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Self-Organizing Maps and Neuro-Fuzzy Classification for Water-Quality Assessment in a Tropical Mangrove–Estuary System

Nuno Avelar Nascimento
State University of Santa Cruz
Thiago Pereira das Chagas
State University of Santa Cruz
Flávio Lima de Sena
State University of Santa Cruz
Mavione de Jesus Primo
State University of Santa Cruz
Fábio Alan Carqueija Amorim
State University of Santa Cruz
Allison Gonçalves Silva
Bahia Federal Institute of Education, Science and Technology
Luana Novaes Santos
State University of Santa Cruz
Erik Galvão Paranhos da Silva
egpsilva@uesc.br
State University of Santa Cruz

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Abstract

Estuarine and mangrove systems exhibit strong spatial and temporal variability, which complicates the interpretation of routine water-quality data and limits the applicability of linear assessment approaches. In this study, an integrated framework combining Self-Organizing Maps (SOM) and a Mamdani Fuzzy Inference System (MFIS) was applied to surface-water samples from Pontal Bay, a tropical mangrove-estuary system in Ilhéus, Bahia, Brazil. Sixty-five samples collected at five monitoring sites were characterized using pH, electrical conductivity (EC), dissolved oxygen (DO), and total dissolved solids (TDS), while site position, tide level, air humidity, rainfall, and temperature were used as explanatory variables. SOM was employed to identify patterns and organize samples into four classes representing distinct hydro-environmental signatures. These groups were subsequently used to train an MFIS classifier for assigning new observations to the SOM-derived classes. The SOM revealed marked heterogeneity among samples, especially for EC and TDS, reflecting estuarine mixing, tidal influence, and local anthropogenic pressure. Group interpretation indicated contrasting signatures associated with higher pH, lower DO, elevated EC/TDS, and comparatively better oxygenation conditions. After optimization, the MFIS classifier improved its hit rate from 0.4285 to 0.6071 and average relevance from 0.3312 to 0.4680. Although the proposed SOM-MFIS strategy did not eliminate the intrinsic variability of the system, it provided an interpretable framework for organizing monitoring complex data and supporting environmental assessment in dynamic coastal transition zones.

1. Introduction

Mangrove–estuary systems are highly dynamic transition environments in which water quality reflects the interaction of freshwater inflow, marine intrusion, tidal oscillation, meteorological forcing, and local anthropogenic inputs. Because these drivers act simultaneously and at short spatial and temporal scales, physicochemical variables such as pH, dissolved oxygen (DO), electrical conductivity (EC), and total dissolved solids (TDS) often exhibit marked heterogeneity, making environmental interpretation difficult when based only on isolated measurements or simple linear relationships. This intrinsic variability has been repeatedly recognized as a central challenge for environmental monitoring in coastal and estuarine systems, where continuous assessment is necessary to support ecosystem protection and management (Mondal, 2024).

In this context, data-driven approaches have become increasingly relevant for organizing complex environmental datasets and supporting water-quality assessment. Among artificial intelligence techniques, artificial neural networks are particularly useful when the system under study is nonlinear, multivariate, and influenced by overlapping environmental controls. Their value lies not only in prediction, but also in pattern recognition and structure detection in datasets where mechanistic relationships are not easily isolated (Haykin 2009; Baum et al. 2021). Hybrid methods combining neural computation and fuzzy logic are also attractive because they allow classification under uncertainty and generate interpretable rule-based outputs, an important feature for environmental monitoring and screening applications (Andonovski et al. 2025; Yan et al. 2010).

Among unsupervised methods, the Self-Organizing Map (SOM) has been widely used to reveal hidden structure in multidimensional environmental data, project complex relationships into low-dimensional representations, and identify clusters of samples with similar signatures. Recent evidence indicates that SOM is especially useful in water-quality studies because it can handle heterogeneity, data overlap, and nonlinear behavior while preserving neighborhood relationships among samples (Almegdadi et al. 2025). In practical terms, SOM does not replace monitoring; it improves interpretation by converting large and noisy datasets into organized similarity patterns that can be linked to environmental states. This characteristic is particularly relevant in estuarine systems, where distinct hydrochemical conditions may emerge even under apparently comparable field conditions.

The use of intelligent classification tools in aquatic systems has already shown potential in different contexts. For example, neuro-fuzzy inference has been successfully applied to classify river water-quality status using physicochemical indicators, demonstrating that fuzzy rule-based structures can convert environmental measurements into operational classes with good interpretability (Yan et al. 2010). Likewise, exploratory multivariate approaches, including Kohonen-based methods, have proven useful in distinguishing impacted and non-impacted aquatic environments and in identifying seasonal and spatial patterns in Brazilian water systems (Santos et al. 2023). These advances suggest that combining unsupervised mapping with fuzzy classification may be especially useful in highly variable transition zones, where direct deterministic prediction is often limited by the overlap of natural and anthropogenic drivers.

Pontal Bay, located in Ilhéus, Bahia, Brazil, is an appropriate case study for this type of approach because it is a mangrove-influenced estuarine environment under simultaneous riverine, tidal, and urban influence. In such settings, variation in EC and TDS may reflect not only estuarine mixing, but also the contribution of wastewater-affected waters, since conductivity has been reported as a useful marker of contamination in surface freshwaters subject to anthropogenic inputs (de Sousa et al. 2014). At the same time, spatial variation in pH and DO may indicate changing oxidation conditions, organic matter decomposition, and local hydrodynamic effects, all of which complicate the interpretation of conventional monitoring datasets. Therefore, a method capable of organizing overlapping signatures into interpretable classes is more useful here than a purely descriptive analysis of individual parameters.

Based on this rationale, the aim of the present study was to apply an integrated framework based on Self-Organizing Maps and a Mamdani Fuzzy Inference System (MFIS) to classify water-quality patterns in Pontal Bay. Specifically, the study sought to identify groups of samples with similar physicochemical signatures using SOM, interpret the environmental meaning of the resulting groups and develop a fuzzy classifier capable of assigning new observations to the SOM-derived classes using site and environmental input variables. The central premise is that the combined SOM–MFIS strategy can provide an interpretable support tool for environmental monitoring in tropical mangrove–estuary systems characterized by strong nonlinearity and short-scale hydrochemical variability.

2. Materials and methods

2.1. Study area

The study was conducted in Pontal Bay, Ilhéus, southern Bahia, Brazil, a tropical estuarine environment influenced by freshwater discharge from the Cachoeira River and by marine intrusion (Fig. 1). The area is characterized by strong tidal influence and by the coexistence of urbanized sectors and mangrove-associated sites, which together promote pronounced hydrochemical variability. Because the bay functions as a river–sea transition zone, its water quality is sensitive to short-term hydrodynamic forcing and local anthropogenic pressures. The coordinate of the location points are P1 center (Ilha do Frade) -14.800227, -39.038120; P2 Jorge Amado Bridge – 14.809513, -39.026204; P3 Nelson Costa – 14.821225, -39.042848; P4 Sapetinga – 14.806845, -39.040895 and P5 Teotônio Vilela – 14.813943, -39.057976.

2.2. Sampling design and measured variables

Surface-water samples were collected at five monitoring sites distributed along Pontal Bay. A total of 65 samples were obtained, including replicate measurements. The monitored physicochemical variables were pH, electrical conductivity (EC), dissolved oxygen (DO), and total dissolved solids (TDS). Measurements were obtained using a multiparameter probe (HANNA HI9829), except for TDS, which was estimated from EC using the adopted conversion relationship reported in the manuscript. For model input, the following explanatory variables were considered: sampling site, parameterized by distance from the source region of the Cachoeira River; tide level; air humidity; rainfall; and air temperature. Meteorological information was obtained from the INMET station for Ilhéus.

2.3. Data organization

To support pattern recognition, samples were coded according to sampling event and collection point. Prior to SOM analysis, the dataset was organized into an input matrix containing the monitored water-quality variables. All variables were standardized before SOM training due to differences in scale and measurement units. This step prevented variables with larger numerical ranges from dominating the map organization and improved the comparability of pH, EC, DO, and TDS in the training stage.

2.4. Self-organizing map (SOM)

The SOM was used as an unsupervised tool to identify similarity patterns among samples based on pH, EC, DO, and TDS. The model was implemented in SOM Toolbox version 2.1 (Aalto University, Finland), using a hexagonal lattice with 8×6 neurons and linear initialization, as reported in the original analysis. After network training, sample distribution was examined using the unified distance matrix (U-matrix), sample hits, component planes, and contextual projection. Four groups were defined from the trained map by considering neuron proximity, neighborhood structure, and visual separation of clusters on the contextual representation. Map quality was assessed using the quantization error (QE) and topographic error (TE), which were 0.603 and 0.036, respectively.

2.5. Mamdani Fuzzy Inference System (MFIS)

A Mamdani Fuzzy Inference System (MFIS) was developed to classify samples into the four water-quality groups previously identified by the SOM. Therefore, the role of the MFIS in this study was not to predict the exact numerical values of pH, EC, DO, or TDS, but rather to assign each observation to one of the SOM-derived hydrochemical classes using monitoring-related explanatory inputs.

The predictor variables used in the MFIS were site position, tide level, air humidity, rainfall, and temperature. Site position was represented according to the relative location of each monitoring point along Pontal Bay, whereas the remaining variables described the meteorological and hydrodynamic context associated with each sampling event. The output variable corresponded exclusively to the class label derived from the SOM clustering structure.

Fuzzy membership functions were defined for each input variable based on the observed data distribution and the classification logic adopted in the original model. The inference structure was implemented using a Mamdani rule-based architecture because this approach is transparent, interpretable, and suitable for environmental classification problems involving gradual transitions rather than sharp boundaries. The rule base was then adjusted to improve the correspondence between predictor conditions and the SOM-based classes.

Classifier performance was evaluated by comparing the initial and optimized rule structures using functional cost, hit rate, and average relevance of the correct class. Optimization improved hit rate from 0.4285 to 0.6071 and average relevance from 0.3312 to 0.4680, indicating a better alignment between environmental input conditions and the class structure identified by the SOM (Table 1). Even so, the classifier should be interpreted as a support tool for environmental screening rather than as a high-precision predictive model, because the strong hydrochemical variability of estuarine systems naturally limits strict class separation.

Table 1
Performance metrics of the MFIS classifier before and after optimization.

Classifier	Functional Cost	$\varvect_{\varvecs}$	$\varvecu_{\varvecm}^{\varvecr}$
Initial	0.4815	0.4285	0.3312
optimal	0.6453	0.6071	0.4680
Source: Prepared by the author			

2.6. Regulatory interpretation

To contextualize the environmental meaning of the monitored variables, observed values were interpreted using the reference ranges adopted in the study, including CONAMA Resolution No. 357/2005 for pH and dissolved oxygen and WHO guidance for TDS (Table 2). These benchmarks were used as interpretive references rather than as the sole basis for class assignment.

Table 2
Regulatory and guideline reference values used for interpreting water-quality variables.

Variable	WHO - Guideline	CONAMA nº357/2005
pH	6,5–8,5	5,0–9,0
Electrical Conductivity (μS cm^{-1})	-	-
Dissolved Oxygen (mg L^{-1})	-	4,0
Total dissolved solids (mg L^{-1})	< 1000	-
Source: Prepared by the author		

2.7. Limitations

Because the study was based on 65 samples from five monitoring sites within a highly dynamic estuarine system, the proposed framework should be interpreted as a classification-support strategy rather than a universal predictive model. In addition, the use of TDS estimated from EC introduces dependency between these two variables, which should be considered when interpreting the resulting cluster structure.

3. Results and discussion

3.1. SOM organization of water quality variability

The SOM provided a compact representation of the physicochemical variability observed in Pontal Bay, allowing samples to be organized according to similarity in pH, EC, DO, and TDS. The U-matrix (Fig. 2) and contextual map (Fig. 3) indicated that the dataset was not distributed as a single homogeneous cloud, but rather as a set of differentiated regions with distinct internal cohesion. This result is consistent with the environmental complexity of estuarine systems, where tidal oscillation, river discharge, meteorological forcing, and local anthropogenic effects interact over short spatial scales.

The contextual representation showed the formation of four groups, later used as the basis for fuzzy classification. Visual inspection of neuron distribution indicated that some groups were more compact, whereas others were more dispersed, suggesting unequal internal heterogeneity among hydrochemical states. In particular, the group represented by more spatially dispersed neurons reflects the instability expected in transitional waters, where similar external conditions may still produce contrasting water-quality responses due to estuarine mixing and local inputs.

Rather than treating this dispersion as a modeling failure, it should be interpreted as evidence that the monitored system does not behave under a simple deterministic structure. In practical terms, the SOM was useful because it reduced the complexity of the monitoring dataset into interpretable environmental classes without imposing linear relationships among variables.

3.2. Environmental meaning of the identified groups

Interpretation of component planes and representative samples revealed that the four SOM-derived groups corresponded to distinct water-quality signatures (Fig. 4). Group 1 was associated with the highest pH values and low DO, indicating a condition that approaches the upper regulatory limit for pH while also suggesting reduced oxygenation. Group 2 was characterized by lower DO and relatively lower EC and TDS, indicating a distinct low-oxygen signature not necessarily linked to the highest dissolved-solids content. Group 3 concentrated the highest EC and TDS values, which is consistent with stronger mineralization and possible influence of estuarine mixing and anthropogenic inputs. Group 4 was associated with the highest DO values and may be interpreted as the comparatively better oxygenated condition within the dataset.

This class-based interpretation is more useful for environmental monitoring than isolated variable inspection because it links multiple physicochemical indicators into coherent states. For example, the samples grouped in the high-EC/TDS class do not simply reflect salt content, in an urbanized estuarine setting, they may also indicate the superposition of marine influence and contamination markers previously associated with wastewater-affected waters. Likewise, spatial variation in pH observed on the same sampling day (Table 2) supports the view that local environmental setting strongly influences water chemistry, particularly in mangrove-associated sectors where decomposition of organic matter can contribute to acidification.

Table 2
Example of spatial pH variability among sites samples under comparable meteorological conditions.

Collection Site (km)	Air Humidity (%)	Rainfall Index (mm)[1]	Temperature (°C)	pH
60	75	6.2	27.10	7.52
62	75	6.2	25.40	7.79
64	75	6.2	25.70	7.17
61	75	6.2	25.40	7.45
57	75	6.2	28.50	7.17
Source: Prepared by the author				

The observed instability in EC and TDS (Table 4), even under apparently similar input conditions, reinforces the importance of using a pattern-recognition approach. In estuarine environments, comparable meteorological conditions do not guarantee comparable hydrochemical outcomes because short-term tidal exchange and local mixing processes may alter conductivity, solids content, and oxygen conditions over narrow spatial scales (Table 5). Therefore, the identified classes should be interpreted as

environmental signatures emerging from interacting drivers rather than as fixed categories controlled by a single factor.

Table 4
Example of EC and TDS variability under similar field conditions.

Sample	Location (km)	EC (µS cm⁻¹)	TDS (ppm)
1	60	29.80	19.07
2	62	45.00	28.80
16	60	45.93	29.40
17	62	40.15	25.70
Source: Prepared by the author			

Table 5
Representative samples and hydrochemical characteristics of the four SOM-derived classes.

Sample	pH	EC (µS cm⁻¹)	DO (mg L⁻¹)	TDS (ppm)	Classification
18	8.70	29.18	2.74	18.68	1
20	8.50	19.18	2.83	12.28	1
17	8.90	40.15	2.92	25.70	1
6	7.69	31.61	1.25	20.23	2
8	7.58	25.15	1.58	16.10	2
9	7.35	22.18	2.99	14.20	2
53	7.04	56.8	2.81	36.35	3
54	7.74	61.8	3.27	39.55	3
55	7.33	54.1	3.84	34.62	3
5	7.97	31.39	6.04	20.09	4
2	7.80	45.00	6.17	28.80	4
3	8.05	14.50	6.40	9.28	4
Source: Prepared by the author					

3.3. MFIS classification performance

The MFIS classifier was developed to translate SOM-derived patterns into an operational classification framework based on monitoring-related predictor variables (Fig. 5). After optimization, classifier improved performance from a hit rate of 0.4285 to 0.6071, while average relevance of the correct class increased from 0.3312 to 0.4680. These gains indicate that rule improved the correspondence between environmental inputs and the SOM-based class structure.

Even so, classifier performance remained moderate rather than high, which is an important point and should not be hidden. This outcome is coherent with the intrinsic variability of Pontal Bay and with the expected overlap among estuarine water-quality states. In other words, the model captured meaningful structure, but the environmental system itself limits sharp class separation. This is precisely why an interpretable fuzzy framework is preferable here: it accommodates gradual transitions better than rigid deterministic classification.

The confusion matrices suggest that optimization reduced class imbalance in prediction and improved recognition of classes 2, 3, and 4 (Fig. 6). However, the present results should be interpreted as proof of concept for environmental screening rather than as definitive predictive validation. The MFIS is therefore better framed as a decision-support tool for assigning new observations to probable water-quality states than as a substitute for field monitoring.

3.4. Implications for environmental monitoring

From a monitoring perspective, the main contribution of the proposed SOM-MFIS framework is not the replacement of direct measurements, but the organization of routine environmental data into interpretable hydrochemical states. In transitional systems such as Pontal Bay, where similar field conditions may produce contrasting responses, this type of classification can help identify areas or periods requiring increased surveillance. For example, classes associated with elevated EC/TDS or reduced DO can be prioritized for follow-up sampling, regulatory attention, or integration with additional contamination indicators.

This approach is particularly relevant for monitoring programs operating under limited resources, because it supports the transformation of heterogeneous datasets into a structured screening system. In that sense, the framework aligns with the logic of environmental monitoring and assessment by linking field measurements to practical decision categories. Its main value lies in supporting early interpretation and prioritization, especially in estuarine environments where natural variability can obscure emerging signs of environmental degradation.

4. Conclusions

The integrated SOM-MFIS framework was effective in organizing the physicochemical variability of Pontal Bay into four interpretable water-quality classes. The SOM stage revealed that the monitored estuarine system is characterized by substantial heterogeneity, especially with respect to conductivity-

and solids-related signatures, while the MFIS stage translated these patterns into an operational classification structure based on environmental input variables.

The identified classes captured contrasting hydrochemical states, including conditions associated with higher pH, lower dissolved oxygen, elevated EC/TDS, and comparatively better oxygenation. Although classification performance improved after optimization, the moderate accuracy obtained indicates that environmental overlap remains substantial, which is expected in a mangrove-estuary transition zone influenced by tide, river discharge, and local anthropogenic pressure.

Therefore, the main contribution of this study is not a high-precision predictive model, but an interpretable support tool for environmental monitoring and screening. Future work should expand the dataset, include independent validation, and incorporate additional indicators of anthropogenic impact in order to strengthen class discrimination and improve transferability to other estuarine systems.

Declarations

Ethical responsibilities of authors

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 of Environmental Monitoring and Assessment. The authors confirm that this manuscript is original, has not been published previously, is not under consideration for publication elsewhere, and that the results are presented clearly, honestly, and without fabrication, falsification, plagiarism, or inappropriate data manipulation. All authors approved the submitted version of the manuscript and agree with its submission to this journal.

Competing interests:

The authors declare no competing interests.

Consent to participate:

Not applicable.

Consent for publication:

All authors approved the final version of the manuscript and agree with its submission to Environmental Monitoring and Assessment.

Ethics approval:

Not applicable.

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Author Contribution

Nuno Avelar Nascimento (nuno.an@hotmail.com): data curation, formal analysis, writing - original draft. Thiago Pereira das Chagas ([tpchagas@uesc.br] (mailto:tpchagas@uesc.br)): methodology, software, formal analysis. Flávio Lima de Sena (fsena9324@gmail.com): investigation, data curation. Mavione de Jesus Primo (mjprimo.ppgquim@uesc.br): investigation. Fábio Alan Carqueija Amorim (facamorim@uesc.br): conceptualization, supervision, writing - review and editing. Allison Gonçalves Silva([allisongoncalves@ifba.edu.br] (mailto:allisongoncalves@ifba.edu.br)): methodology, review. Luana Novaes Santos (lnsantos@uesc.br): investigation, review. Erik Galvão Paranhos da Silva (egpsilva@uesc.br): conceptualization, supervision, project administration, writing - review and editing.

Data Availability

The datasets generated and/or analyzed during the current study are available from the corresponding author on reasonable request.

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Figures

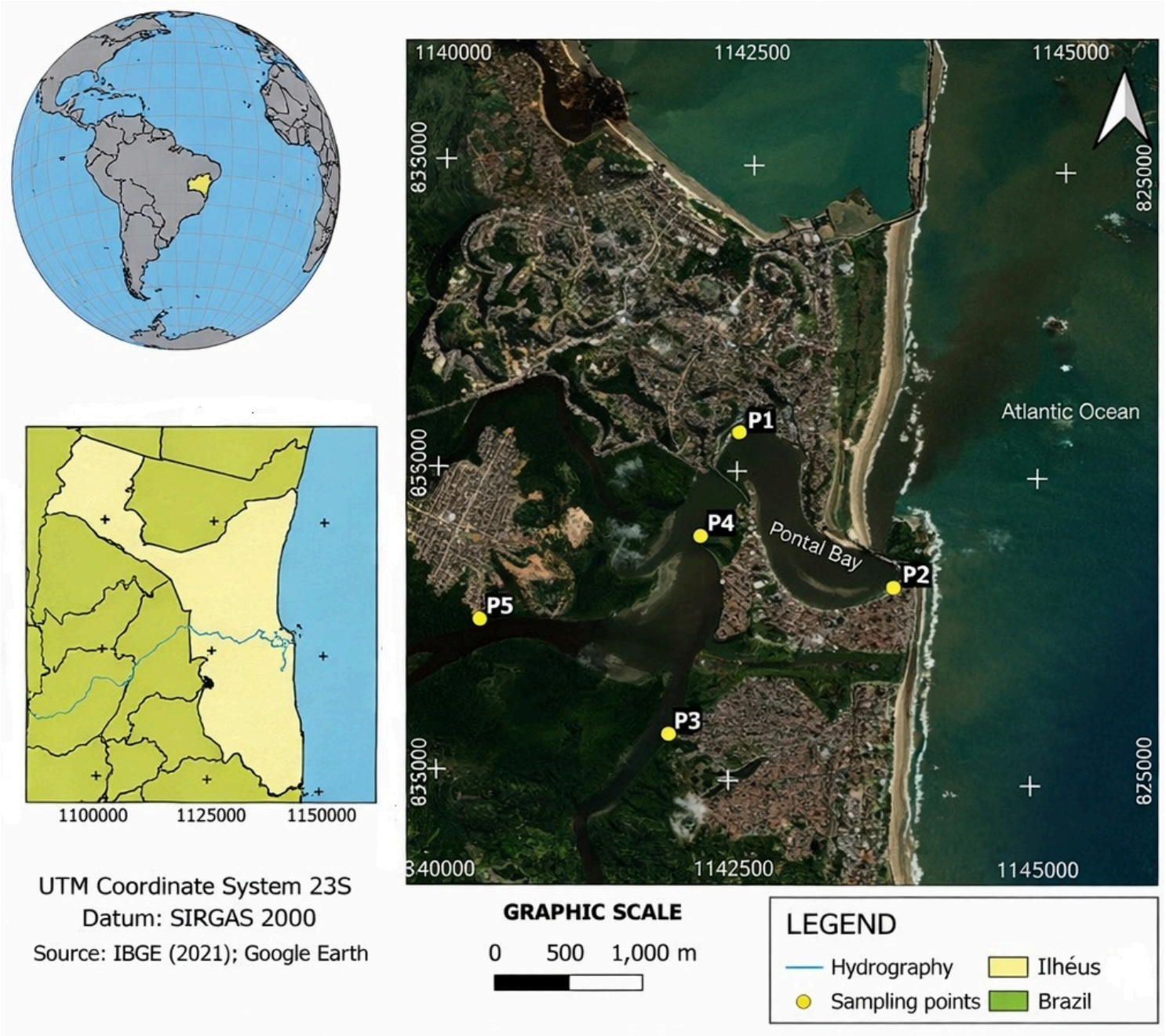


Figure 1

Location of the five monitoring sites in Pontal Bay, Ilhéus, Bahia, Brazil.

Source: Author

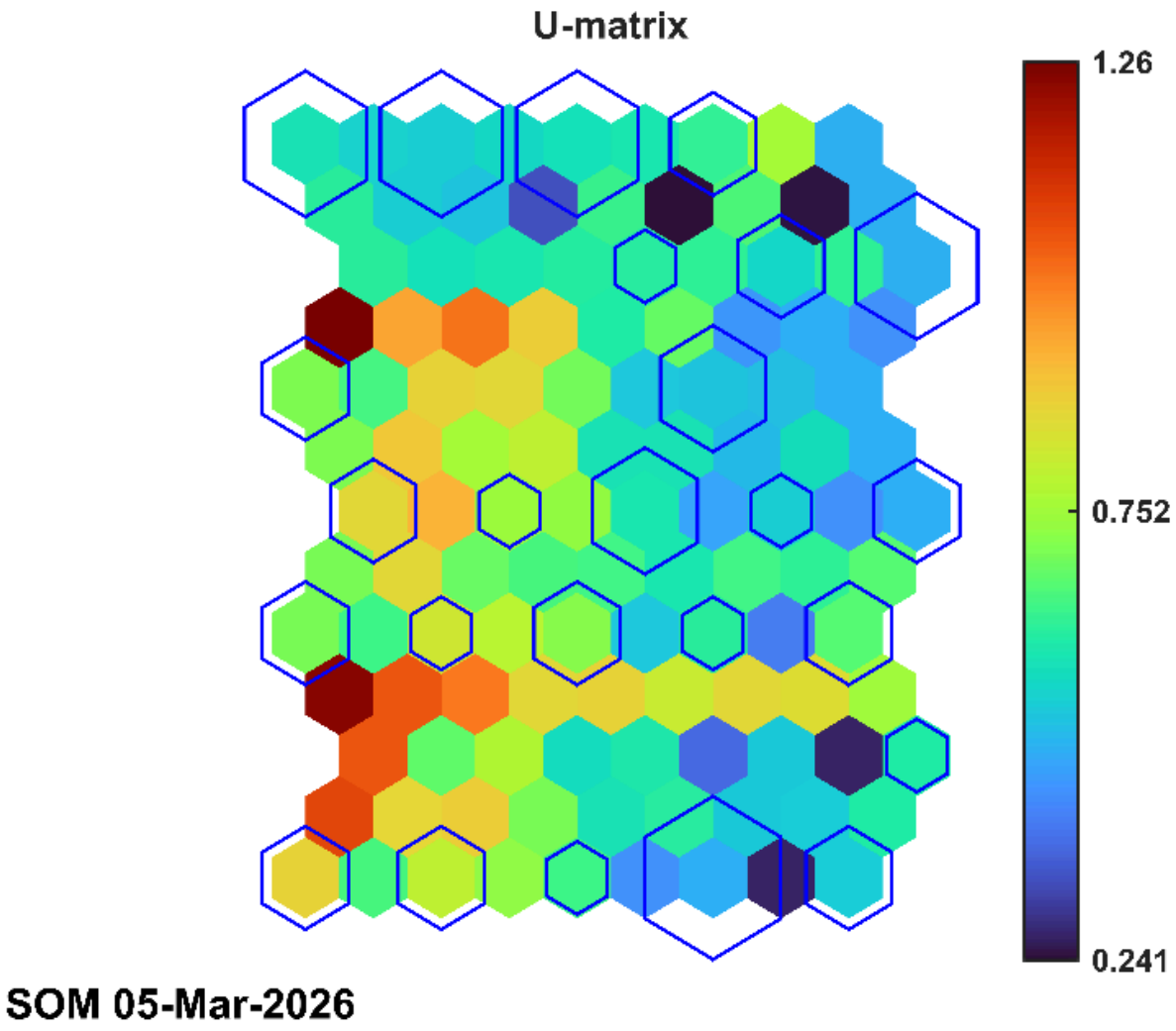


Figure 2

U-matrix representation of the trained SOM showing neighborhood structure of the samples.

Source: Prepared by the author

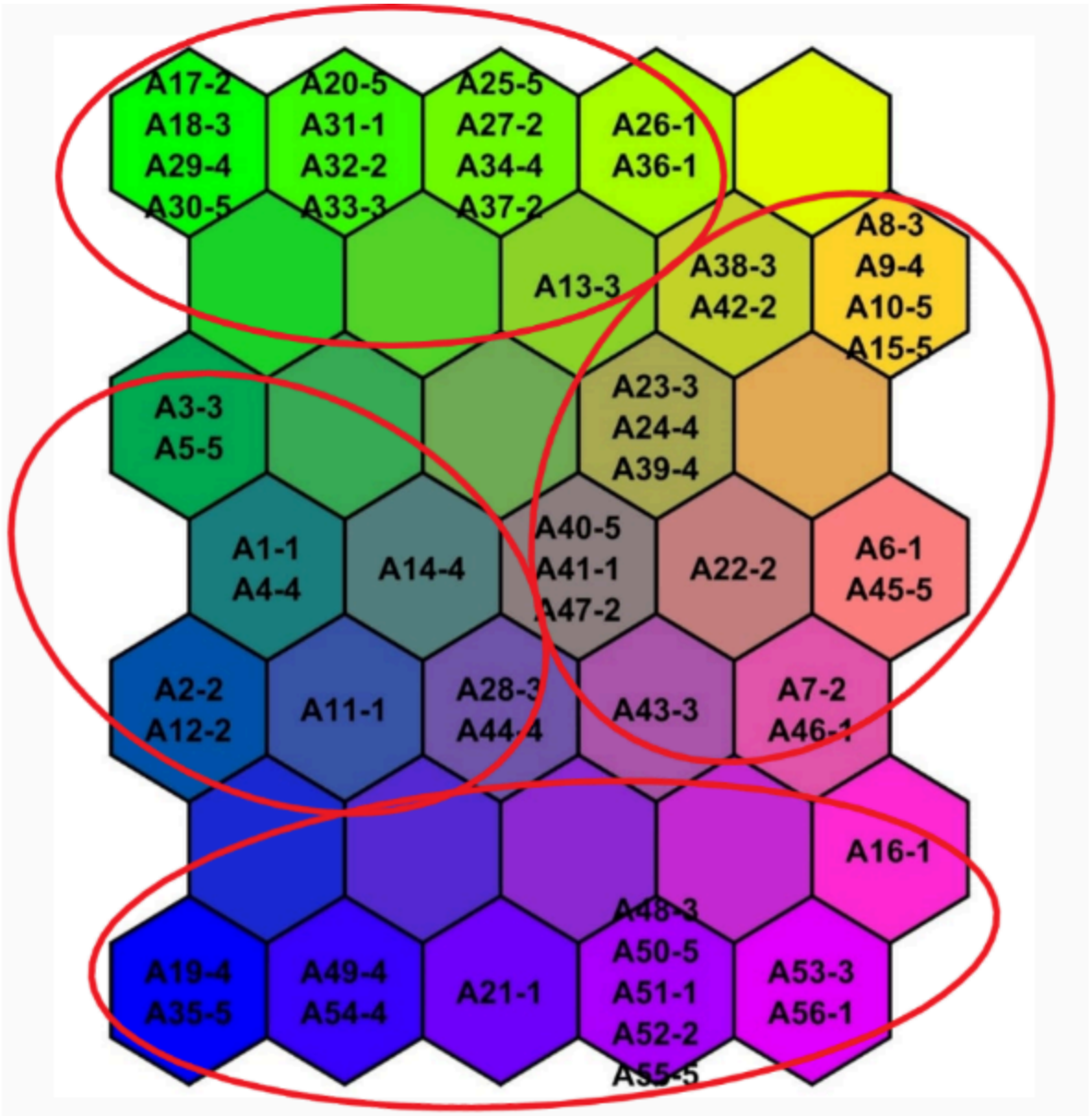


Figure 3

Sample hits on the trained SOM lattice.

Source: Prepared by the author

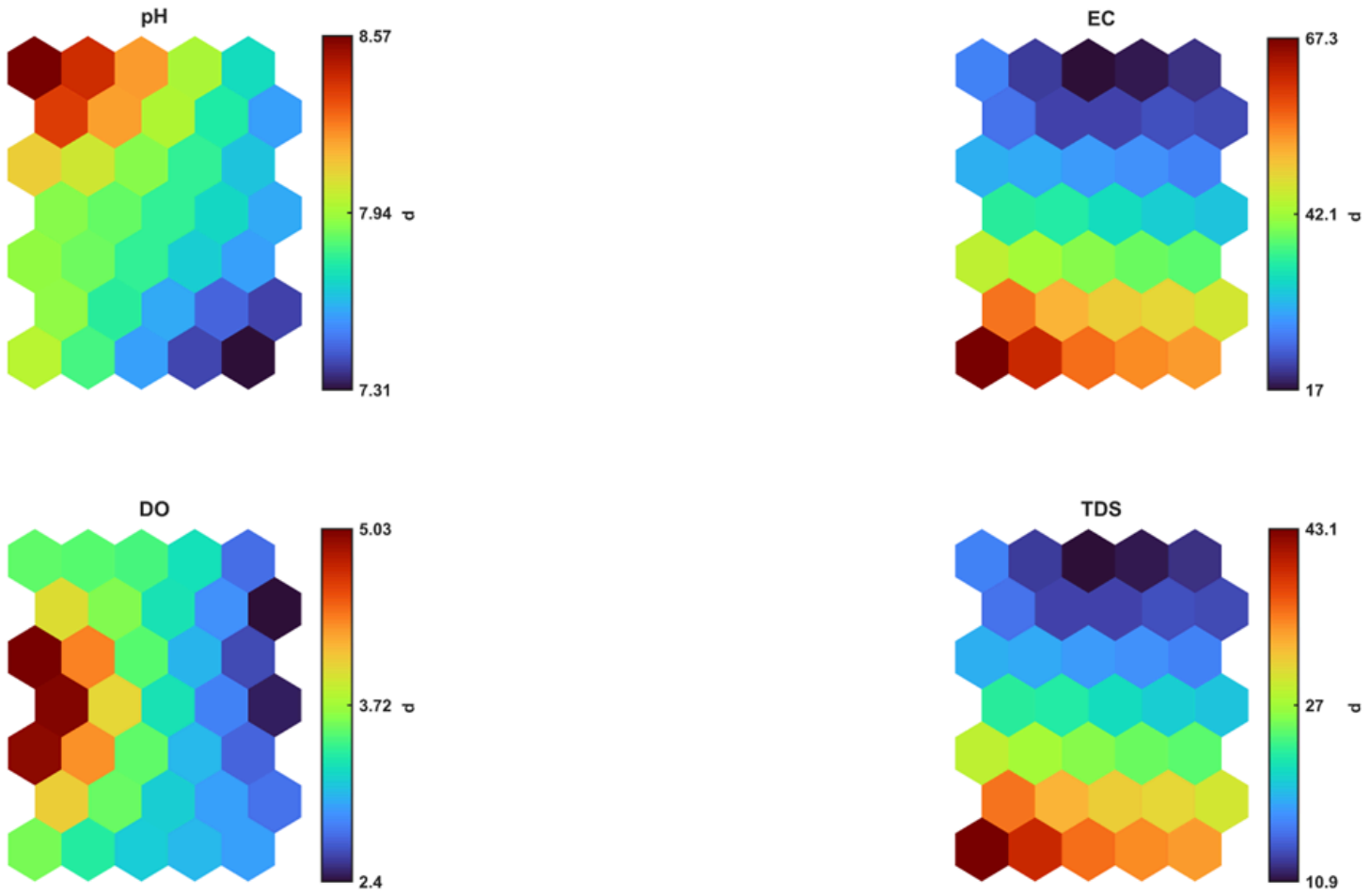


Figure 4

SOM component planes for pH, EC, DO and TDS.

Source: Prepared by the author

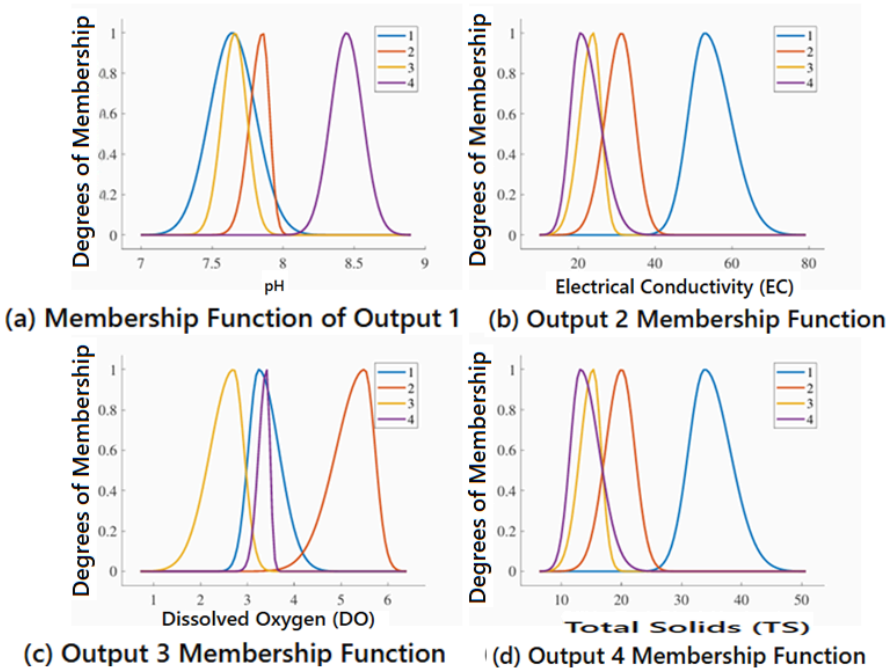


Figure 5

Membership functions and output-group pertinence structure of the optimized MFIS classifier.

Source: Prepared by the author

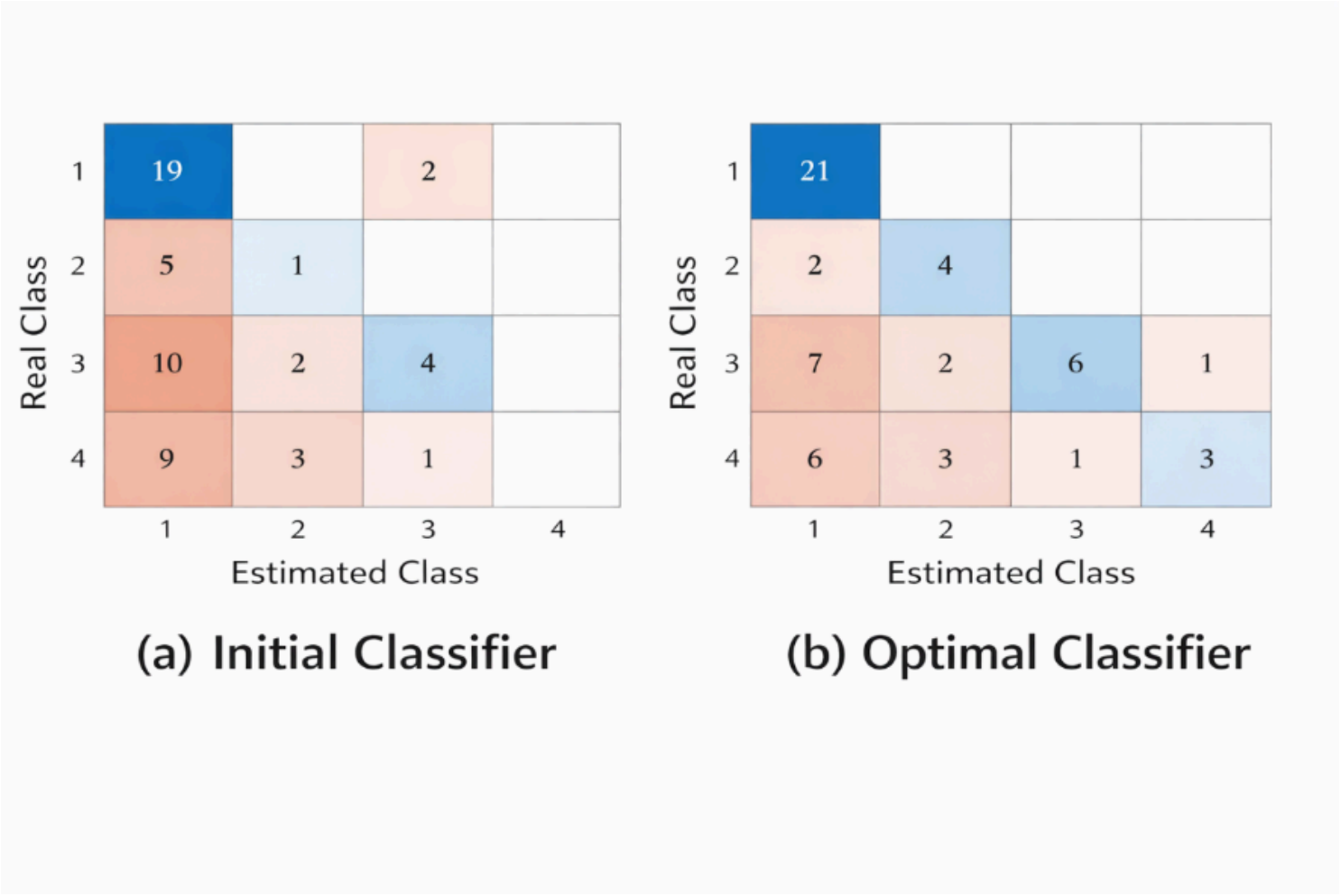


Figure 6

Confusion matrix and classifier output

Source: Prepared by the author