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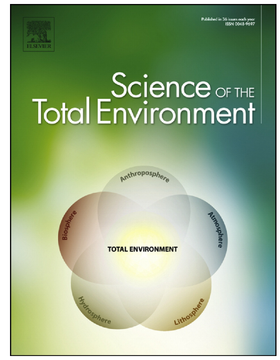

Pattern recognition describing spatio-temporal drivers of catchment classification for water quality

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Title: Pattern recognition describing spatio-temporal drivers of catchment classification for water quality

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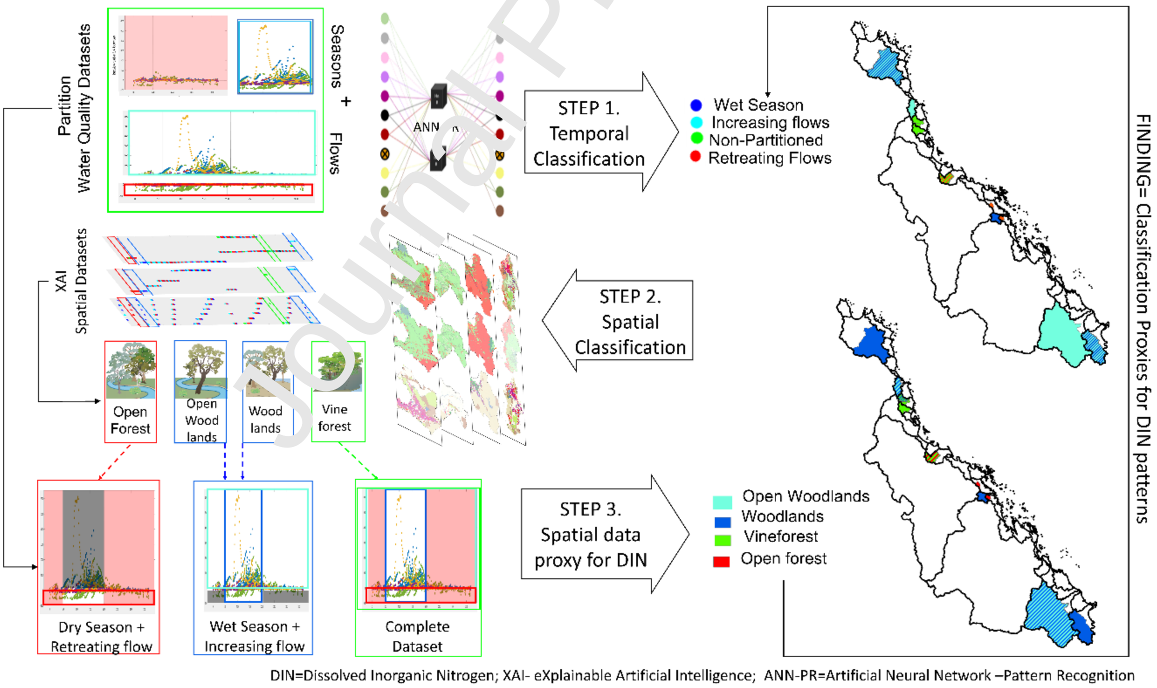
Graphical Abstract



Abstract

Classification using spatial data is foundational for hydrological modelling, particularly for ungauged areas. However, models developed from classified land use drivers deliver inconsistent water quality results for the same land uses and hinder decision-making guided by those models. This paper explores whether the temporal variation of water quality drivers, such as season and flow, influence inconsistency in the classification, and whether variability is captured in spatial datasets that include original vegetation to represent the variability of biotic responses in areas mapped with the same land use. An Artificial Neural Network Pattern Recognition (ANN-PR) method is used to match catchments by Dissolved Inorganic Nitrogen (DIN) patterns in water quality datasets partitioned into Wet vs Dry Seasons and Increasing vs Retreating flows. Explainable artificial intelligence approaches are then used to classify catchments via spatial feature datasets for each catchment. Catchments matched for sharing patterns in both spatial data and DIN datasets were corroborated and the benefit of partitioning the observed DIN dataset evaluated using Kruskal Wallis method. The highest corroboration rates for spatial data classification with DIN classification were achieved with seasonal partitioning of water quality datasets and significant independence ($p<0.001$ to 0.026) from non-partitioned datasets was achieved. This study demonstrated that DIN patterns fall into three categories suited to classification under differing temporal scales with corresponding vegetation types as the indicators. Categories 1 and 3 included dominance of woodlands in their datasets and catchments suited to classify together change depending on temporal scale of the data. Category 2 catchments were dominated by vineforest and classified catchments did not change under different temporal scales. This demonstrates that including original vegetation as a proxy for differences in DIN patterns will help guide future classification where only spatially mapped data is available for ungauged catchments and will better inform data needs for water modelling.

Key words:

Classification, temporal, spatial, water quality, data, XAI (eXplainable Artificial Intelligence), pattern recognition, ANN

Nomenclature

Classifee: Catchment selected as having the most similar data patterns to the Classifier catchment.

Classified catchments: Catchments are paired together where they are matched in both inductive and deductive dataset types.

Classifier: one catchment seeking other catchments with the most similar data patterns.

Deductive: *"the use of alternative data sources as a proxy to deduce the same conclusions as would otherwise be found by the corresponding inductive data. For deductive classification, catchment similarities are inferred from proxy data that represent the process drivers of DIN, in the absence of observed water quality data"*. (O'Sullivan et al., 2022 pg 809)

Inductive: *"the use of observed data to draw inferences regarding that observed data. For inductive classification, catchment similarities are inferred from observed water quality and streamflow data collected from gauging stations and represent the hydrosphere only".* (O'Sullivan et al., 2022 pg 809)

Match(ing)/(es): Catchments paired together for their similarities within a dataset.

SHapley: Method for game theory approach to explanations (Lundberg & Lee 2017; Shapley, 1953)

1. Introduction

Catchment classification using spatial data as a proxy for drivers of water quality or flow is fundamental in hydrological modelling for catchments that are lacking necessary observed data (Nash & Sutcliffe 1970). In such situations, this classification approach based on spatially mapped drivers is referred to as deductive classification (Olden et. al., 2012, O'Sullivan et. al., 2012); it enables the transfer of flow and water quality data from gauged to ungauged catchments (Jaffrés et.

al. 2022, Kanishka & Eldho 2020) and is particularly relevant for the Great Barrier Reef lagoon where 17 of the 35 feeder catchments are ungauged (O'Sullivan et. al., 2022). Land use in these ungauged catchments are perceived to contribute to a disproportionately higher nitrogen load compared to gauged catchments (Wells et al., 2021). To increase certainty in classified models for the Great Barrier Reef catchments as much as possible, identifying the gauged catchments with the most similar nitrogen drivers to the ungauged catchment is important.

Nitrogen process and transport drivers vary in relation to an extensive combination of biotic and productivity influences including ever changing seasons and flows, which affect Dissolved Inorganic Nitrogen (DIN) patterns in water quality observations (Kominoski et al., 2018, and Rodríguez-Castillo et al., 2017). In particular, temporal changes in antecedent vegetation, and water availability drivers are known to contribute to changed responses for DIN in Great Barrier Reef catchments (Liu et al., 2021a and Liu et al., 2021b). These fluctuations in water availability and seasonal variability over space and time make spatial and temporal scales important to consider in classification and data transfer for model development and verification of DIN.

For deductive classification, spatial data is sourced from maps that delineate the area of drivers in each catchment (Olden et al., 2012). The area of the drivers does not change for the period of time the spatial data represents, and so catchments deductively classified using spatial data are matched to the same combination of catchments for the entire mapping period. This approach is reported to be effective for classifying catchments based on most similar flow drivers (Hrachowitz et. al. 2013), however, differing water quality responses from homogenous land uses throughout catchments classified based on those flow drivers are evident (Swain & Patra, 2019, Merz et al., 2020).

Evaluation of overall water quality behaviour throughout catchments, across timescales and in regional contexts is beneficial to make connections between seemingly unrelated or heterogeneous processes (Harman & Troch 2014, Peters-Lidard et al., 2017, Sivapalen et al., 2018). For daily or fine scale data considered in the context of yearly or coarser, dataset periods exceeding 12 years are the minimum to encompass variability affecting water quality on seasonal scales such as floods, low flows and climatic cycles (Ciria & Chiogna, 2020, Howden et. al., 2011). Harris, et al., (2000) also found the length of the water year is not always fixed and classifying catchments on regimes that reflect the full cycle of ecological interactions, rather than the Gregorian calendar time cycles of the day, month and year are more appropriate. Both the magnitude of flows as well as understanding their context in different time periods assist with attributing water quality signatures from short points in time to their respective catchments (Heathwaite et al., 2021). Australia's agroecosystems have evolved to the wet and dry climate cycles of La Nina, and El Nino which circulate over the Pacific Ocean (Holmgren et al., 2001). In response, nutrient production and transport drivers, and associated water quality responses can also fluctuate on fine timescales (Cruz-Ramírez et. al., 2019, Racchetti et. al. 2011, Ciria & Chiogna, 2020, Howden et. al. 2011). An earlier study focused on the Great Barrier Reef Catchments that have regular monthly data over the long term, i.e., exceeding 10 years to cover one full La Nina and El Nino climatic cycle, as well as irregular high frequency sampling that coincides with seasonally influenced rainfall events (O'Sullivan et al., 2022). This study developed a novel approach based on Artificial Neural Network Pattern Recognition (ANN-PR) models to match catchment spatial datasets as a proxy for catchments with corroborating matched Dissolved Inorganic Nitrogen (DIN) patterns. This method uses forward and back propagation to weigh all variables in relation to all others in the dataset and match catchments that share spatial data and water data patterns. In that study, a notable portion of both regular long term and high frequency DIN records for each catchment matched more than one catchment, and this can only be related to heterogeneous patterns for variables of time as a reflection of seasons or flows, that are the only other variables in the DIN dataset. Whilst O'Sullivan et al., (2022) made a significant contribution to catchment classification, the influence of time periods on classification, and assessment of the contribution of spatial drivers towards the classification outcomes remained limited in the proposed ANN-PR corroboration models. Accordingly, the gaps of interest in classification research regarding DIN are the influence of differing time scales on the classification of catchments for DIN, and the relationship of spatial variables as explanatory drivers of DIN under the varying timescale influences.

To address the deficit in knowledge regarding the drivers of DIN classification, variable inputs to ANN models are interrogatable using eXplainable Artificial Intelligence (XAI) approaches. XAI provides transparency and understandability to human end users of artificial intelligence model outputs and further builds trust when used for decision-making (Lundberg et al., 2020). It considers the contributions of each feature individually to overall system outcomes, and therefore each feature variable is uniquely influenced by the presence of the other features in the dataset (Arrieta et al., 2020, Lundberg & Lee, 2017, Wang et al., 2022). The weighted influence of the Shapley method informs on input variable weightings for individual models only (Das & Rad 2020). However, the principle of equal weighting approach applied to traditional hydrological models infact facilitates for catchments that share similar weighted influence of variables as identified by Shapley to be classified.

The objective of this study is therefore to make a novel contribution to classification methods via the application of datasets in new ways to ANN-PR models to explain heterogeneity in DIN water quality patterns observed in previous studies (e.g., O'Sullivan et al., 2022, Liu et al., 2021a) for Great Barrier Reef catchments. We aim to explore variations in DIN patterns that correspond to changes in classified water quality patterns under the different seasons or flow time periods. To identify drivers in the DIN pattern results for future application to ungauged areas we also aim to exploit information in currently mapped spatial feature types that corroborate with the ANN-PR informed results.

The hypothesis evaluated in this study is that: catchments suitable to be classified for DIN differ depending on the periods of time represented in the dataset evaluated for classification, and these differences are influenced by spatial variables that drive DIN. This will be explored here through these research questions: *Do classified patterns induced from water quality data change from* *classification results found by O'Sullivan et al. (2022) where smaller portions of the dataset are considered for a novel aspect to this research*, 1) in different seasons? 2) in high and low flow events? Finally, 3) *do features within currently mapped spatial datasets explain changes in season or flow classification results to identify previously unconsidered drivers and facilitate the future transfer of the method to ungauged areas*?

We explore whether partitioning the full observed dataset included in an Artificial Neural Network Pattern Recognition (ANN-PR) classification evaluation affects catchments matched for similarities in DIN that flow to the Great Barrier Reef. For this study, partitioning included increasing and retreating flows and wet season vs dry season, this is to compare classification results for data collected in different time vs flow scales. To inform future transfer of the results to ungauged areas, we also use an adaption of XAI methods to find spatial variables in datasets that corroborate with catchment response for DIN (O'Sullivan et al., 2022). We finally evaluate whether identified spatial data features drive any changes in classification for different flows and seasons.

2. Methods

2.1. Study area

To evaluate spatio-temporal influences on classification, the study area covered 11 catchments, located in north-eastern Australia, that provide flow to the Great Barrier Reef. These gauged catchments, relative to other gauged and ungauged ones in the region are shown in Fig. 1, and the spatial extent of gauged areas for catchments evaluated in this study are consistent with Khan et al., (2020). Details regarding the observed data available at the respective gauging station, i.e. sample site, for each catchment evaluated in this study, along with sampling frequency and period for DIN collected in each catchment are presented in Table 1.

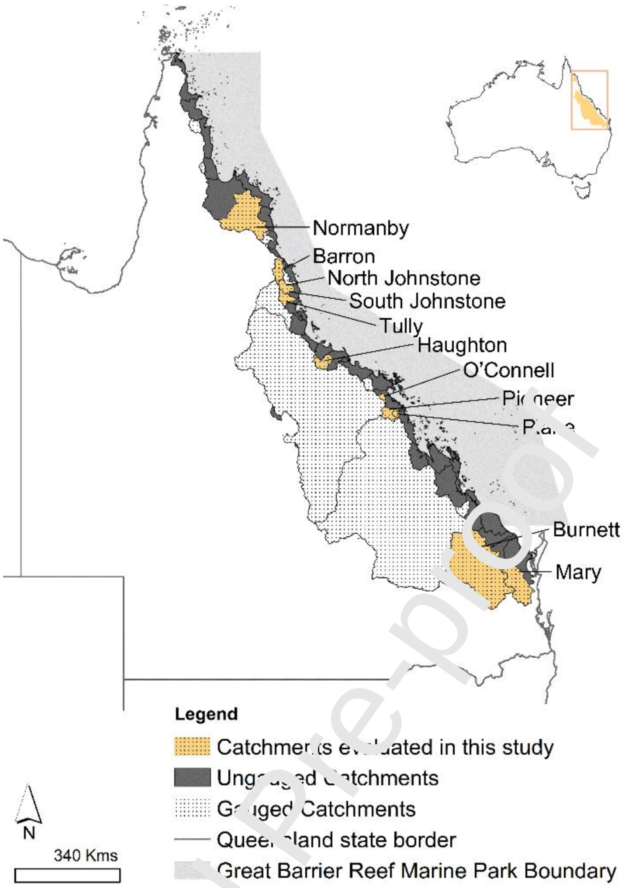


Figure 1: Map of the study area showing the location of catchments evaluated in this study with gauged and ungauged catchments that flow into the Great Barrier Reef

Table 1. Observed data summary for the evaluated catchments. This table includes frequency, and range of all available DIN observations at the gauging stations between 2006-2018 **.** **^** Refer to Figure 2 and Table 2 for definition of records included in Wet Season, Dry Season, Increasing Flows and Retreating Flow datasets

Catchment Name	**Normanby**	**Barron**	**North Johnstone**	**South Johnstone**	**Tully**	**Haughton**	**O'Connell**	**Pioneer**	**Plane**	**Burnett**	**Mary**
Gauging station ID for observed data	105107A	110001D	112004A	112101B	113006A	119003A	124001B	125013A	126001A	136007A	138014A
Gauged catchment area (km^2)	12,828	1,950	926	399	1,386	1,807	336	1,464	327	30,724	6,863
Natural Resource Management Region	Cape York	Wet tropics	Wet tropics	Wet tropics	Wet tropics	Burdekin	Mackay Whitsunday	Mackay Whitsunday	Mackay Whitsunday	Burnett Mary	Burnett Mary
Gauged Catchment Centroid Latitude (decimal °)	-15.46	-17.05	-17.5	-17.66	-17.87	-19.72	-20.77	-21.23	-21.24	-25.73	-26.19
Gauged Catchment Centroid Longitude (decimal °)	144.56	145.51	145.69	145.77	145.72	146.81	148.56	148.74	148.94	151.28	152.49
DIN Record Period)	3/10/2006-25/08/2017	19/01/06-15/09/17	30/01/2006-15/09/2017	24/02/2006-15/09/2017	13/01/2006-1[illegible]/04/2018	20/12/2012-25/09/2017	25/01/2007-24/08/2017	18/10/2006-13/09/2017	4/09/2009-26/08/2017	23/10/20006-15/09/2017	25/09/2013-29/06/2018
DIN sampling frequency	Events Jan-March	Regular (1) monthly, Events Jan-March	Infrequent half yearly, Events Jan-March	Regular (1) monthly Events Jan-March	Frequent (>1) monthly, Events Jan-March	Regular monthly, Events Jan-March	Irregularly One off Events Jan-March	Frequent (>1) monthly, Events Jan-March	Regular (1) monthly, Events Jan-March	Frequent (>1) monthly, Events Jan-March	Frequent (>1) monthly, Events Jan-March
Number of records in DIN record period	244	318	94	414	723	80	87	402	302	400	176
Number of records in Wet Season^	229	233	77	318	523	47	65	292	229	275	111
Number of records in Dry Season^	17	87	17	98	204	33	22	111	75	127	66
Number of records in Increasing flows^	233	146	52	227	420	43	81	321	148	222	103
Number of records in Retreating flows^	12	172	42	187	303	37	6	81	154	178	73
Max DIN (mg/L)	1.70	0.63	0.37	0.37	1.88	0.33	0.83	3.56	3.87	4.66	1.29
Min DIN (mg/L)	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
Mean DIN (mg/L)	0.06	0.12	0.15	0.13	0.24	0.07	0.11	0.23	0.42	0.16	0.20
Median DIN (mg/L)	0.03	0.10	0.14	0.13	0.21	0.03	0.06	0.17	0.21	0.10	0.16
Standard Deviation DIN (mg/L)	0.13	0.09	0.07	0.06	0.15	0.09	0.14	0.28	0.53	0.32	0.20

2.2. *Modelling and Conceptual framework*

Our earlier studies showed that the application of an Artificial Neural Network Pattern Recognition (ANN-PR) is effective in classifying catchments based on patterns in the Dissolved Inorganic Nitrogen (DIN) and the hydrological flow dataset (O'Sullivan et al., 2022). The ANN-PR method facilitates for each DIN observation to be independently classified to another catchment, and so is suited to our evaluation to classify DIN observations depending on the respective season or flow regime. Classification is then characterised through eXplainable Artificial Intelligence approaches. For this study, water quality and flow records from the most downstream gauging station utilised for each gauged catchment (Table 1) were obtained and arranged consistent with methods described in O'Sullivan et al., (2022). Data sets were then partitioned to include data for the following scenarios, to identify whether data included in the partitioned dataset only changed classification results:

Increasing baseflows: positive geomean score, i.e., daily baseflow rates that exceed the average flow calculated from the commencement of the dataset;

Retreating baseflows: negative geomean score, i.e., daily baseflow rates lower than the average calculated from the commencement of the dataset until that point in time;

Wet Season: All dates within the time period following the date after commencement of the water year where all catchments exhibit positive geomean baseflows;

Dry Season: All dates within the time period following commencement of the wet season each water year where all catchments exhibit negative geomean baseflows; and

Non Partitioned: complete data set

Equations for nominating whether DIN observations were allocated to a Wet or Dry Season, or an Increasing and Retreating baseflow dataset are described in Table 2, and a visual example of the records included in each partitioned dataset scenario are shown in Figure 2. For simplicity, this novel research partitioned wet vs dry season for each catchment based on all catchments achieving the criteria for above vs below average flow .

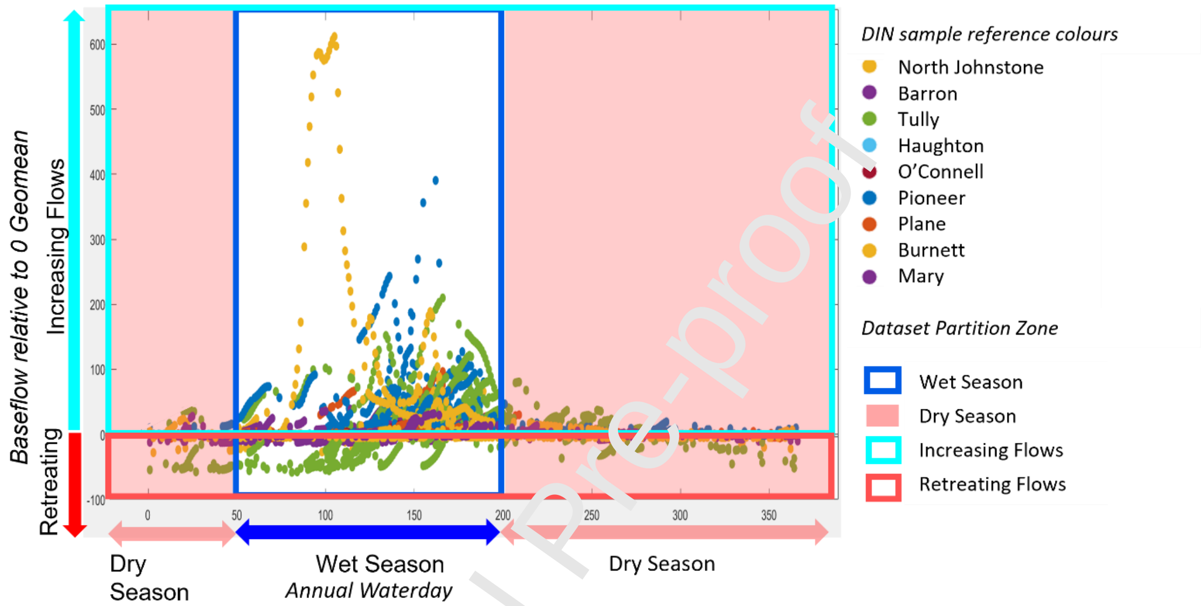


Figure 2: Visual representation of dataset records included in each dataset partition zone.

The partitioned datasets were then classified with other catchments in the study area using the ANN-PR classification method (Figure 4). Because this classification is induced from observed water quality data, i.e. here for Dissolved Inorganic Nitrogen, this classification is referred to hereafter as inductive classification consistent with O'Sullivan et al., (2022).

For this study, we also use feature relevance exploration XAI approaches (Arrieta et al., 2020) to identify similarities in spatial data attributes for catchments and evaluate their match rate with the inductive classification for DIN under differing flow and seasonal scenarios. The purpose of this step is to establish whether it is possible to classify catchments for DIN under differing flows or seasons based on using only spatial data as a surrogate for DIN. The workflow for this study is shown in Figure 3.

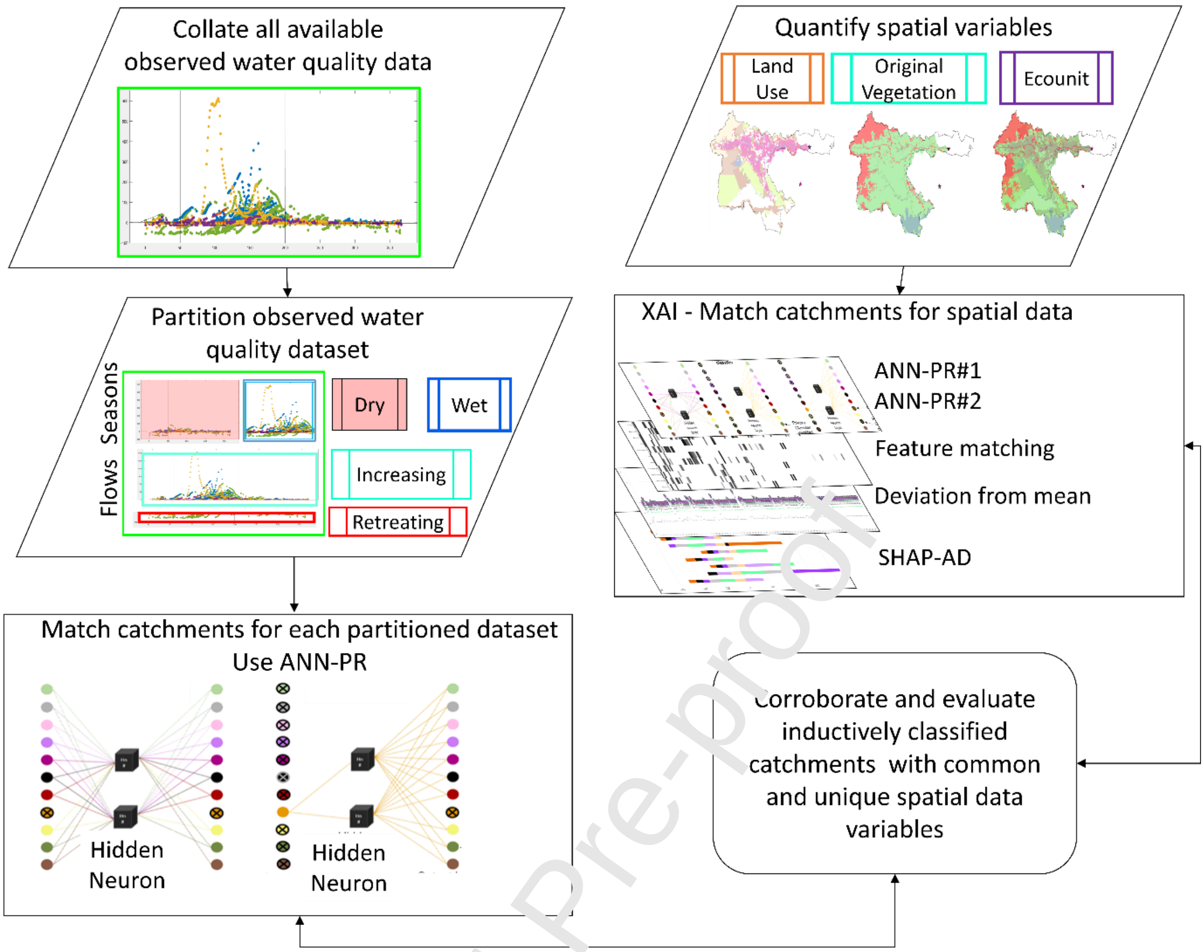


Figure 3: Workflow for identifying the most suitable catchment to classify under flow or seasonal scenarios and corroborating spatial drivers.

2.3. *Water Quality Data Pattern Matching*

A fundamental part of this research is to first partition water quality datasets to establish the catchments that inductively classify together under the different flow or seasonal dataset partitions. Water quality dataset establishment and detailed methodology for subsequent matching of catchments for the inductive classification used similar approach to O'Sullivan et. al., (2022) and is presented in Supplementary Material S1. Criteria for water quality dataset partitioning that is the novel aspect to this research are detailed in Table 2.

Table 2 Dataset partitioning for DIN observations. For this study, the dataset is partitioned by Wet Season vs Dry Season or Increasing vs Retreating flows. This partitioning created four sub datasets, and retained the Non-Partitioned form of the complete dataset used in O'Sullivan et al., (2022).

Data Partitioning	Method of extraction from Complete Dataset	Equation
Non-Partitioned	Complete dataset included for control	$N_A = \in_1 ..... \in_n$ Where: N = Records to be included; $_A$= All; ∈ =dataset record; $_n$ = last dataset record
Dry Season	Dry Season = water days 201-49. Commencement of dry season at day 200 was based on negative geomean for flows for all catchments.	$N_{DS} = \in\omega_{201} ..... \in\omega_{49}$ Where: N = Records to be included; $_{DS}$=Dry Season;∈ =dataset record; ω=waterday;
Wet Season	Wet Season = water days 50 – 200, Commencement at 50 was based on first positive geomean values for surface flows for all catchments after the commencement of the traditional water year on 1 October annually.	$N_{WS} = \in\omega_{50} ..... \in\omega_{200}$ Where: N = Records to be included; $_{WS}$=Wet Season;∈ =dataset record;ω=waterday;$_n$ = last dataset record
Increasing flows	Complete dataset records with baseflow and with a positive geomean score were allocated to this group	$N\cap = \in\cap_1 ..... \in\cap_n$ Where:N = Records to be included; ∈ =dataset record;∩=Geomean value of negative baseflows;$_n$ = last dataset record
Retreating flow	Complete dataset records with baseflow with a negative geomean score were allocated to this group	$N\cup = \in\cup_1 ..... \in\cup_n$ Where: N = Records to be included;∪=Geomean value of negative baseflows; ∈ =dataset record;$_n$ = last dataset record

2.4. Spatial Data Matching

O'Sullivan et al., (2022) demonstrated spatial data as a catchment classification proxy for DIN patterns in water quality datasets. The novel aspect of this research involves adjustment to the ANN-PR method introduced in O'Sullivan et. al. 2022 to pair multiple catchments together based on spatial data. Explainable artificial intelligence (XAI) approach is also used to explore and explain the spatial data similarities.

2.4.1. Spatial Dataset Construction

The mapping data was obtained from the state of Queensland's open access Q-Spatial mapping portal, for Queensland Land Use Mapping which is developed using the approach described in ABARES (2016), and Original Vegetation from Broad Vegetation Group Mapping (Neldner et al., 2017). Broad Vegetation Group mapping represents the combination of mesic, landscape, geological situation, with the natural vegetation response to the unique combination of those influences at each location. Rather than including numerous mapping layers of all elements of the environment known to influence vegetation growth and productivity, Broad Vegetation Group mapping has been used as a proxy for biotic responses to abiotic factors. It is used here as a parsimonious dataset to spatially represent natural biotic (vegetation) responses to abiotic factors commonly used in water quality modelling. Ecounit polygons were also created in this study via a merging of the Land Use and Original Vegetation mapping together. The purpose of the variables created in Ecounit mapping is to account for situations where environmental features that influenced evolution of the original vegetation persist and influence the nutrient responses of the same land uses in areas that naturally evolved different original vegetation types (O'Sullivan et al., 2022). ArcGIS ver 10.6.1 was used to extract the areas of variables in the Land Use, Original Vegetation and Ecounit spatial mapping datasets for each catchment.

2.4.2. Catchment matching using Artificial Neural Network Pattern Recognition

This study investigated whether different catchments classify together under different spatio temporal scales, therefore more than one classifee is needed. Given ANN-PR only classifies one catchment as most similar for each catchment (ANN-PR#1) we repeated the ANN-PR classification as described in O'Sullivan et al., (2022) with the dominant classifee catchment removed to identify the secondary classifee catchment as ANN-PR#2, Figure 4. The benefit of ANN-PR for classification is its capability to facilitate direct comparison of classification results for both water quality and spatial data (O'Sullivan et. al., 2022). The model is designed to match each record in the input layer dataset to one catchment in the classifee dataset with the most similar data patterns as established by algorithms in the supervised training scenario.

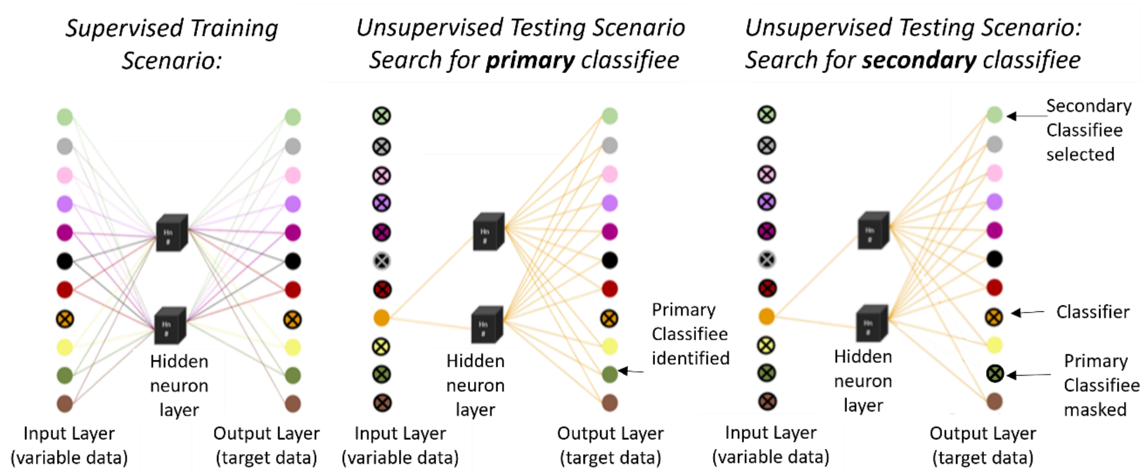


Figure 4: ANN-PR approach developed to identify a secondary classifiee for spatial data. Coloured dots represent datasets for individual catchments. The secondary classifiee is identified based on the trained algorithm by hiding the primary classifee catchment data from the testing dataset.

2.4.3. *An eXplainable Artificial Intelligence* (XAI) Method: *Feature Matching System*

To explain catchments matched using ANN-PR, relative similarities in the proportion of each spatial variable in each catchment were evaluated. The purpose was to identify landscape or ecological reasoning for classification results generated by ANN-PR. The XAI method also classifies catchments based on shared features, but unlike ANN-PR, XAI does not limit the classification to one most similar catchment. All data within the spatial data tables for each catchment was converted to be the fraction of the total for each respective catchment (A from Eq 1). Rapid comparison of catchments with similar variable distributions Land Use, Original Vegetation and Ecounit dataset feature variables were visualised using standard heatmap function in Matlab. Colour scaling was adjusted to logarithmic to expose similarities in small fractions and eliminate zero. Catchments with matching feature dominance for each respective correlation categories of 0.51-0.60, 0.61-0.70, 0.71-0.80, 0.81-0.90 and 9.1-1.0 were identified visually from the heatmaps.

2.4.4. An *eXplainable Artificial Intelligence* (XAI) Method: *Deviations and SHapley additive deviations*

For hydrological classification studies, each variable is traditionally considered to have equal weighting in comparison to all other variables in the dataset, and laws of scaling for positive and negative influences of variables are also considered to average each other out in parameterisation of models after classification has been applied (Jehn, 2020). In contrast, game theory recognises up front that each variable in datasets used for classification is influenced by the additive influence of all variables with each other (Cohen et al., 2007, Lundberg & Lee 2017). For this study, both these approaches are combined whereby the fundamental influence of each variable towards DIN is considered equal, while simultaneously being scaled relative to the deviation of all other spatial feature variables using Eq 1.

$$D_s = A_s - A_\forall \qquad \text{Eq 1}$$

where:

D: deviation of spatial dataset variable

A: proportional area of variable (A= area of variable /total catchment area)

S: subject variable

∀: all dataset variables excluding s

The deviation of the spatial dataset variable was then evaluated in two ways. First, Standard Deviation valuations involved identifying, catchments with the same spatial variables that deviated from the average proportional area of all other spatial variables in their respective datasets. These catchments were then manually recorded as “matched”. Second, consistent with SHapley game theory principles (Lundberg et. al., 2020; Shapley, 1953), the accumulative proportional area of spatial feature deviations were plotted for each spatial dataset type, Land Use, Original Ecosystem and Ecounit for each catchment, as well as accumulatively for the entire dataset to determine which spatial feature deviations fell in the top 10% throughout the datasets for all catchments separately and combined. Spatial features with the highest 10% additive feature deviations for all catchments combined were selected and referred to as SHAP-AD (i.e., SHapley Additive Deviations) deviations for each catchment.

Original Vegetation, Land Use, or Ecounits matched in the heatmap, all standard deviations and SHAP-AD were recorded to facilitate interrogation of the influence of the extraordinary spatial variables towards corresponding catchment matches using water quality patters, i.e. inductive classification.

2.5. Corroboration Metrics

Catchment matching results for all datasets were evaluated to establish the feasibility of the approach for spatial data to be used as a proxy in place of partitioned water quality data for classification. Fifteen catchment match results were identified for each classifier (i.e., five partitioned inductive water quality dataset scenarios of Wet Season, Dry Season, Increasing Flows, Retreating flows and non-partitioned, evaluated separately for each of the three dataset types of SF, BF or SFBF), were visualised on a graph which shows all corroborating classification results for all catchments on one figure. for rapid visual assessment whether matched catchments change under the different season or flow scenarios.

For catchment matching using spatial data, 12 scenarios were evaluated for each classifier. These were three spatial datasets Land Use (LU), Original Vegetation (OV) and Ecounit (EU)) and 4 iterations of the evaluation method (i.e. ANN-PR#1 with ANN-PR#2, Feature Matching, Standard Deviations and SHAP-AD). Catchment match results for each scenario were overlaid on the quilt graph for visual corroboration with the catchment match results for the water quality dataset matches. Where the same classifee was identified for the classifier in both inductive classification (i.e., pattern matching using water quality datasets) and deductive classification (i.e., pattern matching informed by spatial datasets) the classifee and classifiers were nominated as corroborated.

Corroboration rates for each evaluation technique for partitioned datasets scenario were calculated using equation 2.

$$\delta_T = \frac{\sum_{B_{T(FP)n1.....n}}^{B_{TFP}}}{k_{\mathbb{N}}} \qquad \text{Eq 2}$$

where:

δ: Corroboration Rate for evaluation technique

T: evaluation technique

F: Dataset for flow state (BFSF, SF, or BF) with associated DIN

P: Dataset partition for F (Wet Season, Dry Season, Increasing Flows, Retreating Flows)

B: number of catchments corroborated

$k_{\mathbb{N}}$: Number of classifee catchments

Kruskal Wallis nonparametric test was used to evaluate the independence of the corroboration rates for each evaluation technique (i.e., ANN-PR, Feature Matching and Deviation Evaluations), spatial dataset (LU, OV, EU), and partition type (Flows, Increasing flows, Decreasing flows, Season, Wet Season and Dry Season) from each other (Kruskal & Wallis, 1952). The significance level for testing the independence of dataset corroboration rates from each other was set at the default of p<0.05 consistent with O'Sullivan et al., 2022.

3. Results

For inductive datasets, different catchments were matched together under different flow or season scenarios (Figure 5). Corroboration of inductive classification results with the deductive classification informed by spatial data varied for each catchment and dataset partition type (Supplementary Material Figure SF1).

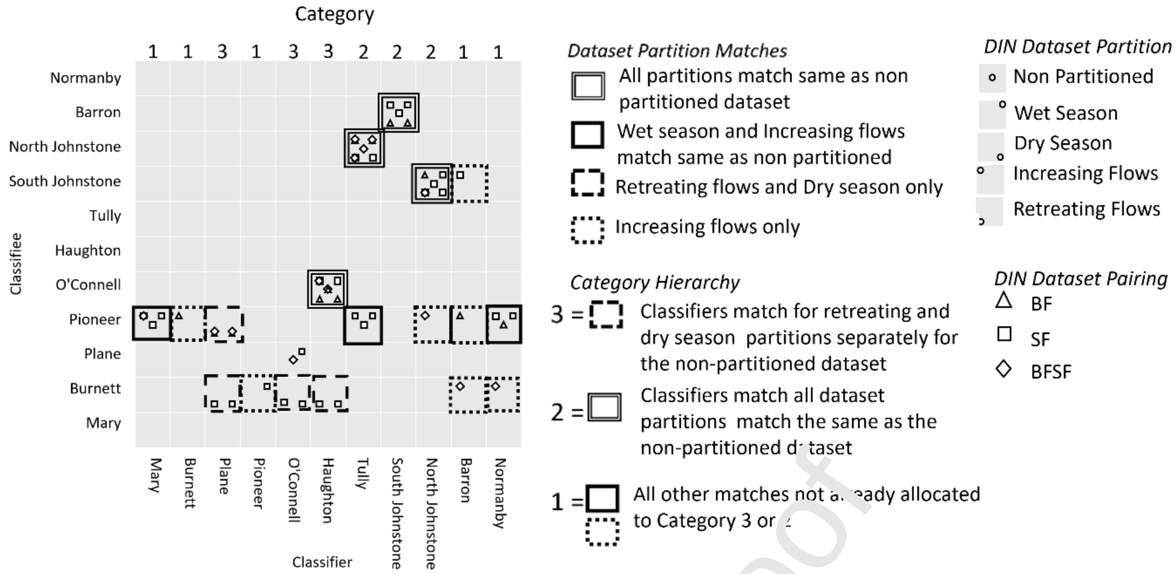


Figure 5: Catchments matched by majority pattern matches for different season and flow data compared to the non-partitioned dataset. DIN dataset colour and shape icons identify catchments that matched together for the respective datasets. Three categories of catchment matches are shown for the combination of dataset partitions and distinguished by cell frames.

3.1. Pattern Matching

Patterns in the datasets partitioned for Increasing flow matched the majority of the patterns observed in another catchment dataset for all 11 catchments. Inductive classification, i.e., classification using observed water quality data, catchment matches vary depending on the dataset partition, and classification fell into one of three categories (Figure 5). The highest inductive classification rate was achieved for Wet Season dataset partitioning with 9 of the 11 catchments (>80%) pattern matching a majority of the dataset with another catchments dataset. Datasets partitioned for Increasing flows and the non-partitioned dataset both matched a majority of dataset patterns for 8 out of the 11 catchments (72%). Finally, datasets partitioned for the Dry Season and Retreating Flows both only matched 6 of the 11 catchments (<55%). Of the catchment matches, North Johnstone and South Johnstone were the only catchments that achieved the same catchment matches through all three Wet Season, Dry Season and Non-Partitioned dataset scenarios. In contrast, while catchment matches for Mary, Pioneer, Haughton and Tully remained consistent through the Wet Season, Increasing flows and the Non-Partitioned dataset, the same matches did not persist for Dry Season or Retreating Flows partitioning of the datasets. Plane is the only catchment that has the same pattern match for both Dry Season and Retreating flows data partitioning, but the Plane catchment did not have a majority pattern match for the non-partitioned dataset. Barron did not have pattern matches for Non-Partitioned, Dry Season or Retreating flows (Figure 5). Collectively ANN-PR pattern matching of partitioned datasets revealed three inductive classifier categories (Figure 5). Plane, O'Connell and Haughton are nominated Category 3 where Dry Season and Retreating flows match to a different catchment than the other dataset partitions. Wet tropics catchments of Tully, South Johnstone and North Johnstone match only to the same catchment as the Non-Partitioned dataset, and Normanby, Barron, Pioneer, Burnett and Mary are nominated as Category 1, where dataset partitioning match catchments for Wet Season or Increasing flows dataset partitions and never for Dry Season or Retreating flow dataset partitions. Both ANN-PR#1 with ANN-PR#2 and XAI Feature Matching methods paired all catchments to at least one other catchment. Matching all deviations achieved 85% match rate, while SHAP-AD (largest 10% of feature deviations) achieved only a 33% match rate (Supplementary Material Figure SF1).

3.2. Corroboration of catchment matches for Water Quality and Spatial datasets

Corroboration between inductive classification for water quality patterns and each spatial data pattern match evaluation varied. The highest frequency of corroboration was achieved for feature matches for Land Use in the Wet Season (Supplementary Material Figure SF1). For feature matching datasets, Ecounit Data which combines both Land Use and Original Vegetation had the highest corroboration frequency with the non-partitioned dataset. For ANN-PR#1, the non-partitioned dataset instead had the highest corroborations with Land Use data, while Wet Season partitioning had the highest corroboration with Ecounits for ANN-PR#1. Addition of ANN-PR#2 facilitated for 9 of the 11 catchments to corroborate a second classifier that was not identified in ANN-PR#1. Excepting Barron, South Johnstone and North Johnstone where ANN-PR#2 did not generate a catchment match for LU, and Plane where there appeared to be an issue in the results generated, because they were a duplicate of ANN-PR#1, the catchment matches generated by ANN-PR#2 for LU only corroborated with Tully for the inductive classification results. In contrast, ANN-PR#2 for Original Vegetation and Ecounit generated secondary catchment matches that successfully corroborated with at least one of the inductive dataset catchment matches for the rest of the catchments (Supplementary Material Figure SF1).

3.2.1. Corroboration for Evaluation Techniques

Pattern Matching Corroboration rates show statistical independence between the three different evaluation techniques ($p=0.015$) and 5 different dataset partitions ($p=0.001$). In the pairwise comparisons, Feature Matching and ANN-PR combined evaluation techniques did not significantly differ from each other ($p=0.879$), however, both had significantly higher corroboration rates than Deviation Evaluations ($p=0.015$ and 0.010 respectively). This result shows that interrelationships between all variables in the spatial dataset collectively, as included in evaluations for ANN-PR and Feature Matching, have a more significant corroboration with water quality patterns for DIN compared to only considering spatial features that deviate the most, i.e., top 10%, from all others in the dataset.

3.2.2. Corroboration for Spatial Datasets

Although Original Vegetation (OV) and Ecounit (EU) had higher median and overall corroboration rates of catchment matches with water quality catchment matches than Land Use (LU), no significant difference in corroboration rates was found between the dataset types (ie. LU, EU or OV) $p=0.067$ (Supplementary Material Figure SF1).

3.2.3. Corroboration for Partitioning

Partitioning the dataset into seasons resulted in the best performing corroboration with a median corroboration rate of 0.3, a maximum corroboration rate of 0.57 and pairwise significance scores for independence from the other dataset partition corroboration results of mostly $p<0.001$ to $p=0.026$. The exceptions were the difference between corroboration rates for combined seasons partition and Non-partitioned datasets that were not classified as significantly independent ($p=0.069$). There was an insignificant difference between corroboration rates for the combined season partition compared to Wet Season partition by itself (p=0.107). The median corroboration rate for seasons combined exceeded maximum corroboration rates for all the other partitions evaluated, with the greatest difference in performance with Retreating flows (Supplementary Material Figure SF1).

3.3. Evaluation of Extraordinary Spatial Variables

Evaluation of spatial features using XAI techniques showed in the wet tropics, corroborated catchments were dominated by spatial deviations for productivity in natural environments as well as all the land uses on land with Original Vegetation mapped as mesophyll and notophyll vine forests (Supplementary Material Figure SF2). In contrast, corroborations for Burnett and Normanby Original Vegetation data were dominated by areas mapped open wood and or depositional areas. This did not persist when the combination of Land Use with Original Vegetation data was considered. Dominant Ecounit features for Burnett instead were more similar to Barron where production of relatively natural systems on open woodland areas (Supplementary Material Figure SF2).

The SHAP-AD method identified that 17 of the 162 spatial variables were in the top 10% largest deviations from the average area for each catchment, compared to all other variables in the dataset. Evaluation of the top 17 spatial variables demonstrates that there are distinct differences between dominant spatial variables in catchments north of Haughton compared to catchments south of and including Haughton (Supplementary Material Figure SF3). Ecounit, 1.2, which is produced from relatively natural environments on lands with complex mesophyll to notophyll vine forests of the wet tropics, was most prominent in the wet tropics catchments. While Ecounit 2.2 with the production from relatively natural environments with complex to simple, semi-deciduous mesophyll to notophyll vine forests sometimes with *Araucaria cunninghamii* (hoop pine), also dominated in all catchments north of Haughton, as well as Burnett. However, the Original Vegetation portions of the dominant Ecounit data were not in the most dominant spatial variables in the Original Vegetation datasets. The land use portion of the dominant Ecounits was, however, consistent with Land Use spatial datasets for the wet tropics. Land Use 2: Production on relatively natural environments dominant in North Johnstone, South Johnstone and Tully catchments, as well as contributing to Barron and a smaller extent, Mary.

For catchments south of Haughton, as well as Barron, Ecounits including 16.3 production from dryland agriculture and plantations on lands mapped with Original Vegetation of *Eucalyptus spp*. dominated open forest and woodlands drainage lines and alluvial plains were most prominent in Haughton, Pioneer, Burnett and to a lesser extent Mary and Barron. Meanwhile, Ecounit 13.3 of production from dryland agriculture and plantations on land originally characterised by dry to moist eucalypt woodlands and open forests, mainly on undulating to the hilly terrain of mainly metamorphic and acid igneous rocks only dominated in Mary, Burnett and Barron.

In contrast to Land Use and Ecounit SHAP-AD results, North Johnstone and South Johnstone SHAP-AD results for Original Vegetation features displayed negative deviations from the mean. Interestingly. Normanby and Burnett shared similarities for variable 21: *Melaleuca spp*. dry woodlands to open woodlands on sandplains or depositional plains, while Mary and Pioneer were the only catchments that shared positive deviations for dry woodlands to open woodlands, mostly on shallow soils in hilly terrain. Haughton, Pioneer and Burnett shared deviations for variable 6: Notophyll vine forests and microphyll fern forests to thickets on high peaks and plateaus. Tully and Normanby shared wetlands associated with permanent lakes and swamps, as well as ephemeral lakes, claypans and swamps. Includes fringing woodlands and shrublands, and Barron, Normanby and Tully shared *Melaleuca spp*. open forests and woodlands on seasonally inundated lowland coastal swamps and fringing drainage lines (Palustrine wetlands). Pioneer and Haughton shared deviations for Complex mesophyll to notophyll vine forests of the wet tropics bioregion. Both these catchments are located outside of the wet tropics, and pre-clearing extent for this vegetation type.

In general, the wet tropics catchments are dominated by Original Vegetation of medium to large-leaved vine thickets, production in relatively natural environments, or intensive uses dominate contrast, Mary, Burnett and Normanby share a large deviation of open forests or dry woodland, with Burnett and Normanby sharing large deviations of depositional areas.

3.4. Evaluation of dominant spatial features

A full evaluation of spatial features and corroborated classification is provided in Supplementary Material S2. Catchments that had mesophyll or notophyll vineforest as a dominant spatial variable consistently shared water quality patterns and dominant spatial features across more than one dataset partition. For example, in the wet tropics, all zones of the partitioned dataset were corroborated to spatial deviations dominated by productivity in natural environments as well as all the land uses mapped on land with Original Vegetation of mesophyll and notophyll vine forests. In contrast, all other catchments with variation of open forest type spatial features corroborated the spatial features with water quality matches for only a partition of the dataset, e.g, Normanby, Haughton or Pioneer with Burnett. In contrast, Mary corroborated with Barron and Pioneer and both corroborations included a variation of mesophyll or notophyll vineforest in the matched dominating spatial data. Evaluation of Feature Matching and Inductive Classification corroborations. Evaluation of the feature matching results is shown in Figure 6 with the record identifiers coloured to the corresponding dataset partition for the matched classifier. Interestingly, Category 2 catchments (All seasons and Flows) were never classified based on Original Vegetation or Ecounits that contained open woodlands or woodlands.

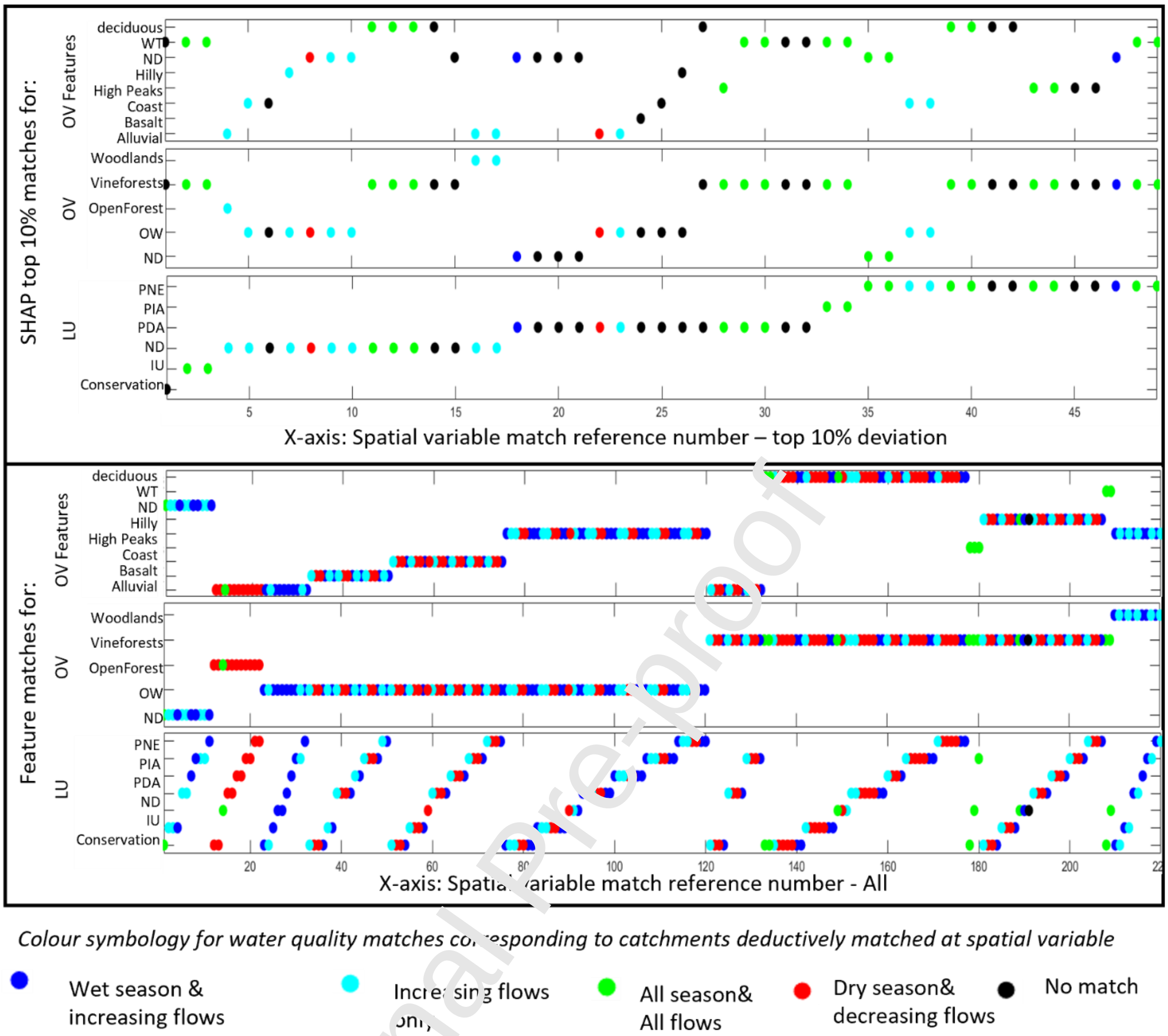


Figure 6: Scatter plots for spatial variables shared for catchment matches as grouped by water quality dataset partitions, evaluated and compare between OV, LU and EU spatial datasets. The top three plots show the most dominant 10% spatial variables using the SHAP-AD method, the bottom three plots show all spatial variables determined by the feature matching method. Y axis abbreviations: ND= Spatial Variable Not Differentiated; W=Water, PNE = Production on Natural Environments, PIA= Production on Irrigated Agriculture, PDA = Production on Dryland Agriculture, OW= Open Woodlands, WT=Wet Tropics.

Feature matching and SHAP-AD revealed that for the wet tropics catchments, corroborated catchment features were relevant for all 5 dataset partitions where spatial variables included elevation (Figure 6). In contrast, while Feature Matching identified catchments matches for Wet Season and Increasing flows, but not Dry Season or Retreating flows (Category 1) identified that, these categories only corresponded to all identified land uses on Original Vegetation of Woodlands on Hilly Terrain and Open Woodlands on Alluvial areas this distinction was not exposed in the SHAP-

AD evaluation. Likewise, excepting Intensive Uses and Not Disclosed, Feature Matching exposed for all other land uses on originally Open Forest on Woodland Areas, the catchments only matched for Dry Season and Retreating flows, i.e. Category 3 (Figure 6).

3.5. Result Summary

Results for all catchments, except for North Johnstone and Tully, supported the hypothesis that the best catchment to classify changes depends on the season or flow zone in the observed water quality dataset. Catchments matched together for DIN patterns in North Johnstone and Tully persisted regardless of the partitioning of the dataset. In contrast, pattern matching for all the other catchments changed depending on the season, or flow zone of the partitioned dataset. Likewise, spatial data deviation matches for Category 2 classified catchments (i.e. North Johnstone and Tully, as well as South Johnstone), uniquely did not include any open woodland original vegetation types in the corroborated catchment spatial data deviations. Instead, the deviations were dominated by original vegetation of notophyll or mesophyll vine forests regardless of Land Use spatial data and dataset partitions. While mesophyll and notophyll vine forest appeared in spatial data deviations shared between catchment classifications for O'Connell, Plane, the corroboration only applied during the Wet Season and Increasing flows zone for O'Connell.

4. Discussion

4.1 Influence of data timescale on classification

The study results support the hypothesis that data from different time periods, i.e., dataset partitioned for different flow or seasons, influence the catchments that ANN-PR match together for inductive classification, but the application depends on the catchment. In particular, we found partitioned water quality datasets matched catchments to one of three categories. Category 1 supported the hypothesis in full, whereby catchment matches alternated under differing flow or season dataset partitions, Category 2 the hypothesis was not supported, instead the same catchments matched together for all dataset partitions, including non-partitioned dataset, and Category 3 matched a dataset to one catchment only in some partitioning of the dataset, but the majority pattern matching threshold was not achieved for other partitions of the dataset. These three catchment response patterns to DIN are consistent with studies which also found dominating drivers of nitrogen patterns vary in different catchments depending on the season, flows and natural landscape variations (Liu et al., 2021a, Zhang et al., 2022a,b). These findings demonstrate that that application of classified catchments for water modelling need to consider the time scale and time period of the intended model outputs, as well as the data availability of the donor catchment.

4.2 Timescale drivers of DIN variability

The second part of the hypothesis that differences between season and flows are driven by spatial variables was supported by the finding that catchment matches using the partitioned datasets corroborated with catchment matches found via interrogation of spatial patterns. This finding was significantly stronger for datasets partitioned for season compared to the non-partitioned dataset. Datasets partitioned for Retreating flows had the lowest corroboration. This is consistent with previous observations for Great Barrier Reef catchments where differences in nitrogen have been attributed to temperature effects on biological processes in conjunction with the lower mobility of nutrients during dry and colder seasons, while the mobility of nitrogen and therefore pattern variation is known to become restricted on dryer environments (Liu et al., 2021a). The alignment between these studies and our findings suggests that the use of water quality data from distinctive seasons and periods of increasing flows provides more value to identifying catchments suitable for classification than all water quality data collected or compared for periods of retreating flows only.

4.3 Spatial data proxies for variable classification

In this study, XAI Feature Matching and XAI SHAP-AD deviation evaluations of the variables in the corroborated spatial datasets identified spatial variable proxies of the likely drivers of DIN under various season and flow regimes in the Great Barrier Reef catchments. The clear delineation for dominant Land Use data north of Haughton compared to south of and including Haughton, based only on mapped Land Use data, did not corroborate with the three classification categories for the observed water quality data. This result of three water quality categories compared to the two Land Use groups aligns with Jehn et al., (2020) who found heterogeneity exists among catchments classified for the same Land Use spatial variables. In contrast, SHAP-AD graphs that included other Original Vegetation and Ecounit spatial variables corroborated more closely with the three water quality categories. Although using the top 10 % of dominant features was useful for rapid comparison of catchment matches and similarities to general regions, the SHAP-AD evaluations had the lowest median corroboration rate of all the spatial data evaluation techniques. Significantly higher corroboration scores for the evaluation technique of Feature Matching, which included all spatial variables demonstrate important combinations that influence DIN patterns. Evaluation of the top 10% of features, as used in the SHAP-AD method overlooked the wholistic influence of all explanatory features.

Category 2 classification was the only category that contradicted the hypothesis whereby the classified catchment persisted regardless of the dataset partition and was restricted to the wet tropics catchments. The persistence of the same catchment classifier across all dataset partitions indicates that the drivers of DIN in the Natural Resource Management Region catchments of the wet tropics (Table 1) areas may respond consistently, or be unaffected by changes in season or flows, and therefore be inconsequential for classification purposes. The unique response of DIN in the wet tropic's catchments to Retreating and Increasing flows has also been noted in O'Sullivan et al., 2022 which used the same water quality datasets and demonstrated that DIN to flow ratios remained elevated in the Retreating flows for a larger portion of the flow profile in comparison to category 1 and 3 catchments. Likewise, Liu et al., (2021a) found the wetter profile for the wet tropics catchments corresponded to different nitrogen patterns in these areas compared to the rest of the Great Barrier Reef catchments. While mineralisation of nitrogen is influenced by seasons through both temperature and water availability (Maxwell et al., 2022), the influence of soils on nitrogen balances in rainforest environments, typical to wet tropics, are uniquely related to rainforest soils (Vallicrosa et al., 2022). The absence of alteration to catchment classification responses for only the wet tropics catchments suggest the nitrogen drivers unique to rainforest soils, or continually wetter environments that are characterised by vineforests, particularly at elevation, could be masking the seasonal influences of nitrogen mineralisation that are otherwise observed in the catchments that allocated to Category 1 and 3 classifications. Implications of these findings for water quality models is that data transfer between classified catchments in originally wet rainforest type environments characterised by vineforests may not need to consider flow or seasonal changes for classification. However, flow or seasonal variations do need consideration for catchments outside these areas.

In contrast to Category 2 trends, Category 1 catchments matched for Increasing flows only, all shared similar deviations for primary production on original vegetation of open woodland. The corroboration did not continue to Dry Season or Retreating flows zone of partitioned datasets. This phenomenon of indistinguishable nitrogen patterns during times of Retreating flow has been observed by Liu et al., 2021a. Likewise, Jackson and Ash, (1998) found for production open woodlands landscapes, open woodland trees influence soil carbon making nitrogen more available during wet years for pasture uptake, with trees outcompeting pasture for nitrogen in dry years.

Feature matching corroborated classifications for ANN-PR#1 were consistent with O'Sullivan et al., (2022). Additional catchments that are more suitable to classify for data transfer or different zones of partitioned water quality datasets were also identified using the ANN-PR#2 method. Here we found while classification results for the Non-Partitioned dataset persist, and are also consistent with corroborations shown for the dominating spatial features, as demonstrated by the SHAP-AD evaluation, Feature Matching classification can more appropriately reflect the season or flow regime scenario of most influence.

Our results for multiple catchment classification under differing dataset partition zones support the notion that the same approach for transfer of data from each of the classified catchments for nutrient modelling is not appropriate for all catchments over differing temporal (season or flow) scales, and that spatial data can explain the catchment responses. This study demonstrates that Original Vegetation spatial data of vineforests are indicators for Category 2 classification dynamics. In comparison, Category 1 classification is more appropriate in catchments with matching spatial patterns for primary production on Original Vegetation of woodland.

5. Conclusion

Practical implications of the ANN-PR - XAI coupled methodology approach of this study is the finding that catchments most suitable to classify for DIN can change over seasons and spatial features can serve as a proxy indicator for the most suitable catchment to classify depending on data application. Here we found for gauged catchments that flow to the Great Barrier Reef, periods of data suitable to transfer, and catchments to classify for drivers of DIN altered depending on the relative deviation of spatial data, i.e. vine forests or woodland from the areas of all other original vegetation types in the catchment. This finding will help inform future classification to the gauged catchments evaluated in this study where only spatially mapped data is available for ungauged catchments.

Limitations for future application of findings of this study are that the suitability of spatial features identified as a proxy for drivers of DIN are specific only to the catchments evaluated and therefore transfer to other catchments require site specific verification. Further research on whether the deviation of vineforest and woodland spatial drivers exists in ungauged catchments that also flow to the Great Barrier Reef will confirm the suitability of this classification method for application to those ungauged areas. Research on how to best apply spatial data as a proxy for changing classified catchments in different flow or season scenarios has potential practical outcomes to increase certainty in parameter transfer used in process based models for DIN simulations for ungauged catchments.

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Declaration of interests

☒The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Highlights

a) Flow vs season data expose biosphere and hydrosphere variability on DIN drivers
b) ANN-PR coupled with XAI expose spatial data features to classify for DIN
c) DIN classification varies on season/flow scales, explained by original vegetation
d) Original vegetation maybe a proxy for alternating/heterogeneous classification