Automating Historic Nutrient Delivery Model Calibration to Assess Nutrient Retention Services in Puerto Rico

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Abstract

Nutrient retention is an essential ecosystem service that plays a critical role in maintaining water quality by reducing nutrient runoff, particularly in ecologically sensitive regions such as Puerto Rico. Existing literature indicates significant shortcomings in the calibration and validation processes of nutrient retention models, notably the widely used InVEST (Integrated Valuation of Ecosystem Services and Tradeoffs). This study aimed to enhance the reliability of nutrient retention estimates by employing an automated calibration process for the InVEST Nutrient Delivery Ratio (NDR) model and applied it to examine the historical changes in nutrient retention across Puerto Rican watersheds from 1951 to 2000. Utilizing Land Use Land Cover maps and relevant biophysical and topographical inputs, the study implements an automated batch calibration approach to identify optimal calibration values, focusing on the threshold flow accumulation parameter. Results indicated significant changes in nutrient retention capacity, with phosphorus exports decreasing by up to 31% in low-erosion potential watersheds. However, nitrogen exports showed minimal changes, particularly in high-erosion potential areas. The study found that model calibration sensitivity varied spatially and temporally, highlighting the need for watershed-specific parameterization. The findings of this study indicate the relevance of watershed-specific nutrient management strategies, particularly in high-risk erosion areas where nitrogen exports remain a persistent challenge. By providing a comprehensive analysis of nutrient dynamics, this research offers actionable insights for policymakers, ensuring more effective and sustainable interventions to protect water quality in Puerto Rico's diverse watersheds.

Introduction

Ecosystem services (ES) refer to the benefits that humans derive from nature, encompassing a broad range of ecological processes that support well-being (Boyd & Banzhaf, 2007). These services arise from complex ecological interactions involving biophysical structures, organisms, and climate, and include functions such as nutrient cycling, water filtration, and carbon sequestration (Xepapadeas, 2011). For instance, the nutrient retention capacity (NRC) of ecosystems is a critical ecosystem service that helps maintain water quality by mitigating the inflow of nutrients into aquatic systems (Keeler et al., 2012). Improving water quality, in turn, supports human activities such as swimming, fishing, and the provision of safe drinking water, which are integral to public health and local economies (European Commission et al., 2016). However, the long-term provision of nutrient retention services is vulnerable to disturbances, particularly those arising from Land Use and Land Cover (LULC) change. Such changes alter the structure and function of ecosystems, potentially diminishing their capacity to provide essential services (Liu et al., 2018).

Recent advances in ES modeling tools have improved our ability to estimate the effects of land use and land cover changes in ecosystem services. Tools such as InVEST (Tallis & Polasky, 2009), SWAT (Arnold, 1994), and ARIES (Villa et al., 2009) have been instrumental in identifying critical areas for ecosystem restoration and understanding the potential implications of land cover changes on water quality (Jackson et al., 2013). However, the utility of these models is often limited by uncertainties in input data, model assumptions, and spatial resolution that require robust calibration and validation procedures (Olander et al., 2017). Notably, many of these models lack location-specific validation and rely on generalized parameterizations that may not reflect the true local ecological conditions (Agudelo et al., 2020). Accurate predictions of nutrient retention services are essential for effective water quality management, especially in ecologically sensitive areas like Puerto Rico. Thus, there is a pressing need for more robust, and reproducible frameworks for model validation to improve transparency and enhance the reliability of decision-support tools.

Previous research has highlighted a significant gap in the calibration and validation processes of ecosystem service models, particularly in the most widely used one InVEST (Integrated Valuation of Ecosystem Services and Tradeoffs) (Ochoa & Urbina-Cardona, 2017). Within the InVEST workbench, the Nutrient Delivery Ratio model (NDR) designed to predict nutrient retention ecosystem services, is sensitive to the model parameters governing streamflow delineation. Streamflow delineation is crucial to derive the areas in which water flow routes drain to the streams, such delineation can change considerably based on the value of the parameter selected (Redhead et al., 2018). However, despite the model sensitivity to such parameters, less than 15% of scientific publications using the InVEST NDR model report conducting model calibration or validation procedures relying solely on default calibration parameters (Agudelo et al., 2020). For the fewer studies that do perform calibration and validation, they tend to focus on discrete watersheds with a static or fixed time interval, potentially overlooking the complex interactions that affect ecosystem services which limits their broader applicability. While static parameter calibration can be useful, it does not meet the dynamic needs required for effective decision-making.

To gain a comprehensive understanding of historical changes in nutrient retention, a more expansive and dynamic approach to model calibration is necessary. There is an urgent need for methods that allow for thorough evaluations of these variations to ensure model predictions are reliable. However, evaluating the accuracy of multiple parameters can be challenging and labor-intensive when done manually. This highlights the need for an automated calibration process, especially when using widely accepted ecosystem service estimation tools like InVEST across regions and periods.

This study sets an example of such calibration tools to examine the historical differences in nutrient retention services across Puerto Rican watersheds from 1951 to 2000. By employing an automated batch calibration process and evaluating suitable model parameters, I enhanced the model processing efficiency and evaluated its accuracy, thereby providing effective watershed management and conservation strategies. The main objectives of the research were to: 1) Identify the InVEST NDR model sensitivity to changes in stream network delineation values for using an automatized calibration function. 2) Understand how the nutrient retention capacity in Puerto Rico's watersheds has changed between 1951 and 2000, and 3) if there are differences in the nutrient retention capacity changes between watersheds with higher slopes and erosion potential, compared to watersheds with lower slopes, and lower erosion potential. The study hypothesized that the nutrient retention capacity in Puerto Rico watersheds has increased driven primarily by increases in herbaceous areas, and evolving watershed management practices that promoted increases in nutrient retention functions.

Methods

The study demonstrates an automated calibration function for nutrient retention estimates derived from the InVEST Nutrient Delivery Ratio (NDR) model using the Python package (natcap.invest). The workflow of the model construction, calibration, and suitable parameter selection is represented in Figure 1.

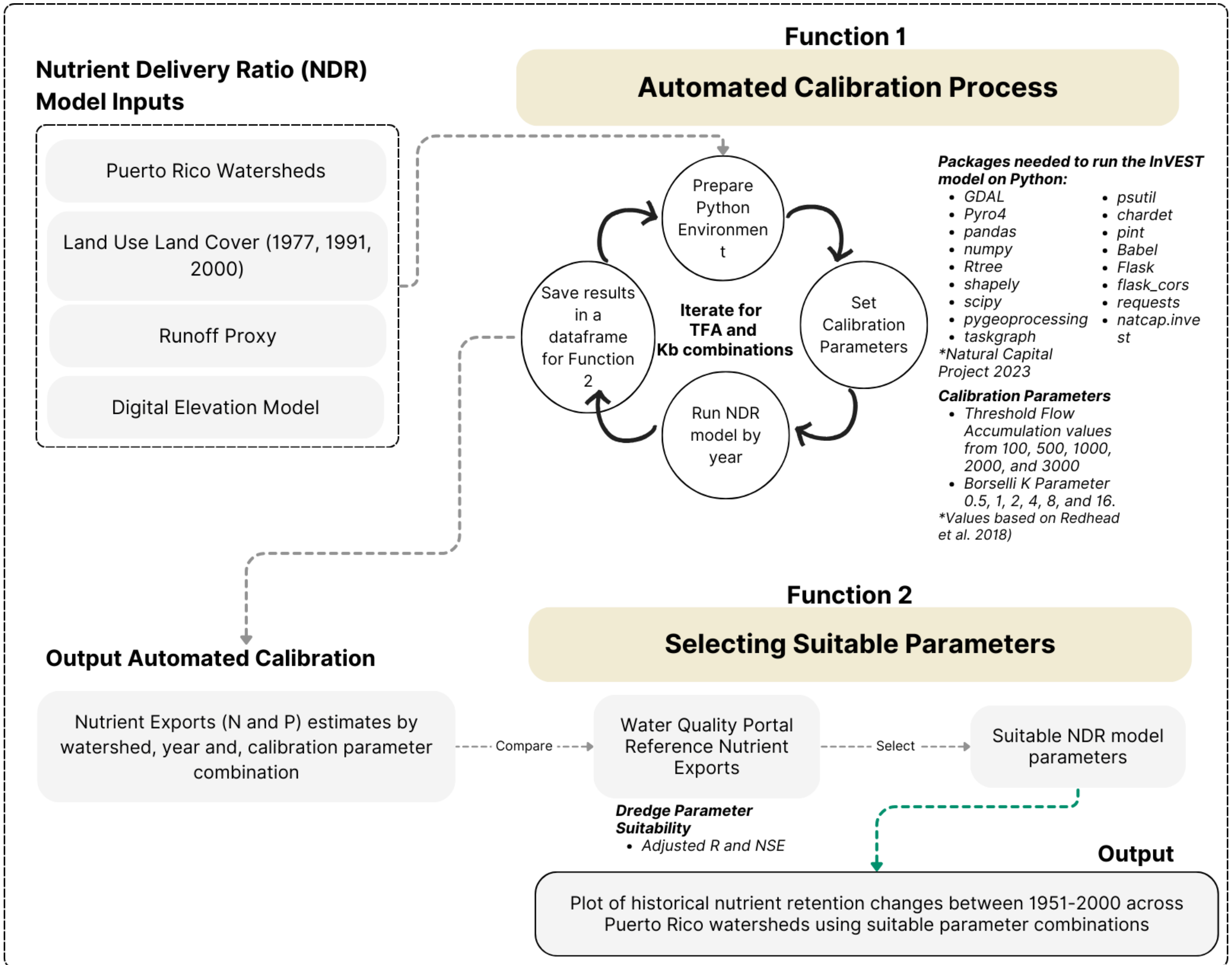

Figure 2. Workflow illustrating the process for establishing an automated calibration function to execute the natcap.invest NDR model, along with a secondary function for selecting optimal parameter combinations when comparing estimates to reference observations.

Estimating Nutrient Retention Services

The InVEST Nutrient Delivery Model (NDR), referred to as the water purification model in the InVEST workbench, quantifies and maps the nutrient retention capacity provided by a watershed's vegetation and the nutrient exports to the river streams (Natural Capital Project, 2023). Mapping nutrient retention services enables identifying critical areas to enhance water quality and prevent nutrient over-enrichment downstream that could impact fisheries, drinking water, and recreation uses. The NDR model utilizes a mass balance to assess total nitrogen and total phosphorus exports from upland drainage areas into the streams. By incorporating landscape, elevation, and runoff features, the NDR model calculates the fraction of nutrients that drain into streams by surface and subsurface flow, defined as the Nutrient Delivery Ratio (Perrine et al., 2015). The model output is the nutrient exports per pixel measured as $Kg \cdot yr^{-1}$. In contrast, the nutrient retained by each pixel is the difference between the nutrient loadings and the nutrient exports from non-point sources.

InVEST NDR Model Parameterization

In this study, the InVEST NDR model was executed using the Python package *natcap.invest* developed by the Natural Capital Project (2023). The inputs for the model were first, 30-meter resolution Land Use Land Cover (LULC) maps from the years 1951 and 2000, sourced from USDA-IITF files (Helmer et al., 2002). The maps were reclassified into seven primary categories based on the Anderson Classification system using ArcGIS Pro 3.0, as outlined by Beck et al. (2013). The LULC classes considered urban areas, bare ground, pasture, wetland, agriculture, forestland, and water. Second, the biophysical parameter tables which are essential for establishing baseline nutrient values for each LULC class were adapted from Smith et al. (2017). Third, a 30-meter Digital Elevation Model (DEM) was acquired from the Advanced Spaceborne Thermal Emission and Reflection Radiometer ASTER (2019) product. Fourth, the runoff proxy layer was derived from the InVEST Urban Flood Mitigation using a 43 mm storm layer following De Jesus Crespo et al. (2019) guidelines to represent an average rainfall-runoff event for the island. Finally, the watershed input for the model was delineated using the USGS Stream Stats v4.16.1 tool (Ries Iii et al., 2008), with the resulting watershed shapefiles employed to summarize the model estimates. The watersheds were clustered in two groups based on their slope gradient, erosivity (the capacity of the rain to cause soil erosion), erodibility (the resistance of the soil to be eroded by rain or wind), and stream density characteristics using a K means clustering algorithm using ArcGIS Pro 3.0 (Figure 2).

InVEST NDR model calibration

An automated batch calibration function was built in Python to execute the *natcap.invest* NDR model for each year under consideration (1951 and 2000), selecting for each iteration a new set of calibration parameter values across the two groups of watersheds in Puerto Rico. Calibration in this context focuses on evaluating the model's relative performance in response to changes in the selected parameter. The model estimates resulting from each watershed-year-parameter iteration were stored in a data frame for comparison against observed nutrient loads.

For this study, the calibration parameter evaluated was the threshold flow accumulation (TFA). TFA indicates the minimum number of pixels required to define a stream, and therefore directly impacts the stream network delineation. As previously mentioned, the streamflow delineation is crucial to derive the areas in which water flow routes drain to the streams, such delineation can change considerably based on the TFA value used. Based on preliminary analyses TFA values evaluated were: 50,100, and 150 while keeping additional calibration parameters constant (Anjinho et al., 2022; Redhead et al., 2018).

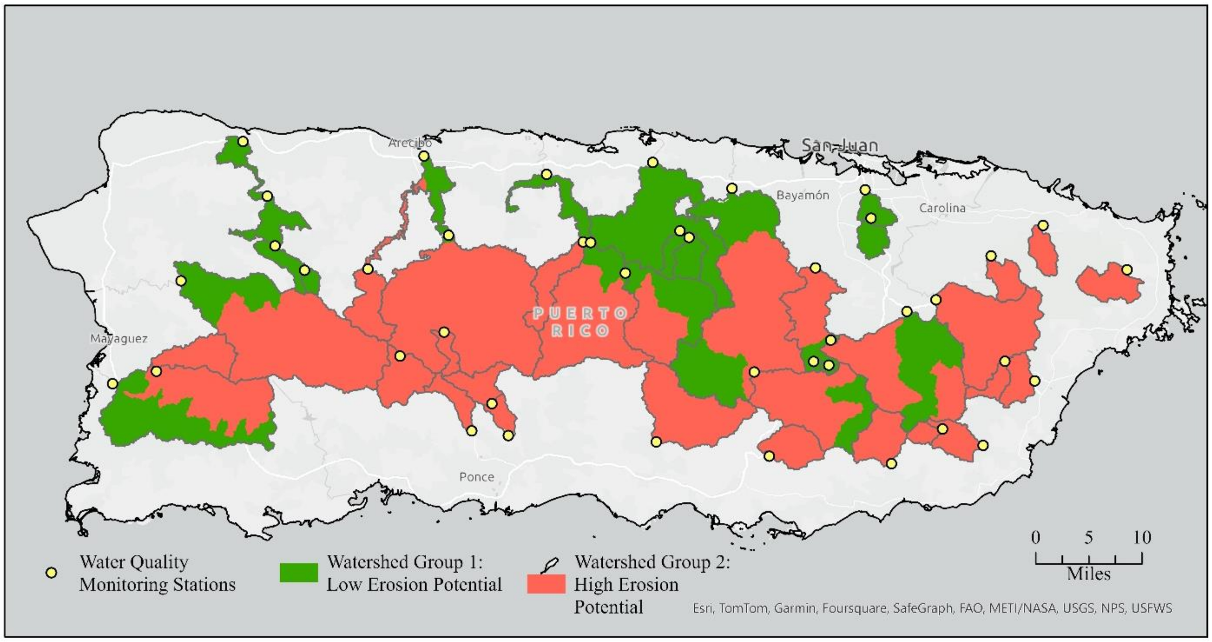

Figure 2. Map showing the watersheds included in the study. Watersheds shaded in green represent areas with low erodibility, erosivity, and gentle slopes, indicating a low potential for erosion. In contrast, watersheds shaded in red represent areas with high erodibility, erosivity, and steep slopes, associated with a high erosion potential. Yellow dots mark the locations of water quality monitoring stations.

Evaluating Model Accuracy

To validate the InVEST NDR model, the main requirement is the availability of long-term monitoring data on nutrient exports. The reference nutrient exports for total nitrogen, total phosphorus, and streamflow, spanning from January 1, 1950, to December 31, 2020, were acquired from the Water Quality Portal (WQP) (National Water Quality Monitoring Council, 2020). Any gaps in the reference data were addressed using a random forest machine learning method, wherein 70% of observed data was used to train the random forest algorithm, while the remaining 30% for validation. Reference nutrient exports were calculated by multiplying daily nutrient concentrations by streamflow. The loads were aggregated in ten-year blocks to estimate the mean nutrient load per year (1951 and 2000).

The model outputs were stored in data frames that were used to build boxplot visualizations comparing the differences between 1951 and 2000 model estimates and observed reference values in Python using the *matplotlib* and *seaborn* packages. In addition, the spatially explicit output of the models was used to build maps using ArcGIS Pro 3.0

Results

Sensitivity of the InVEST NDR Model to Changes in Stream Network Delineation Values

The sensitivity of the InVEST NDR model to changes in the TFA (threshold flow accumulation) parameter varies depending on watershed erosion risk and land-use/land-cover characteristics (Table 1). In 1951, doubling the TFA parameter had a more pronounced effect on watersheds with a high erosion potential compared to those with low erosion potential. Specifically, increasing the TFA from 50 to 100 led to a 6% reduction in nutrient export estimates for both nitrogen and phosphorus. Conversely, increasing TFA from 100 to 150 resulted in a 5% increase in nutrient export estimates. In low-erosion-potential watersheds, changes in TFA produced consistent 4% increments in nutrient export estimates across both TFA ranges (50–100 and 100–150), regardless of nutrient type.

By 2000, the effect of doubling the TFA was greater in both high- and low-erosion-risk watersheds than it was in 1951. For these watersheds, increasing the TFA from 50 to 100 resulted in a 10% increase in model estimates, while further increasing the TFA from 100 to 150 led to a 15% increase. These findings suggest that the model's sensitivity to TFA values has intensified over time.

The calibration process identified suitable TFA values depending on erosion potential. For low-erosion-potential watersheds, a TFA value of 50 was optimal for both nitrogen and phosphorus. However, in high-erosion-potential watersheds, a TFA value of 150 yielded better results. Despite these adjustments, the NDR model demonstrated greater predictive accuracy in low-erosion-potential watersheds compared to high-risk areas. In high-erosion-potential watersheds, even with the most suitable TFA parameter, the model overestimated changes in nitrogen exports between 1951 and 2000 by 55% (Table 2). These discrepancies highlight the challenges of accurately modeling nutrient exports in areas with complex erosion dynamics.

Changes in Nutrient Retention Capacity in Puerto Rico's Watersheds (1951–2000)

Between 1951 and 2000, Puerto Rico's watersheds experienced notable shifts in their nutrient retention capacity, with phosphorus exports showing significant reductions and nitrogen exports remaining largely unchanged on average (Figure 3). When analyzing watershed groups, phosphorus exports decreased by 29–31% in both low- and high-erosion-potential watersheds (Table 3). In contrast, nitrogen exports exhibited divergent trends: watersheds with low erosion risk experienced reductions of up to 35%, while high-erosion-potential watersheds showed negligible changes (<1%).

Spatially, nutrient export dynamics revealed contrasting trends between high- and low-erosion-potential watersheds over time. In high-risk watersheds, the overall pattern of nutrient export hotspots remained stable, but the intensity of these exports declined significantly between 1951 and 2000 (Figure 4). Areas that were major nutrient sources in 1951 exhibited reduced export magnitudes by 2000, suggesting that consistent spatial patterns were accompanied by diminished nutrient export capacity. These reductions may be linked to changes in land use, vegetation cover, or watershed management practices. In contrast, watersheds with low erosion potential not only experienced a reduction in nutrient export intensity but also showed increased spatial dispersion of nutrient-exporting areas (Figure 5). This indicates a broader distribution of nutrient retention capacity over the landscape, potentially reflecting more widespread improvements in land management or other environmental changes that redistribute nutrient retention functionality. These divergent spatial trends underscore the role of erosion risk in shaping how watersheds respond to long-term environmental and land-use changes. These results highlight the interplay between erosion risk and watershed dynamics in shaping nutrient retention over time.

Table 1. Differences in estimated nutrient exports (nitrogen and phosphorus) among threshold flow accumulation (TFA) values between 1951 and 2000.

		1951			2000		
Nutrient	Watershed	TFA 50	TFA 100	TFA 150	TFA 50	TFA 100	TFA 150
Nitrogen	Group 1: Low Erosion Potential (Kg Year-1)	4152.13	4342.82	4524.66	2651.33	2897.06	3320.45
	Group 2: High Erosion Potential (Kg Year-1)	22700.49	21420.78	22705.49	7853.13	8668.62	10032.26
	Group 1 Model estimate variability (%)	Baseline	4.59	4.19	Baseline	9.27	14.61
	Group 2 Model estimate variability (%)	Baseline	-5.64	5.97	Baseline	10.38	15.73
Phosphorus	Group 1: Low Erosion Potential (Kg Year-1)	809.43	846.49	882.27	679.70	742.68	850.83
	Group 2: High Erosion Potential (Kg Year-1)	4379.70	4134.37	4385.70	1943.29	2139.50	2467.53
	Group 1 Model estimate variability (%)	Baseline	4.58	4.23	Baseline	9.27	14.56
	Group 2 Model estimate variability (%)	Baseline	-5.60	5.93	Baseline	10.10	15.33

Table 2. Changes in the model nutrient estimates between 1951-2000. Values in bold represent the most suitable parameter selected during the calibration process.

		1951 - 2000 Changes (%)		
Nutrient	Watershed	TFA50	TFA100	TFA150
Nitrogen	Group 1: Low Erosion Potential	**-36.15**	-33.29	-26.61
	Group 2: High Erosion Potential	-65.41	-59.53	**-55.81**
Phosphorus	Group 1: Low Erosion Potential	**-16.03**	-12.26	-3.56
	Group 2: High Erosion Potential	-55.63	-48.25	**-43.66**

Table 3. Changes in observed nitrogen and phosphorus exports between 1951 and 2000 in Puerto Rico Watersheds.

	1951		2000		Change (%)	
Watersheds	Phosphorus (Kg Year -1)	Nitrogen (Kg Year -1)	Phosphorus (Kg Year -1)	Nitrogen (Kg Year -1)	Phosphorus	Nitrogen
Group 1: Low Erosion Potential	148787.87	1516890.98	104240.47	985588.87	-29.94	-35.03
Group 2: High Erosion Potential	434802.61	3884093.76	298427.73	3920739.36	-31.36	0.94

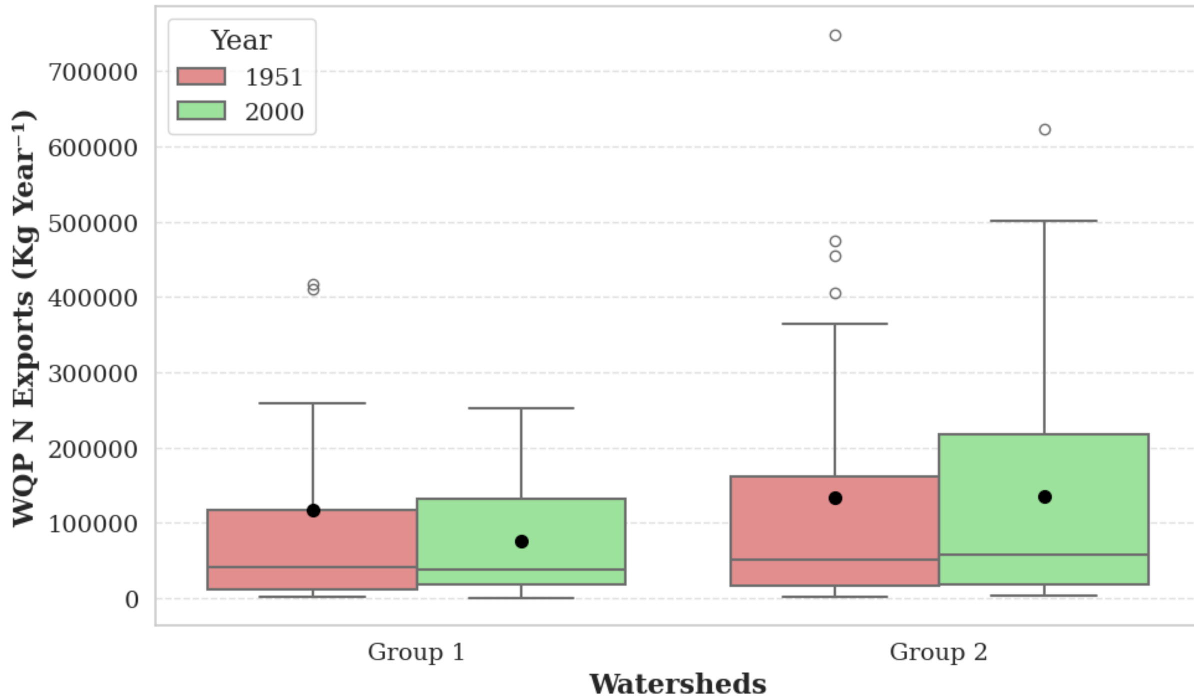

Figure 3. Differences in 1951 and 2000 in the observed nitrogen exports. Mean values are represented by the black dots inside the boxplots.

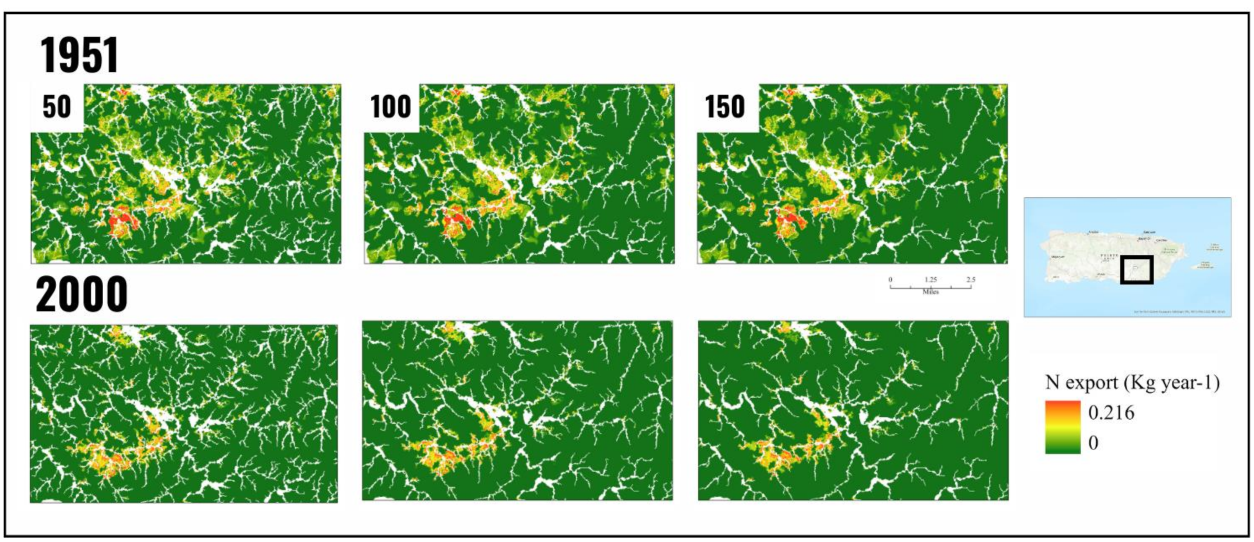

Figure 4. Representation of the spatial distribution of nitrogen exports in one example watershed with a high risk of erosion showing the differences in nutrient export magnitude between 1951 and 2000. Red colors represent major nutrient export areas in 1951. The number listed in the upper left corner of the panels represents the threshold flow accumulation parameters used in each nutrient estimation.

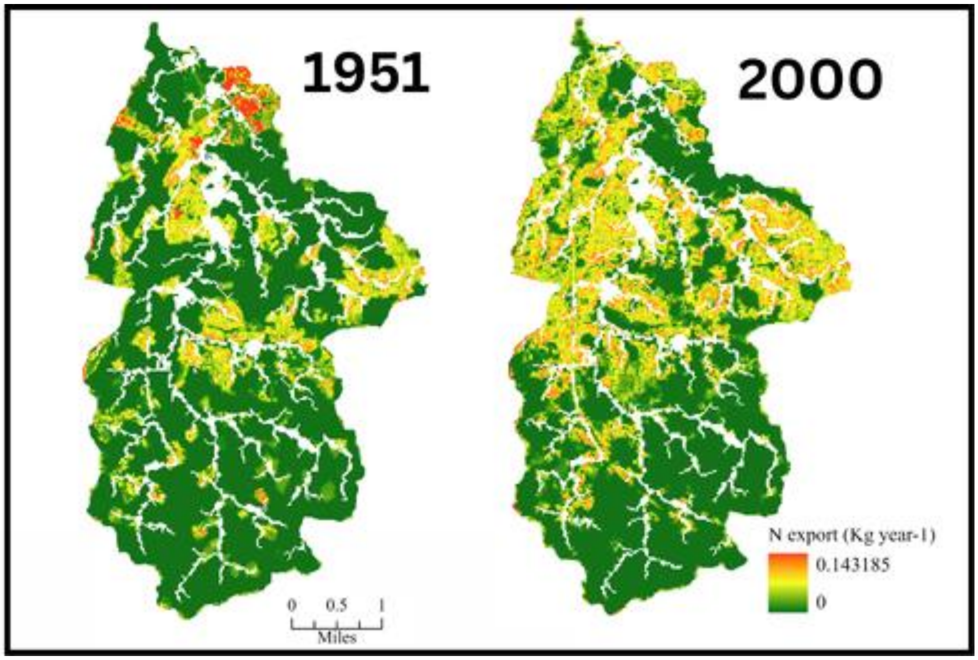

Figure 5. Representation of the spatial distribution of nitrogen exports in one example watershed with a low risk of erosion showing the differences in nutrient export magnitude and spatial dispersion between 1951 and 2000. Red colors represent major nutrient export areas in 1951.

Discussion

Nutrient Model Parameter Sensitivity to Changes Over Time and Space

The results demonstrate that the sensitivity of the InVEST NDR model to the threshold flow accumulation (TFA) parameter varies both temporally and spatially. For example, nutrient export estimates in high-erosion-potential watersheds were more affected by changes in TFA values than those in low-risk watersheds. This variability suggests that applying a uniform calibration parameter across all watersheds could lead to nutrient estimate discrepancies exceeding 15%, as seen in the observed increases in sensitivity between 1951 and 2000. To improve model reliability, it is critical to validate TFA parameters by year and watershed group, as shown in this study. For instance, high-risk watersheds required higher TFA values (150), whereas low-risk watersheds performed better with lower TFA values (50). These findings emphasize the importance of localized calibration to enhance the model's applicability to diverse watershed characteristics.

Additionally, the higher accuracy of the InVEST NDR model in predicting nutrient exports for low-erosion-potential areas highlights its limitations in steeper, high-risk watersheds. These regions, characterized by greater slopes and rainfall-driven soil movement, presented overestimations of nitrogen exports, even with optimized parameters. This discrepancy suggests the need for further evaluation of the model's sensitivity to the runoff proxy parameter. A more refined understanding of runoff processes and erosion dynamics in steep terrains could help bridge this gap, enabling more accurate predictions and tailored management strategies.

Nutrient Retention Capacity Trends and Implications

As hypothesized, nutrient retention capacity across Puerto Rico's watersheds has generally increased since 1951, as evidenced by the overall reduction in nutrient exports from non-point source pollution. However, this improvement is not uniform across the island. Watersheds with low erosion potential experienced notable reductions in both nitrogen and phosphorus exports, likely due to gentler slopes and reduced soil displacement. In contrast, high-erosion- potential watersheds showed minimal changes in nitrogen exports (<1%), indicating that nitrogen remains a persistent nutrient export source in these areas. This persistence underscores the importance of targeting nitrogen management strategies in the island's upper watersheds, where nutrient sources are likely concentrated.

The spatial trends observed in this study further suggest that traditional nutrient export hotspots, particularly in high-risk watersheds, may have improved their retention capacity over time. For example, areas identified as significant nutrient sources in 1951 exhibited reduced export intensity by 2000 potentially due to abandonment of agriculture areas. Meanwhile, low-risk watersheds displayed a dispersion of nutrient-exporting areas potentially due to changes in watershed management practices. These trends provide critical insights for designing future nutrient management practices. For instance, prioritizing reforestation, erosion control, or precision agriculture in high-risk watersheds could help address nitrogen export issues.

This study demonstrates the critical importance of tailoring nutrient management strategies to watershed-specific conditions and advancing ecosystem service model calibration. By automating the calibration process, we provided a comprehensive analysis of historical nutrient dynamics across diverse watersheds, highlighting spatial and temporal variability in retention capacities. These findings enhance model precision and offer actionable insights for policymakers to design targeted, sustainable interventions, particularly in high-risk erosion areas where nitrogen remains a persistent issue. This research provides a robust foundation for improving water quality and preserving essential water resources in Puerto Rico, offering a scalable approach for broader applications in watershed management.

Appendix

Sample code availability**:**

https://github.com/chsharrison/Sci_comp_F24/blob/main/Mariam_Valladares/Final_report_Valladares_Appendix.ipynb

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