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Watershed urbanization drives nonlinear water-quality responses across mangrove-associated coastal systems.

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Abstract

Coastal watersheds connect terrestrial land-use pressures with estuarine receiving environments, but long-term assessments of this connectivity are often constrained by fragmented monitoring records. We compiled 31 years of surface-water monitoring data from four subtropical watersheds draining into protected mangrove systems in southern Brazil to examine how watershed conditions were associated with coastal water quality. Overall conditions across 2,603 sampling events were summarized using a standardized Nemerow Pollution Index (StdNPI), and XGBoost models combined with SHapley Additive exPlanations (SHAP) were used to identify the main predictors of water-quality classes and interpret nonlinear responses. The model discriminated among pollution classes with a mean AUC of 0.841 and identified watershed urban cover and population as the predominant predictors. The modeled probability of clean-water conditions declined markedly around 10% urban cover within the observed study domain. Mangrove cover was associated with a greater probability of clean conditions principally under lower watershed pressures, while contrasting patterns inside the Ratones and Tavares mangroves suggested that downstream water-quality responses depended on the surrounding watershed context. Frequent exceedances of regulatory criteria for fecal indicators, organic-matter-related variables, nutrients, and dissolved oxygen were consistent with substantial wastewater influence. Scenario projections indicated increasing probabilities of polluted conditions under the urban expansion permitted by current zoning. These findings show that the condition of protected estuarine wetlands cannot be evaluated independently of their hydrologically connected watersheds and demonstrate how heterogeneous long-term records can support integrated land-to-estuary assessment and management.

Keywords: Catchment-to-coast connectivity; coastal watershed; mangrove; water quality; urbanization; long-term monitoring.

Introduction

Estuarine water quality is strongly conditioned by processes occurring throughout the hydrologically connected watershed, where land-use changes, population growth, sanitation deficits, and stormwater networks regulate the delivery of nutrients, organic matter, and fecal contaminants to receiving coastal waters (Kennish, 2002; Tuholske et al., 2021). Accelerated urbanization is reshaping coastal watersheds worldwide, altering hydrological connectivity, increasing pollutant loads, and progressively degrading estuarine ecosystems (Freeman et al., 2019). Coastal zones support a

disproportionate and rapidly growing share of the global population: in 2018, approximately two billion people lived within 50 km of the shoreline and about one billion within 10 km, with coastal populations growing faster than inland populations (Cosby et al., 2024). This demographic concentration and continued growth intensify pressure for urban expansion and infrastructure development in coastal watersheds, often outpacing the provision of sanitation infrastructure, particularly in developing countries, and resulting in chronic contamination of receiving waters by nutrients, pathogens, and organic pollutants (Alberti, 2005; Parkinson, 2002; McGrane, 2016; Garbossa et al., 2017). These pressures are particularly pronounced in estuarine environments, where urban development frequently converges with ecologically sensitive habitats such as mangroves, amplifying environmental degradation while eroding the capacity of coastal ecosystems to regulate water quality and sustain critical ecosystem services (Wolanski and Elliott, 2015; Andres et al., 2018; Pardal et al., 2024).

Long-term water-quality assessments often rely on data compiled from multiple institutions, research projects, and regulatory monitoring programs. Such multi-source datasets can substantially expand spatial and temporal coverage, bridging critical information gaps that individual monitoring campaigns cannot address alone. However, systematic differences in sampling design, sampling frequency, monitored variables, analytical methods, and program objectives may compromise comparability among sites and periods (Hering et al., 2010). These limitations are particularly relevant in regional-scale assessments, where incomplete and heterogeneous monitoring records can obscure environmental gradients and hinder the identification of major anthropogenic pressures (Sprague et al., 2017). Despite these methodological hurdles, aggregating and interpreting disparate data remains essential to track long-term ecological trends, evaluate policy effectiveness, and establish reliable baselines for aquatic ecosystems (Read et al., 2017). Therefore, robust analytical approaches that harmonize heterogeneous observations into interpretable water-quality indicators are vital to transform fragmented raw measurements into actionable knowledge for sustainable environmental monitoring and management (Lumb et al., 2011).

Although urbanization is widely recognized as a major driver of water-quality degradation (Walsh et al., 2005; Schueler et al., 2009; Fletcher et al., 2013; McGrane, 2016), it remains unclear how long-term conditions across hydrologically connected coastal watersheds change along gradients of urban development and whether downstream mangrove-associated waters exhibit similar responses

under contrasting levels of watershed pressure. Land-use planning in rapidly urbanizing coastal regions rarely incorporates the assimilative capacity of receiving estuarine ecosystems. Development limits are commonly defined by administrative zoning and building-density criteria, with limited consideration of watershed connectivity, sanitation deficits, or the cumulative delivery of pollutants to downstream wetlands and estuaries (Yigitcanlar et al., 2018; Figueiroa and Scherer, 2016; Rodrigues et al., 2026). This disconnect is particularly important in subtropical coastal cities of the Global South, where rapid urbanization and infrastructure limitations coincide with protected and biodiverse receiving environments (Cabral et al., 2020).

To address these gaps, we integrated 31 years of water-quality monitoring data from 26 independent sources, encompassing 120 sampling locations and 46,965 individual analyses across four subtropical coastal watersheds in Florianópolis, southern Brazil. Although all watersheds contain mangroves protected by environmental legislation, they differ markedly in urbanization intensity, population density, and sanitation coverage, providing a natural gradient of anthropogenic pressure. Accordingly, this study aimed to develop an integrated assessment of long-term water-quality conditions across four urbanizing coastal watersheds. Specifically, we sought to: (i) compile and harmonize water-quality measurements from multiple monitoring sources; (ii) assess parameter-specific compliance with regulatory standards and characterize overall pollution using the standardized Nemerow Pollution Index; (iii) identify the principal environmental and anthropogenic predictors of water-quality classes using explainable machine learning; (iv) examine whether modeled water-quality responses exhibited nonlinear transitions along urbanization and population gradients; and (v) evaluate the potential implications of projected land-use change for future monitoring and watershed management. We hypothesized that increasing watershed urbanization would be associated with nonlinear deterioration in water quality across the catchment-to-estuary continuum and that mangrove-associated waters would exhibit contrasting conditions depending on the intensity of upstream anthropogenic pressure. By identifying nonlinear water-quality responses along urbanization gradients and linking them to plausible future development scenarios, this study provides a transferable framework for integrating ecological resilience and the assimilative capacity of receiving ecosystems into the planning and management of rapidly urbanizing coastal watersheds.

Materials and Methods

Study area

Florianópolis, the capital of Santa Catarina State, is a coastal municipality in southern Brazil (Fig. 1), of which approximately two-thirds lies on Santa Catarina Island and one-third on the adjacent mainland. Approximately 39.7% of the municipal territory is designated as protected areas, whereas 19.1% is urbanized (MapBiomas, 2023). The landscape comprises forested hillslopes dominated by Atlantic Forest, flat sandy plains supporting sandbank vegetation (*restinga*), and clayey, saline environments at river mouths that sustain mangroves (Reis, 2012; Luiz, 2015). These land-cover types correspond to the forest, sandbank vegetation, and mangrove classes considered in the analyses, while urban and rural areas represent the principal anthropogenic land-use categories. The climate is humid subtropical (Cfa), with abundant rainfall throughout the year, no pronounced dry season, and precipitation concentrated in spring and summer (Peel et al., 2007). Mean temperatures range from approximately 18 to 24°C (Luiz, 2015). The tidal regime is semidiurnal and microtidal, with a mean range of approximately 0.7 m (Cruz, 1998). The island's watersheds are relatively small, and their rivers have low discharge, conditions that constrain dilution and flushing and may increase the sensitivity of receiving waters to urban pollutant inputs (Luiz, 2015; Rodrigues et al., 2021). The monitoring network encompassed the hydrologically connected continuum from freshwater tributaries and urban drainage channels to brackish and saline mangrove-associated receiving waters. This spatial arrangement allowed watershed pressures to be examined in relation to downstream coastal systems rather than treating upstream and estuarine environments as independent units.

We focused on four coastal watersheds on the western side of Santa Catarina Island: Ratonés, Saco Grande, Itacorubi, and Tavares. Together, these watersheds encompass approximately 44% of the island and contain major mangrove ecosystems within the municipality. The mangroves of the Ratonés and Saco Grande watersheds are protected within the Carijós Ecological Station, established in 1987; the Tavares River mangrove is protected within the Pirajubaé Marine Extractive Reserve, established in 1992; and the Itacorubi mangrove is protected within the Itacorubi Mangrove Municipal Park, established in 2002. Thus, all four study watersheds contain mangrove ecosystems under formal legal protection, while differing substantially in urbanization intensity and other forms of anthropogenic pressure (Fig. 1). The four watersheds are small (17.7 – 100.7 km²), with mean annual discharge ranging from 0.31 to 2.06 m³ s⁻¹ (Table 1).

Florianópolis had an estimated population of 576,361 inhabitants in 2024 (IBGE, 2026),

147 while sewerage services reached approximately 56% of the population according to available
148 municipal-scale data (ANA, 2017). The four watersheds differ in population size, urbanization, forest,
149 rural, and sandbank vegetation covers, mangrove extent, and sanitation and drainage infrastructure
150 (Table 1), providing a spatial gradient of anthropogenic pressure for assessing variation in water
151 quality. Future urban expansion and densification are also expected to substantially increase both
152 the extent of developed areas and population, with the municipal Master Plan projecting a 135%
153 increase in urbanized area, primarily through the conversion of rural land and sandbank vegetation
154 environments (Rodrigues et al., 2026). This combination of contrasting present-day watershed conditions
155 and projected future urban expansion provides a suitable setting for evaluating how watershed
156 characteristics and anthropogenic pressure shape coastal water quality and for assessing the potential
157 consequences of continued urban expansion for mangrove-associated coastal ecosystems.

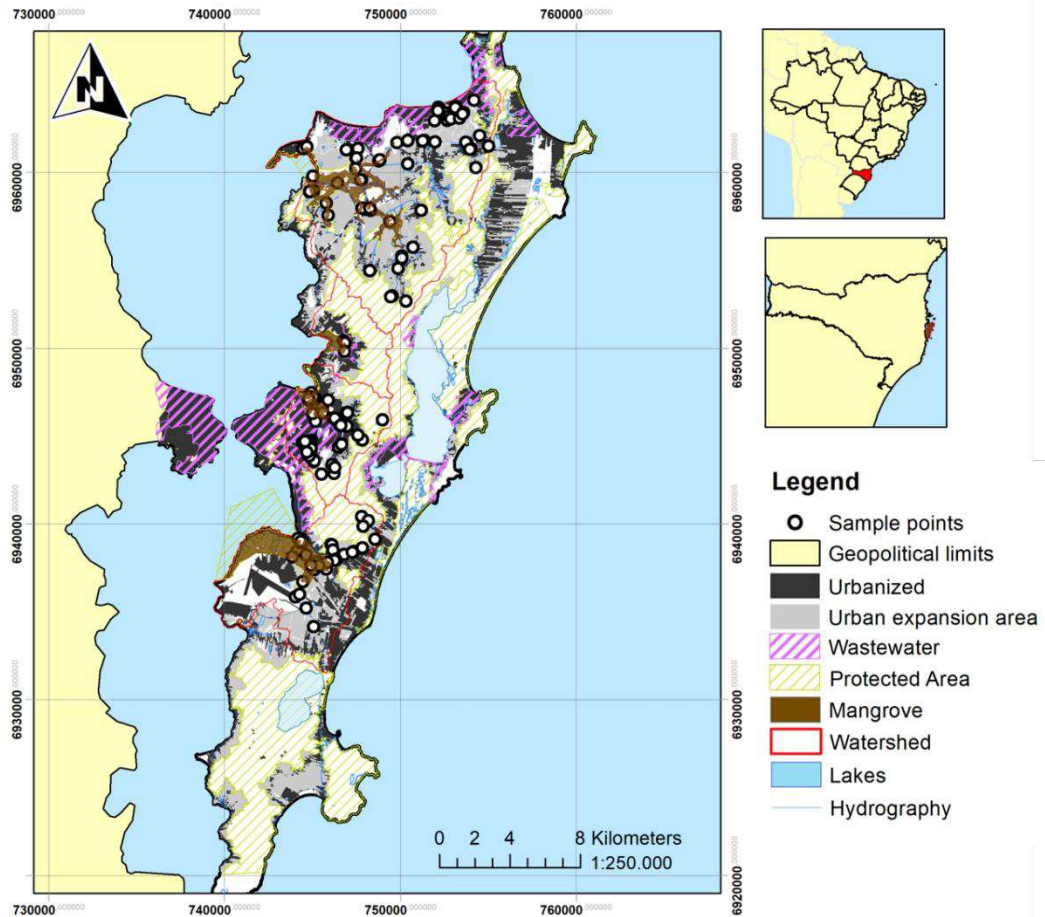


Fig. 1. Map of Florianópolis, southern Brazil, showing urbanized and developable areas, sewerage coverage, and sampling locations represented in the compiled secondary water-quality database for the Ratones, Saco Grande, Itacorubi, and Tavares watersheds.

Table 1. Physical, environmental, land-use, demographic, and sanitation characteristics of Florianópolis and the four study watersheds.

City/Watershed	Florianópolis	Ratones	Saco Grande	Tavares	Itacorubi
Area (km ²) ^a	443.1	100.7	17.7	49.6	28.3
Average flow rate (m ³ s ⁻¹) ^b	—	2.06	0.31	0.95	0.52
Resident population (inhabitants) ^c	537,031	36,383	19,634	49,700	85,870
Population density (inhabitants/km ²)	1,212	361	1,109	1,002	3,034
Urbanized area (%) ^a	19.11	14.6	17.9	28.1	36.7
Sewage coverage (%) ^c	56	37	13.2	0	61.3
Sewage deficit density (housing equivalents/km ²)	533	228	963	1,002	1,174
Streets with drainage (%) ^d	10.4	25.8	13.7	40.0	13.7
Mangrove area (%) ^a	3.2	5.8	4.6	12.6	3.9
Inhabitants without sewage service per km ² of mangrove forest	167	39	209	80	301

<i>Urbanization planned in the Master Plan (%)</i>	45	58	34	52	50
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^a Mapbiomas (2023)

^b Santa Catarina (2006)

^c PMF (2019)

^d Finotti et al. (2021).

Land use, demographic, and climate predictors

Land-use and land-cover (LULC) data from 1985 to 2023 were obtained from the MapBiomas Project (Collection 9; Souza Jr. et al., 2020; MapBiomas, 2023). LULC classes were aggregated into the categories used as predictor variables in the models: urban areas, forest, rural areas (sum of the pasture and agricultural mosaic categories), and sandbank vegetation. For each watershed and year, the proportional cover of each class was calculated to represent landscape composition and the degree of anthropogenic modification. Spatial information on sanitation infrastructure was obtained from municipal databases, including sewerage coverage (PMF, 2019) and stormwater drainage networks (Finotti et al., 2021). These variables were used to characterize differences in wastewater management and urban infrastructure among watersheds. Population estimates were obtained from the Brazilian Institute of Geography and Statistics (IBGE, 2025) demographic censuses for census years 1992, 2000, 2010, and 2022. Population density and total population per watershed were estimated from census-tract information and used as indicators of demographic pressure. Values between census years were interpolated to match the temporal resolution of the water-quality database.

Daily precipitation records from four meteorological stations were obtained from DECEA station 83899 (-27.67, -48.55), EPAGRI stations 1006 (-27.58, -48.51) and 2024 (-27.47, -48.49), and INMET station A806 (-27.60, -48.62). Precipitation data were used to characterize climatic variability among sampling dates. The Multivariate ENSO Index (MEI; Wolter and Timlin, 2011) was obtained from NOAA (2025) to represent the influence of El Niño Southern Oscillation variability on regional climate conditions. MEI values range from approximately -3 to +3, with positive values representing El Niño conditions and negative values representing La Niña conditions. For each water-quality observation, the corresponding MEI value was assigned according to sampling date.

Water-quality database compilation

Surface water-quality data were identified through previous regional literature surveys (Lopes et al., 2020; Cabral et al., 2020) and a complementary search of technical and administrative records maintained by the Chico Mendes Institute for Biodiversity Conservation (ICMBio). The resulting database integrated original event-level measurements from 26 monitoring sources conducted between 1992 and 2023, comprising 17 academic studies and 9 technical studies or monitoring reports. When original measurements were not available in academic publications or their supplementary materials, the authors were contacted and asked to provide the underlying datasets. Parameter names and units were standardized across sources, with molar concentrations converted to mass concentrations according to the chemical species originally reported. Sampling coordinates were organized as a spatial point layer in QGIS® v.3.40.7 and assigned to the corresponding watersheds and contributing sub-basins. The total database comprised 46,965 measurements of 40 water-quality variables from 3,371 sampling events at 120 locations. Sampling locations represented different portions of the catchment-to-estuary continuum, including freshwater tributaries, transitional waters and mangrove-associated receiving environments. Water type and applicable regulatory criteria were defined for each sampling event according to salinity and Brazilian Resolution CONAMA No. 357/2005, using criteria for Class 2 freshwaters and Class 1 brackish and saline waters. Detailed procedures for data acquisition, standardization, unit conversion, spatial organization, regulatory classification, and traceability are provided in the Supplementary Material.

To synthesize multiple water-quality parameters into a single measure of overall pollution, we calculated the Nemerow Pollution Index (NPI; Nemerow and Sumitomo, 1971). The NPI expresses observed concentrations relative to the maximum values permitted by Brazilian water-quality legislation, integrating multiple contaminants while preserving the influence of the most impaired parameter (Abbasi and Abbasi, 2012). This property makes the index particularly suitable for assessing complex pollution patterns in estuarine and mangrove environments, where water quality is influenced by multiple interacting stressors (Liu and Myat, 2021). The NPI was calculated according to Eqs. 1 and 2:

$$RPC = \frac{c_i}{L_{ij}} \quad \text{Eq. 1}$$

$$NPI = \sqrt{\frac{(RPC)_{max}^2 + (RPC)_{average}^2}{2}} \quad \text{Eq. 2}$$

226

227 where RPC is the relative pollution contribution of each parameter, C_i is the measured
 228 concentration, and L_{ij} is the corresponding maximum value permitted by legislation.

229 The NPI was calculated separately for each sampling event, defined as a unique combination
 230 of sampling location and sampling date. Each sampling event therefore generated a single NPI value,
 231 although the number of water-quality variables measured varied among events. To ensure that the
 232 index provided a representative assessment of overall water quality, sampling events were retained
 233 only if they met three criteria: (i) at least four water-quality variables were available for NPI
 234 calculation; (ii) the resulting NPI value was not identified as an outlier ($Q1-1.5 \times IQR$; $Q3+1.5 \times IQR$;
 235 $Q1$ and $Q3$ are first and third quartiles; IQR = interquartile range); and (iii) salinity measurements
 236 were available to evaluate potential dilution effects associated with seawater intrusion. After applying
 237 these criteria, the final analytical dataset comprised 2,603 sampling events distributed across the four
 238 watersheds between 1992 and 2023.

239 Because NPI values are unbounded ($0 - \infty$), we applied a base-10 logarithmic transformation
 240 to compress the scale while preserving the relative ordering of observations. Log-transformed values
 241 were subsequently standardized (Eq. 3), producing the standardized Nemerow Pollution Index
 242 (StdNPI), which ranges from 0 to 100 and facilitates comparisons among sampling events. Higher
 243 StdNPI values indicate better water quality, whereas lower values indicate greater pollution.

$$StdNPI_i = 100 - \left[\frac{\log_{10}(NPI_i) - \log_{10}(NPI_{\min})}{\log_{10}(NPI_{\max}) - \log_{10}(NPI_{\min})} \times 100 \right] \quad \text{Eq. 3}$$

244

245 where $NPI_{\min}$ and $NPI_{\max}$ are the minimum and maximum observed NPI values, respectively.

246 The original formulation of the NPI does not define qualitative water-quality classes.
 247 Therefore, following thresholds commonly adopted in previous applications of the index (e.g., Su et
 248 al., 2022), NPI values were classified into four categories: Clean ($NPI \leq 1$), Light pollution ($1 <$
 249 $NPI \leq 2$), Pollution ($2 < NPI \leq 5$), and Heavy pollution ($NPI > 5$) (Table 2).

250

251 **Table 2:** Water-quality categories, in terms of pollution levels, according to the NPI values

<i>NPI</i>	<i>StdNPI</i> (standardized)	<i>Pollution levels</i>
$NPI \leq 1,0$	100 – 64	Clean
$1,0 < NPI \leq 2,0$	63 – 55	Light pollution
$2,0 < NPI \leq 5,0$	54 – 45	Pollution

Data analysis

Water quality was assessed using two complementary approaches. First, compliance with the maximum concentrations established by Brazilian water-quality legislation (Brazil, 2005) was evaluated for each monitored parameter. Second, overall water quality was synthesized using the standardized Nemerow Pollution Index (StdNPI; Eq. 3), which integrates multiple pollutants into a single event-level metric. To evaluate how anthropogenic pressures at the watershed scale influenced water quality, we compared StdNPI values across gradients of watershed urbanized area, sewerage coverage, population size, and mangrove presence using the non-parametric Kruskal–Wallis test followed by Dunn's multiple comparisons with Bonferroni correction ($\alpha = 0.05$). To distinguish ecological buffering from simple seawater dilution, Spearman's rank correlation ($\alpha = 0.01$) was used to examine the relationship between salinity and StdNPI.

To identify the environmental and anthropogenic drivers of water quality, quantify their relative importance, detect nonlinear ecological thresholds, and project future scenarios, we developed supervised machine-learning models using Extreme Gradient Boosting (XGBoost; Chen and Guestrin, 2016). Because water quality was classified into four pollution categories, XGBoost was implemented as a multiclass classification model. XGBoost sequentially combines decision trees while incorporating regularization to reduce overfitting, making it well suited to heterogeneous environmental datasets and nonlinear ecological relationships. The response variable comprised the four NPI-based water-quality classes (“clean”, “light pollution”, “pollution”, and “heavy pollution”).

Candidate predictors represented four classes of watershed predictors: (i) landscape composition (urban, forest, rural, sandbank, and mangrove cover); (ii) anthropogenic pressure (log-transformed population, sewerage coverage, and stormwater drainage coverage); (iii) climatic and hydrological conditions (water temperature, salinity, previous-day rainfall, and the Multivariate ENSO Index); and (iv) categorical descriptors of environmental condition, including sampling location (inside or outside mangroves), ENSO phase and intensity, salinity class (Venice classification), and watershed imperviousness classes following Schueler et al. (2009). Watershed-scale predictors were quantified for each sampling location by delineating 24 contributing sub-basins across the four study watersheds (Fig. 2). Land-use composition, demographic variables, and sanitation infrastructure were then

quantified within each contributing area, ensuring that all predictors represented the hydrologically connected watershed upstream of each sampling site.

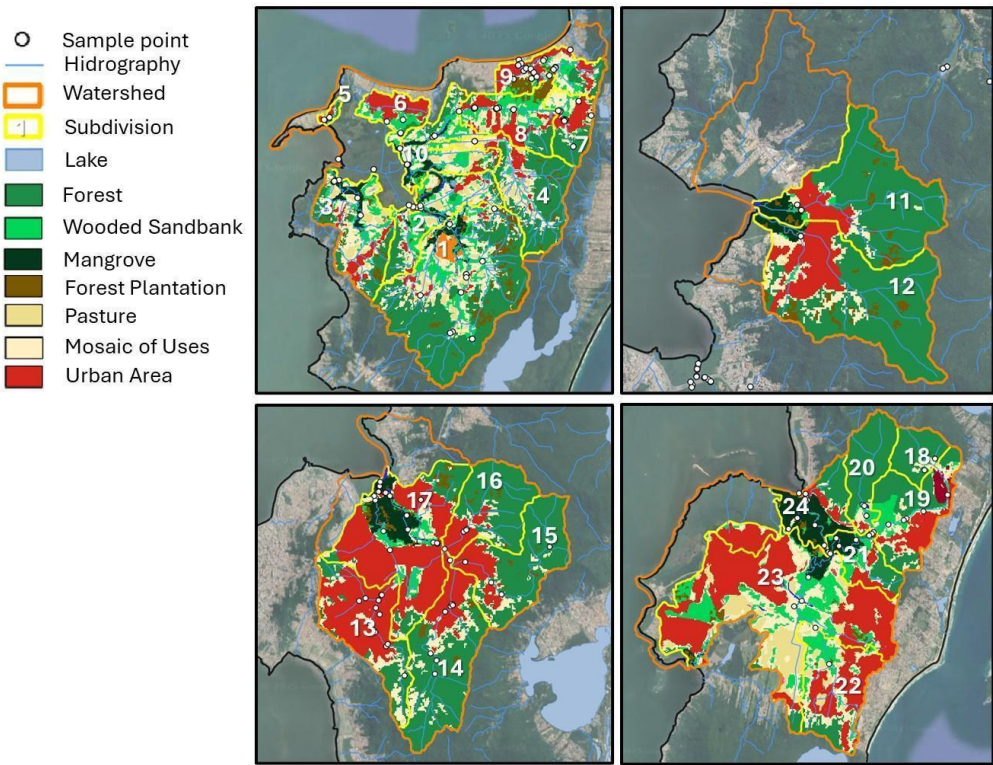


Figure 2. Study watersheds, sampling locations, and contributing sub-basins used to assign watershed-scale predictors. Orange lines delineate watershed boundaries, whereas yellow lines indicate the 24 contributing sub-basins used to quantify watershed-scale predictors for each sampling location (numbered in the figure).

Model development comprised six sequential stages (Fig. 3). First, the dataset was randomly partitioned into stratified training (75%) and testing (25%) subsets while preserving the original distribution of water-quality classes. Second, numerical variables were standardized, categorical predictors were converted to dummy variables, and class imbalance in the training dataset was corrected using the Synthetic Minority Over-sampling Technique (SMOTE; Chawla et al., 2002). An initial XGBoost model including all candidate predictors was optimized using Bayesian hyperparameter optimization (Snoek et al., 2012), with multinomial log-loss as the objective function. Predictor selection was based on the gain metric, retaining variables that together accounted for 70% of cumulative model importance. A second Bayesian optimization was then performed to calibrate the final model using only the selected predictors. Model performance was evaluated exclusively using

the independent test dataset. Because SMOTE alters class frequencies during model training, predicted class probabilities were corrected to account for prior probabilities before evaluation. Predictive performance was assessed using receiver operating characteristic (ROC) curves and the corresponding area under the curve (AUC), overall accuracy, F1-score, Cohen's kappa, Brier score, confusion matrices, and calibration curves based on Spiegelhalter's Z statistic (Spiegelhalter, 1986). Spatial autocorrelation in the model prediction residuals in the test set was evaluated using Moran's I test (Moran, 1950). The temporal structure of these residuals was then investigated using the Ljung-Box Q test (Ljung & Box, 1978) applied to the annual mean residuals. To improve model interpretability, we applied SHapley Additive exPlanations (SHAP) to quantify the magnitude and direction of each predictor's contribution to the model's predictions, enabling the identification of key environmental determinants and non-linear ecological thresholds (Ponce-Bobadilla et al., 2024).

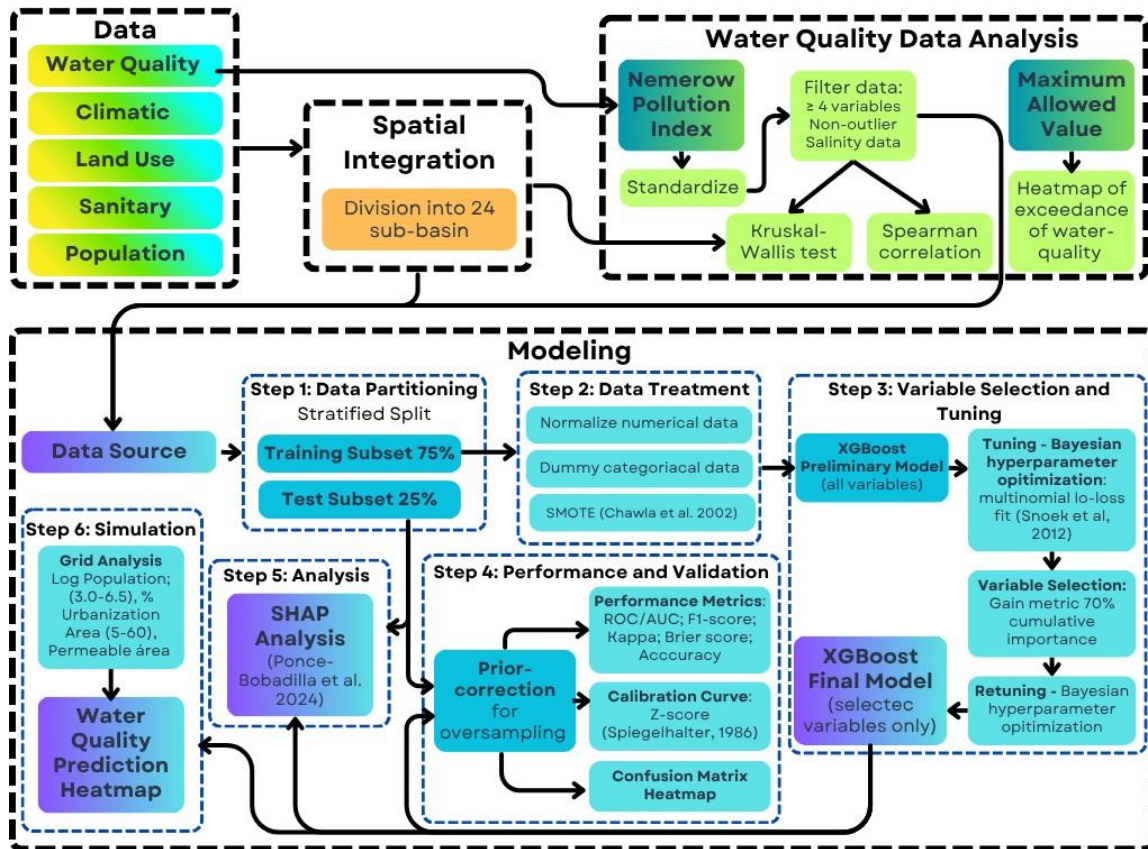


Figure 3. Analytical workflow summarizing database compilation, water-quality assessment, XGBoost model development and validation, SHAP-based model interpretation, and simulation of future urbanization scenarios.

Finally, the calibrated model was used to simulate water-quality conditions under projected

urbanization scenarios. Predictions were generated over a scenario grid defined by log-transformed population (3.0–6.5), urban land cover (5–60%), the observed proportional composition of the remaining land-use classes, and median values for all other predictors. Current watershed conditions and projected future urbanization scenarios were subsequently projected onto this prediction surface to evaluate the potential consequences of continued urban expansion for coastal water quality (Supplementary Material, Table S2). All analyses were performed in R 4.5.2 (R Core Team, 2025).

Results

Between 1985 and 2023, urban land cover in Florianópolis increased by 74%, primarily through the conversion of rural and pasture areas (–47%) and heterogeneous land-use mosaics (–39%) (Supplementary Material, Fig. S1). During the same period, mangrove (+12%) and forest (+7%) cover increased slightly, whereas sandbank vegetation declined by 6%, indicating that urban expansion occurred predominantly at the expense of other terrestrial land-cover classes.

Exceedances of Brazilian water-quality standards were frequent across all watersheds (Fig. 4). Total organic carbon (98%), surfactants (72%), *Escherichia coli* (71%), total phosphorus (64%), and dissolved oxygen (60%) exhibited the highest frequencies of non-compliance, indicating widespread organic enrichment associated with domestic sewage inputs. Among watersheds, Itacorubi recorded the highest proportion of samples exceeding legal standards (54%), followed by Saco Grande (41%), Ratones (38%), and Tavares (33%). Ratones and Tavares, which had the lowest densities of inhabitants lacking sewerage per square kilometre of mangrove (Table 1), also exhibited lower exceedance frequencies for ammoniacal nitrogen and higher frequencies for nitrite and nitrate, suggesting more effective nitrification and pollutant transformation within mangrove ecosystems.

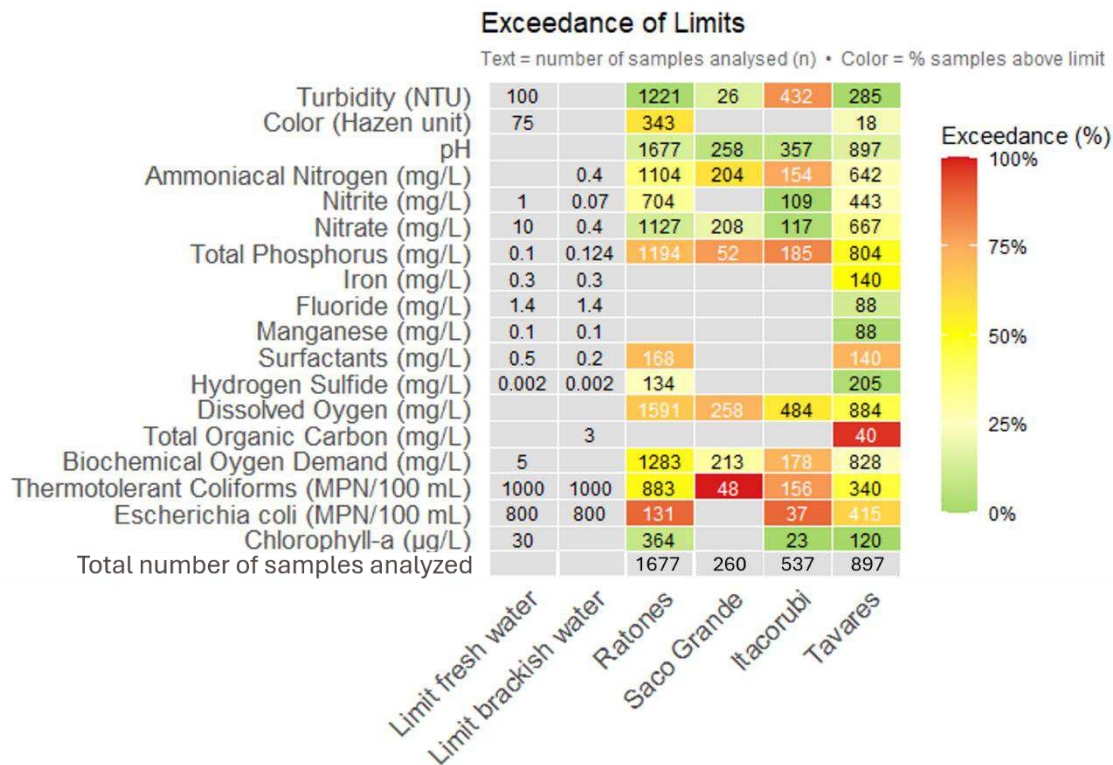


Figure 4. Heatmap of exceedance of water-quality parameters relative to the limits set by Brazilian Resolution CONAMA 357/2005.

After quality filtering, 2,603 sampling events were classified using the standardized Nemerow Pollution Index (StdNPI) as “Clean” ($n = 451$), “Light pollution” ($n = 803$), “Pollution” ($n = 807$), or “Heavy pollution” ($n = 542$). Ratones, Saco Grande, and Tavares were dominated by the intermediate water-quality classes, whereas Itacorubi was characterized predominantly by “Heavy pollution” (Fig. 5A). Water-quality classes shifted systematically along gradients of watershed urbanization and population size (urbanized area $X^2 = 345.3$, $df = 3$, $p < 0.001$; population $X^2 = 368.7$, $df = 3$, $p < 0.001$; Fig. 5B,C; Supplementary Material, Table S3), with progressively poorer water quality observed in more urbanized and densely populated watersheds. Water quality also deteriorated with increasing stormwater drainage

coverage, although the “Pollution” and “Heavy pollution” classes did not differ significantly (Fig. 5D). Differences between the “Light pollution” and “Pollution” classes were likewise not significant along the sewerage coverage gradient (Fig. 5E). Water-quality classes also varied significantly with mangrove extent within watersheds, except between the “Clean” and “Pollution” classes (Fig. 5F; Supplementary Material, Table S3).

In Ratones, StdNPI values were significantly higher inside the mangrove than at upstream locations. In contrast, StdNPI values were lower inside the Tavares mangrove (Fig. 5G). These opposing patterns indicate that downstream water-quality conditions varied according to watershed context rather than responding uniformly to mangrove presence. StdNPI showed only a negligible association with salinity (Spearman correlation, $\rho = -0.04$; $p = 0.041$; Supplementary Material, Fig. S2), which was not statistically significant under the predefined $\alpha = 0.01$. Thus, salinity alone did not explain the broad water-quality patterns observed across the dataset.

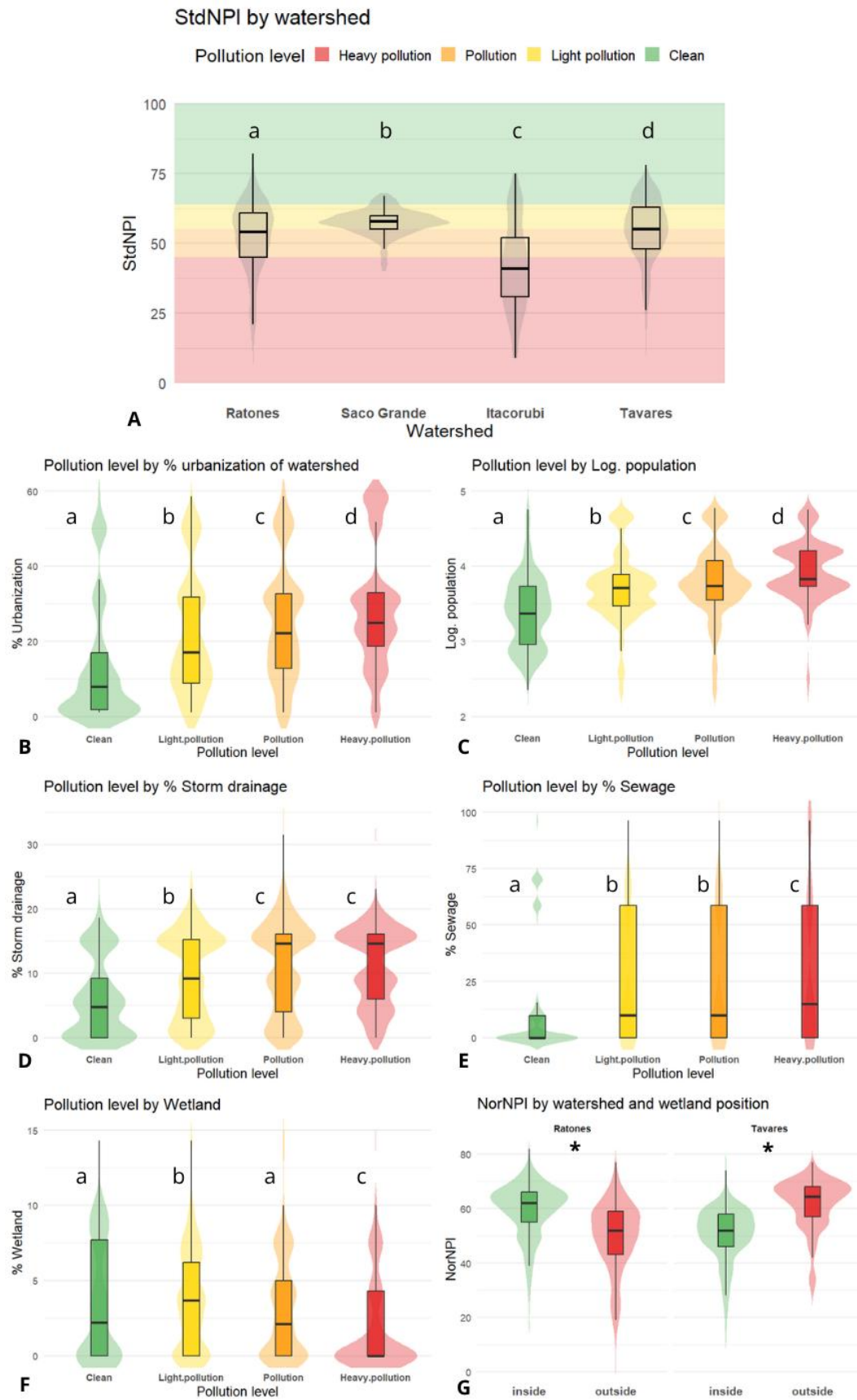


Figure 5: Violin plots with over-laid box-plots showing the distribution of the StdNPI index (y-axis). A) StdNPI in the evaluated watersheds. Pollution levels in relation to: B) percentage of

urbanization in the watershed; C) the log-transformed watershed population; D) the percentage of storm drainage network in the watershed; E) the percentage of sewage network in the watershed; F) the percentage of wetland area (mangrove) in the contributing watershed; G) comparison regarding the sampling position relative to mangrove habitat (inside vs. outside) in the watershed with data available for comparison (Ratones and Tavares). The violin outline depicts data density; the box shows the interquartile range, and the central line marks the median. Kruskal-Wallis test (*) Dunn *post hoc* test with Bonferroni adjustment for groups (a, b, c, d).

The optimized XGBoost model retained nine predictors that together accounted for 70% of cumulative model importance: water temperature (Temp), the Multivariate ENSO Index (MEI), salinity (Salt), log-transformed population (LogPop), and the percentage cover of urban, forest, rural, restinga, and mangrove (AU) land uses (Supplementary Material, Fig. S3). The optimized hyperparameter values are reported in Supplementary Material (Table. S4). The final model showed good predictive performance on the independent test dataset, achieving a mean ROC/AUC of 0.841 across the four water-quality classes (Supplementary Material, Fig. S4). Overall accuracy was 0.607, with a mean F1-score of 0.610 and Cohen's κ of 0.463. Probabilistic performance was also satisfactory, with a Brier score of 0.259. Calibration curves closely followed the 1:1 reference line (Supplementary Material, Fig. S5), and Spiegelhalter's Z tests indicated no significant lack of calibration for any water-quality class ("Clean": $Z = -0.285$, $p = 0.776$; "Light pollution": $Z = -0.388$, $p = 0.698$; "Pollution": $Z = -0.586$, $p = 0.558$; "Heavy pollution": $Z = 1.514$, $p = 0.130$). The confusion matrix confirmed that classification accuracy was consistently higher than expected by chance across all four pollution classes (Fig. 6), supporting the ability of the model to discriminate among water-quality conditions in heterogeneous estuarine environments. Residual diagnostics indicated significant spatial autocorrelation in the prediction errors (Moran's $I = 0.067$, $p < 0.001$), suggesting that some spatially structured variation remained unexplained by the model. In contrast, the Ljung-Box test applied to annual mean residuals showed no evidence of temporal autocorrelation ($X^2 = 6.14$, $df = 10$, $p = 0.80$).

Having established the predictive performance of the model, we used SHAP analyses to quantify the relative influence of individual predictors and identify nonlinear thresholds associated with water-quality degradation.

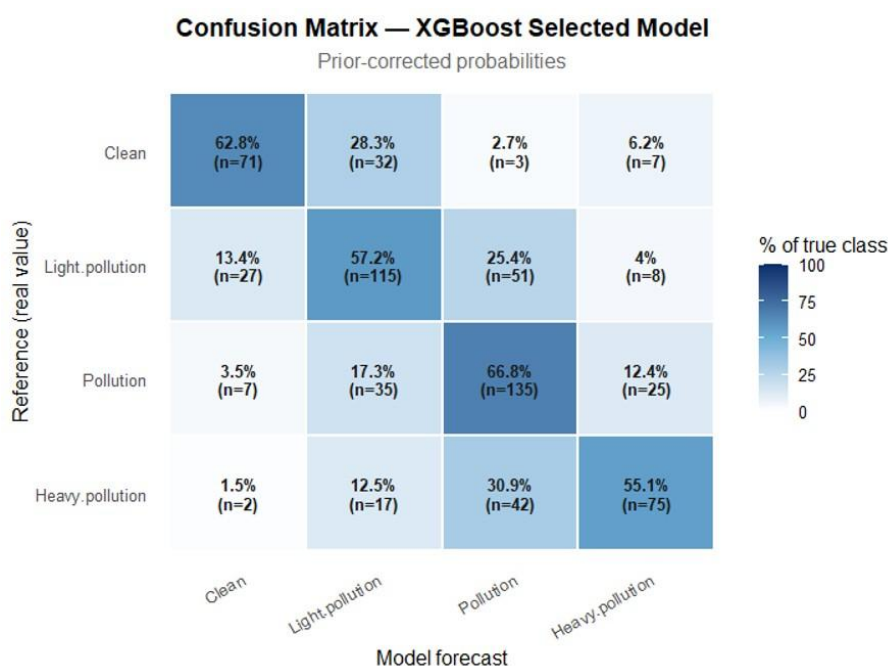


Figure 6: Confusion matrix of the XGBoost model on the test set, values within the cells represent the percentage of observations per true class.

Global SHAP analysis confirmed that watershed urbanization (Urban) was the dominant predictor of water-quality classification, followed by log-transformed population (LogPop), mangrove cover (AU), the Multivariate ENSO Index (MEI), and the proportions of rural, forest, and sandbank land cover, whereas salinity and water temperature showed comparatively smaller contributions (Supplementary Material, Fig. S6). Beyond ranking predictor importance, SHAP analyses quantified both the direction and magnitude of each predictor's contribution to the probability of each water-quality class.

For the “Clean” class, low levels of urbanization and population exerted the strongest positive influence on model predictions (SHAP values approaching +1), indicating that watersheds with limited human occupation were consistently associated with high water quality (Fig. 7). An apparent transition at around 10% urban cover and a population of approximately 3,000 inhabitants (log 3.5), above this level, urbanization and population progressively reduced the modeled probability of clean water conditions (Fig. 8). These values represent a model-derived transition within the observed environmental domain rather than a universal ecological or regulatory threshold. Higher salinity also increased the probability of this class. Mangrove cover (AU) contributed positively to the probability of clean conditions, particularly under low levels of watershed urbanization. The “Light pollution” class

exhibited the smallest SHAP magnitudes (approximately -0.5 to $+0.5$), indicating that no individual predictor dominated model predictions. Instead, this class emerged under intermediate combinations of anthropogenic and environmental conditions, representing a transitional state between preserved and degraded watersheds. For the "Pollution" class, positive MEI values, associated with El Niño conditions, substantially increased the probability of classification (SHAP values approaching $+0.75$). Intermediate levels of watershed urbanized area combined with relatively high population density also increased the probability of this class. The "Heavy pollution" class was primarily associated with highly urbanized watersheds characterized by high population density and reduced mangrove cover. Under these conditions, increasing urbanization and population produced the largest positive SHAP values, whereas decreasing AU further increased the probability of severe pollution, identifying extreme watershed urbanization as the dominant driver of the most degraded water-quality conditions. Overall, SHAP analyses showed that increasing watershed urbanization and population consistently shifted model predictions from the "Clean" toward the "Heavy pollution" class (Fig. 7)

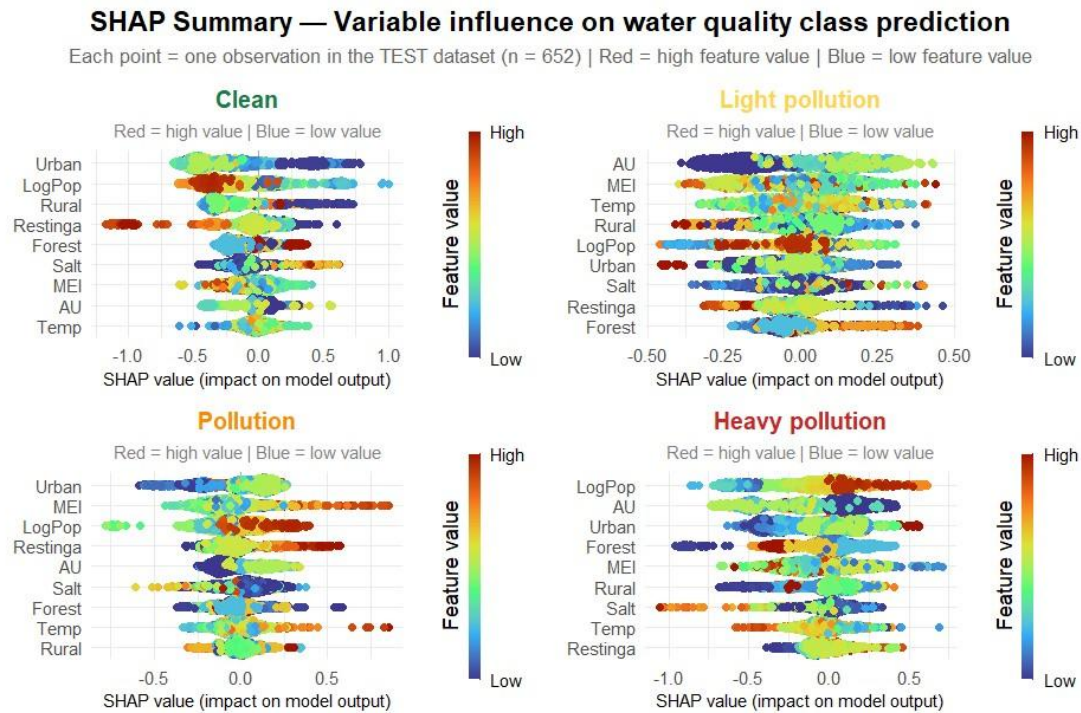


Figure 7. SHAP (SHapley Additive exPlanations) summary beeswarm plots showing the contribution of each predictor to the four water-quality classes in the final XGBoost model. Each point represents one sampling event. Horizontal position indicates the SHAP value, where positive values increase and negative values decrease the probability of the corresponding class. Point color

represents the standardized predictor value (red = high; blue = low).

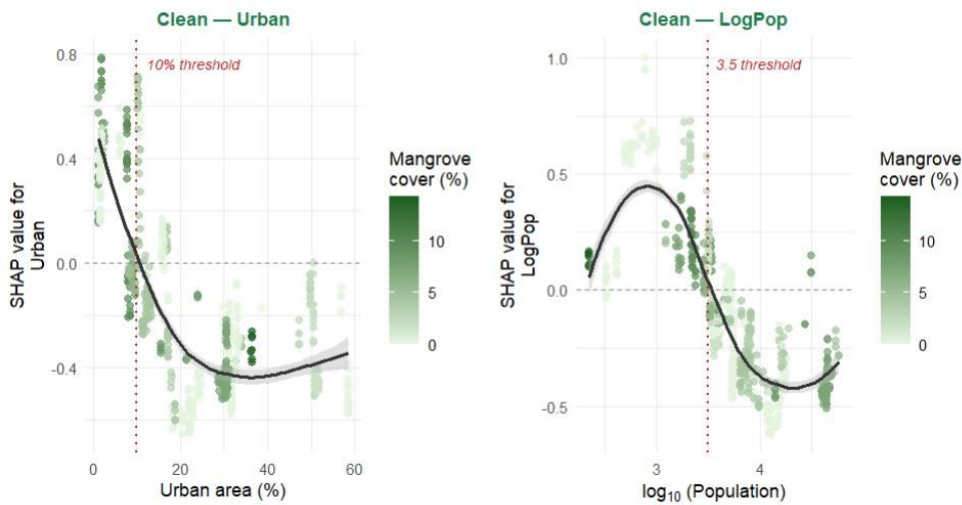


Figure 8. SHAP dependence plots showing the interaction effects of watershed urbanization and population density with mangrove cover on the probability of clean water quality.

The dominant predictors of water-quality classification identified by SHAP (urbanization and population) were subsequently used to simulate future water-quality responses under increasing urbanization (Fig. 9). Simulations incorporating projected population growth and proportional conversion of permeable land to urban areas (39.2% rural, 39.5% forest, 18.0% restinga, and 3.2% mangrove) predicted a marked shift toward poorer water quality. Across the scenario space, the predicted distribution of water-quality classes was 3.6% “Clean”, 50.0% “Light pollution”, 19.6% “Pollution”, and 26.8% “Heavy pollution”. Overlaying current watershed conditions and projected future scenarios onto the prediction surface revealed consistent deterioration in water quality across all watersheds (Fig. 9). Ratones, Saco Grande, and Tavares shifted toward more degraded water-quality classes under projected urban expansion, whereas Itacorubi remained within the “Heavy pollution” category, reflecting its already highly urbanized condition.

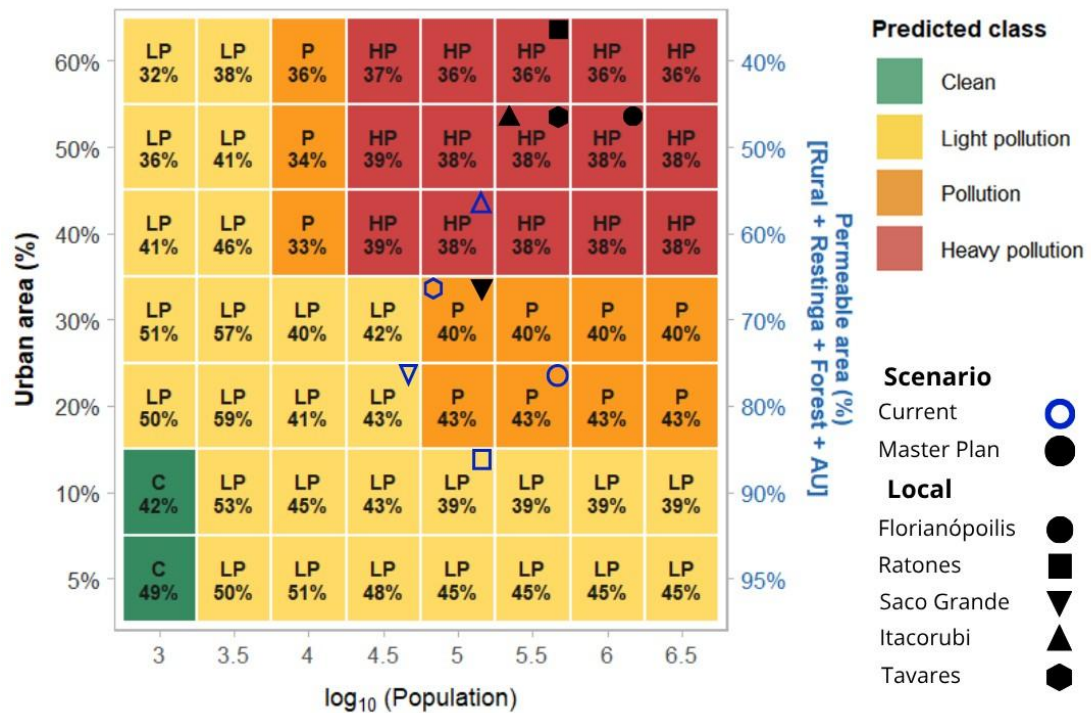


Figure 9. Predicted probabilities of water-quality classes generated by the calibrated

XGBoost model across gradients of watershed population and urban land cover. Current watershed conditions and projected urbanization scenarios are overlaid on the prediction surface to illustrate expected water quality transitions under continued urban expansion.

Discussion

Our results show that water-quality conditions across four mangrove-associated coastal watersheds were structured primarily by anthropogenic pressures in the hydrologically connected contributing areas. Urban cover and population were the predominant predictors of pollution classes, and the modeled probability of clean-water conditions declined nonlinearly along the urbanization gradient. However, mangrove-associated water-quality responses were not uniform among watersheds. Conditions improved inside the Ratones mangrove but deteriorated inside the Tavares mangrove, indicating that downstream wetland condition depends on the magnitude and configuration of upstream pressures rather than on protected status or mangrove extent alone. Scenario projections further suggested that urban expansion permitted under current zoning would move the studied watersheds toward landscape conditions associated with poorer water quality. Together, these findings demonstrate that estuarine conservation cannot be separated from management of the connected watershed and that legal protection

of downstream habitats may be insufficient where urban development and inadequate sanitation maintain chronic pollutant delivery.

The observed deterioration in water quality was primarily driven by untreated or insufficiently treated domestic wastewater. Across the four watersheds, the highest frequencies of non-compliance with Brazilian water-quality standards were observed for *E. coli*, thermotolerant coliforms, total organic carbon, biochemical oxygen demand, total phosphorus, ammoniacal nitrogen, and surfactants, all characteristic indicators of domestic sewage inputs. These patterns were most pronounced in the Itacorubi watershed, where legal exceedances reached 54% of all analyses. Florianópolis still relies heavily on onsite sanitation systems, with approximately 36% of the population served by septic tanks and soakaways (ANA, 2017). Such systems generally provide lower treatment efficiency than conventional networked sewerage systems and become particularly vulnerable during periods of intense rainfall, when soil saturation and flooding increase the likelihood of wastewater reaching stormwater networks and receiving waters (Wear et al., 2024). This interpretation is further supported by the XGBoost model, which identified positive MEI values, indicative of El Niño conditions, as important predictors of degraded water quality. Because El Niño increases rainfall over southern Brazil, projected increases in extreme precipitation are likely to amplify this climatic influence by increasing pollutant transport and placing additional pressure on the assimilative capacity of these coastal watersheds (Caprario et al., 2022). These projections reinforce the need for watershed planning that explicitly incorporates climate variability and future climate change into sanitation design and coastal water-quality management, rather than treating them as exceptional or secondary considerations (Howard et al., 2016; Hyde-Smith et al., 2022).

Contrary to expectations, sewerage coverage explained relatively little of the observed variation in water quality. Although the Itacorubi watershed had the highest proportion of households connected to the sewerage network (61.3%), it consistently exhibited the poorest water quality among the four watersheds. This apparent contradiction reflects the limitations of using infrastructure coverage as a proxy for environmental protection. Itacorubi also has the largest absolute sewerage deficit and the highest number of inhabitants without sewerage service per square kilometer of mangrove, resulting in pollutant loads that are likely to exceed the assimilative capacity of the receiving ecosystem. Consequently, the effectiveness of sanitation infrastructure depends not only on the proportion of the population served, but also on the balance between pollutant inputs

and the capacity of downstream ecosystems to retain, transform, or remove contaminants. This interpretation is consistent with the comparatively low importance of sewerage coverage in the XGBoost model and suggests that sanitation policies based solely on coverage targets may substantially overestimate environmental protection in densely populated coastal watersheds (Cabral et al., 2019; Rodrigues et al., 2021; Buttner et al., 2022).

Stormwater drainage emerged as a stronger predictor of water-quality degradation than sewerage coverage, highlighting the critical role of pollutant transport pathways in urban watersheds. Although Brazilian legislation requires separate sewerage and stormwater systems, inspections in Florianópolis indicate that approximately 75% of inspected household connections contain irregular cross-connections (PMF, 2026), allowing untreated wastewater to enter stormwater networks or rainfall runoff to overload sewerage infrastructure. Previous studies have similarly identified stormwater drainage as a major pathway for contaminant delivery to rivers and estuaries in the municipality (Garbossa et al., 2017; Cabral et al., 2019). Our results further indicate that watersheds with stormwater drainage coverage exceeding approximately 15% were consistently associated with the most degraded water-quality classes. This relationship is likely reinforced by the predominance of conventional stormwater systems in the studied watersheds, which are designed to rapidly convey surface runoff and associated pollutants to receiving waters rather than promoting infiltration or retention. In the short, low-discharge rivers that characterize Santa Catarina Island, where assimilative capacity is inherently limited (Luiz, 2015; Rodrigues et al., 2021), this rapid hydraulic transfer reduces opportunities for dilution and natural attenuation, amplifying the effects of urbanization on water quality. Together, these findings indicate that improving coastal water quality will require not only expanding sewerage infrastructure but also reducing pollutant transport through improved drainage system operation and greater adoption of infiltration-based and other nature-based stormwater management strategies (Rech, 2019).

The results indicated a marked nonlinear response to watershed urbanization, where the probability of maintaining clean water conditions dropped sharply once urban land cover exceeded approximately 10% of the watershed area, suggesting an apparent nonlinear transition in modeled water-quality probability. The ecological significance of this threshold is illustrated by the contrasting responses of the Ratones and Tavares watersheds. Although lower mangrove cover was generally associated with poorer water quality, mangrove extent alone did not determine downstream water-

quality condition. Instead, the capacity of mangroves to improve water quality depended strongly on watershed context. In Ratonés, higher StdNPI values inside the mangrove were consistent with net attenuation along the upstream-to-estuary continuum, although the compiled observations do not distinguish among retention, transformation, mixing and dilution processes. In contrast, lower StdNPI values inside the Tavares mangrove were consistent with cumulative upstream inputs exceeding the net attenuation detectable from the compiled monitoring records. This watershed combines high population density, concentrated urban occupation immediately upstream of the estuary, and widespread reliance on site sanitation systems, conditions that likely increase pollutant delivery while reducing the time available for natural attenuation before runoff reaches the mangrove. Together, these contrasting responses indicate that mangroves function as effective biogeochemical filters only as long as external pollutant loads remain within their assimilative capacity. Under watershed pressures above the observed transition range, increasing mangrove extent alone is unlikely to offset continued watershed degradation. This interpretation is consistent with experimental and field studies demonstrating that chronic anthropogenic loading progressively reduces mangrove nutrient retention and pollutant removal capacity (Bimrah et al., 2022; Lovelock et al., 2024).

Multiple lines of evidence indicate that some of the studied watersheds may already be approaching or exceeding the assimilative capacity identified by our analyses. Across the 31-year monitoring period, 17% of dissolved oxygen measurements were classified as hypoxic ($< 2 \text{ mg L}^{-1}$) and 4% as anoxic ($< 0.5 \text{ mg L}^{-1}$), frequently coinciding with elevated nutrient concentrations. These conditions are consistent with chronic inputs of untreated or insufficiently treated wastewater and can fundamentally alter sediment biogeochemistry by reducing oxygen availability, disrupting microbial processes, and promoting the remobilization of sediment-bound nutrients and metals (Stumm and Morgan, 2013; Testa and Kemp, 2011). As these processes intensify, mangroves may progressively shift from effective nutrient sinks to systems that increasingly recycle accumulated contaminants back into the water column, thereby weakening the ecosystem functions responsible for water-quality regulation. Experimental nutrient-enrichment studies support this mechanism, showing that chronic organic loading alters microbial communities, impairs benthic ecosystem functioning, and reduces resilience to additional environmental stressors (Bartolini et al., 2009; Craig et al., 2021; Theuerkauff et al., 2020). Such changes can ultimately compromise biodiversity and erode the regulating ecosystem services that make mangroves effective nature-based solutions for coastal water-quality

567 protection.

568 Despite rapid urban expansion (74.2% between 1985 and 2023), Florianópolis also
569 experienced increases in forest (+7.2%) and mangrove (+12.4%) cover, primarily within legally protected
570 areas. These gains indicate that protected areas have been effective in promoting ecosystem recovery
571 and partially reversing the historical decline in mangrove extent. Nevertheless, mangroves still occupy
572 only 3.2% of the municipal territory following an estimated 42% loss between 1938 and 1998, a decline
573 exceeding the global average (Trindade, 2009; Polidoro et al., 2010). Our findings therefore reinforce,
574 rather than challenge, the importance of protected areas. However, they also demonstrate that
575 conserving mangrove fragments alone is insufficient to sustain ecosystem functioning when
576 watershed-scale urbanization exceeds ecological limits. Protected areas should therefore be
577 integrated with watershed-scale planning that explicitly considers pollutant loads, assimilative
578 capacity, and future urban expansion (Rezende et al., 2018; Friess et al., 2020).

579 The predictive scenarios generated by the XGBoost model indicate that the urban expansion
580 permitted under the current Florianópolis Master Plan would move several watersheds into
581 combinations of urban cover and population associated with lower modeled probabilities of clean-water
582 conditions, shifting predicted water quality from Light pollution to Heavy pollution and increasing
583 pollutant concentrations to more than five times the limits established by Brazilian legislation. Under
584 these scenarios, ecosystems that currently retain pollutant-removal capacity, particularly the Ratonas
585 mangrove, may experience increasing water-quality pressure and reduced potential for net attenuation as
586 upstream pollutant delivery increases. These projections suggest that the principal challenge is not the
587 degree of urbanized area itself, but urban development that proceeds without accounting for watershed
588 assimilative capacity, ecological thresholds, and the cumulative effects of soil sealing and diffuse
589 pollutant runoff (Walsh et al., 2005; Schueler et al., 2009). More broadly, our study demonstrates that
590 integrating long-term environmental monitoring with explainable machine learning approaches provides
591 a complementary framework for interpreting non-linear associations in heterogeneous long-term coastal
592 monitoring records, directly supporting urban planning and environmental policies. Rather than relying
593 solely on infrastructure coverage targets, sustainable watershed management should explicitly
594 incorporate ecosystem assimilative capacity into land-use planning, sanitation strategies, and
595 stormwater management (Santana et al., 2026). Because coastal water quality underpins
596 economically important activities such as tourism, oyster farming, and artisanal fisheries in

Florianópolis, exceeding these ecological thresholds represents not only an environmental liability but also a socioeconomic risk. More broadly, our findings suggest that urban management, specifically land-use, sanitation, and stormwater planning, must incorporate ecological limits as a precautionary framework to safeguard vital coastal ecosystem services that sustain both biodiversity and human well-being.

By integrating monitoring records collected over three decades, this study provides a regional perspective on the relationships between watershed urbanization and water quality in connected coastal environments. Differences among the original monitoring programs, including their objectives, sampling frequencies, analytical methods, and parameter combinations, were addressed through data harmonization and event-selection procedures. However, some variation among sampling events remained because the NPI was calculated from the parameters available in each event, and the resulting standardized values are specific to this dataset. The findings should therefore be interpreted primarily in terms of broad response patterns rather than direct comparisons with standardized index values from other regions. The observational nature of the study also means that wastewater influence, mangrove attenuation, and assimilative processes are inferred from convergent water-quality patterns rather than measured directly. Similarly, the transition observed along the urbanization gradient represents an approximate model-derived response within the study domain, not a universal ecological or regulatory threshold. Model performance reflects discrimination among sampling events, as the training and testing subsets were not composed of entirely independent watersheds, and the small residual spatial autocorrelation suggests that some spatially structured variation remained. Within these interpretive boundaries, the study provides consistent evidence that pressures across contributing watersheds are associated with downstream water-quality conditions in mangrove-associated coastal systems.

Although the numerical transition observed here is specific to the studied watersheds and the monitoring framework, the broader pattern is relevant to other rapidly urbanizing coastal systems. Small coastal watersheds can transfer land-use pressures to receiving estuarine environments over short hydrological distances, while deficiencies in sanitation and stormwater connectivity can increase pollutant loads even where downstream wetlands remain legally protected. The contrasting responses of Ratones and Tavares further demonstrate why the extent of mangroves is an insufficient indicator of estuarine condition. Assessments of coastal wetland resilience must, therefore, incorporate the intensity and spatial configuration of pressures across the contributing watershed.

Conclusion

By integrating 31 years of monitoring records, this study examined how conditions across hydrologically connected coastal watersheds were associated with water quality in systems draining into protected mangrove environments. Frequent exceedances of regulatory criteria for fecal indicators, organic-matter-related variables, nutrients, surfactants, and dissolved oxygen were consistent with chronic wastewater influence. Watershed urban cover and population were the predominant predictors of water-quality classes, and the modeled probability of clean conditions declined nonlinearly around 10% urban cover within the observed study domain. Contrasting conditions inside the Ratoes and Tavares mangroves indicated that downstream water-quality responses depended on the broader watershed context and were not determined by mangrove extent or protected status alone. Urban-expansion scenarios moved the watersheds toward combinations of land use and population associated with higher probabilities of degraded water quality. These findings support an integrated land-to-estuary perspective in which management of protected coastal wetlands includes their hydrologically connected contributing areas. More broadly, the study demonstrates how heterogeneous long-term monitoring records can be used to identify watershed pressures, interpret context-dependent responses of receiving coastal systems, and support precautionary management in rapidly urbanizing coastal regions.

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Conflicts of interest and ethical responsibilities: The authors declare no conflict of interest. All authors have read, understood, and have complied as applicable with the statement on “Ethical responsibilities of Authors” as found in the Instructions for Authors

Availability of data: The harmonized dataset, derived from publicly accessible sources and analytical scripts, will be deposited in Zenodo.org upon acceptance. Data provided by CASAN under a restricted-use agreement cannot be directly redistributed. A reproducible version of the analytical dataset, excluding restricted records, along with the scripts used for data processing, index calculation, model fitting, validation, and figure generation, will be made publicly available.

Code availability: All R scripts used for data harmonization, quality control, StdNPI calculation, statistical analyses, model optimization, probability correction, performance assessment, SHAP interpretation, and scenario simulation will be deposited in Zenodo.org.

Author contributions (CRediT)

Claudinei José Rodrigues: Writing – review & editing, Writing – original draft, Validation, Supervision, Project administration, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Bruno Renaly Souza Figueiredo:** Writing – review & editing, Supervision, Investigation. **Paulo Roberto Pagliosa:** Conceptualization, Investigation Methodology, Supervision, Writing – review & editing. **Michelle das Neves Lopes:** Writing – review & editing, Investigation. **Alexandra Rodrigues Finotti:** Writing – review & editing, Investigation. **Aichely Rodrigues da Silva:** Writing – review & editing, Investigation. **José Ripper Kós:** Writing – review & editing, Investigation. **Schayana Bonin dos Santos:** Data curation, Writing – review & editing. **Nei Kavaguichi Leite:** Conceptualization, Investigation Methodology, Supervision, Writing – review & editing.

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Supplementary material

Land-use

Land use data for the Tavares River watershed were obtained from the MapBiomias Project collection 9 (<https://brasil.mapbiomas.org/produtos/>), with a spatial resolution of 30 meters (Souza Jr. et al. 2020). The following classes were used: forest, mangrove, sandbank vegetation (restinga), forest plantation, pasture, mosaic of use and urban area. The data covers the period from 1985 to 2023.

Souza Jr, C. M., Z. Shimbo, J., Rosa, M. R., Parente, L. L., A. Alencar, A., Rudorff, B. F., ... and Azevedo, T., 2020. Reconstructing three decades of land use and land cover changes in brazilian biomes with landsat archive and earth engine. *Remote Sensing*, 12(17), 2735.

Data sources and harmonization

Potential data sources regarding surface water quality on Santa Catarina Island were identified through previous regional literature reviews (Lopes et al., 2020; Cabral et al., 2020) and a supplementary survey of technical and administrative records held by the Chico Mendes Institute for Biodiversity Conservation (ICMBio), the federal agency responsible for managing two of the protected areas (Carijós Ecological Station and Pirajubáé Marine Extractive Reserve) included in this study. The search identified 26 monitoring data sources covering the period from 1992 to 2023, comprising 17 academic studies (including peer-reviewed articles, dissertations, and theses) and 9 technical studies or monitoring reports obtained from ICMBio records. When original numerical measurements were not included in the academic publication or its supplementary material, the authors were contacted via email and asked to provide the original dataset. All technical studies and reports obtained from ICMBio contained spreadsheets with the original measurements and sampling site coordinates.

Only original analytical measurements corresponding to specific sampling events were incorporated into the database. Values extracted from figures, as well as results available only as ranges, means, or other aggregated statistics, were excluded. None of the measurements in the obtained datasets were reported as being below the corresponding analytical detection limit. Data were manually consolidated into a structured Microsoft Excel database, preserving information on the data source, sampling location, collection date, parameter, measured value, reported unit, and analytical method, whenever available.

Parameter names, abbreviations, and units of measurement were standardized prior to analysis.

Measurements reported in different units were converted to common units. Chemical forms were taken into account during conversion to avoid combining concentrations reported as elemental mass with those reported as the corresponding ion or compound. The analytical methods reported by the various data sources are summarized in Supplementary Table S1.

Sampling coordinates were organized as a spatial point layer in QGIS and linked to the boundaries of the four study watersheds and their respective contributing sub-basins. Water type was assigned to each sampling event based on measured salinity and the classification established by CONAMA Resolution No. 357/2005. Samples were classified as fresh water (salinity up to 0.5‰), brackish water (salinity above 0.5‰ and below 30‰), and saline water (salinity equal to or greater than 30‰). The total database comprised 46,965 measurements of 40 water-quality variables from 3,371 sampling events at 120 locations. Applicable regulatory criteria were defined based on both the measured parameter and the water type, using standards established for Class 2 fresh waters and Class 1 brackish and saline waters. The resulting harmonized database contained 22,467 individual measurements of 18 water quality variables, derived from 3,371 sampling events conducted at 120 sampling sites.

Tabela S1. Surface water-quality dataset used for all analyses, including 31 years of monitoring data from the four subtropical coastal watersheds investigated in this study.

<i>Watershed</i>	<i>Author</i>	<i>Period</i>	<i>Parameters</i>	<i>Analytical method</i>
<i>Ratones</i>	Bittencourt (2013)	2012-2013	T°; pH; OD; Sal; Condu.; Secchi; DBO	APHA et al. (2012)
	FLORAM/ARESC (2017)	2016-2017	T°; pH; OD; Sal; Turb.; DBO; Cla; Coli Tot.; NH ₄ ; NO ₃ ; NT; PT; Surfactantes.	APHA et al. (2012)
	Rezende (2013)	2008-2009	T°; pH; OD; Condu.	APHA et al. (2012)
	ICMBio (2010)	2013-2019	T°; pH; OD; Condu.; Turb.; DBO; Cla; Coli Termo.; Coli Tot. PT; NT; NO ₃ ; NO ₂ ; NH ₄ ; MPS	APHA et al. (2012)
	Silva et al. (2013)	2005-2007	Secchi; T°; pH; Sal; OD; DBO; PID; NO ₃ ; NH ₄ ; SiO ₄ ; Cla; MPS	Grasshoff et al. (1999)
	Souza (2022)	2009-2018	T°; pH; OD; Turb.; Condu.;	APHA et al. (2012)

			Coli Termo.; Coli Tot.; PT; NO3; NH4	
	Parizotto (2009)	2007	T°; pH; Sal; OD; PT; PID; NT; NO3; NO2; NH4; Cla; Turb.; Coli Termo.; Coli Tot.	APHA et al. (2012), Grasshoff et al. (1999)
	Brentano et al. (2013)	2008-2009; 2011-2012	T°; pH; OD; DBO; PID; NO2; Condutiv.; Turb.; Coli Termo.; Coli Tot.	Grasshoff et al. (1999)
	Fuzzinatto (2009)	2008	T°; pH; Sal; OD; DBO; PT; NT; Turb.; Coli Termo.	APHA et al. (1998)
	ICMBio (2025)	2009-2023	T°; pH; OD; DBO; DQO; PT; NT; NO3; NO2; NH4; Condut.; Turb.; Coli Termo.; Coli Tot.; Cla	APHA et al. (1998)
	Rodrigues (2016)	2011-2012; 2014-2015	T°; pH; Sal; OD; DBO; PID; PT; NO2; MPS; Condut.; Turb.	APHA et al. (1998)
	Silva et al. (2016)	2013-2014	T°; pH; Sal; OD; PID; PT; NO3; NH4; Cla; MPS; Turb.	Grasshoff et al. (1999)
	Steinwandter (2019)	2015-2018	T°; pH; Sal; OD; DBO; DQO; PT; NT; NO3; NH4; MPS; Cor; Turb.; Coli. Termo.; Coli Tot.	APHA et al. (1998)
	Freitas (2020)	2017	T°; pH; Sal; OD; PID; NO3; NH4; Cla; MPS; Turb.; Condutiv.	Grasshoff et al. (1999)
<i>Saco Grande</i>	Silva et al. (2013)	2013-2014	T°; pH; Sal; OD; PID; PT; NO3; NH4; Cla; MPS; Turb.	Grasshoff et al. (1999)
	Rodrigues (2016)	2011-2012; 2014-2015	T°; pH; Sal; OD; DBO; PID; PT; NO2; MPS; Condut.; Turb.	APHA et al. (2012)
<i>Tavares</i>	Araujo (1993)	1992	T°; pH; OD; Sal; Condut.; Secchi; DBO; NT; PT	APHA et al. (1985)
	UNIVALI (2012)	1996-2008	Sal; NH4; NO3; PID	APHA et al. (1985)

	Cabral (2020)	2010	T°; pH; OD; Sal; Cla; NH4; NO;; PID; MPS	Grasshoff et al. (1999)
	CASAN (2009)*	2014-2020	T°; pH; OD; Sal; Turb; DBO; DQO; Coli Tot.; E coli; PT; NT; NO3; NO2; NH4; S; SO4	APHA et al. (2017)
	Engelplus /CASAN (2022)*	2019-2020	T°; pH; OD; Sal; Turb; DBO; DQO; Coli Tot.; E coli; PT; NT; NO3; NO2; NH4; SO4; Secchi; COT; Cla; PID; Fe; Surfactantes; SO4; S; MPS	APHA et al. (2017)
	Infraero (2014)	2014-2015	T°; pH; OD; Turb.; DBO; DQO; Coli Tot.; Coli Termo.; NO3; NT; PT	APHA et al. (2012)
	Pagliosa (2004)	2002	T°; pH; OD; Sal; Cla; NH4; NO3; PID; MPS	Grasshoff et al. (1999)
	Parizotto (2009)	2007	T°; pH; Sal; OD; PT; PID; NT; NO3; NO2; NH4; Cla; Turb.; Coli Termo.; Coli Tot.	Grasshoff et al. (1999)
	Fuzzinatto (2009)	2008	T°; pH; Sal; OD; DBO; PT; NT; Turb.; Coli Termo.	APHA et al. (1998)
	PMF/Secr. de Pesca (2015)	2015	T°; pH; OD; Sal; Turb.; Coli Termo.; E.coli;	APHA et al. (2012)
	ICMBio (2018)	2018-2020	T°; pH; OD; Cl; Sal; Turb.; DBO; DQO; PT; NT; NO3; NO2; NH4; Coli Termo; Coli Tot.; Fe; F; SO4	APHA et al. (1998)
<i>Itacorubi</i>	Bittencourt (2013)	2012-2013	T°; pH; OD; Sal; Condu.; Secchi; DBO	APHA et al. (2012)
	Cabral (2020)	2010	T°; pH; OD; Sal; Cla; NH4; NO;; PID; MPS	Grasshoff et al. (1999)
	Parizotto (2009)	2007	T°; pH; Sal; OD; PT; PID; NT; NO3; NO2; NH4; Cla; Turb.; Coli Termo.; Coli Tot.	APHA et al. (1992), Grasshoff et al. (1999)

Fuzzinatto 2009	2008	T°; pH; Sal; OD; DBO; PT; NT; Turb.; Coli Termo.	APHA et al. (1998)
Laut (2007)	2007	T°; pH; OD; Sal; Turb.; NO3; NO2; NH4; PID; SiO4	APHA et al. (1992)
Olberg (2018)	2018	Coli Termo.; E coli	APHA et al. (2012)
Pagliosa (2004)	2002	T°; pH; OD; Sal; Cla; NH4; NO3; PID; MPS	Grasshoff et al. (1999)
Rezende (2013)	2008-2009	T°; pH; OD; Conduct.	APHA et al. (2012), pH and conductivity (YSI multi-analyzer, model 85), and dissolved oxygen (oxymeter AT170)
Rigotti (2019)	2013-2014	T°; pH; OD; Conduct.; Turb.; Cla; PID	APHA et al. (2012), temperature and conductivity (YSI- EC300), dissolved oxygen (YSI – 55), and pH (YSI – 100 AC), Grasshoff et al. (1999)
UFSC (2016)	2015-2016	T°; pH; OD; Conduct.; Turb.; DBO; COT; Coli Tot.; Coli Termo.; NO3; NO2; NH4; PT.	APHA et al. (2012)
Fuzzinatto (2009)	2008	T°; pH; Sal; OD; DBO; PT; NT; Turb.; Coli Termo.	APHA et al. (1998)

*Data provided by CASAN for exclusive use in this investigation. The

remaining data are public and will be made available upon request.

Where: T°, temperature; pH, potential of hydrogen ions; DO, dissolved oxygen;
BOD, biochemical oxygen demand; COD, chemical oxygen demand; TOC, total organic
carbon; Sal, salinity; TP, total phosphorus; TN, total nitrogen; DIP, dissolved inorganic
phosphorus; NO3, nitrate; NO2, nitrite; NH4, total ammoniacal nitrogen; SiO4, silicate; Fe,
iron; F, fluoride; SO4, sulfate; Secchi, Secchi disk transparency depth; Conduct, conductivity;
Turb, turbidity; SPM, suspended particulate matter; Coli Tot, total coliforms; Coli Termo,
thermotolerant coliforms;

E. coli, *Escherichia coli*; Cla, chlorophyll-a; S, sulfide.

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1100 **Table S2:** Locations and scenarios to be applied to the heatmap.
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<i>Local</i>	<i>Scenario</i>	<i>Urbanization % (rounded value)</i>	<i>Log. Population (rounded value)</i>
<i>Florianópolis city</i>	Current	19,11 (20)	5,73 (5,5)
	Master Plan	45,25 (50)	6,24 (6,0)
<i>Watershed Ratonas</i>	Current	14,66 (10)	4,77 (5,0)
	Master Plan	58,10 (60)	5,49 (5,5)
<i>Watershed Tavares</i>	Current	28,12 (30)	4,80 (5,0)
	Master Plan	49,81 (50)	5,25 (5,5)
<i>Watershed Itacorubi</i>	Current	36,71 (40)	4,96 (5,0)
	Master Plan	52,46 (50)	5,29 (5,5)
<i>Watershed Saco Grande</i>	Current	17,92 (20)	4,36 (4,5)
	Master Plan	33,83 (30)	4,86 (5,0)

1104 **Table S3:** Results of non-parametric Kruskal-Wallis tests with Dunn's post hoc analysis, with p-values
1105 adjusted using the Bonferroni method.

Test comparing StdNPI values across river basins – Figure 5A			
<i>Kruskal-Wallis</i>	$X^2 = 126.81$	df = 3	p-value = $< 2.2 \times 10^{-16}$
<i>Comparison using Dunn's test</i>	<i>Z</i>	<i>p – unadjusted</i>	<i>p – Bonferroni-adjusted</i>
Itacorubi vs Ratonos	-7.832	4.82×10^{-15}	2.89×10^{-14}
Itacorubi vs Saco Grande	-10.332	5.04×10^{-25}	3.02×10^{-24}
Ratonos vs Saco Grande	-5.764	8.19×10^{-09}	4.91×10^{-08}
Itacorubi vs Tavares	-9.669	4.09×10^{-22}	2.45×10^{-21}
Ratonos vs Tavares	-4.227	2.37×10^{-05}	1.42×10^{-04}
Saco Grande - Tavares	2.864	4.18×10^{-03}	2.51×10^{-02}
Test of the relationship between pollution levels and the percentage of urbanization – Figure 5B			
<i>Kruskal-Wallis</i>	$X^2 = 345.32$	df = 3	p-value $< 2.2 \times 10^{-16}$
<i>Comparison using Dunn's test</i>	<i>Z</i>	<i>p – unadjusted</i>	<i>p – Bonferroni-adjusted</i>
Clean vs Heavy pollution	-17.518	1.04×10^{-68}	6.25×10^{-68}
Clean vs Light pollution	-10.993	4.14×10^{-28}	2.48×10^{-27}
Heavy pollution vs Light pollution	8.449	2.94×10^{-17}	1.76×10^{-16}
Clean vs Pollution	-15.083	2.08×10^{-51}	1.25×10^{-50}
Heavy pollution vs Pollution	4.137	3.51×10^{-05}	2.11×10^{-04}
Light pollution vs Pollution	-4.813	1.48×10^{-06}	8.91×10^{-06}
Test between pollution levels and the logarithm of the population – Figure 5C			
<i>Kruskal-Wallis</i>	$X^2 = 362.68$	df = 3	p-value $< 2.2 \times 10^{-16}$
<i>Comparison using Dunn's test</i>	<i>Z</i>	<i>p – unadjusted</i>	<i>p – Bonferroni-adjusted</i>
Clean vs Heavy pollution	-18.309	6.98×10^{-75}	4.186×10^{-74}
Clean vs Light pollution	-9.897	4.27×10^{-23}	2.57×10^{-22}
Heavy pollution vs Light pollution	10.515	7.33×10^{-26}	4.40×10^{-25}
Clean vs Pollution	-14.104	3.59×10^{-45}	2.15×10^{-44}
Heavy pollution vs Pollution	6.082	1.19×10^{-09}	7.11×10^{-09}
Light pollution vs Pollution	-4.951	7.37×10^{-07}	4.42×10^{-06}
Test of the relationship between pollution levels and the percentage of stormwater drainage – Figure 5D			
<i>Kruskal-Wallis</i>	$X^2 = 230.19$	df = 3	p-value $< 2.2 \times 10^{-16}$
<i>Comparison using Dunn's test</i>	<i>Z</i>	<i>p – unadjusted</i>	<i>p – Bonferroni-adjusted</i>
Clean vs Heavy pollution	-13.567	6.05×10^{-42}	3.63×10^{-41}
Clean vs Light pollution	-9.529	1.59×10^{-21}	9.53×10^{-21}
Heavy pollution vs Light pollution	5.471	4.46×10^{-08}	2.68×10^{-07}
Clean vs Pollution	-13.406	5.55×10^{-41}	3.33×10^{-40}
Heavy pollution vs Pollution	1.382	1.67×10^{-01}	1.00
Light pollution vs Pollution	-4.563	5.04×10^{-06}	3.02×10^{-05}
Test of the relationship between pollution levels and the percentage of the sewerage coverage – Figure 5E			
<i>Kruskal-Wallis</i>	$X^2 = 148.54$	df = 3	p-value $< 2.2 \times 10^{-16}$
<i>Comparison using Dunn's test</i>	<i>Z</i>	<i>p – unadjusted</i>	<i>p – Bonferroni-adjusted</i>
Clean vs Heavy pollution	-12.068	1.57×10^{-33}	9.40×10^{-33}
Clean vs Light pollution	-7.906	2.65×10^{-15}	1.59×10^{-14}
Heavy pollution vs Light pollution	5.467	4.58×10^{-08}	2.75×10^{-07}
Clean vs Pollution	-8.505	1.81×10^{-17}	1.09×10^{-16}
Heavy pollution vs Pollution	4.846	1.26×10^{-06}	7.57×10^{-06}
Light pollution vs Pollution	-0.698	4.85×10^{-01}	1.00

Test between pollution levels and the percentage of wetland area – Figure 5F			
<i>Kruskal-Wallis</i>	$X^2 = 125.38$	df = 3	p-value < 2.2×10^{-16}
<i>Comparison using Dunn's test</i>	<i>Z</i>	<i>p – unadjusted</i>	<i>p – Bonferroni-adjusted</i>
Clean vs Heavy pollution	6.982	2.90×10^{-12}	1.74×10^{-11}
Clean vs Light pollution	-2.874	4.04×10^{-03}	2.43×10^{-02}
Heavy pollution vs Light pollution	-11.048	2.23×10^{-28}	1.34×10^{-27}
Clean vs Pollution	0.196	8.44×10^{-01}	1.00
Heavy pollution vs Pollution	-7.806	5.91×10^{-15}	3.54×10^{-14}
Light pollution vs Pollution	3.625	2.89×10^{-04}	1.73×10^{-03}
Comparison of StdNPI inside and outside the wetland area – Figure 5G			
<i>Ratones - Kruskal-Wallis</i>	$X^2 = 185.65$	df = 1	p-value < 2.2×10^{-16}
<i>Tavares - Kruskal-Wallis</i>	$X^2 = 228.35$	df = 1	p-value < 2.2×10^{-16}

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Table S4: Calibration hyperparameters and model performance metrics.

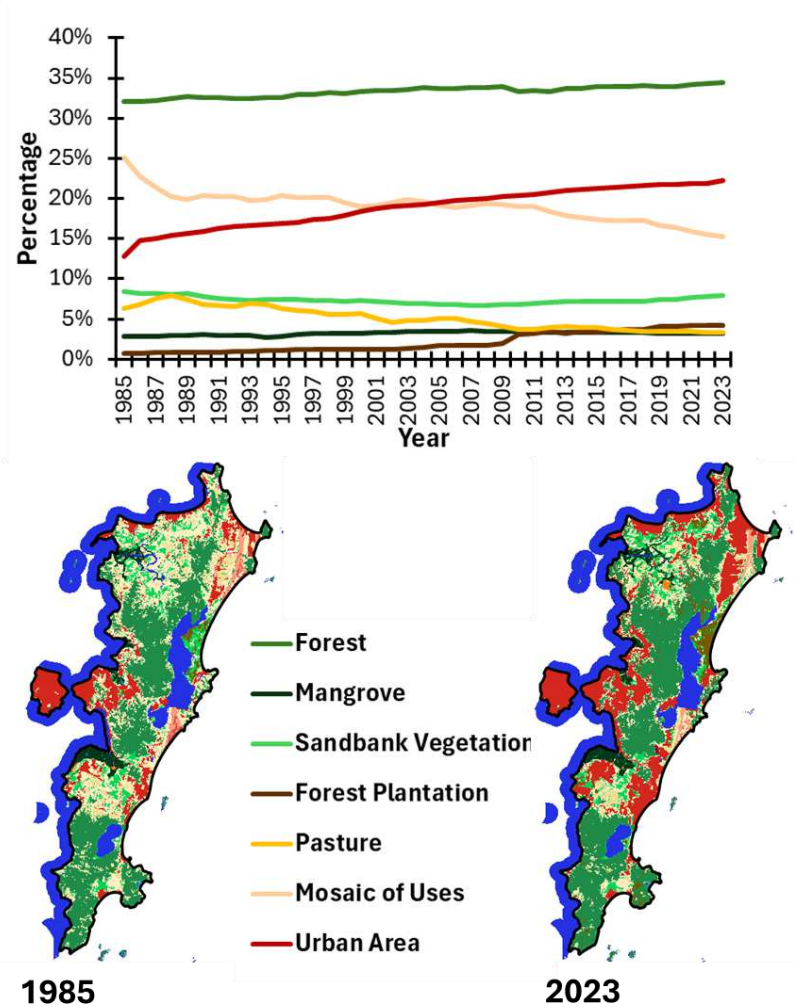
<i>Hyperparameter</i>	<i>Value Used</i>	<i>Explanation</i>	<i>Range Used in Calibration</i>
<i>mtry</i>	2	Number of predictor variables randomly sampled as candidates at each tree split.	2 a 8 (number of selected variables – 1)
<i>trees</i>	163	Total number of trees (boosting iterations) built sequentially in the model.	100 – 800
<i>min_n</i>	5	Minimum number of observations required in a node to allow a new split.	1 – 8
<i>tree_depth</i>	9	Maximum depth allowed for each decision tree.	4 – 12
<i>learn_rate</i>	0.0434	Learning rate; controls how much each new tree corrects the errors of the previous trees.	$10^{-1.5}$ – $10^{-0.5}$
<i>loss_reduction</i>	0.0303	Minimum reduction in the loss function required to justify a new split (equivalent to the gamma parameter).	10^{-3} – 10^1
<i>sample_size</i>	0.626	Proportion of training data randomly sampled to build each tree.	0.30 – 0.90
<i>Index</i>	<i>Obtained Value</i>	<i>Meaning</i>	<i>Reference value</i>
<i>Accuracy</i>	0.607	Total proportion of correct model classifications.	0 – 1
<i>Cohen's Kappa</i>	0.463	Agreement between predicted and observed outcomes, corrected for chance.	–1 – 1
<i>ROC/AUC</i>	0.841	Model's ability to correctly discriminate between classes (one-vs-all average).	0 – 1
<i>Brier score</i>	0.259	Mean squared error between predicted probabilities and observed outcomes; simultaneously evaluates discrimination and probabilistic calibration (multiclass, summed over 4 classes).	0 – 1
<i>LogLoss</i>	0.933	Penalizes incorrect probabilistic predictions with greater weight the more confident the model's error is.	0 (ideal) – no upper limit
<i>Precision</i>	0.620	Reliability of the classifications assigned to each class (macro average).	0 – 1

<i>Recall</i>	0.605	Model's ability to correctly retrieve cases belonging to each class (macro average).	0 – 1
<i>F1 score</i>	0.610	Harmonic mean between precision and recall (macro average).	0 – 1

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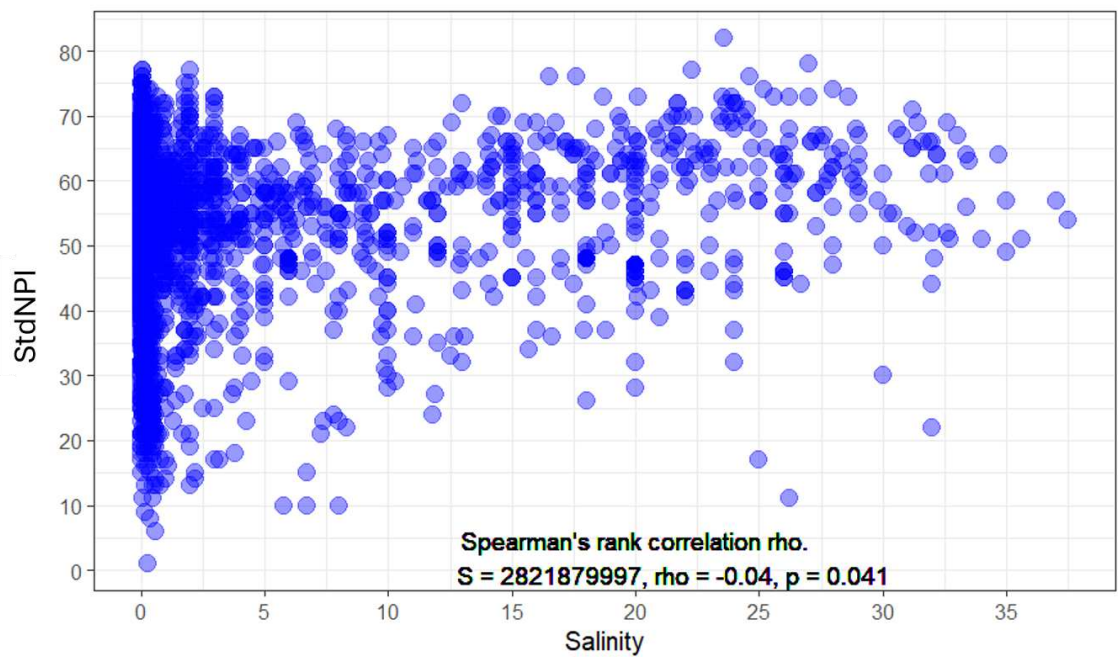


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Figure S1: Evolution of land use and occupation in Florianópolis city between 1985 and 2023.

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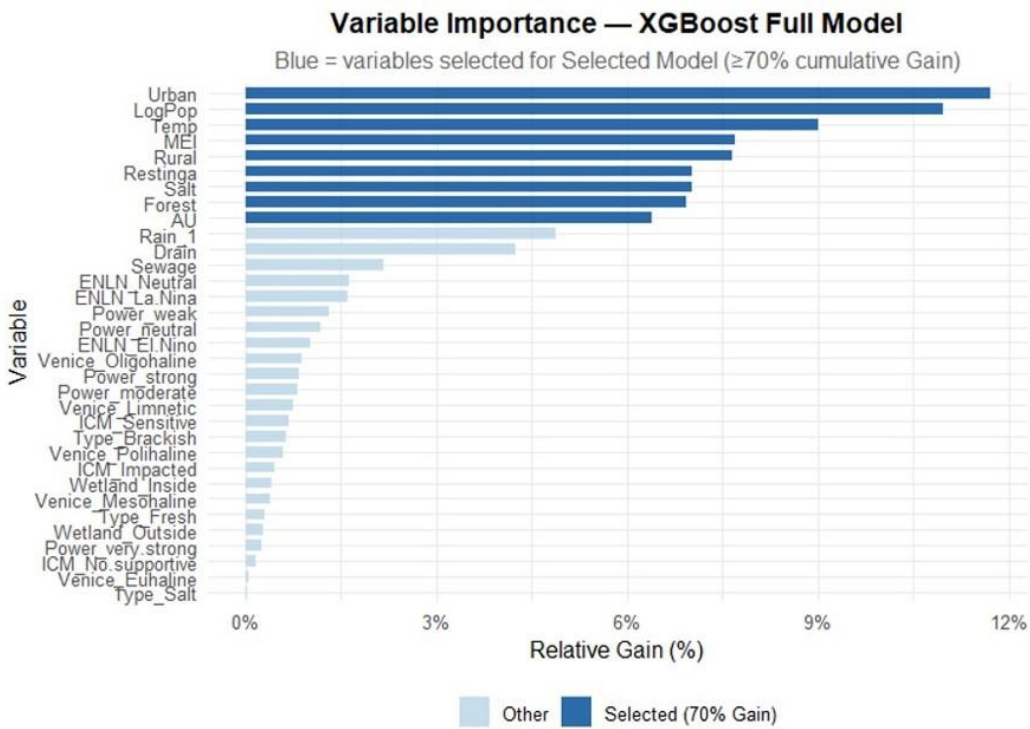


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1119 **Figure S2:** Scatterplot between StdNPI and salinity and Spearman’s rank correlation.

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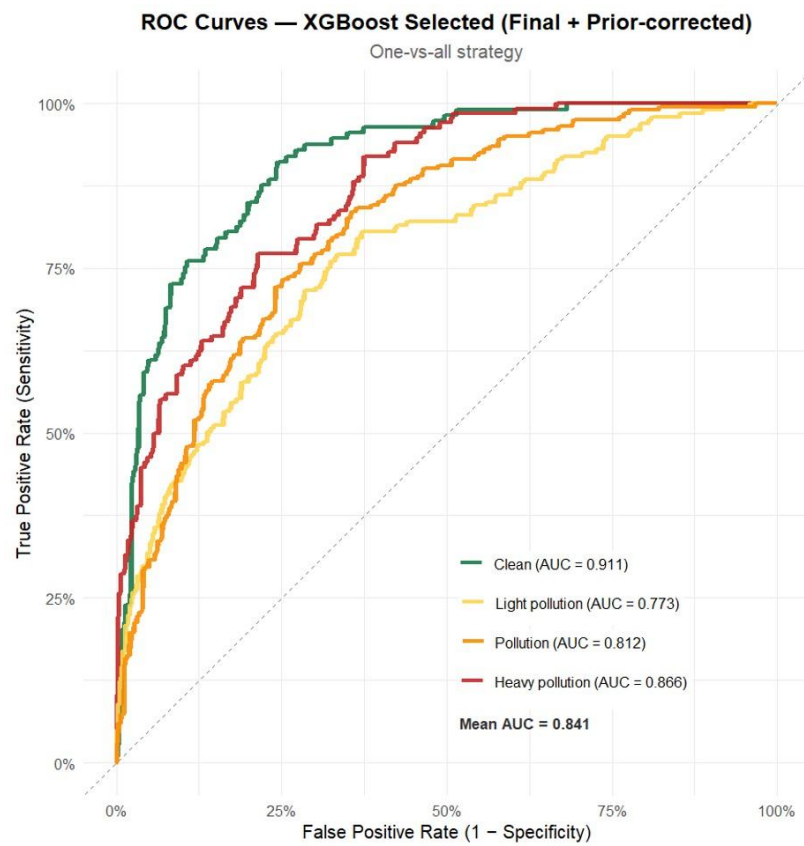


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1123 **Figure S3:** Ranked variable importance obtained from the final XGBoost classification model. Bar
1124 length represents each predictor’s relative contribution (gain), and darker shades indicate higher

1125 importance (70%).

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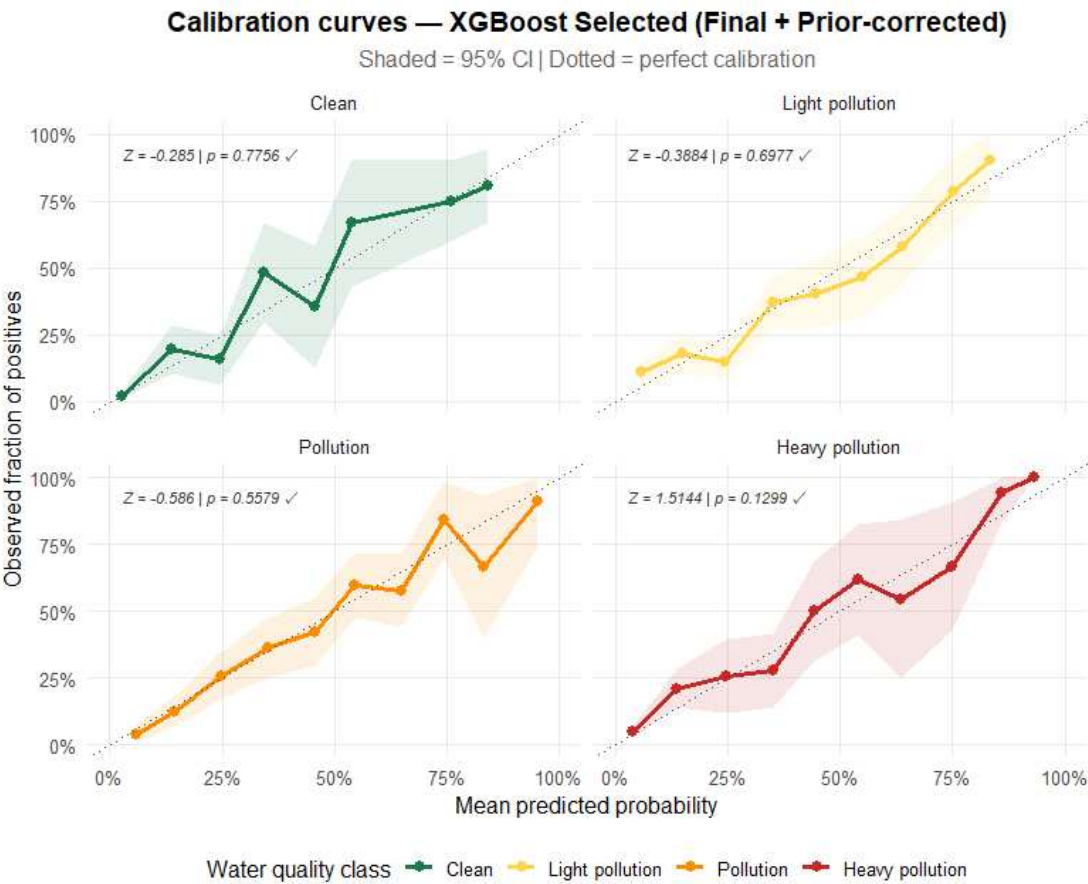


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1128 **Figure S4:** ROC curves and overall value for each category, where the diagonal dashed line marks

1129 random performance.

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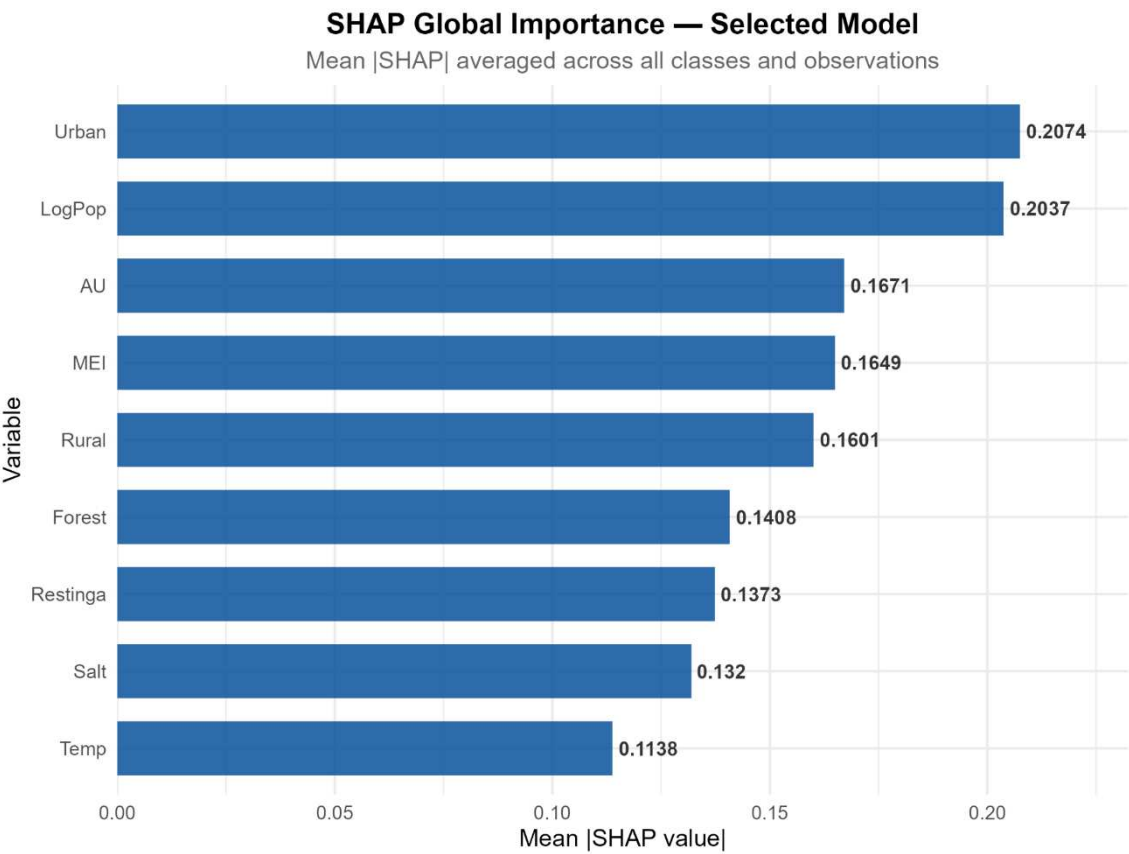


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1132 **Figure S5:** Calibration curves and Spiegelhalter Z-test for each class, with 95% confidence intervals;
1133 the 1:1 dashed line indicates perfect calibration.

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1137 **Figure S6:** SHAP (Shapley Additive exPlanations) global importance of the variables present in the
1138 selected model.