From Global to Station-Centric Models: Improved Chlorophyll-a Prediction in the Gulf of İzmir Using Sentinel-2

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Abstract

Chlorophyll-a (Chl-a) serves as a primary indicator of phytoplankton abundance and plays a central role in assessing coastal water quality and eutrophication processes. As an optically active substance, its concentration modulates water-leaving radiance, enabling retrieval from multispectral satellite observations. Conventional remote sensing models typically rely solely on spectral information derived from reflectance bands. This study extends this approach by integrating spectral information with spatial context using Geographically Weighted Regression (GWR). Nevertheless, standard GWR faces practical constraints such as high computational cost and challenges in conducting unbiased performance evaluations across heterogeneous areas. To address these limitations, we introduce a Station-Centric GWR (SCGWR) framework. SCGWR constructs separate locally calibrated regression models centred on each *in-situ* sampling station, thereby capturing site-specific relationships between Sentinel-2 reflectance bands and measured Chl-a concentrations. The performance of SCGWR was evaluated in the Gulf of İzmir using Sentinel-2A surface reflectance data together with synchronous *in-situ* Chl-a observations. Comparative analysis with Multiple Linear Regression (MLR) showed that SCGWR provides improved prediction accuracy while better representing local spatial variability. In particular, SCGWR produced a lower test RMSE (6.26) compared to MLR (6.95), together with higher correlation and concordance coefficients. Visual inspection of the predicted maps further indicated that SCGWR generates spatially coherent Chl-a patterns that correspond more closely with *in-situ* measurements. These results demonstrate the potential of the SCGWR framework as a reliable spatial modelling approach for improving satellite-based monitoring of coastal eutrophication and water quality dynamics.

1. Introduction

Coastal ecosystems are highly vulnerable to nutrient enrichment and pollution, which directly affect water quality and ecological balance. Among optically active constituents (OACs), chlorophyll-a (Chl-a) concentration is widely used as a proxy for eutrophication and phytoplankton biomass, making its monitoring crucial for sustainable coastal management (Matthews, 2011). High Chl-a concentrations are commonly associated with excessive nutrient loading and phytoplankton blooms, which may lead to reduced water transparency, oxygen depletion, and broader ecosystem degradation in coastal waters (Cloern, 2001; Bricker et al., 2008). These processes are particularly evident in semi-enclosed coastal basins where limited water circulation can intensify the effects of nutrient inputs. The Gulf of İzmir, located in the eastern Aegean Sea, represents one such system where anthropogenic activities and riverine discharges have long contributed to water quality deterioration.

Satellite remote sensing has become an effective tool for monitoring spatial and temporal variations in water quality parameters across large coastal and inland water bodies. In particular, the Sentinel-2 MultiSpectral Instrument (MSI) has been widely used for aquatic applications due to its spectral capability to detect variations in optically active constituents such as chlorophyll, suspended particulate matter, and colored dissolved organic matter (Pahlevan et al., 2017). Nevertheless, artifacts such as sun glint and product-related anomalies may affect the reliability of satellite-derived reflectance and therefore require appropriate atmospheric and radiometric corrections (Vanhellemont and Ruddick, 2016; Yagmur et al., 2022). After these corrections, statistical and spatial modeling approaches are commonly employed to estimate water quality parameters such as chlorophyll-a.

Many satellite-based water quality studies rely on empirical or semi-empirical regression models that establish relationships between spectral reflectance and *in-situ* measurements. Global approaches such as Multiple Linear Regression (MLR) assume spatially stationary relationships between predictors and the target parameter, which may limit their ability to represent local variability in heterogeneous coastal environments. To address this limitation, spatially adaptive models such as Geographically Weighted Regression (GWR) have been increasingly applied in environmental studies. GWR estimates local regression parameters using distance-based weighting, allowing relationships between variables to vary across space (Fotheringham et al., 2002). However, when the number of observations is limited, local models may become strongly influenced by nearby samples, potentially leading to unstable parameter estimates and overfitting.

Building on these considerations, this study introduces a Station-Centric Geographically Weighted Regression (SCGWR) framework, which modifies the traditional GWR concept by structuring the regression around measurement stations rather than relying solely on spatial bandwidth optimization (Özkan et al., 2026). This station-based strategy aims to improve the stability of local regression estimates while preserving the ability to represent spatial variability in water quality conditions.

This study evaluates the performance of the SCGWR framework for predicting Chl-a concentrations in the Gulf of İzmir. *In-situ* measurements were integrated with Sentinel-2 MSI observations to establish the modeling dataset. Model outputs from SCGWR were compared against a global MLR baseline to assess the contribution of the station-based spatial modeling strategy and to examine whether locally constrained regression structures improve prediction reliability under limited sampling conditions.

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2. Study Area

The Gulf of İzmir is a semi-enclosed coastal gulf in the eastern Aegean Sea, spanning approximately 64 km in length and 32 km in width, with a maximum depth of about 100 m. The gulf receives freshwater and pollutant inputs mainly from the Gediz River and several smaller creeks, and it is bordered by the densely urbanized and industrialized metropolitan area of İzmir (Figure 1).

Previous investigations have reported high nutrient and heavy metal concentrations in water, sediments, and biota, with distinct gradients from the inner to the outer gulf (Kontaş et al., 2004; Kucuksezgin et al., 2006; Kucuksezgin, 2011). Despite improvements in wastewater treatment, pollution signals and ecological pressures have persisted, especially in nearshore and river-influenced zones. In recent years, several remote sensing studies have also examined the ecological dynamics of the gulf and have shown significant spatial and temporal heterogeneity. For example, analyses based on Sentinel-2 observations have shown that chlorophyll-sensitive metrics such as the Normalized Difference Chlorophyll Index (NDCI) can successfully capture algal bloom development and help explain events such as the fish mortality recorded in the summer of 2024 (Yılmaz et al., 2025). Furthermore, long-term time-series studies have revealed clear seasonal cycles in Chl-a and suspended matter, together with localized hotspots particularly in river-influenced and nearshore areas (Altuntaş et al., 2025). These findings indicate the importance of spatial modeling approaches that can better represent local variability, which motivates the use of SCGWR in this study.

3. Data & Pre-processing

A total of 20 *in-situ* Chl-a samples were collected across the Gulf of İzmir on 23 May 2025, coinciding with a cloud-free Sentinel-2 overpass (Figure 1). Sentinel-2 Level-1C (L1C) data were processed using ACOLITE with the Dark Spectrum Fitting plus Glint Correction (DSF+GC) approach to minimize sun glint effects, which were clearly visible in this acquisition.

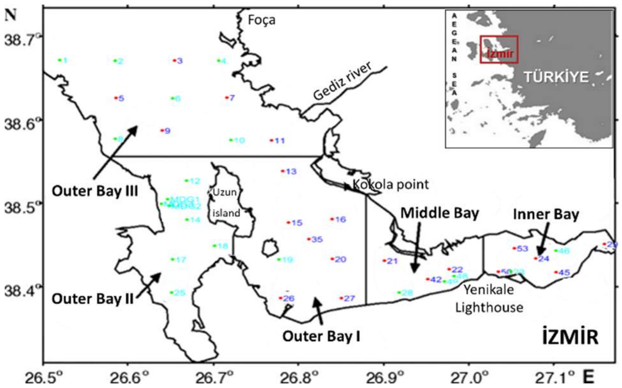

Figure 1. Location of the Gulf of İzmir with its Inner, Middle, and Outer Gulf (I–III) sections, major landmarks, and sampling stations. Blue points indicate training stations, while cyan points represent test stations.

In addition to sun glint effects, Sentinel-2 imagery contained stripe anomalies, visible in several spectral bands. These artifacts have been documented in Copernicus support resources and user forums under "Product anomalies and features" (Copernicus Dataspace Forum, 2023; SentiWiki, 2024).

An additional 20 in-situ Chl-a samples were collected on the following day (24 May 2025). These samples were used to test the model performance, assuming minimal short-term variability (Figure 1).

Table 1 summarizes descriptive statistics of *in-situ* Chl-a concentrations (µg/L) of training and test data, including the number of measurements (n), minimum and maximum values, mean, standard deviation (std) and quartiles. Outliers were identified using the 1.5× interquartile range (IQR) criterion (Navidi, 2010). The distributions show differences in dispersion and skewness. The test data show highly positive skewed distribution with four outliers, whereas the training data exhibit a more symmetric distribution with no outliers. These statistical patterns were visualized in a boxplot (Figure 2).

Data	Training	Test
Number of Stations	20	20
Minimum	0.083	0.083
Maximum	6.358	29.281
Mean	2.234	3.772
Standard deviation	2.284	7.788
The first quartile	0.363	0.142
Median	1.097	0.300
The third quartile	4.786	2.308

Table 1 Descriptive statistics of *in-situ* Chl-a concentrations (µg/L) for the training and test datasets.

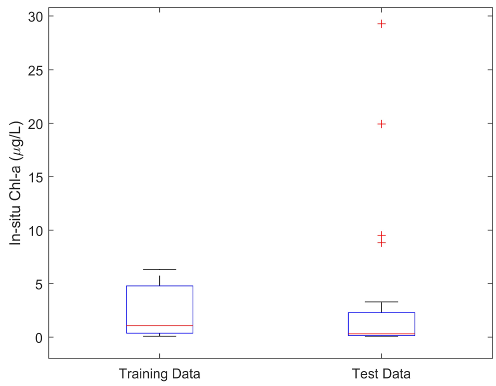

Figure 2. Boxplots of training and test Chl-a datasets.

4. Methodology

Conventional spatial analysis techniques, including ordinary least squares regression and numerous algorithms from the machine learning literature, operate under the premise of spatial stationarity. They assume that the relationship between dependent and independent variables is uniform across the entire geographic extent of the study area. However, many environmental processes exhibit spatial heterogeneity, meaning that relationships between variables may vary depending on location. A well-established alternative is GWR, which relaxes the stationarity assumption by calibrating local regression models (Fotheringham et al., 2002). GWR employs a distance-based weighting matrix to prioritize nearby data points, thereby generating location-specific parameter estimates. The efficacy of this localized calibration hinges on the selection of a kernel function and its bandwidth. While GWR provides valuable insights into spatially varying processes, its practical application is frequently hindered by substantial computational overhead, a marked sensitivity to hyperparameter configurations, and inherent difficulties in conducting robust, unbiased model validation due to the non-independent nature of the local models.

SCGWR builds on the principles of GWR but incorporates a station-centric modeling strategy to reduce overfitting and spatial adjacency biases (Özkan et al., 2026):

- Each station is treated as a local modeling center.

- The outer sixteen Moore-neighbor pixels (range= 2; Figure 3) are used for validation to support unbiased optimization of each station centric model. The inner eight neighboring pixels are excluded to avoid adjacency bias.

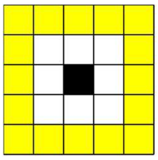

Figure 3. Moore-neighbor configuration used for validation.

- Multiple localized models are generated, and their predictions are aggregated using Inverse Spectral Distance Weighted Averaging (ISDWA), which assign weights based on spectral rather than geographic proximity. ISDWA is a modified form of the conventional Inverse Distance Weighted (IDW) interpolation, computing weights based on spectral Euclidean distances between regression points and station points (Amidror, 2002). This ensures that predictions from spectrally similar stations have a greater influence on the result, thereby enhancing spatial representativeness.

Overall, this framework enables locally adaptive modelling while providing a more robust validation strategy than conventional GWR. Further methodological details on the SCGWR framework are provided in Özkan et al. (2026).

As shown in Equation (1), three complementary accuracy metrics were used to evaluate the predictive performance of the models. Root Mean Square Error (RMSE) quantified the magnitude of prediction errors, while Pearson's correlation coefficient (r) described the strength of the linear relationship between observed and predicted values. Lin's concordance coefficient (r_c) was used to jointly assess precision and accuracy by measuring the agreement between predicted and observed values.

$$RMSE = \frac{1}{n}\sum_{i=1}^{n}(z_i - \hat{z}_i)^2$$

$$r = \frac{s_{z\hat{z}}}{s_z s_{\hat{z}}} \tag{1}$$

$$r_C = r\frac{2s_z s_{\hat{z}}}{s_z^2 + s_{\hat{z}}^2 + \left(\bar{z} - \bar{\hat{z}}\right)^2}$$

In these equations, z_i and $\hat{z}_i$ denote the observed and predicted Chl-a values for the i-th sample, respectively. The terms $\bar{z}$ and $\bar{\hat{z}}$ represent the corresponding mean values, s_z and $s_{\hat{z}}$ are standard deviations of z and $\hat{z}$, and n indicates the total number of samples.

5. Results

MLR was applied as a global model to establish empirical relationships between selected Sentinel-2 reflectance bands and *in-situ* Chl-a concentrations. While computationally simple, MLR does not account for local spatial heterogeneity and therefore provides a useful baseline for comparison. SCGWR addresses these limitations by incorporating both spatial proximity and spectral similarity into its design. Instead of generating a model for every point in space, SCGWR develops a dedicated regression model for each station. A key aspect of this architecture is the explicit separation of training and validation data: the target station is excluded from the model-building process and used only for testing, allowing model performance to be assessed using independent data.

Two approaches were used to assess the model performance: i) evaluation with the training dataset (*in-situ* measurements collected on 23 May 2025) and ii) evaluation with the test dataset (*in-situ* measurements collected on 24 May 2025). While Leave-One-Out Cross-Validation (LOOCV) was deliberately chosen to evaluate the performance of the MLR model using the training dataset, the SCGWR approach inherently relies on LOOCV as part of its algorithmic design.

The performance assessment showed that the SCGWR framework yielded more accurate Chl-a estimates than the global MLR benchmark. As presented in Table 2, SCGWR achieved a lower RMSE and higher Pearson's correlation coefficient (r) and Lin's concordance coefficient (r_c), reflecting closer agreement between predicted and observed values in the test dataset. This indicates that accounting for local variability provides measurable benefits compared with a single global regression model.

Dataset	Method	RMSE	r	r_c
Training	MLR	0.6418	0.9577	0.9575
	SCGWR	0.1565	0.9975	0.9975
Test	MLR	6.9450	0.7676	0.2628
	SCGWR	6.2616	0.8777	0.4044

Table 2. Performance comparison of MLR and SCGWR for Chl-a prediction using the training and test datasets (n = 20 each).

Scatter plots comparing predicted Chl-a concentrations from the MLR and SCGWR models with *in-situ* measurements are shown in Figure 4. The axes are displayed on a square-root scale to accommodate the wide dynamic range of Chl-a values. The 1:1 reference line helps illustrate agreement between predicted and observed values, as well as potential over- or underestimation, and the influence of outliers. These visualizations reveal error patterns and model behavior across the concentration range that may not be fully reflected by summary statistics such as RMSE and correlation coefficients.

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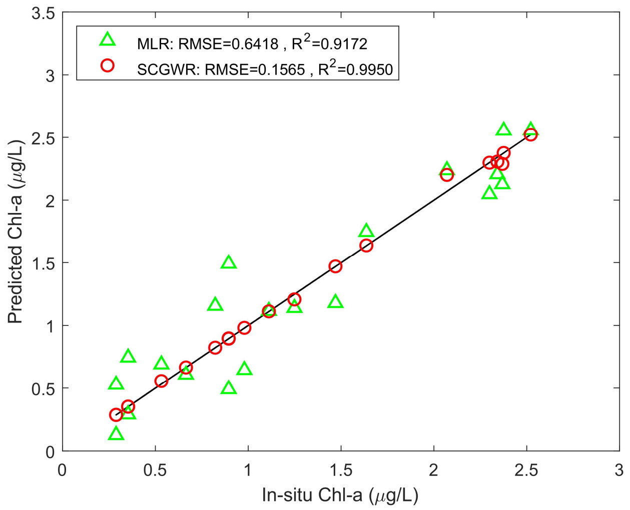
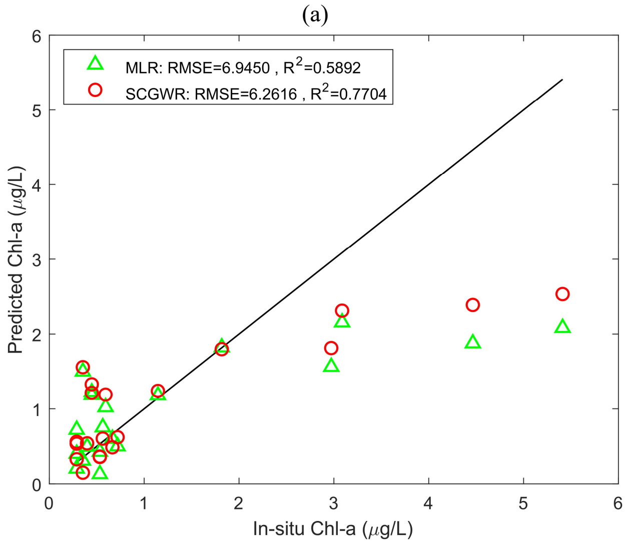


(a)



(b)

Figure 4. Scatter plots of predicted versus *in-situ* Chl-a concentrations (µg/L) for the MLR (green triangles) and SCGWR (red circles) models for (a) the training dataset and (b) the test dataset. The axes are displayed on a square-root scale and the black line indicates the 1:1 reference line.

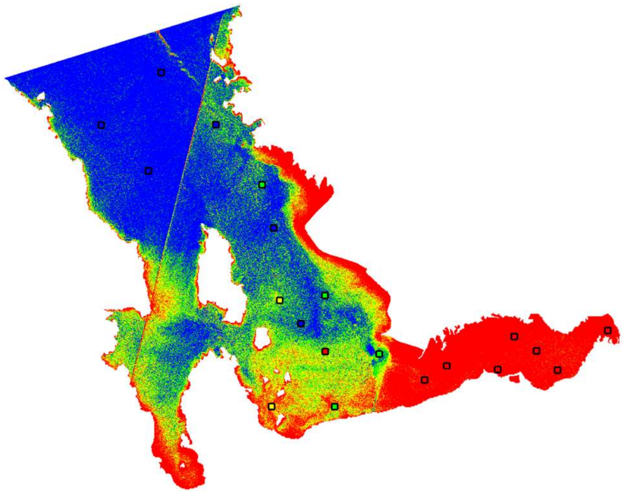
In the training dataset, SCGWR shows noticeably tighter clustering along the 1:1 line, reflecting superior local fit compared with MLR. For the test dataset, the models diverge clearly, especially for the extreme high-concentration points associated with the intense algal bloom events. While both models underestimate these values, falling well below the 1:1 line, the underestimation by SCGWR is less severe than that of MLR. SCGWR also maintains better alignment when representing both oligotrophic conditions and hypertrophic blooms. Overall, Figure 4 indicates that SCGWR provides more stable agreement with *in-situ* measurements across the study area, supporting its suitability for capturing spatially varying Chl-a dynamics in the Gulf of İzmir.

After model development, Chl-a concentrations were predicted for the entire study area. In addition to the quantitative assessment of model accuracy, a complementary qualitative evaluation was conducted through visual examination of the predicted Chl-a maps. This analysis, informed by domain knowledge and cross-checked with *in-situ* measurements, provided additional insight into model performance. Predicted Chl-a values were categorized according to the eutrophication criteria listed in Table 3 and visualized using a color-coded classification scheme. *In-situ* measurement locations were overlaid on the maps as black squares to enable direct comparison between observed and predicted values, as shown in Figure 5. This visualization approach enhanced spatial interpretability and strengthened confidence in the model outputs.

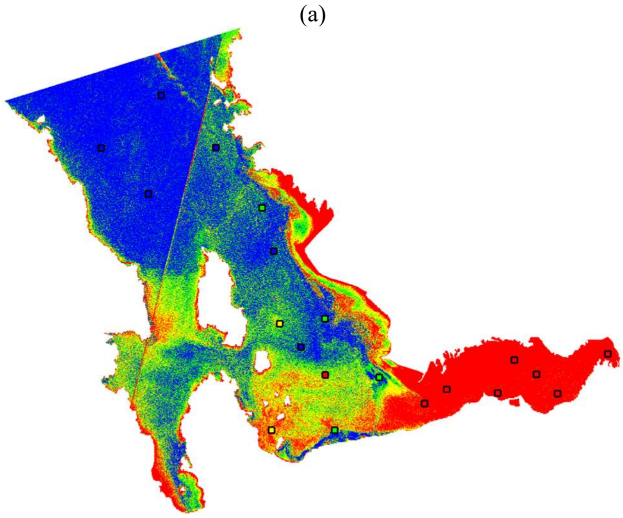
Water Quality	Chl-a (µg/L)	Color Code	Number Code
Oligotrophic	0 < Chl-a < 0.5	Blue	1
Mesotrophic	0.5 ≤ Chl-a ≤ 1	Green	2
Eutrophic	1 < Chl-a ≤ 2	Yellow	3
Hypertrophic	Chl-a >2	Red	4

Table 3 Seasonal eutrophication thresholds for the Gulf of İzmir based on Chl-a concentrations during the spring period (adapted from YSKY, 2023).

The spatial distribution maps (Figure 5) show broadly similar large-scale patterns for both models; however, SCGWR provides a more realistic depiction of local variations in several ecologically sensitive zones.



(a)



(b)

Figure 5. Spatial distribution of eutrophication classes predicted by MLR (a) and SCGWR (b). The black squares indicate *in-situ* measurement locations, with classes derived from measured Chl-a concentrations according to Table 3.

In particular, areas influenced by wastewater treatment outfalls, river inputs, and nearshore mixing—where sharp gradients in water quality are typically observed—were represented more consistently with in-situ observations when modeled with SCGWR. Unlike the globally fitted MLR, which tends to smooth these localized transitions, SCGWR retains small-scale contrasts that are characteristic of the Gulf of İzmir’s heterogeneous coastal dynamics. This behavior is consistent with observations from ongoing monitoring programs in the region.

Moreover, to assess categorical consistency across models, a paired contingency matrix was constructed for MLR and SCGWR, using classified outputs for all pixels in the study area. This matrix, presented in Table 4, quantifies joint classification patterns across the four eutrophication classes.

		SCGWR			
	Classes	1	2	3	4
MLR	1	35.19	6.16	0.60	0.34
	2	4.10	9.84	3.67	0.51
	3	1.18	2.85	9.71	2.06
	4	0.58	1.10	3.30	18.81

Table 4. Concordance ratios of eutrophication classes between MLR and SCGWR (%). Total number of pixels: 9,280,611.

The paired contingency matrix enabled evaluation of consistency beyond chance. However, due to the large dataset size (over 9 million pixels), formal statistical tests such as the McNemar–Bowker test were not applied. Instead, the analysis focused on overall classification consistency. Cohen’s Kappa coefficient (κ) (Cohen, 1960) was therefore used to quantify inter-model agreement. For example, if one model classifies an area as oligotrophic while the other assigns a hypertrophic class to the same pixels, the κ value approaches zero, indicating poor agreement. In contrast, values near 1 indicate strong classification agreement between models.

The Kappa value was computed as 0.63, indicating moderate agreement according to the thresholds proposed by Congalton and Green (2008) and Landis and Koch (1977). This result indicates that MLR and SCGWR produce broadly similar eutrophication classifications across the study area, although local differences remain in certain areas.

To emphasize methodological differences, the eutrophication classifications shown in Figure 5 were compared by calculating the difference between corresponding class values for each pixel. The resulting class differences are visualized in Figure 6, where green areas indicate identical classifications (no difference), while yellow, red, and black represent absolute differences of one, two, and three classes, respectively. Agreement was concentrated mainly in the inner (I), middle (II) and outer gulf (III) regions, while larger discrepancies occurred in the southern parts of the outer gulf regions (I and II) and the eastern part of the outer gulf (III).

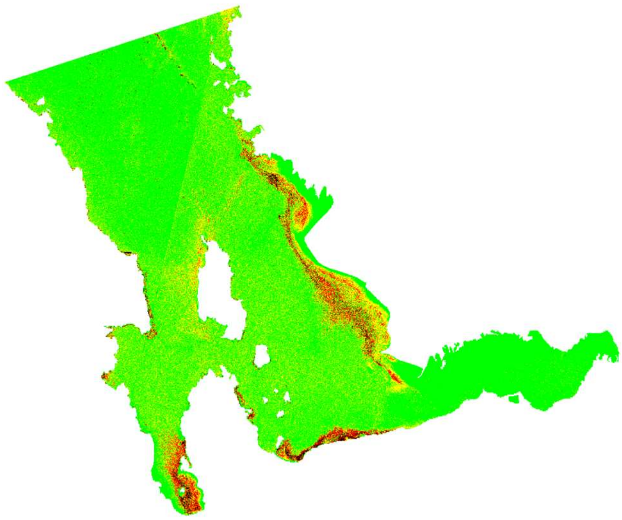


Figure 6. Map of eutrophication class differences between MLR and SCGWR predictions. Colors indicate class differences between the two models (green = 0, yellow = ±1, red = ±2, black = ±3).

6. Conclusion

This study presents an initial evaluation of the SCGWR framework for predicting chlorophyll-a concentrations from Sentinel-2 imagery in the Gulf of İzmir. The results demonstrate the potential of a station-based spatial regression approach for modeling water quality in heterogeneous coastal environments.

The main findings of this study can be summarized as follows:

• SCGWR produced more accurate Chl-a estimates than the global MLR model, achieving lower RMSE and higher correlation and concordance coefficients.
• Scatter plot analyses indicated that SCGWR better preserved the relationship between predicted and *in-situ* Chl-a values, particularly under low and moderate concentration conditions.
• Spatial classification maps showed that SCGWR captured local eutrophication patterns more clearly, especially in nearshore and river-influenced areas.
• The contingency matrix and Kappa analysis (κ = 0.63) indicated moderate agreement between MLR and SCGWR, suggesting that the two models produce similar large-scale patterns while differing in several localized regions.

Future work will focus on applying the SCGWR framework to other coastal regions of Türkiye, testing its stability with larger datasets, and evaluating the generalizability of the station-centric modeling approach across diverse coastal environments.

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