

Article

Spatial Modeling of Olive Oil Polyphenol Content and Phenolic Terroirs Using Empirical Bayesian Kriging Regression Prediction

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Abstract

Following the 2021 Montiferru wildfire, one of the largest wildfire events in modern Italian history, assessing the suitability of olive-growing environments for high-quality extra virgin olive oil (EVOO) production is crucial for supporting sustainable agricultural restoration. This study models the spatial distribution and temporal stability of total polyphenol concentration in EVOO (cv. Bosana) across a complex Mediterranean landscape. Olive samples from georeferenced sites were collected during the 2022 (22 samples) and 2023 (37 samples) harvest seasons and processed using a standardized protocol. Spatial modeling was performed via Empirical Bayesian Kriging Regression Prediction (EBKRP), integrating seven bioclimatic and topographic covariates. Cross-validation demonstrated high predictive accuracy with negligible bias (RMSE = 53.3 and 58.8 mg kg^{−1} for 2022 and 2023, respectively). While single-predictor correlations were weak, multi-variable analysis highlighted a strong interaction between topography and water balance driving phenolic accumulation. The mean prediction map identified regional hotspots approaching 600 mg kg^{−1} of polyphenols content in the obtained olive oils. Spatial overlay analysis successfully delineated “Stable High-Phenolic Core Areas” (>500 mg kg^{−1} with interannual variation < 100 mg kg^{−1}), filtering out high-altitude marginal zones. This geostatistical approach provides a valuable territorial decision-making tool to support post-fire agricultural reconversion and the valorization of high-quality monovarietal EVOO terroirs.

Keywords: GIS; precision agriculture; environmental covariates; Mediterranean olive cultivation; phenolic terroir



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1. Introduction

Extra virgin olive oil (EVOO) is one of the most relevant products of Mediterranean agriculture and a fundamental component of the Mediterranean diet. In addition to its nutritional value, EVOO is recognized as an important source of bioactive compounds that contribute to both technological quality (shelf life) and human health. Among these compounds, phenolic substances play a central role because they are responsible for antioxidant activity, oxidative stability, bitterness, pungency and several health-promoting properties associated with olive oil consumption [1–4]. Phenolic compounds are recognized as key determinants of the nutritional, oxidative, technological and sensory quality of virgin olive

oil, although they do not alone define the overall commercial quality classification of olive oil. Their concentration influences shelf-life by protecting the lipid fraction from oxidative degradation by photo-oxidation and auto-oxidation and contributes significantly to quality attributes, particularly through bitterness and pungency, which are recognized as positive sensory descriptors of high-quality oils. Furthermore, extensive biomedical research has demonstrated their antioxidant, anti-inflammatory, anti-atherogenic and cardioprotective properties, leading the European Food Safety Authority [5] to approve a specific health claim relating olive oil polyphenols to the protection of blood lipids from oxidative stress. The accumulation of phenolic compounds in olive fruits and oils is regulated by a complex interaction among genetic, physiological, agronomic and environmental factors. Among these, genotype plays a major role, and significant differences in phenolic content have been reported among cultivars grown under similar environmental conditions [6–8]. Because of their strong influence on nutritional, technological and sensory quality, phenolic compounds are increasingly considered important traits in olive breeding and varietal selection programs aimed at improving olive oil quality, even if consumer preference for highly phenolic oils may vary according to market segment and familiarity with bitter and pungent sensory attributes [6,9]. However, cultivar alone cannot explain the large variability commonly observed in olive oil phenolic composition. Numerous studies have demonstrated that environmental conditions substantially affect both the biosynthesis and accumulation of phenolic compounds in olive fruits [10–13]. In Mediterranean environments, water availability is considered one of the most influential drivers of phenolic variability. Several irrigation experiments have shown that moderate water deficit frequently promotes phenolic accumulation, whereas increased water availability and full irrigation often lead to lower concentrations of phenolic compounds in virgin olive oil [14]. The physiological mechanisms underlying this response are associated with the activation of plant stress pathways and secondary metabolism under moderate drought conditions. Water stress can stimulate the synthesis of phenolic compounds as part of the plant defense response, while excessive water availability may reduce phenolic concentration through both metabolic and dilution effects. Consequently, indicators describing seasonal and pre-harvest water balance are expected to play a major role in determining the spatial variability of olive oil phenolic concentration. Temperature is another major environmental determinant of olive oil quality. Several studies have reported significant relationships between thermal conditions during fruit development and phenolic accumulation [11,15,16]. High temperatures may alter fruit growth, oil biosynthesis and ripening dynamics, ultimately affecting phenolic metabolism. In Mediterranean olive-growing areas, where drought and heat stress frequently occur simultaneously, the interaction between water availability and temperature becomes particularly important for determining final oil quality [16]. Solar radiation also influences olive fruit metabolism through its effects on photosynthesis, carbon assimilation and secondary metabolite production. Variations in radiation load can modify fruit exposure, ripening dynamics and biochemical composition, contributing to spatial differences in olive oil quality across heterogeneous landscapes [10,17]. Topography further contributes to this variability by regulating local microclimatic conditions. Elevation affects thermal regimes and phenological development, whereas slope influences drainage patterns, soil depth and water redistribution processes. Terrain-derived indices such as the Topographic Wetness Index (TWI) have been successfully used to represent potential soil moisture accumulation and hydrological behavior, providing valuable information on local environmental conditions that influence crop performance and quality attributes [18]. The combined influence of climate, topography, soil and management practices is commonly described through the concept of “terroir”. Although originally developed in viticulture, the terroir concept has increasingly been applied to olive-growing systems, where growing environment strongly influences the chemical

and sensory properties of olive oil [11,15]. Understanding the spatial distribution of olive oil phenolic potential is therefore essential for identifying high-value production areas and supporting territorial characterization strategies. The present study extends beyond olive oil quality assessment and is closely connected to the ecological and socio-economic consequences of the 2021 “Montiferru” wildfire. The Montiferru–Planargia district represents one of the most important traditional olive-growing areas of Sardinia, characterized by extensive cultivation of the cv. Bosana and the presence of historical and centuries-old olive groves. The study area includes territories affected by the 2021 Montiferru wildfire [19–22], although wildfire effects were not explicitly modeled. Within this context, the identification of environmentally suitable areas characterized by high potential for olive oil quality assumes strategic importance. Spatial modeling of olive oil polyphenol concentration can therefore contribute not only to understanding the environmental controls of phenolic accumulation, but also to supporting post-fire territorial recovery through the identification of areas with favorable bioclimatic conditions for high-quality olive production. The rapid development of Geographic Information Systems (GISs), remote sensing and spatial modeling techniques has created new opportunities for investigating the environmental determinants of crop quality. Spatially explicit approaches enable the integration of georeferenced analytical measurements with environmental raster datasets, allowing the characterization of continuous quality gradients across agricultural landscapes [18,23]. Among the available geostatistical approaches, Empirical Bayesian Kriging Regression Prediction (EBKRP) is particularly suitable for modeling complex environmental variables because it combines regression on explanatory covariates with Bayesian estimation of residual spatial dependence. Unlike conventional kriging methods, EBKRP explicitly incorporates uncertainty associated with semivariogram estimation through repeated simulations, thereby improving uncertainty quantification and predictive performance [24]. The objective of the present study was to investigate the spatial distribution of total polyphenol concentration in olive oil through the integration of analytical measurements and environmental predictors describing water balance, thermal regime, solar radiation and terrain morphology (Figure S1). Specifically, EBKRP was applied to two consecutive growing seasons (2022 and 2023) in order to evaluate the spatial drivers of phenolic variability and provide the basis for identifying stable areas of high phenolic potential associated with olive-growing terroir. To the best of our knowledge, no previous studies have integrated standardized olive oil production protocols and EBKRP to investigate the spatial distribution of olive oil polyphenols across heterogeneous olive-growing landscapes. Within this framework, the present study was initiated to identify the environmental factors associated with olive oil quality and to support the restoration and sustainable development of local olive-growing systems.

2. Materials and Methods

2.1. Study Area

The study was conducted in the Montiferru–Planargia olive-growing district, located in western Sardinia (Italy), covering a surface of 59,742.87 ha. The study area encompasses a wide altitudinal gradient extending from coastal zones to the volcanic reliefs of the Montiferru massif. This environmental heterogeneity generates marked spatial variability in temperature regimes, solar radiation, water availability and terrain morphology, providing an ideal framework for investigating the environmental determinants of olive oil phenolic composition. The region hosts one of the most important volcanic complexes in Sardinia. In the mountainous areas, elevations reach a maximum of 1052 m a.s.l. The landscape is characterized by imposing volcanic domes with rugged morphologies, interconnected by exposed ridges with limited vegetation cover. Slopes frequently reach gradients of 40–50%, favoring the occurrence of both sheet runoff and concentrated erosion processes. This environmental heterogeneity generates marked spatial variability in temperature regimes, solar

radiation, water availability and terrain morphology, providing an ideal framework for investigating the environmental determinants of olive oil phenolic composition. The area represents one of the most important traditional olive-growing regions of the island, especially in the municipalities of Cuglieri, Bosa, Scano Montiferru, Seneghe, Bonarcado, Riola Sardo, and Narbolia, and is characterized by a strong interaction between Mediterranean climatic conditions, complex topography and a long-established olive-growing heritage.

2.2. Plant Material and Sampling

The study focused exclusively on the Sardinian olive cultivar “Bosana”, which represents the dominant olive variety cultivated throughout the study area and one of the most important cultivars for virgin olive oil production in Sardinia. Olive samples were collected manually in rain-fed olive orchards during two consecutive harvest seasons (2022 and 2023) in order to evaluate the consistency of the observed spatial patterns under different annual environmental conditions. Sampling sites (Figure 1), both inside and outside the fire perimeter, were georeferenced and distributed across the study area to capture the environmental variability associated with climatic and topographic gradients. A total of 59 samples (22 in 2022 and 37 in 2023) were taken and processed. To minimize variability unrelated to environmental conditions, olives were harvested manually (6 kg of olives collected from all over the canopy, from 5 plants) at a comparable physiological ripening stage. Fruit maturity was assessed according to [25] (Jaén’s Maturity Index 2.8 ± 0.3) to ensure consistency among sampling locations.

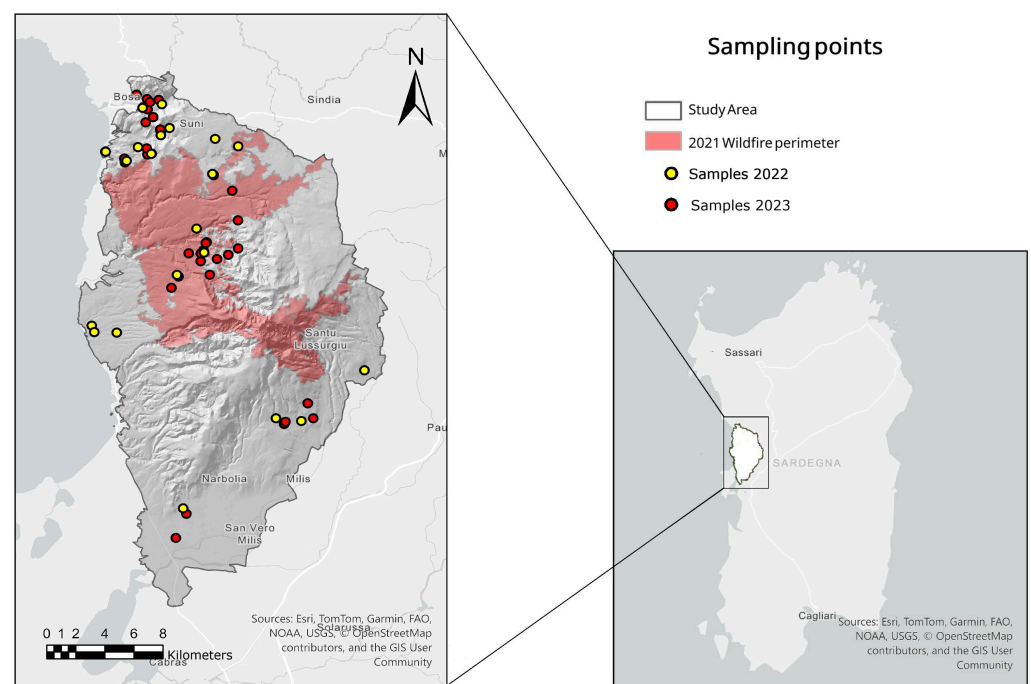


Figure 1. Location of the study area within the Montiferru–Planargia olive-growing district (western Sardinia, Italy), including the 2021 wildfire perimeter (red colored shape) and the sampling sites surveyed during the 2022 (yellow spots) and 2023 (red spots) seasons.

2.3. Experimental Olive Oil Extraction

For each sampling site, olives were transported to the laboratory under refrigerated conditions and processed on the same day as the sampling. Approximately 3 kg of olives were processed for each sample. For each olive sample, three independent oil extraction replicates were performed using the Abencor system, yielding three separate olive oil samples. Oil was extracted using an Abencor system small-quantity mill, simulating commercial

oil extraction systems (MC2 Ingeniería y Sistemas, Seville, Spain). The Abencor system reproduces the main mechanical phases of industrial olive oil extraction, including crushing, malaxation and centrifugation, allowing the processing of small quantities of olives under controlled laboratory conditions. The olives were crushed with the Abencor hammer mill equipped with a 4 mm sieve, then 700 g of paste were processed using the Abencor system's malaxer and centrifuge. Malaxation conditions were: time 30 min, temperature 25 °C, and with no water addition. The malaxed olive paste was centrifuged with the Abencor centrifuge for 60 s. at 3500 rpm. Oil samples were then centrifuged in a laboratory centrifuge (Heraeus megafuge, 40R, Thermo Scientific, Waltham, MA, USA) at 3600 rpm, 20 °C, for 15 min. to eliminate residual water and solid traces. Oils were kept at +15 °C, in the dark, until time of analysis (1 day). All samples were processed following an identical and standardized extraction protocol in order to minimize technological variability and ensure comparability among samples, thus allowing the measured differences in oil composition to be primarily attributed to environmental and biological factors rather than processing effects.

2.4. Determination of Oil Commercial Category and Total Polyphenols

The determination of the basic quality indices was performed primarily to verify the commercial category of the investigated oils. Free acidity, peroxide value, and UV spectrophotometric indices (K232, K268, and ΔK) were measured according to standard methods [8]. Sensory panel test was conducted by the AGRIS Sardegna sensory panel, an officially accredited panel recognized by the Italian Ministry of Agriculture, Food Sovereignty and Forestry (MASAF) for the sensory assessment of virgin olive oils. All samples met the legal requirements for classification as “extra virgin olive oil” and were therefore included in the subsequent analyses of polyphenol content and spatial variability. Total phenolic content was determined independently for each oil sample by means of two independent Folin–Ciocalteu assays. The mean phenolic concentration obtained from the three oil extraction replicates was subsequently used for the statistical and geostatistical analyses.

Phenolic extracts were obtained from olive oil samples according to standard analytical procedures [17]. Absorbance was measured at 765 nm using a UV–visible spectrophotometer (Cary 50, Varian, Palo Alto, CA, USA) and total phenolic concentration and results were expressed as mg gallic acid equivalents (GAE) per kg of olive oil using a gallic acid calibration curve. ($\geq 97.5\%$ titration, Product No. G7384, CAS 149-91-7, Sigma-Aldrich, St. Louis, MO, USA). The Folin–Ciocalteu assay is widely employed in olive oil quality studies and provides a robust estimate of the total reducing phenolic fraction associated with antioxidant capacity and sensory characteristics of virgin olive oil [17].

2.5. Climatic Data Sources

Environmental predictors were derived from climatic and topographic datasets. Climatic variables, including maximum summer temperature, precipitation, and reference evapotranspiration (E_t0), were obtained from georeferenced raster layers produced by the Regional Environmental Protection Agency of Sardinia (ARPAS Sardegna) through spatial interpolation of data collected by its meteorological station network. The raster had a resolution of 250×250 m and were calculated from the climatic data of 10 climatic stations, 7 inside and 3 outside the study area. These datasets, unpublished raster datasets specifically developed by ARPAS Sardegna for the purposes of the present study, constituted the basis for the derivation of the water-balance indicators used in the study, including the net irrigation requirement calculated for the May–December period (NIR-MD) and for the September–November period (NIR-SN). The latter was specifically included to characterize the balance between autumn precipitation and atmospheric evaporative demand during the final stages of fruit development and oil accumulation. Net irrigation requirements

(NIR-MD and NIR-SN) and annual solar radiation were calculated separately for each study year (2022 and 2023), generating year-specific raster layers used as environmental covariates in the spatial modeling workflow. Topographic predictors were derived from a Digital Elevation Model (DEM) of the study area. Elevation, slope, and the Topographic Wetness Index (TWI) were computed using standard terrain and hydrological analysis tools implemented in ArcGIS Pro (version 3.6.3, Esri Inc., Redlands, CA, USA). Annual solar radiation was estimated using the ArcGIS Pro Area Solar Radiation tool, which accounts for terrain geometry, slope, aspect, and topographic shading. The resulting raster represents the potential annual incoming solar energy and provides an integrated measure of the radiative environment experienced by olive trees across the landscape. In detail, the seven environmental raster covariates (Figure 2, NIR Sep–Nov) included in the regression component of the EBKRP model were:

1. Net irrigation requirement (May–December, mm):

$$NIR = \sum_{1May}^{31Dec} (ET_c - PE)$$

where

$$ET_c : ET_0 \times K_c$$

where ET_c = crop evapotranspiration; K_c = crop coefficient. ET_0 was estimated using the Hargreaves–Samani equation following FAO-56 procedures [26,27]. Groundwater contributions and soil water storage were not available for NIR calculation and were indirectly accounted for through the Topographic Wetness Index (TWI). Effective precipitation (PE) was estimated according to the simplified FAO method [28], using the following equations:

$$PE = (0.8 \times P) - 25 \quad \text{if } P > 75 \text{ mm/month}$$

$$PE = (0.6 \times P) - 10 \quad \text{if } P < 75 \text{ mm/month}$$

with

P = rainfall or precipitation (mm/month);

PE = effective rainfall or effective precipitation (mm/month).

2. Net irrigation requirement (September–November, mm):

$$NIR = \sum_{1Sep}^{30Nov} (Etc - PE)$$

3. Maximum temperature of the warmest month ($^{\circ}\text{C}$).
4. Annual global solar radiation ($\text{KWh m}^2 \text{ yr}^{-1}$):

$$R_a = \sum_{d=1}^{26} \sum_{h=1}^{48} (R_{dir} + R_{dif} + R_{ref})$$

where

R_a = cumulative annual solar radiation;

R_{dir} = direct solar radiation component;

R_{dif} = diffuse solar radiation component;

R_{ref} = reflected solar radiation component;

d = sampled days used for annual integration;

h = hourly intervals used for daily integration.

$$R_{dir} = S_0 \tau \cos \theta(\theta_i)$$

S_0 = solar constant;

τ = atmospheric transmissivity coefficient;

θ_i = angle of incidence of solar radiation on the terrain surface.

$$R_{dif} = R_{sky} \times SVF$$

R_{sky} = diffuse radiation received from the sky hemisphere;

SVF = Sky View Factor, representing the proportion of visible sky from a given location.

$$R_{ref} = \rho R_g$$

ρ = surface albedo coefficient;

R_g = incoming global solar radiation.

5. Elevation (m).
6. Slope ($^{\circ}$).
7. Topographic Wetness Index (TWI):

$$TWI = \ln \left(\frac{A_s}{\tan \beta} \right)$$

where

A_s : specific catchment area ($\text{m}^2 \text{m}^{-1}$);

β = local slope angle (radians).

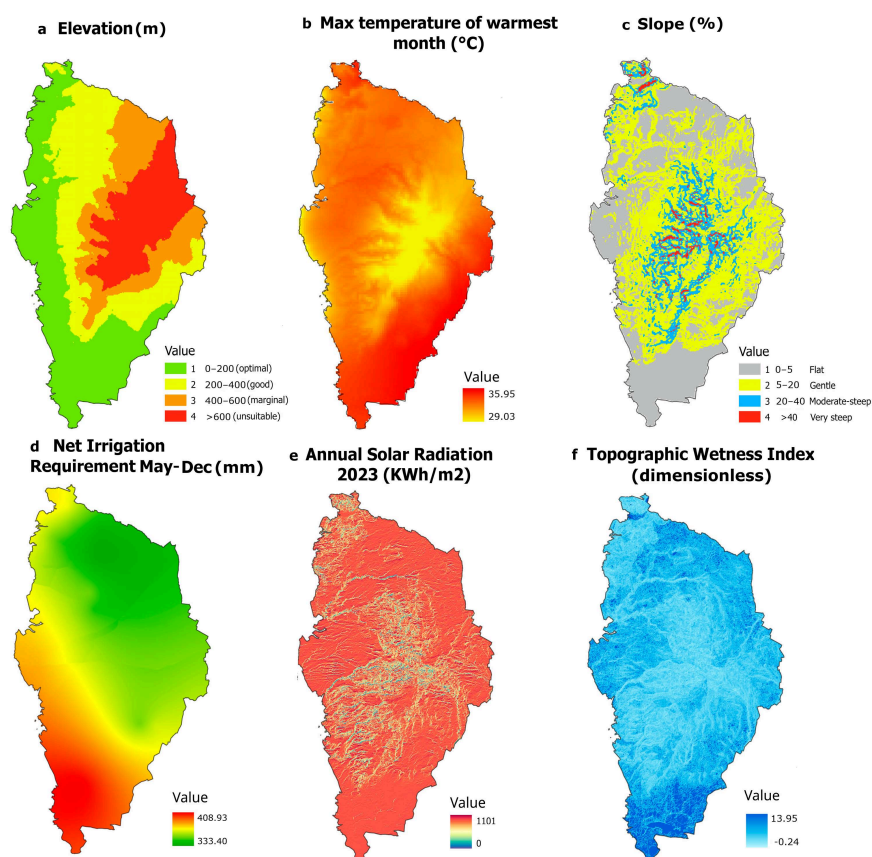


Figure 2. Environmental covariates included in the EBKRP regression model.

All raster layers were projected in the same coordinate reference system (WGS 1984 UTM Zone 32N), resampled to a common spatial resolution and aligned prior to predictor extraction and geostatistical modeling.

2.6. Exploratory Statistical Analysis and Predictor Screening

Prior to geostatistical modeling, an exploratory statistical analysis was performed to assess the relationships among environmental predictors and to identify potential multicollinearity issues. Pairwise Pearson correlation coefficients were calculated to evaluate linear associations among predictors and between predictors and olive oil total polyphenol concentration. Multicollinearity among predictors was assessed using the Variance Inflation Factor (VIF) following commonly adopted thresholds [29,30]. Variables with VIF values lower than 5 were considered acceptable and retained for subsequent analyses. Since all predictors showed acceptable VIF values (<5), no variables were excluded and all environmental predictors were included in the PCA. To explore the multivariate structure of the environmental space, Principal Component Analysis (PCA) was performed on standardized predictors. PCA was used to identify dominant environmental gradients and to evaluate potential clustering of observations according to growing season. PCA Dataset included all samples from 2022 and 2023 harvest seasons. All exploratory statistical analyses, including Pearson correlation analysis, Variance Inflation Factor (VIF), and Principal Component Analysis (PCA), were performed prior to geostatistical modeling in order to verify predictor suitability and ensure compliance with best practices for spatial predictive modeling [18,23]. All exploratory statistical analyses were performed using Python 3.11. Pearson correlation coefficients were calculated using the SciPy statistical package, while multicollinearity diagnostics (Variance Inflation Factor, VIF) and Principal Component Analysis (PCA) were implemented using scikit-learn and pandas libraries. Data visualization was produced using Matplotlib version 3.11.1.

2.7. Geostatistical Modeling

Spatial modeling procedures were performed in ArcGIS Pro using the EBKRP framework [24]. EBKRP was selected because it combines regression-based modeling of environmental predictors with Empirical Bayesian Kriging of regression residuals, allowing both deterministic environmental gradients and local spatial autocorrelation to be represented simultaneously. Compared with conventional regression approaches, EBKRP explicitly accounts for uncertainty in semivariogram estimation through repeated Bayesian simulations, improving prediction robustness when sample size is moderate and spatial autocorrelation is present. Unlike ordinary kriging, EBKRP incorporates explanatory environmental variables; while compared with machine-learning approaches it produces fully geostatistical prediction uncertainty estimates.

This approach combines a regression component based on explanatory raster covariates with Empirical Bayesian Kriging of the residual spatial structure, allowing the prediction surface to account simultaneously for environmental gradients and local spatial autocorrelation. All seven environmental predictors were retained in the EBK Regression Prediction models, since none exceeded the adopted VIF threshold and therefore no variable was excluded from the modeling procedure. The spatial distribution of total polyphenol concentration in olive oil was modeled separately for the 2022 and 2023 growing seasons. The two growing seasons were modeled separately because the measured polyphenol concentrations and the climatic covariates represented year-specific conditions. This approach was required to generate independent annual prediction surfaces and to distinguish spatial patterns from interannual differences. All elaborations were made using the total polyphenol concentration measured in olive oil samples obtained from georeferenced sampling

points as the dependent variable. The 2022 dataset included 22 sampling locations, whereas the 2023 dataset included 37 sampling locations.

For both 2022 and 2023 models, EBKRP was performed using a K-Bessel semivariogram model, 100 simulations, subset size of 100, overlap factor of 1, and 95% cumulative variance. The search neighborhood was Standard Circular, including a minimum of 10 and a maximum of 15 neighbors and one sector. No transformation was applied prior to EBK Regression Prediction because exploratory analysis indicated that data transformation was not necessary. In contrast, environmental predictors were standardized exclusively for the Principal Component Analysis (PCA), where standardization was required to place variables measured on different scales onto a common standardized scale. Model performance was assessed through leave-one-out cross-validation. The following diagnostics were evaluated: Mean Error (ME), Root Mean Square Error (RMSE), Average Standard Error (ASE), Mean Standardized Error (MSE), Root Mean Square Standardized Error (RMSSE), Continuous Ranked Probability Score (CRPS), and the percentage of observations falling within the 90% and 95% prediction intervals. Model calibration was considered optimal when ME and MSE approached zero, ASE was close to RMSE, and RMSSE approached one. Observed-versus-predicted scatterplots and standardized error QQ plots were also inspected to evaluate agreement between measured and predicted values and the distributional behavior of standardized residuals.

2.8. Mean Predicted Polyphenol Content

To evaluate the average phenolic potential independently of year-specific climatic conditions, a mean prediction raster was calculated as the arithmetic mean of the 2022 and 2023 predicted surfaces:

$$P_{mean} = \frac{P_{2022} + P_{2023}}{2}$$

where P2022 and P2023 are the predicted polyphenol concentrations for the 2022 and 2023 growing seasons, respectively. The resulting raster represents the average predicted phenolic potential across the study area.

2.9. Interannual Stability Analysis

To assess the temporal consistency of phenolic expression, an interannual difference raster was calculated using the absolute difference between yearly predictions:

$$D = |P_{2023} - P_{2022}|$$

where D represents the absolute magnitude of variation in predicted polyphenol concentration between years (in mg kg^{−1}).

The resulting map was classified into five variability classes (Table 1).

Table 1. Stability classes.

Difference (mg kg ^{−1})	Stability Level
<50	Very high
50–100	High
100–150	Moderate
150–250	Low
>250	Very low

Lower values indicate greater temporal stability and therefore a stronger expression of terroir-related effects. These classes were subsequently combined with the mean predicted polyphenol raster to identify stable high-phenolic areas, as described in the following section.

2.10. Identification of Stable High-Phenolic Terroirs

A spatial overlay analysis was performed between the mean predicted polyphenol raster (Pmean) and the interannual difference raster (D). Areas were classified according to both phenolic potential and temporal stability.

Three classes of high-phenolic terroirs were identified:

Stable High-Phenolic Core Areas

$P_{\text{mean}} > 500 \text{ mg kg}^{-1}$ and $D < 100 \text{ mg kg}^{-1}$

High Phenolic with Moderate Stability

$P_{\text{mean}} > 500 \text{ mg kg}^{-1}$ and $100 \leq D \leq 150 \text{ mg kg}^{-1}$

High-Phenolic Areas with Low Stability

$P_{\text{mean}} > 500 \text{ mg kg}^{-1}$ and $D > 150 \text{ mg kg}^{-1}$

These classes were used to delineate areas combining elevated phenolic potential and temporal consistency.

3. Results

3.1. Exploratory Analysis of Environmental Predictors

Variance Inflation Factors ranged from 1.19 to 3.43, indicating low levels of multicollinearity among predictors and confirming that all variables provided complementary environmental information. The highest VIF values were observed for elevation (3.43) and NIR-MD (3.04), although both remained well below commonly accepted thresholds. Pairwise correlations among environmental variables (Figure 3) revealed moderate relationships between elevation and NIR-MD ($r = -0.779$), reflecting the influence of topography on atmospheric demand and water balance. Most predictor pairs exhibited weak or non-significant correlations, whereas only a limited number of relationships were statistically significant (Figure 4). However, significant interannual differences emerged. In 2022, no statistically significant correlations were detected between polyphenol concentration and environmental variables. In contrast, the 2023 season showed significant relationships with elevation ($r = -0.440$, $p = 0.006$), slope ($r = 0.355$, $p = 0.031$) and Topographic Wetness Index ($r = -0.336$, $p = 0.042$). These results suggest that local topographic controls on water availability played a stronger role during the 2023 growing season.

The first two principal components explained 61.64% of the total environmental variance, with PC1 accounting for 36.46% and PC2 accounting for 25.18%. PC1 was primarily associated with water availability and topographic gradients, showing the strongest positive loadings for NIR May–December and solar radiation and negative loadings for elevation and slope, as detailed in Table 2 and illustrated in Figure 5. This component can therefore be interpreted as a “hydro-climatic environmental gradient integrating terrain position, atmospheric demand, solar energy and water balance”. PC2 was mainly influenced by slope and elevation, together with secondary contributions from TWI, Tmax and solar radiation (Table 2). This component reflects a “topographic exposure gradient related to terrain morphology and local redistribution of water resources”.

Table 2. Loadings of environmental predictors on the first two principal components.

Variable	PC1	PC2
NIR May–December	0.787	0.396
NIR September–November	0.575	0.459
Elevation	−0.696	−0.623
Slope	−0.596	0.656
TWI	0.589	−0.481
Solar Radiation	0.670	−0.429
T max Summer	0.107	−0.439

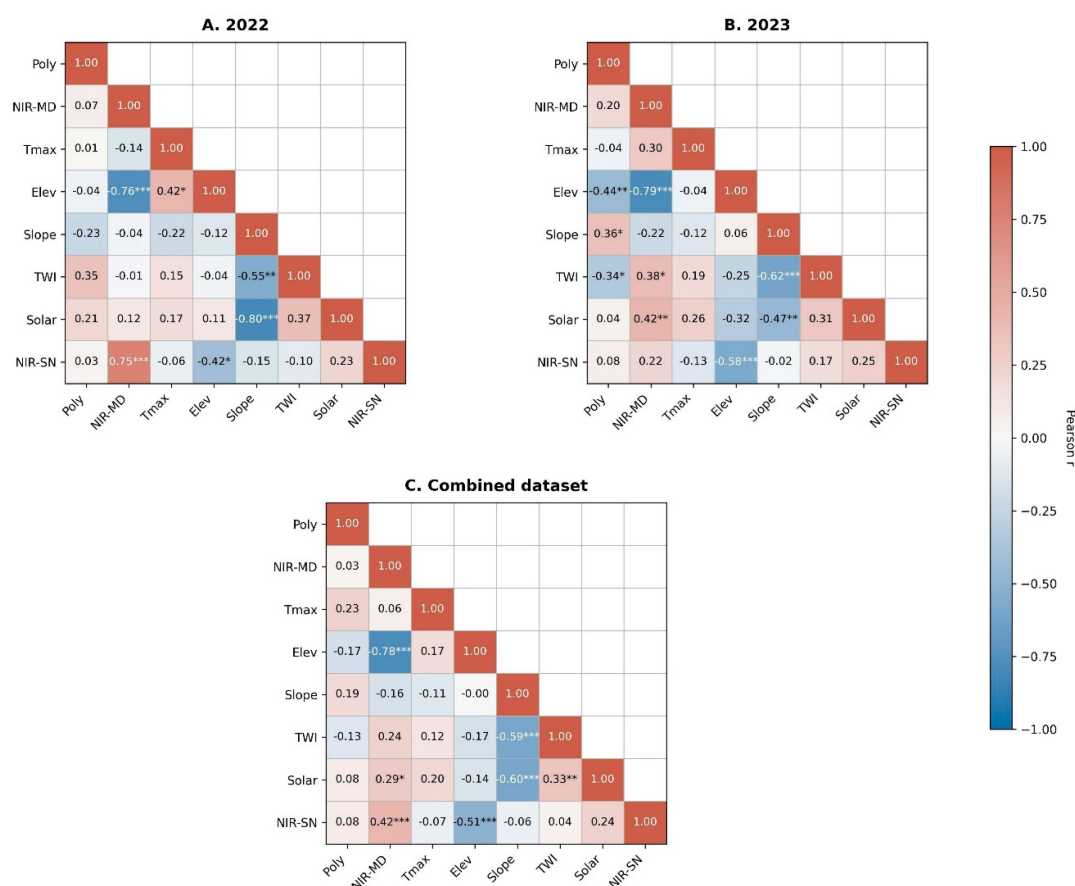


Figure 3. Pearson Correlation matrices among polyphenols and environmental predictors. Cell values are Pearson correlation coefficients; significance level: * $p < 0.05$; ** $p < 0.01$; *** $p < 0.001$.

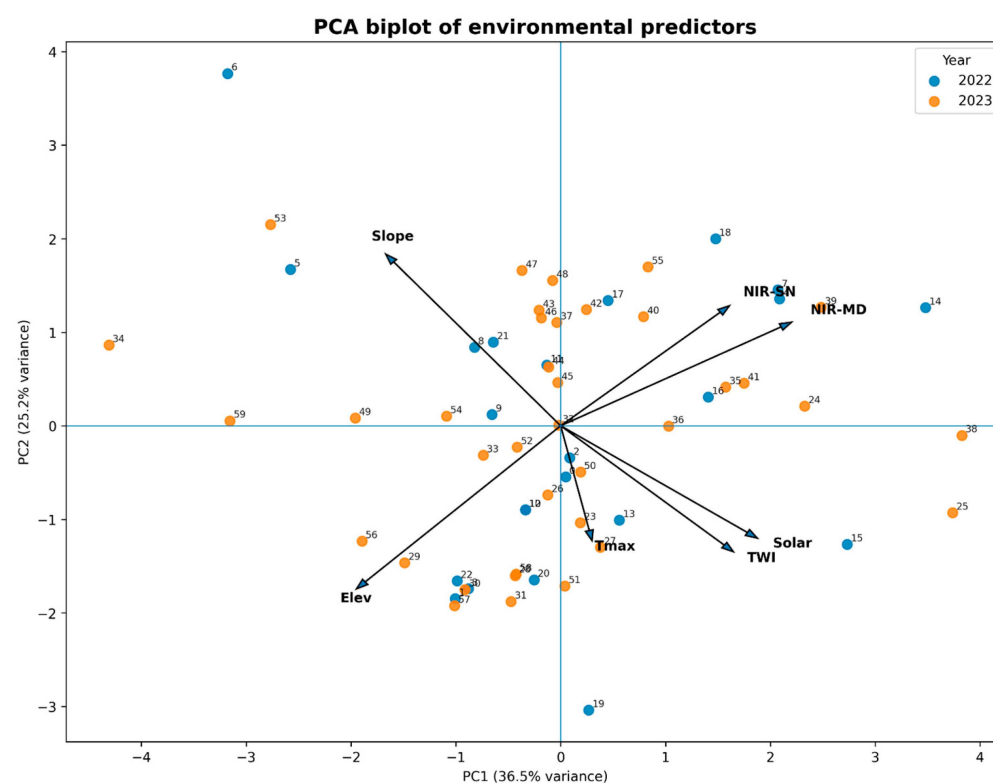


Figure 4. Principal Component Analysis (PCA) biplot of environmental predictors. Points represent sampling locations colored according to growing season (2022 and 2023). Sample identifiers are reported next to each observation.

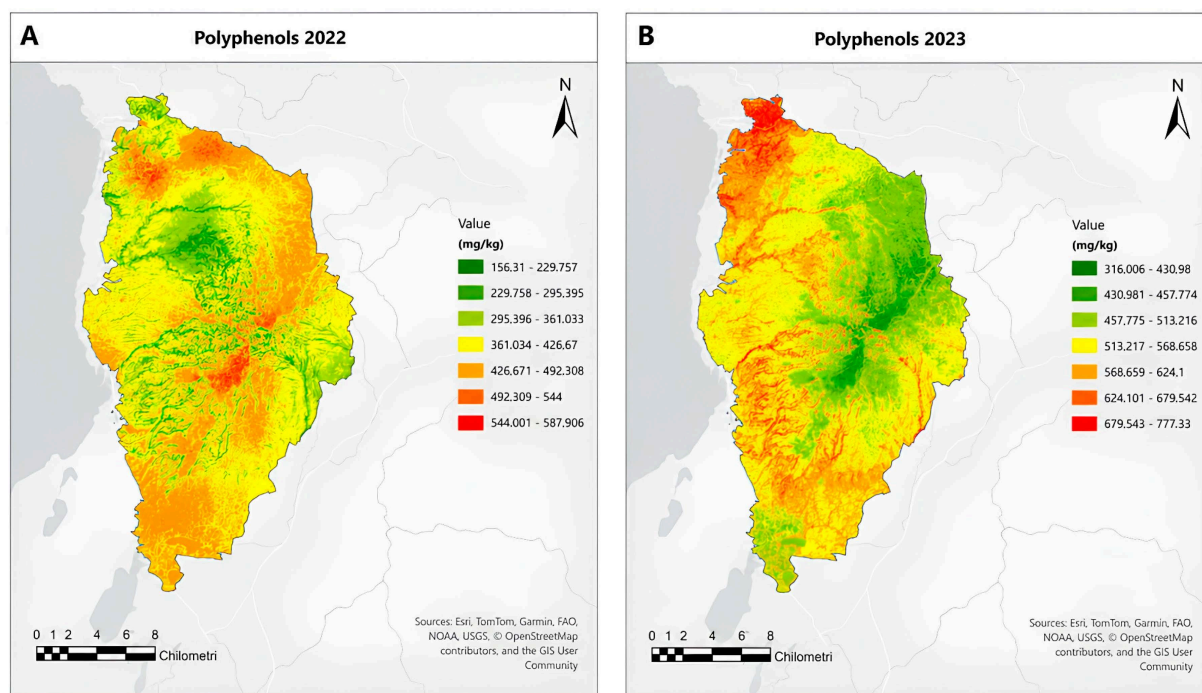


Figure 5. EBKRP-predicted spatial distribution of olive oil total polyphenol content (mg kg^{-1}) in the study area (Sardinia, Italy) for the 2022 (A) and 2023 (B) growing seasons.

The PCA biplot (Figure 4) revealed a continuous distribution of sampling sites across the environmental space, without clear clustering of observations. Samples from 2022 and 2023 partially overlapped, suggesting that both growing seasons were characterized by the same underlying environmental gradients, although the magnitude of their contribution differed between the 2022 and 2023 models.

3.2. Cross-Validation Performance of the 2022 Model

The EBKRP models showed satisfactory predictive performance in both growing seasons (Table 3). Although minor differences were observed among the validation statistics, the overall cross-validation results indicated good model reliability and consistent predictive accuracy. This conservative behavior was also reflected by the prediction interval diagnostics, with 100% of observations falling within both the 90% and 95% prediction intervals. The observed-versus-predicted scatterplot showed a positive linear relationship, with regression equation $y = 1.187x - 75.34$. Although the slope was higher than the ideal value of 1, the general agreement between measured and predicted values confirmed that the model captured the main spatial trend of polyphenol variability. The Q-Q plot of standardized errors showed an approximately normal distribution, with moderate deviations in the tails.

Table 3. Cross-validation performance metrics of the EBKRP models for olive oil total polyphenol concentration mapping in 2022 and 2023.

Metric	Ideal Value	2022	2023	Interpretation
Number of samples	-	22	37	Number of observations used for model calibration and validation
Mean Error (ME) (mg kg^{-1})	0	1.31	−0.77	Values close to zero indicate absence of systematic prediction bias
Root Mean Square Error (RMSE) (mg kg^{-1})	As low as possible	53.30	58.77	Overall prediction error

Table 3. Cont.

Metric	Ideal Value	2022	2023	Interpretation
Average Standard Error (ASE) (mg kg^{-1})	Similar to RMSE	76.56	64.32	Estimated prediction uncertainty
RMSE/ASE ratio	≈ 1	0.70	0.91	Measures consistency between observed and estimated uncertainty
Mean Standardized Error (MSE)	0	0.017	−0.018	Standardized measure of prediction bias
Root Mean Square Standardized Error (RMSSE)	1	0.742	0.927	Indicates calibration of prediction variances
Continuous Ranked Probability Score (CRPS)	Lower values indicate better performance	31.86	33.06	Probabilistic accuracy of the model
Coverage of 90% confidence interval (%)	90	100.0	94.6	Reliability of uncertainty estimates
Coverage of 95% confidence interval (%)	95	100.0	97.3	Reliability of uncertainty estimates
Regression equation (Observed vs. Predicted)	$y = x$	$y = 1.187x - 75.34$	$y = 1.048x - 34.85$	Agreement between observed and predicted values
Semivariogram model	–	K-Bessel	K-Bessel	Spatial covariance structure
Simulations	–	100	100	Number of EBK simulations

3.3. Cross-Validation Performance of the 2023 Model

The 2023 EBKRP model also showed robust predictive behavior (Table 3). The close agreement between these two values suggests that the model provided a realistic estimate of prediction uncertainty. The RMSSE was 0.927, very close to the theoretical optimum of 1, indicating better uncertainty calibration than in 2022. The 90% and 95% prediction intervals contained 94.6% and 97.3% of observations, respectively. The observed-versus-predicted regression equation was $y = 1.048x - 34.85$, with a slope very close to unity, indicating strong agreement between predicted and measured polyphenol concentrations.

3.4. Comparison Between Years

The two annual models showed the spatial distribution of predicted polyphenol content (Table 3, Figure 5). The 2022 model had a slightly lower RMSE, suggesting marginally smaller prediction error, but its RMSSE value indicated a marked overestimation of uncertainty. Conversely, the 2023 model showed a slightly higher RMSE but better calibration of prediction uncertainty, as indicated by an RMSSE close to 1 and prediction interval coverage consistent with the expected values. Overall, both annual models were unbiased and suitable for spatial prediction of olive oil polyphenol concentration, although the 2023 model exhibited the best overall geostatistical performance.

3.5. Mean Predicted Polyphenol Content

The mean prediction map (Figure 6A) revealed marked spatial variability in olive oil phenolic potential across the study area. The highest predicted concentrations were predominantly located in the central and north-central sectors of the study area, whereas lower values were observed in the central plateau and in some eastern sectors. Several localized hotspots approach 600 mg kg^{-1} as the average for the two years under consideration, indicating areas characterized by a particularly favorable combination of environmental and topographic conditions. Overall, most of the territory expresses medium-high polyphenol

contents (400–500 mg kg⁻¹), suggesting a generally high suitability for the production of phenolic-rich olive oils.

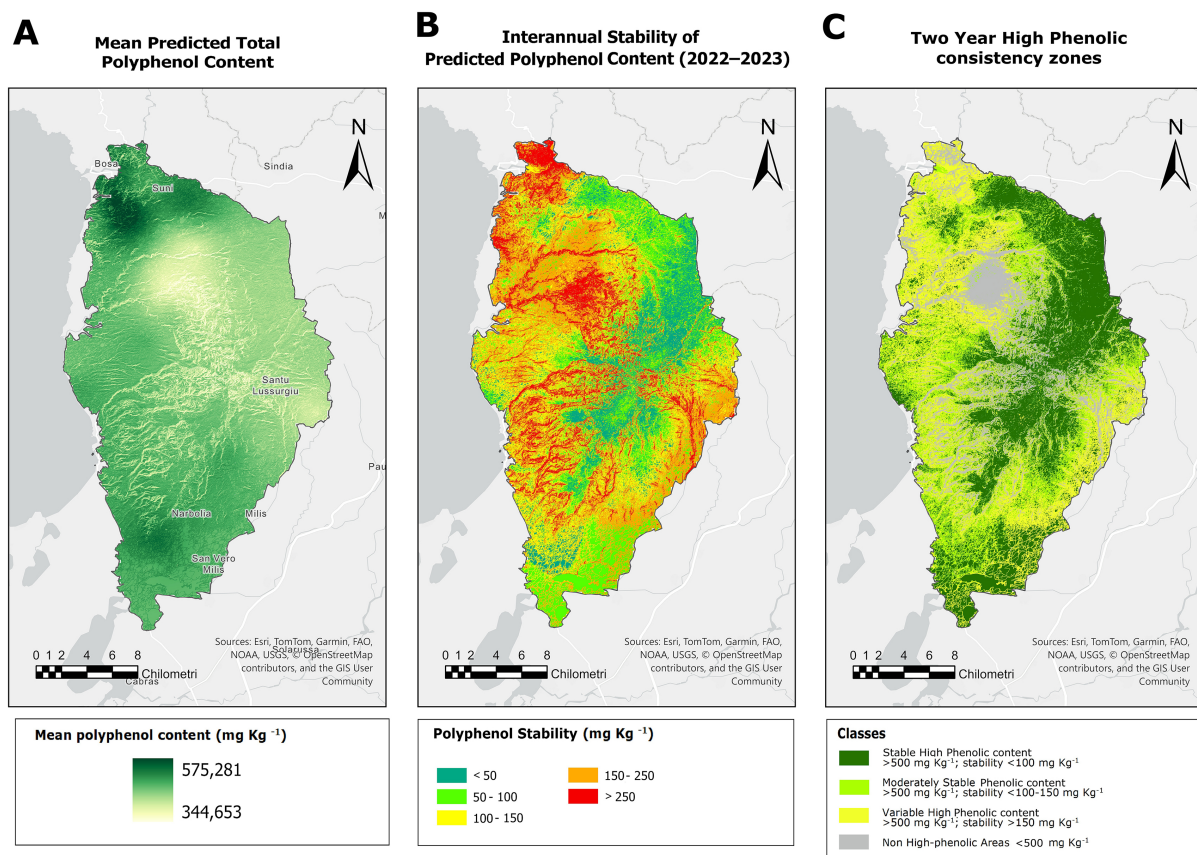


Figure 6. Identification of two-year stable high polyphenol zones in the study area olive-growing area. (A) Mean predicted total polyphenol content derived from EBK interpolation of 2022 and 2023 analytical data. (B) Interannual variability of predicted polyphenol content expressed as the absolute difference between yearly prediction surfaces. (C) Stable High-Polyphenol Terroirs identified through the integration of phenolic potential and temporal stability.

3.6. Interannual Stability

The interannual variability map (Figure 6B) highlighted substantial differences in the temporal stability of phenolic expression. The most stable areas of predicted high polyphenol content (difference < 100 mg kg⁻¹) were concentrated mainly in the eastern and southern portions of the study area, while higher variability characterized portions of the central mountainous sector and some north-western areas. Linear landscape features associated with steep slopes and drainage networks exhibited the greatest variability, suggesting a stronger influence of annual climatic fluctuations. Despite local variability, extensive portions of the territory maintained relatively consistent phenolic levels across the two production seasons (Figure 6A,B).

3.7. Stable High-Phenolic Terroirs

The overlay analysis identified several spatially coherent zones characterized by both high phenolic potential and strong temporal stability. These areas were concentrated primarily in:

- north-central area;
- central-eastern slopes;
- southern sectors.

Two-year high-phenolic consistency zones (Figure 6C) represented the most potentially valuable terroirs because they simultaneously exhibited:

- elevated predicted polyphenol concentrations ($>500 \text{ mg kg}^{-1}$);
- limited interannual difference ($<100 \text{ mg kg}^{-1}$).

Conversely, some areas with high phenolic potential displayed substantial year-to-year variability and were therefore classified as secondary phenolic zones.

Notably, some areas, classified as potentially valuable terroirs may have limits regarding altitude and slopes, therefore terroir mapping potential should be carefully compared with altitude maps regarding potential marginality of the cultivation due to excessive altitudes and slopes. In the region, increasing elevation is generally associated with lower temperatures and a higher probability of frost events. Consequently, the suitability of these areas for commercial olive cultivation should be evaluated jointly with agronomic and climatic constraints, rather than on phenolic potential alone.

4. Discussion

The exploratory statistical analyses revealed that olive oil polyphenol concentration was only weakly correlated with individual environmental variables when considered separately. This finding suggests that phenolic accumulation is controlled by complex interactions among multiple environmental drivers rather than by a single dominant factor. The dominant topographic–hydrological gradient identified by PC1 reflects the main structure of the environmental predictor dataset. The ecological relevance of this gradient is consistent with the well-established role of plant water status in influencing olive fruit metabolism, as discussed below. Moderate water limitation has been shown to enhance the synthesis of phenolic compounds through the activation of stress-responsive pathways and increased allocation of carbon towards secondary metabolites [10,12,13]. The second component, associated with solar radiation and thermal conditions, represents an environmental gradient related to energy availability and oxidative stress. Increased exposure to solar radiation may stimulate antioxidant defense mechanisms and influence the expression of genes involved in the phenylpropanoid pathway, ultimately affecting the concentration of phenolic compounds in olive fruits and oils [31,32]. The PCA identified these major environmental gradients within the study area, while their relevance for olive oil phenolic accumulation is supported by the EBK Regression Prediction results together with the available physiological literature. Such complexity helps explain the relatively weak bivariate correlations observed between polyphenols and individual predictors and further justifies the adoption of multivariate geostatistical approaches such as EBKRP. The significant relationships observed during the 2023 season provide further insight into the ecophysiological mechanisms underlying phenolic variability. The negative correlation with elevation and TWI, together with the positive correlation with slope, consistently point toward the role of water availability as a major environmental regulator of phenolic metabolism. Areas characterized by lower TWI values and steeper slopes are typically associated with reduced soil moisture accumulation and increased drainage. These conditions can induce moderate water deficit, which is known to stimulate antioxidant responses and phenylpropanoid metabolism in olive trees. The resulting activation of secondary metabolic pathways may contribute to increased accumulation of phenolic compounds in fruits and oils [10,12,13]. The absence of similar relationships during the 2022 season suggests that environmental controls on phenolic accumulation are strongly modulated by annual climatic conditions. The environmental predictors included in the EBKRP models can be interpreted not only as spatial covariates, but also as proxies of ecophysiological processes involved in olive fruit development and phenolic metabolism. Olive oil phenolic compounds derive mainly from the shikimate and phenylpropanoid pathways, with secoiridoid derivatives such as

oleuropein- and ligstroside-derived compounds representing the most distinctive phenolic fraction of virgin olive oil [4,31,32]. Their final concentration in the oil is therefore the result of biosynthesis, degradation, enzymatic transformation during ripening and mechanical extraction, and partitioning between fruit tissues, vegetation water and oil phases. Water availability, represented in the model by the net irrigation requirement from May (fruit set) to December (full ripening), net irrigation requirement from September to November (or net effective rainfall, i.e., the effective rainfall minus the Etc), and TWI, is one of the most ecophysiological meaningful drivers of phenolic variability. Under moderate water deficit, olive trees activate stress-response mechanisms involving oxidative signaling, osmotic adjustment and secondary metabolism. Irrigation experiments have repeatedly shown that oils from trees under deficit or rainfed conditions often contain higher concentrations of total phenols and secoiridoid derivatives than oils from fully irrigated trees [10,12–14]. This supports the inclusion of water-balance predictors as mechanistic variables rather than merely empirical spatial descriptors. The May–December net irrigation requirement integrates water deficit over most of the fruit development cycle, from fruit set to harvest. This period includes cell division, mesocarp growth, pit hardening, oil accumulation and ripening, all of which can influence phenolic dynamics. The September–November water-balance variable is especially relevant because late fruit development and ripening are characterized by intense biochemical reorganization of the drupe. During ripening, oleuropein and related secoiridoids are progressively transformed into downstream derivatives, while the phenolic profile changes markedly with maturity stage [7,31,33]. High autumn water availability may reduce phenolic concentration through dilution effects, reduced stress signaling and altered ripening dynamics, whereas moderate pre-harvest deficit may maintain stronger antioxidant and secoiridoid-related responses. Areas with high TWI are more likely to retain water, whereas low-TWI areas tend to be better drained and more prone to water deficit. From an olive ecophysiology perspective, this variable may indirectly capture differences in root-zone water availability, stomatal regulation, leaf water potential and oxidative stress intensity. Since olive is a drought-adapted species capable of strong stomatal control and osmotic adjustment [34–36], local differences in soil water status can substantially affect carbon allocation and the balance between primary metabolism, oil biosynthesis and secondary metabolite production. Summer maximum temperature represents the thermal stress component of the model. Temperature affects photosynthesis, respiration, enzyme kinetics, flowering and fruit development, as well as oil accumulation and final oil quality. [16]. Moderate thermal stress may stimulate antioxidant metabolism, whereas excessive heat can impair photosynthetic performance and disrupt normal fruit development, potentially reducing the accumulation of quality-related metabolites [37–41]. Solar radiation represents the energetic component of the olive-growing environment. Phenolic compounds are carbon-based secondary metabolites, and their synthesis is linked to the availability of carbon skeletons generated through photosynthesis. Higher radiation can increase carbon assimilation and may enhance the metabolic resources available for phenylpropanoid and secoiridoid biosynthesis. At the same time, high irradiance can induce photooxidative stress, increasing the need for antioxidant compounds. Elevation and slope represent the geomorphological control of local microclimate and hydrology. Elevation modifies temperature regimes, thermal amplitude and phenological timing, while slope affects runoff, infiltration, drainage and soil depth. The relevance of pedoclimatic variables for olive fruit and oil traits has also been reported in studies on Mediterranean olive-growing environments, including Sardinian conditions [11]. The spatial distribution of mean predicted polyphenol content suggests that environmental conditions exert a strong influence on the accumulation of phenolic compounds in olive oil. The concentration of high-value areas in elevated and topographically complex sectors supports

previous findings indicating that altitude, thermal regime, solar radiation and moderate water stress can promote phenolic biosynthesis. The stability analysis provides additional insight beyond simple concentration mapping. While many studies focus exclusively on absolute phenolic levels, the present approach incorporates temporal consistency, allowing identification of terroirs capable of maintaining high phenolic expression under different climatic conditions. The observed instability along steep drainage systems and highly heterogeneous landscapes suggests that local hydrological processes and microclimatic variability contribute significantly to year-to-year fluctuations in phenolic content. Taken together, the predictors used in the EBKRP models describe an integrated ecophysiological system in which water deficit, thermal regime, solar radiation and terrain morphology jointly regulate phenolic accumulation. Although both EBKRP models showed satisfactory predictive performance, the relatively limited number of observations available for each year (22 and 37 samples, respectively) should be considered when interpreting the results. The leave-one-out cross-validation approach was specifically adopted because it provides an efficient internal validation strategy for datasets of limited size while maximizing the information extracted from each observation. Nevertheless, additional sampling campaigns covering a larger number of orchards and production years would further improve model robustness and allow an independent external validation of the predicted spatial patterns. Previous studies have demonstrated that geographical origin, growing site and environmental conditions significantly influence olive oil composition and quality attributes, while GIS-based approaches have been increasingly used to characterize olive-growing territories and assess land suitability for olive cultivation [42–45]. The threshold of 500 mg kg^{−1} was adopted to identify areas with high phenolic potential. This value is consistent with previous classifications of virgin olive oils, where phenolic concentrations above 500 mg kg^{−1} are considered indicative of high phenolic content, and with the definition proposed by [46] for high-phenolic olive oils. Even when environmental predictors are ecophysologically meaningful, a certain residual variability is expected because the final oil phenolic concentration reflects both field-level metabolism and processing-related transformations [47–53]. The proposed integrated framework provides a spatially explicit basis for understanding the environmental drivers of olive oil quality and supports evidence-based strategies for the restoration and valorization of Mediterranean olive-growing landscapes.

5. Conclusions

The annual EBKRP models provided unbiased and reliable spatial predictions of olive oil polyphenol concentration. The 2022 model showed conservative uncertainty estimates, while the 2023 model achieved stronger calibration between observed errors and predicted uncertainty. Cross-validation procedure implemented within EBKRP may be influenced by spatial autocorrelation among neighboring observations and therefore may provide optimistic estimates of predictive performance compared with spatially independent validation methods. Nevertheless, the two models demonstrate that the spatial variability of olive oil polyphenols can be effectively modeled using the proposed geostatistical framework. The consistency among RMSE, ASE, CRPS, and prediction interval coverage indicates that the models provide reliable regional-scale predictions under the available sampling conditions. The mean prediction map identified extensive sectors with high suitability for the production of phenolic-rich olive oils, while the stability analysis revealed marked spatial differences in the persistence of phenolic expression between years. The overlay of these datasets allowed the delineation of potentially stable high-phenolic zones, representing areas that combine elevated polyphenol concentrations with low interannual variability.

These zones constitute promising targets for:

- polyphenol-rich olive oil production;
- territorial valorization strategies;
- precision agriculture applications;
- future studies on olive oil terroir characterization.

The proposed methodology demonstrates the usefulness of integrating spatial prediction and temporal stability analyses for the identification of environmentally resilient olive-growing terroirs. From an applied perspective, this approach provides a spatial decision-support tool for identifying areas with higher potential for producing oils rich in phenolic compounds. Such maps may support terroir characterization, targeted sampling, valorization of high-quality production zones, precision agronomy, irrigation planning and the development of territorial quality labels. The results also open the way to a multi-year analysis aimed at distinguishing stable spatial patterns from year-specific climatic effects. A limitation of the present study is the availability of only two consecutive growing seasons. Olive oil phenolic composition is known to be strongly influenced by annual climatic variability, and longer monitoring periods would improve the characterization of temporal stability. The study provides a first robust framework for terroir delineation and supports the application of the proposed methodology in olive-growing planning. Future studies including additional growing seasons will allow further refinement and validation of the identified phenolic terroirs.

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Abbreviations

Abbreviation	Definition
ASE	Average Standard Error
CI	Confidence Interval
CRPS	Continuous Ranked Probability Score
DEM	Digital Elevation Model

EBKRP	Empirical Bayesian Kriging Regression Prediction
ET ₀	Reference Evapotranspiration
ET _c	Crop Evapotranspiration
GIS	Geographic Information System
K _c	Crop Coefficient
NIR	Net Irrigation Requirement
NIR-MD	Net Irrigation Requirement (May–December)
NIR-SN	Net Irrigation Requirement (September–November)
R _a	Cumulative annual solar radiation
R _{dir}	Direct solar radiation component
R _{dif}	Diffuse solar radiation component
R _{ref}	Reflected solar radiation component
d	Sampled days used for annual integration
h	Hourly intervals used for daily integration
S ₀	Solar constant
τ	Atmospheric transmissivity coefficient
θ _i	Angle of incidence of solar radiation on the terrain surface
R _{sky}	Diffuse radiation received from the sky hemisphere
ρ	Surface albedo coefficient
R _g	Incoming global solar radiation
A _s	Specific catchment area (m ² m ^{−1})
PCA	Principal Component Analysis
PET	Potential Evapotranspiration
RMSE	Root Mean Square Error
RMSSE	Root Mean Square Standardized Error
SVF	Sky View Factor
TWI	Topographic Wetness Index
UTM	Universal Transverse Mercator
VIF	Variance Inflation Factor
WGS84	World Geodetic System 1984

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