio Claro and 1.4 km from the center in La 149 Esperanza, respectively.

150 2.2. Deficit Irrigation

151 The local producer's irrigation in both orchards involves drip irrigation with two lines per row, 152 operating from October to April (spring–summer) and halting during the winter dormancy period. In 153 order to enhance the variability of plant water status, we implemented five different irrigation 154 repositioning treatments in each orchard. To manage the irrigation amount, we used the ETO and Ψ_s 155 as references. Thus, we have T1, T2, T3, and T4 irrigation treatments, with T1 being the least 156 restrictive and T4 the most restrictive regarding water supply (Fig. 1c and 1d). We also have a 157 control treatment (T0) that receives standard irrigation from the local producer. Each treatment plot 158 contained 60 trees and covered 0.048 ha. We applied the treatments during the consecutive 159 growing seasons of 2022–2023 and 2023–2024. However, we did not irrigate treatments T1 to T4 in 160 *La Esperanza* during the second season, as the previous season's results did not demonstrate any 161 significant impact from the water restriction treatments. Table 1 shows the total volume of 162 reference water demand (ET0), the total volume of water applied by the local producer in the 163 control treatment (T0), and the total volume applied in deficit irrigation treatments, while Fig. 2 164 illustrates the cumulative water depth (mm) for each treatment during irrigation, and the 165 percentage relative to ET0.

166 Table 1. Total volume of reference evapotranspiration (ETO) and the volume of water applied in treatments for each **167** orchard during the 2022-2023 and 2023-2024 seasons.

	Total volume of water (m ³ ha ⁻¹)			
Treatment	Rio Claro		La Esperanza	
	2022-2023	2023-2024	2022-2023	2023-2024
ET0	6,178	6,233	8,119	8,056
Т0	5,128	4,066	3,840	3,740
T1	3,749	1,958	2,350	46
T2	2,937	1,333	1,504	25
Т3	2,083	979	875	16
T4	1,312	625	456	46



169 Figure 2. Variation of daily cumulative water depth (mm) applied by irrigation per treatment in comparison with reference **170** evapotranspiration (ET0). The starting point for the accumulation of ET0 corresponds to the first day of irrigation for each **171** orchard and season.

172 2.3. Data

173 2.3.1. In-situ midday stem water potential

174 Ψ_s was measured using a Scholander (Scholander et al., 1964) pressure chamber (Model 3000, Soil 175 Moisture Equipment, Santa Barbara, CA, USA) connected to a nitrogen cylinder, following the 176 procedures described by Turner (1981). Measurements were performed on mature leaves from the 177 middle to the upper part of the tree on the north-facing side. We selected three trees per treatment 178 in each orchard. One leaf per tree was sampled, totaling 15 measurements per orchard. In order to 179 equilibrate the leaf water potential with the Ψ s, leaves were wrapped in aluminum foil bags at least 180 one hour before measurement. These measurements were conducted weekly between 12:00 and 181 14:00 h during both seasons, resulting in total measurement counts of 412 for Rio Claro (212 for 182 2022-2023; 200 for 2023-2024) and 486 for La Esperanza (176 for 2022-2023; 310 for 2023-2024).

183 2.3.2. Sentinel-2

184 S2 mission consists of two identical satellites, S2A and S2B, both equipped with a multispectral 185 sensor featuring 13 spectral bands covering visible, near-infrared, and shortwave infrared regions, 186 with spatial resolutions of 10, 20, and 60m (see Table S2). In this study, we utilized a total of 106 S2 187 (A/B) images, 54 for the 2022-2023 and 52 for the 2023-2024 season, captured between October 188 and May in both orchards, tiles T19HCB for *La Esperanza* and T19HBB for *Río Claro*. The images were 189 obtained from the atmospherically corrected S2 Level-2A collection from Planetary Computer 190 (Microsoft Open Source et al., 2022), with a frequency of 5 days, at approximately 14:30 local time 191 (UTC-4). A mask was applied based on the Scene Classification Layer (SCL) for values corresponding 192 to "Cloud Shadows," "Cloud Medium Probability," and "Cloud High Probability," respectively.

193 2.4. Deriving spatio-temporal predictors

194 2.4.1. In-situ weather variables

195 The automatic weather stations within both orchards recorded data on weather variables utilizing 196 the ATMOS-41 model of METER group. These stations provided measurements of multiple 197 meteorological variables every 15 minutes. We selected five meteorological variables that may 198 affect water availability and plant physiological functionality: temperature (T°), relative humidity 199 (RH), vapor pressure deficit (VPD), precipitation (PP), and reference evapotranspiration (ETO) (Fig. 3). 200 We summed the precipitation and averaged the other variables daily.



Figure 3. Time series of weather variables at the orchard sites *Rio Claro* and *La Esperanza* and the seasons 2022-2023 and 203 2023-2024. Vertical dashed lines indicate the harvest date for each orchard and season.

204 2.4.2. Vegetation indices derived from Sentinel-2

205 Sixteen VIs related to plant condition—vigor, stress, photosynthetic functionality, and water 206 content—were derived from S2 data, as shown in Table 2. Nine indices do not include red-edge 207 information, originating solely from the visible, NIR, and SWIR wavelength bands: NDVI, EVI, GCI, 208 NDWI, NBR, NDMI, MSI, NMDI and DWSI. In contrast, seven indices—CLr, Clg, NDRE1, NDRE2, NDCI, 209 mSR705, and RESI—were derived from red-edge information. The indices were calculated from the 210 preprocessed images of S2 bands, obtaining time series for each VI across both orchards and 211 seasons.

212 We applied a smoothing process using local polynomial regression (LOESS) (Cleveland, 1979) to 213 reconstruct the time series (e.g., masked cause of cloudiness) of VIs. The LOESS was implemented 214 with a smoothing parameter (span) set to 0.3. As a result, a smooth, continuous daily predicted 215 series for each index was obtained and then extracted for every measured tree. A correlation 216 analysis was performed to evaluate the relationship between these smooth series and the observed 217 Ψ_s (see Fig. S2). The Pearson correlation coefficient (r) was calculated across the trees for each day, 218 orchard and season, and only daily significant correlations (p-value < 0.05) were used to compute a 219 mean.

220 2.4.3. Biophysical parameters estimated from Sentinel-2

The Sentinel Application Platform (SNAP) is an integrated development environment (IDE) created the European Space Agency (ESA, 2024) for analyzing and processing satellite data. SNAP provides a versatile suite of tools and functionalities for handling data from various Sentinel and missions, including a biophysical parameter algorithm. This algorithm consists of two key components: (1) a radiative transfer model that inverts radiative properties from S2's multispectral imagery to retrieve vegetation parameters, and (2) a neural network model that further refines these parameters using empirical data. By applying these models and empirical relationships, SNAP extracts detailed information about the vegetation's physiological status (Weiss et al., 2020).

229 Using SNAP, we calculated various biophysical parameters, including LAI—leaf area index; 230 FAPAR—fraction of absorbed photosynthetically active radiation; FVC—fraction of vegetation cover; 231 CCC—canopy chlorophyll content; and CWC—canopy water content. These parameters were 232 processed at 20 m for both seasons and orchard sites, and the same smoothing process used for 233 reconstructing the time series of VIs was applied. The resulting biophysical parameters were used as 234 predictors for modeling Ψ_{sr} along with the VIs and weather data (Table 2).

Table 2. Predictor variables for Ψ_s modeling. Weather variables from automatic stations (15 min frequency): T (°C), RH (%), (%), WPD (mbar), PP (mm), ETO (mm). Vegetation indices (VIs) derived from Sentinel-2 bands (10 m resolution) and biophysical parameters from SNAP (20 m resolution), both at 5-day intervals. B2 to B12 refer to Sentinel-2 MSI band reflectance.

Classification	Name	Description	Algorithm/Formula	Reference	
Weather variables	Т	Temperature			
	RH	Relative Humidity			
	VPD	Vapor Pressure Deficit	e ^s -e ^a	Allen et al. (1998)	
	РР	Precipitation			
	ET0	Reference Evapotranspiration	FAO-Penman-Monteith	Allen et al. (1998)	
	NDVI	Normalized Difference Vegetation Index	$\frac{B8-B4}{B8+B4}$	Rouse et al. (1974)	
	EVI	Enhanced Vegetation index	$\frac{2.5 \cdot (B8 - B4)}{(B8 + 6 \cdot B4 - 7.5 \cdot B2 + 1)}$	Huete et al. (2002)	
	GCI	Green Coverage Index	$\frac{B9}{B3} - 1$	Gitelson et al. (2003)	
	NBR	Normalized Burn Ratio	$\frac{B8 - B12}{B8 + B12}$	García and Caselles (1991)	
	NDWI	Normalized Difference Water Index	$\frac{B3 - B8}{B3 + B8}$	McFeeters (1996)	
	NDMI	Normalized Difference Moisture Index	$\frac{B8 - B11}{B8 + B11}$	Gao (1996)	
	MSI	Moisture Stress Index	<u>B11</u> B8	Huntjr and Rock (1989)	
Vagatation indicas	NMDI	Normalized Multi-band Drought Index	$\frac{B8 - (B11 - B12)}{B8 + (B11 - B12)}$	Wang and Qu (2007)	
Vegetation indices	DWSI	Disease and Water Stress Index	$\frac{B8+B3}{B11+B4}$	Apan et al. (2004)	
	Clr	Red Edge Chlorophyll	$\frac{B7}{B5} - 1$	Gitelson et al. (2003)	
	Clg	Green Chlorophyll Index	$\frac{B7}{B3} - 1$		
	NDRE1	Normal Deviation Index of the Red Edge 1	$\frac{B6 - B5}{B6 + B5}$	Sims and Gamon (2002)	
	NDRE2	Normal Deviation Index of the Red Edge 2	$\frac{B8-B5}{B8+B5}$	Barnes et al. (2000)	
	NDCI	Normalized Difference Chlorophyll Index	$\frac{B5 - B4}{B5 + B4}$	Mishra and Mishra (2012)	
	mSR705	Red Edge modified Simple Ratio	$\frac{(B6/B5) - 1}{\sqrt{(B6/B5) + 1}}$	Wu et al. (2008)	
	RESI	Red Edge Spectral Index	$\frac{B7 + B6 - B5}{B7 + B6 + B5}$	Xiao et al. (2020)	

Classification	Name	Description	Algorithm/Formula	Reference
Biophysical parameters	LAI	Leaf Area Index	PROSPECT + SAIL coupled model Baret and Bu	Marie Weiss et al. (2020)
	fAPAR	Fraction of Absorbed Photosynthetically Active Radiation		
	FVC	Fraction of Vegetation Cover		Baret and Buis (2008)
	CCC	Canopy Chlorophyll Content		
	CWC	Canopy Water Content		

238 2.6. Modeling the daily spatial $\Psi_{ m s}$

239 2.6.1. Machine learning models (ML)

240 For Ψ_s modeling, we tested three machine learning algorithms (ML) : 1) Extreme Gradient Boosting 241 (XGBoost; Chen and Guestrin, 2016); 2) Random Forest (RF; Ho, 1995); and 3) Support Vector 242 Machine (SVM; Cortes and Vapnik, 1995). The first two methods utilize decision trees, while the 243 latter employs support vectors. We selected these models because they are state-of-the-art, require 244 few training samples (compared to neural networks), and are interpretable. These ML algorithms 245 can be used for both classification and regression. We carried out a regression analysis, using the Ψ_s 246 as the outcome and using 26 predictors: five of weather, 16 VIs, and five biophysical parameters 247 (Table 2). We used 26 dates from seasons 2022–2023 and 34 from 2023–2024, totaling 60 dates. For 248 each date, we take 30 measurements, 15 per orchard (*Río Claro* and *La Esperanza*). Thus, the 249 complete dataset has 883 observations. For the modeling process, we proceed as follows: i) prepare 250 and split the dataset into training and testing; ii) use the training dataset to adjust the algorithms' 251 parameters by hyperparameter optimization; iii) resampling to account for reliability and recognize 252 the most relevant variables to estimate Ψ_s , and iv) evaluate the model to gather the performance.



253

254 Figure 4. Split schemes used for grouping in training and testing datasets for the random split (rnd_split) and the **255** independent time split (ind split).

256 We trained the three models using two splitting schemes (Fig. 4), one in which we considered a 257 random split taking testing and training data randomly (*rnd_split*) and a second one in which we 258 used independent dates for training and testing (*tme_split*). We chose 75% of the data for training 259 and 25% for testing in both cases. We used three types of feature engineering on the training data: 260 i) we removed the predictors whose values remain constant by removing the zero-variance 261 variables; ii) we normalized the predictors as they have a mean of zero and a standard deviation of 262 one; and iii) we tested a model version that used partial least squares (PLS) (Wold, 1966) to cut 263 down on the number of dimensions and used the five principal components as predictors. As a 264 result, we used models with normalized predictors and others with the five principal components265 estimated by PLS.

266 To adjust the parameters of the models (XGBoost, RF, SVM) we used hyperparameter optimization. 267 We start by setting each parameter's range (Table 3). We used five folds for resampling for both 268 splitting schemes (rnd_splt and tme_splt). The hyperparameter optimization used a set of ten 269 combinations of parameters per model. To evaluate the performance of the models, we used the 270 metrics R², root-mean-square error (RMSE), and mean absolute error (MAE). Finally, we ranked the 271 models based on the RMSE and R², selecting the models with the lowest RMSE and higher R².

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Table 3. Range of initial values for the parameters adjusted in the tuning process for the models Extreme Gradient Boosting (XGBoost), Random Forest (RF), and Support Vector Machines (SVM).

Model	Parameter description	Identifier	Range
XGBoost and Random Forest	The number of trees contained in a random forest or boosted ensemble	trees	1000
	Number of randomly sampled predictors	mtry	1 - 28
	The minimum number of data points in a node that is required for the node to be split further	n_min	2 - 40
XGBoost	The maximum depth of the tree	tree_depth	1 - 15
	Learning rate	learn_rate	-30.5
	The reduction in the loss function required to split further	gamma	-10 - 1.5
	The size of the data set used for modeling within an iteration of the modeling algorithm	sample_size	0.1 - 1
Support Vector Machines	Regularization parameter	cost	-10 - 5
	Radial basis function sigma	rbf_sigma	-10 - 0

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276 2.6.3. Evaluation and variable importance for the models

277 To evaluate the performance of the models, we used resampling over the training dataset for both
278 splitting schemes (*rnd_split* and *tme_split*). We selected five folds, and calculated the metrics R²,
279 MAE, and RMSE for each fold.

To estimate the variable importance of each predictor on the model's performance, RF employs an 281 out-of-bag permutation method in each tree, permuting over the predictors, and calculates the 282 mean-square-error for each instance. For XGBoost, we estimate the fractional contribution of each 283 feature to the model based on the total gain of the corresponding feature's splits. In the case of 284 SVM, we compute permutation-based variable importance scores for the predictors (for more 285 detail, see Greenwell and Boehmke, 2020).

286 2.7. Spatio-temporal variation of estimated $\Psi_{ m s}$

To estimate the daily spatial variation in the orchards of *Rio Claro* and *La Esperanza*, we selected the best-performing model from those generated with the random split (*rnd_split*). This was done for all the days within each season. To analyze the spatial variation, we identified the days with the highest coefficient of variation. To assess the temporal variation we averaged the Ψ_s within each irrigation 291 treatment and compared the difference between them for the two seasons. Also, using boxplot 292 graphs, we compared the monthly distribution of values of Ψ_s for the five treatments.

293 2.8. Software

For downloading, processing, analyzing spatio-temporal data, and machine learning modeling, we used the R programming language for statistical computing and graphics (R Core Team, 2022). We used the data available in Planetary Computer (Microsoft Open Source et al., 2022), which we arcessed via the {rstac} package (Simoes et al., 2021). Preprocessing tasks, such as applying cloud coverage masks and cropping to the orchard plots, were performed using {gdalcubes} (Appel et al., 299 2021). For processing raster data, we used {terra} (Hijmans, 2024). To manage vectorial data, we used {sf} (Pebesma, 2018). For mapping, we used {tmap} (Tennekes, 2018). For data analysis and visualization, the suite {tidyverse} (Wickham et al., 2019) was used. For the machine learning 202 modeling, we used the {tidymodels} (Kuhn and Wickham, 2020), {workflowsets} (Kuhn and Couch, 303 2024), {recipes} (Kuhn et al., 2024), {ranger} (Wright and Ziegler, 2017), {xgboost} (Chen et al., 2024), 304 and {kernlab} (Karatzoglou et al., 2004) packages.

305 4. Results

306 4.1. Predictors and their relation to Ψ s

307 4.1.2. Smoothing of Sentinel-2 derived indicators

308 Fig. 5 shows the raw and smoothed-interpolated values of the most important satellite indicators in 309 the model's performance for a representative tree across both seasons and orchard sites. The values 310 of the indices indicate variations in behavior throughout the various growing seasons. In both 311 orchards, CCC, DWSI, mSR705, and NDMI increase during leaf expansion and higher water demand 312 months (summer), peaking around or shortly after harvest dates between Jan-Mar and decreasing 313 with leaf loss in Mar-Abr. In contrast, MSI exhibits opposite seasonal variability, reaching its lowest 314 point after the harvest dates. NMDI shows unique behavior, with a tendency to decrease in the 315 summer but with variable peaks throughout most months. The resulting series reveals a difference 316 in magnitudes between the two orchards, with *La Esperanza* exhibiting higher values compared to 317 *Rio Claro*, except for MSI, in which the behavior is opposite. Regarding both seasons, there are 318 similarities in magnitude and variability, except for a sudden peak in *La Esperanza* during the second 319 season between Jan-Mar and for NMDI in general.



320

321 Figure 5. Time series of raw and smoothed-interpolated Sentinel-2 derived indicators most important to the model's **322** performance at both orchard sites and seasons. Red points and lines correspond to Río Claro, while blue represents La **323** Esperanza. Vertical dashed lines indicate the harvest dates for each orchard and season.

324 4.1.3. Correlation between predictors and Ψ_{s}

325 Table 4 presents the Pearson correlation coefficients between the daily mean values of each 326 weather variable and the observed daily mean Ψ_s . The results indicate that ETO, VPD, and T are 327 negatively correlated with Ψ_s , while RH shows a positive correlation, and PP only exhibits weak 328 correlations ranging between 0.1 and -0.1 for both sites during the 2022-2023 season. ETO 329 demonstrates a strong correlation (r \leq -0.7) at *La Esperanza* in both seasons, but not at *Río Claro*. In 330 contrast, VPD, T, and RH generally exhibit strong correlations in most cases.

	Pearson correlation coefficient (r)			
Variable	Rio Claro		La Esperanza	
	2022-2023	2023-2024	2022-2023	2023-2024
ET0	-0.38	0	-0.77	-0.86
VPD	-0.75	-0.39	-0.66	-0.89
т	-0.8	-0.45	-0.81	-0.88
RH	0.75	0.43	0.53	0.83
РР	0.11		-0.1	

331 Table 4. Pearson correlation coefficient (r) between daily weather data and daily observed Ψ_s (MPa).

332 Regarding S2 derived predictors, Table 5 presents the mean of daily significant Pearson correlation 333 coefficients (r; $p \le 0.05$) between these predictors and the observed Ψ_s (MPa) for the 15 trees at 334 both orchard sites and seasons. The results reflect differences between indices with positive and 335 negative correlations, consistent with the seasonal behavior of these shown in Fig. 5. For CCC, DWSI, 336 mSR705, and NDMI, the mean correlations were positive and moderate (≥ 0.5) in all cases except 337 for *La Esperanza* season 2023-2024, where CCC exhibited both positive and negative correlations on 338 different days (Table 5). The same situation occurs with NMDI, which, along with MSI, averaged 339 negative and moderate correlations (≤ -0.5) in all cases except for this specific group, where NMDI 340 showed a positive correlation. Regarding the seasons, more significant correlations were found in 341 the first season than in the second. In terms of orchards, more significant correlations were 342 observed in *Río Claro* compared to *La Esperanza*.

Orchard site	Season	Variable	r ± sd	n
Rio Claro	2022 2022	ССС	0.69 ± 0.11	5
		MSI	-0.66 ± 0.13	5
		DWSI	0.65 ± 0.12	4
	2022-2023	mSR705	0.69 ± 0.13	9
		NDMI	0.66 ± 0.13	5
		NMDI	-0.69 ± 0.1	6
	2023-2024	ССС	0.66 ± 0.01	2
		mSR705	0.63 ± 0.04	2
		NMDI	-0.55	1
La Esperanza	2022-2023	MSI	-0.59	1
		DWSI	0.61	1
		mSR705	0.52	1
		NDMI	0.59	1
	2023-2024	CCC*	0.03*± 0.88	2*
		NMDI	0.54	1

343 Table 5. Mean of daily significant Pearson correlation coefficients (r) between Sentinel-2 derived predictors and observed **344** Ψ_s (MPa) for the 15 trees across both orchard sites and seasons. n denotes the number of daily significant r obtained.

345 4.3. Modeling the daily spatial Ψ s

346 4.3.1. Evaluation and variable importance of the models

Fig. 6 displays the R² ranking for each of the twelve different models trained with resampling (three all algorithms, two splittings, and with or without partial least squares). Using the RMSE metric, the ranking behaves equally. With *rnd_split*, the R² range is 0.45 to 0.8, and with *tme_split*, it decreases to a range of 0.25 to 0.52. In the case of *rnd_split*, XGBoost and RF reached the highest R² with a mean of 0.77 and 0.76, respectively, followed by SVM with a R² of 0.68. On the *tme_split*, the R² difference between models is minor in comparison to those trained on the *rnd_split*. The three models that reached the maximum R² on *tme_split* are XGBoost, pls_SVM (trained with the five principal components obtained from the partial least squares analysis as predictors), and SVM, store around 0.45. We selected the three models that reached the highest performance in the store around per splitting scheme, hereafter named RF, XGBoost, and SVM.



Model - pls_RF - pls_SVM - pls_XGBoost - RF - SVM - XGBoost

357

358 Figure 6. Ranking of machine learning models in the resampling according to the R² metric. The models are Random forest **359** (RF), extreme gradient boosting (XGBoost), and support vector machines (SVM). The "pls" acronym beside the model name **360** stands for partial least squares. Each panel corresponds to a splitting scheme: a random split (*rnd_split*) and a **361** time-independent split (*tme_split*).

362

363 Fig. 7 shows the eleven most important variables in the model's performance. In the two splitting 364 schemes, the meteorological data, specifically ETO, VPD, and temperature, hold the highest 365 importance and reach their maximum weight. In SVM, RH is the only predictor in the *rnd_split*, and 366 RH, VPD, and temperature are the predictors with higher importance in the *tme_split*. The 367 S2-derived predictors came in second place after meteorological data. In the *rnd_split*, MSI, DWSI, 368 mSR705, NDMI, and NMDI are the most relevant predictors for RF and XGBoost. When considering 369 the *tme_split*, the MSI, DWSI, and NDMI are the most contributing variables to the model's 370 performance. In the case of the SVM model for *tme_split*, the biophysical parameter CCC holds the 371 highest importance. As expected, the S2 predictors that were more closely related to Ψ_s were those 372 using the SWIR wavelength, which is the spectral region more sensitive to water.

373



375 **Figure 7.** Scaled variable importance (0–1) per machine learning models: random forest (RF), extreme gradient boosting 376 (XGBoost), and support vector machines (SVM); for the two splitting schemes: random split (*rnd_split*) and time 377 independent split (*tme_split*).

After the resampling evaluation, we trained the models on the testing dataset. In the *rnd_split*, the 379 R² was 0.76, 0.76, and 0.62 for XGBoost, RF, and SVM, respectively (Fig. 8). The RMSE was between 380 0.24 MPa (XGBoost and RF) and 0.3 MPa (SVM). In the *rnd_split*, RF and XGBoost improve 381 significantly over SVM. When trained in the *tme_split*, the model's performance decreases in 382 comparison to those trained with *rnd_split*. Between them the models behave equally, with an R² of 383 0.59 for the three models. The RMSE was found to be between 0.36 MPa for XGBoost and 0.39 MPa 384 for SVM. In Fig. 8, it can be seen that the error (observed minus estimated) increases for values 385 lower than -1.5 MPa, corresponding to fewer points. Thus, the models do not have enough data to 386 allow them to increase their performance. The reason for the fewer data in this range is that it 387 corresponds to higher water stress levels. Critical stress can lead to plant stomatal closure, which 388 can impact both production and quality.



389

Figure 8. Predicted values into the testing dataset versus observed values of stem water potential (Ψ_s) for La **Sec. 1** Esperanza and Río Claro orchards. The vertical panels correspond to the machine learning model: random **Sec. 1** forest (RF), extreme gradient boosting (XGBoost), and support vector machines (SVM). The horizontal panels **Sec. 1** correspond to the splitting schemes: random split (rnd_split) and time-independent split (tme_split). The metrics **Sec. 1** of performance used are r-squared (R²), mean absolute error (MAE), and root mean squared error (RMSE).

395 4.4. Spatio-temporal variation of estimated $\Psi_{ m s}$

We used the XGBoost model trained over the *rnd_tme* (best-performing model) to estimate the 397 daily spatial variation of Ψ_s over the orchard sites. Figs. 9 and 10 show the spatial variation of Ψ_s for 398 the six dates that had the highest spatial variation (i.e., coefficient of variation) for the two orchard 399 sites. The major spatial variation occurred in December and early January, corresponding to the 400 higher water demand months (summer). The estimation of the whole orchard includes roads and 401 infrastructure (see Fig. 1), which the model detects as the ones with lower Ψ_s . Despite that, the 402 spatial estimation allows us to identify sectors with different plant water statuses. Figs. 9 and 10 403 show that in the Rio Claro orchard there is a higher spatial variation in comparison with La 404 Esperanza. In Rio Claro, from the center to the north-east, a sector persists with lower pressures 405 below -2 MPa. In La Esperanza, the response of Ψ_s is more uniform, with December 11th showing 406 major spatial variation. However, given that this date coincides with harvest days, other factors such 407 as the presence of people in the area could potentially influence the variation.



409

410 Figure 9. Midday stem water potential (Ψ_s) estimated by the extreme gradient boosting (XGBoost) model over the Río **411** Claro orchard. The days selected correspond to the six with the maximum coefficient of variation.



412

413 Figure 10. Midday stem water potential (Ψ_s) estimated by the extreme gradient boosting (XGBoost) model over the La **414** Esperanza orchard. The days selected correspond to the six with the maximum coefficient of variation. **415**

416 The averaged values of Ψ_s per treatment shown in Fig. 11 allow us to observe the temporal variation 417 of the plant water status through the irrigation season (October to April) and the difference 418 between treatments. The Ψ_s has been decreasing since October, reaching its lowest values between 419 December and February, and then increasing until April, in line with the plant's water demand. For 420 the two sites, the differences are most evident during the season 2022-2023 (Fig. 12), especially 421 from December to February. For 2023–2024, during November–December, the Ψ_s is higher in 422 comparison to the previous season, this could be due to the precipitation fall during those months. 423 The dispersion of values of Ψ_s is higher for October, November, and April, and it is tighter for the 424 summer months (December–February) (Fig. 12). Additionally, the disparity between the various 425 irrigation levels is more pronounced for the years 2022–2023, with a noticeable decrease in Ψ_s from 426 T0 to T4, particularly in November and December. This could be attributed to the harsher climatic 427 conditions during the first season, which included higher temperatures and less precipitation, 428 leading to increased stress on the orchards.



429

430 Figure 11. Averaged values of stem water potential (Ψ_s) estimated by the extreme gradient boosting model (XGBoost). The **431** lines are the smoothed series for the five irrigation treatments, the seasons 2022-2023 and 2023-2024, as well as the **432** orchards of Río Claro and La Esperanza.



434

435 Figure 12. Distribution of daily values of estimated stem water potential (Ψ_s) by the extreme gradient boosting model **436** (XGBoost) per month within the irrigation treatments for the seasons 2022-2023 and 2023-2024, as well as the orchards **437** Río Claro and La Esperanza.

438

439 5. Discussion

440 5.1. Sources of uncertainty in the models

441 Some of the major sources of error in the model's prediction are the spatial resolution of the S2 442 images (10/20 meters), the temporal reconstruction of the time series of vegetation predictors, and, 443 to a lesser extent, the null spatial representation of the weather data. The satellite passes over the 444 orchards near the time of the measurements, allowing for timely capture of the plant water status. 445 However, one S2 pixel covers approximately 12 trees. Then, the cover area takes into account cherry 446 canopy as well as background soil. Thus, the reflectance retrieved per pixel is a mixture of canopy 447 and soil. This problem could be faced by spatial fusion techniques of S2 with high-resolution images 448 (Dong et al., 2023; Galar et al., 2020) which will diminish the error due to this issue. Further, we 449 used a simple low pass filter to interpolate daily values of vegetation predictors, which is a 450 technique usually used for gap-filling in cloudy days (Mo et al., 2023), but not for interpolation. 451 When assessing vegetation development, this technique may prove more beneficial as the 452 physiological changes in development span more than a single day. However, the plant's water 453 status changes on an hourly basis. A better approach to estimating daily values is the 454 spatio-temporal fusion with Sentinel-3 (Wang and Atkinson, 2018) which takes into account the 455 spectral reflectance. However, in this instance, a machine learning model that utilizes all predictors 456 gathers temporal variation from weather data and spatial variability from S2 predictors. Therefore, 457 the model operates effectively when the interpolated S2 predictors sustain the spatial variation 458 related to plant water status. We test a different model that uses original spectral vegetation indices 459 as predictors and only fill gaps on cloudy dates, but the results decrease significantly for the 460 tme split (Figs. S4 and S5).

461 Because we have fewer measurements in the range of -1.75 to -2.5 MPa, our model performs poorly 462 for lower values of SWP. To increase the performance of the model, future studies should consider 463 collecting more points in this range. Other research that wasn't included in this article shows that 464 for this species, the turgor loss point, or the point at which the plant stomatal closure happens, is 465 less than -2 MPa. Therefore, if we intend to utilize this model for irrigation optimization, we must 466 accurately estimate the SWP within this range.

467 Another source of uncertainty is regarding the values of SWP on cloudy days. In this study, we only 468 take measurements on clear days. However, we use the LOESS to reconstruct the time series of 469 spectral vegetation indices. Thus, in future work we need to consider taking measurements on 470 cloudy days to evaluate the performance of the model on those days.

471 5.2. Sentinel-2 predictors most related to $\Psi_{ m s}$

472 The resulting S2 derived indices used as predictors for the model can be categorized based on their 473 behavior between November and February, which corresponds to the period of rising temperatures, 474 peak vegetative growth, and leaf expansion in cherry trees. Among the most significant of those 475 affecting the model's performance, were DWSI, mSR705, and NDMI increasing during this period. 476 Except for DWSI, these indices positively correlate with LAI, water and chlorophyll content in leaf 477 and vegetation expansion (Gitelson et al., 2006; Wu et al., 2008; Gao 1996), while DWSI increases in 478 summer due to higher temperatures and water stress (Apan et al., 2004). In contrast, MSI and NMDI 479 exhibit opposite seasonal variability. Some studies indicate that the MSI negatively correlates with 480 Equivalent Water Thickness (EWT) and positively with LAI, increasing as LAI decreases and remaining 481 lower during vegetative growth and leaf expansion (Huntjr and Rock, 1989). NMDI values rise in 482 response to decreasing soil moisture during the leaf dormancy stage, while during foliar expansion, 483 the values show minimal fluctuations according to variations in canopy water content (Wang and 484 Qu, 2007). 485 Between the two seasons, we observe an extension of the peaks and troughs of the index values 486 during the summer, indicating a prolongation of the period of vegetative growth and photosynthetic 487 activity in the second season. Overall, the behavior of these indices suggests that in both *Río Claro* 488 and *La Esperanza*, the trees are healthy, with high water and chlorophyll content and dense canopy 489 cover. However, these conditions are more pronounced in *La Esperanza* compared to *Río Claro*. In 490 relation to the two seasons, we observe an extension of the peaks and troughs of the values during 491 the second season, suggesting a delay in the productive period.

492 5.3. Comparison with other approaches

493 Some studies (Abrisqueta et al., 2015; Blanco et al., 2018) have correlated weather data, such as 494 VPD, with plant water status in tree crops, achieving R² values of 0.72 and 0.88, making it a reliable 495 indicator. The primary drawback is that stations that typically collect weather data lack spatial 496 variation. Seamlessly, in our case, the VPD, ETO, and temperature were the predictors with a higher 497 impact on the model's performance. The three predictors are interdependent, as VPD is dependent 498 on temperature, and ETO is also dependent on both VPD and temperature. To estimate the spatial 499 variation of $\Psi_{
m s}$, one of the most used techniques is the use of UAS (Unmanned Air System) and 500 thermal infrared imagery to derive the Crop Water Stress Index (CWSI). Thermal imagery (Alghory 501 and Yazar, 2019; Blanco et al., 2023; Carrasco-Benavides et al., 2022; Park et al., 2021) offers a 502 significant advantage due to its ability to capture high spatial resolution. Carrasco-Benavides et al. 503 (2022) used the CWSI on cherry trees; they used neural networks and achieved a correlation 504 coefficient of 0.83. Nevertheless, they used a random split for selecting the training and testing 505 datasets; thus, their model allows estimation of Ψ_s but not prediction. Our model outperforms 506 theirs, boasting an R^2 of 0.77 for estimation. Furthermore, the applicability of our methodology 507 depends on remote data to run the model; in the case of CWSI models, it depends on the UAS unit 508 and human staff to collect the imagery in the field, which makes it a costly and time-consuming 509 alternative.

510 6. Conclusion

511 The best-performing models to estimate and predict Ψ_s were the RF and XGBoost algorithms. We 512 used station weather variables and S2 satellite vegetation indicators as predictors. The model for 513 estimation reached a high performance, having an R² = 0.76 and an RMSE = 0.24 MPa. The 514 prediction model (*tme_split*) reduces the performance to R² = 0.59 and RMSE = 0.36 MPa. The 515 weather variables VPD, ETO, and temperature were the most important predictors of temporal 516 behavior, and the vegetation indices that measure in the SWIR region, MSI, DWSI, NMDI, and NDMI 517 were the most important predictors of spatial variation.

518 The model offers an alternative method for optimizing irrigation in cherry orchards, compared to 519 utilizing evapotranspiration. More measurements of Ψ s at higher plant water stress levels, both 520 near and below stomatal closure, could enhance the model's effectiveness. Additionally, in future 521 research, incorporating measurements on cloudy days could enhance the evaluation of performance 522 on those days.

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