

### A Bayesian approach to understanding the key factors influencing temporal variability in stream water quality – a case study in the Great Barrier Reef catchments

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Abstract. Stream water quality is highly variable both across space and time. Water quality monitoring programmes have collected a large amount of data that provide a good basis for investigating the key drivers of spatial and temporal variability. Event-based water quality monitoring data in the Great Barrier Reef catchments in northern Australia provide an opportunity to further our understanding of water quality dynamics in subtropical and tropical regions. This study investigated nine water quality constituents, including sediments, nutrients and salinity, with the aim of (1) identifying the influential environmental drivers of temporal variation in flow event concentrations and (2) developing a modelling framework to predict the temporal variation in water quality at multiple sites simultaneously. This study used a hierarchical Bayesian model averaging framework to explore the relationship between event concentration and catchment-scale environmental variables (e.g. runoff, rainfall and groundcover conditions). Key factors affecting the temporal changes in water quality varied among constituent concentrations and between catchments. Catchment rainfall and runoff affected in-stream particulate constituents, while catchment wetness and vegetation cover had more impact on dissolved nutrient concentration and salinity. In addition, in large dry catchments, antecedent catchment soil moisture and vegetation had a large influence on dissolved nutrients, which highlights the important effect of catchment hydrological connectivity on pollutant mobilisation and delivery.

### 1 Introduction

In-stream water quality plays a vital role in influencing the health of freshwater ecosystems (Pérez-Gutiérrez et al., 2017), which in turn underpins environmental, social and economic sustainability (McGrane, 2016; Ustaoğlu et al., 2020). Pollution derived from agricultural land and urban development has led to water quality degradation in streams and lakes in many regions of the world (Ren et al., 2003). Among these water quality issues, coastal regions with high agricultural production have been delivering large amounts of pollutants to the ocean, where marine ecosystems are vulnerable to the evaluated levels of nutrients and sediments (Gorman et al., 2009). It is estimated that 60 % of coastal rivers in the USA have been moderately to severely degraded (Gorman et al., 2009; Howarth et al., 2002). Therefore, to protect both freshwater and marine ecosystems, better management of catchment-derived pollutants is needed.

Surface water quality is highly variable across spatial and temporal scales (Guo et al., 2019; Lintern et al., 2018a). These spatial and temporal variations are the result of complex interactions between four key pollutant processes in catchments, namely, sources (e.g. atmospheric deposition or anthropogenic inputs), mobilisation (e.g. detachment from the sources), delivery (e.g. transport from sources to receiving waters) and transformation (e.g. biogeochemical processes; Granger et al., 2010; Harris, 2001; Lintern et al., 2018a). Across different catchments, spatial differences in water quality concentration can vary markedly due, in part, to heterogeneity of natural landscapes in catchments (e.g. geology, topography and climate) and human-induced activities (e.g. agricultural and urban development; Liu et al., 2018; Mainali et al., 2019). At a site, water quality concentrations can also exhibit significant daily, event, seasonal and annual variability driven by variations in climatic conditions, in-stream biogeochemical processes and hydrological transport (Thompson et al., 2011). Thus, it can be challenging to design effective catchment water quality management strategies without a sound understanding of the spatial and temporal variation in water quality and the associated driving factors.

While it has been acknowledged that both spatial and temporal variations in water quality are of great importance for effective water resources management (Guo et al., 2020), this study focused on identifying key drivers of the temporal variability in water quality. It follows our previous study investigating spatial variation in water quality in the same region (Liu et al., 2018). A wide range of environmental factors may affect temporal changes in water quality. Runoff and rainfall have been considered as important factors and the most commonly used explanatory variables to describe temporal variation in water quality (Deletic and Maksimovic, 1998), for example, early work by Hem (1948) and Walling (1984). Studies considering hydrometeorological drivers have been typically related to the mobilisation and delivery of pollutants. Catchment soil moisture and evapotranspiration can also have an important role in determining the hydrological cycle (e.g. runoff generation), such as sediments (Bieger et al., 2014), nutrients (Lam et al., 2010) and salinity (Brevik et al., 2006; Tweed et al., 2007), thereby affecting the surface water quality. In addition, riverine water quality has been found to be strongly influenced by seasonal changes in vegetation cover (de Mello et al., 2018; Griffith et al., 2002; Shi et al., 2017). For instance, satellite-derived vegetation indices have provided an opportunity to explore the relationship between land cover and water quality temporal dynamics (Griffith, 2002; Singh et al., 2013). Even though significant research efforts have been made to explore the relationship between water quality and these environmental conditions, a comprehensive understanding of their relative importance in diverse environments and at large scales is still lacking.

Process-based and statistical modelling approaches have been widely used to investigate water quality temporal dynamics in response to changes in the above-mentioned environmental factors (Fu et al., 2019; Wellen et al., 2015). Process-based water quality models use complex mass balance structures describing the water quality source, mobilisation and transport processes (Abbott et al., 1986; Merritt et al., 2003). They are typically based on hydrological and biogeochemical processes that can affect the generation and transport of pollutants into receiving waters. These models (e.g. Soil and Water Assessment Tool – SWAT – and source catchments) have been applied to assess the impact of land use management and climate on sediment and pollutant concentrations (Arnold and Fohrer, 2005; Francesconi et al., 2016; Qi et al., 2018), optimise water management and delivery for agriculture, industry and environmental uses (Ly et al., 2019), and estimate pollutant generation, loss and transport processes (Jayakrishnan et al., 2005; McCloskey et al., 2021). However, the complexity of process-based models results in intensive data and calibration requirements, and large-scale application has been limited (Abbaspour et al., 2015; Arnold and Fohrer, 2005). These models may also have large uncertainties in the interpretability of the parameters and their characterisation of the effects of specific processes (Wade et al., 2002), such as denitrification in streams (Filoso et al., 2004).

On the other hand, statistical water quality models have a relatively simple mathematical structure, an ability to quantify predictive uncertainty (Kasiviswanathan and Sudheer, 2013; Srivastav et al., 2007) and low requirement for a priori information on distinct processes (Letcher et al., 2002; Mainali et al., 2019; Schwarz et al., 2006). However, existing statistical water quality modelling studies have limitations. First, water quality monitoring data have often been limited to low sampling frequencies, typically using monthly grab samples. This can result in a lack of information on water quality dynamics over runoff and/or storm events, which is when a significant proportion of nutrients and sediment loads are transported (Lloyd et al., 2016; Sherriff et al., 2015). Second, most studies on statistical water quality modelling have only investigated the relationship between water quality and explanatory variables in a single or limited number of catchments in small regions (Chang et al., 2015; Khan et al., 2020; Koci et al., 2020). Few studies have investigated water quality at multiple locations using the same modelling framework. Lastly, studies have usually relied on a single best model with an assumption that it best approximated the true drivers of water quality (Paliwal et al., 2007; Zhang et al., 2009). This ignores the issue of selection uncertainty. Furthermore, relying on a single model structure might result in misleading conclusions or overconfidence in the results (Wintle et al., 2003).

This study attempted to address these knowledge gaps in statistical water quality models, taking advantages of eventbased water quality monitoring data from the Great Barrier Reef (GBR) catchments in northern Australia, where landderived pollutants have posed threats to ecosystem health of the GBR lagoon (Brodie et al., 2012; McKergow et al., 2005b). We address the limitations in statistical water quality models by using the following: (1) Bayesian hierarchical modelling was used to investigate water quality temporal variation, which allowed the prediction of water quality in multiple catchments and, simultaneously, quantified parameter uncertainty (Gelman et al., 2013; Rode et al., 2010; Webb and King, 2009); and (2) Bayesian model averaging (BMA) approaches were used to identify the relative importance of the different environmental factors and provide multi-model weighted predictions, which have been shown to better quantify the uncertainty arising from model selection (Höge et al., 2019; Raftery et al., 1997; Wang et al., 2012). We targeted nine common water quality indicators, including sediments, nutrients and salinity. This is a subset of the constituents that have been monitored in the GBR water quality monitoring programme. Our analyses are conducted on constituents that are of great concern to the coral reef ecosystem (McCloskey et al., 2017) and could provide a useful comprehensive picture on the overall water quality status. Finally, we have constrained the variables to only the real parameters that can be directly measured (with the exception of  $NO_x$ ), which helps to understand full sediment and nutrient loads being exported to the GBR lagoon. Overall, this study aimed to (1) identify the key drivers of temporal variation in water quality and (2) predict water quality temporal variation using a Bayesian multi-model approach.

#### 2 Materials and methods

#### 2.1 Study area

The GBR catchments, situated in northeastern Australia (Fig. 1), consist of six natural resource management regions whose streams and rivers discharge into the Great Barrier Reef lagoon. These catchments cover a 437 354 km<sup>2</sup>, approximately a quarter of the state of Queensland, and exhibit significant diversity in climatic, geological and topographical landscape characteristics, as well as in land use and land management (Bartley et al., 2018; Gilbert and Brodie, 2001). The GBR catchments range from small, steep, high-energy streams in the wet tropics, which are dominated by sugarcane crops and rainforest, to large inland catchments used for savannah grazing and crops (e.g. grain) and with extensive low-energy floodplains in the dry tropics (Table 1; Davis et al., 2017; Koci et al., 2019; McKergow et al., 2005a). Spatial and temporal variations in rainfall in the GBR catchments are a major cause of the diversity in land use patterns. Annual rainfall ranges from less than 500 mm in the southwest to more than 8000 mm in the northeast (Fig. 2c; Davis et al., 2017; Kuhnert et al., 2009). Distinct wet (November to April) and dry (May to October) seasons result in high seasonal variation in runoff, and the El Niño-Southern Oscillation (ENSO) leads to high interannual variability (Day and McKeon, 2018). In the dry tropics, a few large events in the wet season contribute the majority of annual runoff, and constant low flow dominates during the dry season (Jarihani et al., 2017).

A total of 32 sites within the GBR catchments were selected as case study catchments (Fig. 1 and Table S1 in the Supplement). Previous multivariate analysis of the patterns of time-averaged concentrations indicated that there were two groups of sites (Table 1 and Fig. 2a). We found that differences in geographic and/or hydroclimatic catchment characteristics (Fig. 2b–d) are the key factors that distinguished



**Figure 1.** The Great Barrier Reef (GBR) catchments, monitoring sites, land uses and the six natural resource management (NRM) regions. Land uses have the following characteristics: (1) conservation (forest, woodland, savannah, etc., for conservation purposes), (2) dryland (rainfed agriculture, including cereals but excluding grazing and sugar cane), (3) grazing (primarily cattle grazing of native and introduced vegetation), (4) intensive (urban areas, roads, etc.); (5) irrigated (irrigated cropping, excluding sugar cane); (6) sugar (rainfed and irrigated sugar cane) and (7) water (water bodies, including lake, river and marsh/wetland).

the two clusters of sites (e.g. small wet areas, i.e. cluster 1, near the coast where topography, or orography, plays an important role in rainfall generation; Liu et al., 2018). Such geographic differences also lead to more dispersed sites in the drier area (cluster 2).

#### 2.2 Data collection and preparation

#### 2.2.1 Water quality data

The nine studied constituents were total suspended solids (TSSs), particulate nitrogen (PN), oxidised nitrogen ( $NO_x$ ), ammonium nitrogen ( $NH_4$ ), dissolved organic nitrogen (DON), filterable reactive phosphorus (FRP), dissolved organic phosphorus (DOP), particulate phosphorus (PP), and



Figure 2. Spatial information of the GBR catchments northeastern Australia. (a) Site locations showing two groups based on the clustering analysis of spatial variability in time-averaged water quality (Liu et al., 2018). (b) Topographic elevation (250 m resolution; Geoscience Australia, 2008). (c) Annual average rainfall (Atkinson et al., 2008, 2012). (d) Updated Köppen–Geiger climate zone classification (Peel et al., 2007).

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Cluster	Climate	Hydrology	Land use or land cover	Topography
1	Wet tropics region, with high annual rainfall	Perennial, high-energy rivers	Dominated by conservation (e.g. rainforest) and cropping (e.g. sugar)	Small and steep
2	Mostly dry tropics and rela- tively dry areas, with clear sea- sonal variability in rainfall	Ephemeral, low-energy rivers that cease to flow in dry periods	Dominated by brigalow na- tive vegetation and pastures for grazing	Large and flat

Table 1. Summary of differences in landscape characteristics between the two clusters of sites (Liu et al., 2018).

electrical conductivity (EC). Water quality monitoring data collected for the 32 GBR catchments over the 11-year period of 2006 to 2016 were obtained from the loads monitoring programme (Turner et al., 2012). This data set contained both high-frequency event-based samples (e.g. daily or every few hours by automatic samplers) that were taken during runoff events and grab samples (e.g. monthly) that were taken under baseflow conditions (Orr et al., 2014; Waters and Packett, 2007). As EC data from the loads monitoring programme were limited, we extracted additional EC data from the Water Monitoring Information Portal provided by the Department of Natural Resources, Mines and Energy of Queensland (DNRME, 2016) to complement the loads monitoring programme records.

#### 2.2.2 Event mean concentration

We extracted continuous discharge records for each site from the Water Monitoring Information Portal (DNRME, 2016) to identify individual runoff events. An automated hydrograph analysis tool - HydRun (Tang and Carey, 2017) - was used to delineate runoff events. This approach allowed us to extract runoff event on the baseflow-free hydrograph by specifying a set of parameters (e.g.  $\beta$  filter coefficient – ReTh difference between two flows to set the local minima for event extraction). This toolbox directly returned the start and end points of an event, thereby avoiding time-consuming and subjective inconsistent outcomes. The key parameters used for the HydRun toolbox are provided in Table S2 in the Supplement, and an example hydrograph output is provided in Fig. S1. These parameters are determined based on recommended values from the literature (Garzon-Garcia et al., 2016; Ladson et al., 2013; Zhang et al., 2017) and a manual review of all event hydrographs ensured overall consistency. The event mean concentration (EMC) was then calculated for each event that had at least two samples on each of the rising and falling limbs of the hydrograph. Thus, for each EMC, a minimum of four samples was achieved, which is above the standard (three samples per event) set by Bartley et al. (2012). On average, there were 14 samples per event across the nine constituents (ranging from 12 for DOP to 16 for EC; Table S3 in the Supplement). This ensured that the water quality dynamics over a runoff event were reasonably well captured and that the derived EMCs were reliable (Waters and Packett, 2007). For each event, the EMC of a constituent was calculated as the total load per unit flow volume within the event using the following (Bartley et al., 2012):

$$EMC = \frac{Event \ Load}{Event \ Flow \ Volume} = \frac{\sum_{j=0}^{n} \frac{c_j + c_{j+1}}{2} \cdot q_{j+1/2} \cdot t_{j+1/2}}{\sum_{j=0}^{n} q_{j+1/2} \cdot t_{j+1/2}}, \quad (1)$$

where *n* is the total number of samples for a given event,  $c_j$  is concentration of the *j*th sample, and  $q_{j+1/2}$  and  $t_{j+1/2}$  are the intersample mean discharge and time interval between *j*th and (j + 1)th samples. The concentrations at the start and end of the event  $(c_0 \text{ and } c_{n+1})$  are assumed to be the averaged value for samples during baseflow (with baseflow identified in the previous section). The EMCs were essentially flow-weighted mean concentrations over individual runoff events, which allowed the comparison of water quality across catchments with contrasting flow regimes (e.g. two clusters of sites in Fig. 2; Cooke et al., 2000; Richards and Baker, 1993). A total of 1412 events was identified across the 32 sites, and depending on data availability, EMCs were calculated for between 21 % (DOP) and 43 % (TSS) of these identified runoff events (Table S2).

The derived EMCs (i.e. rather than the individual water quality samples) were Box-Cox transformed to improve the symmetry of the response variable (Box and Cox, 1964). The normalisation of the predictand is necessary to facilitate the fitting process and fulfil the statistical assumption of our model. This is because we use a Bayesian linear regression with the response variable sampled from a normal distribution (Sect. 2.3.1; Atkinson, 2021; Castillo et al., 2015; Hoeting et al., 2002). The site-level Box-Cox transformation parameter  $\lambda$  for each constituent was first identified, using the car package in R (Fox et al., 2012; R Core Team, 2013). Then, for each constituent, the average  $\lambda$  from the 32 sites was used to transform all available EMCs for that specific constituent. This ensured that an identical transformation parameter was applied across the different sites for each constituent (Guo et al., 2019).

#### 2.2.3 Explanatory variables

This study investigated the effect of various hydrologic, climatic and vegetation cover characteristics for different

Explanatory variable	Unit	Spatial resolution	Source
Daily runoff	$\mathrm{mm}\mathrm{d}^{-1}$	Point measurements	Queensland Department of Natural Resources, Mines and En- ergy (DNRME, 2016). Available at https://water-monitoring. information.qld.gov.au/ (last access: 1 September 2016)
Daily rainfall	mm	$5 \text{ km} \times 5 \text{ km}$	Australia Water Availability Project (AWAP; Raupach et al., 2009). Available at http://www.csiro.au/awap/ (last access: 1 June 2017)
Daily temperature	°C		
16 d normalised difference vegetation index (NDVI)	_	1 km × 1 km	Moderate Resolution Imaging Spectroradiometer (MODIS) – MOD13A2v006 (Didan, 2015). Available at https://earthdata.nasa. gov/ (last access: 24 October 2016)
Daily soil moisture (root zone 0–100 cm)	mm	5 km × 5 km	Australia Landscape Water Balance model (AWRA-L; Frost et al., 2016). Available at http://www.bom.gov.au/water/landscape (last access: 1 March 2017)
Daily actual ET	mm	-	

Table 2. Explanatory variables and their data sources.

The term ET refers to evapotranspiration.

events. These characteristics included runoff, catchment root zone soil moisture, actual evapotranspiration rainfall, air temperature and vegetation cover. The continuous streamflow monitoring data, gridded weather and climatic products and remotely sensed imagery were used to derive catchment average conditions for each event (Table 2).

For individual runoff events identified in the previous section, three groups of event characteristics were prepared, characterising pre-event, during-event and post-event conditions (Table 3). Except for runoff, data for all explanatory variables were first extracted from gridded data using catchment boundaries were delineated using the Geofabric (Australian Hydrological Geospatial Fabric) tool provided by the Australian Bureau of Meteorology (Atkinson et al., 2008; Fig. 1). The catchment-average time series data were then averaged over the specific time window related to the event (Table 3).

The explanatory variables in the during-event conditions were averaged over the duration of the event. For the preevent and post-event conditions, the 7 d prior to and after the event were used as the time window (except NDVI). The 7 d period was the median of the time of concentration (i.e. the time for runoff to travel from the most remote point of the catchment to the monitoring site) across all catchments. These were estimated from catchment topography using the Bransby-William's equation, following its wide application in Australian catchments for flood estimation (Pilgrim et al., 1987). The ground cover was quantified by NDVI, an indicator of the biophysical condition of the vegetation canopy (Griffith et al., 2002). Previous studies have also shown that there is a time lag between water availability and a change in ground cover, which is typically 3 months for Australian catchments (De Keersmaecker et al., 2015). Therefore, to

represent the pre-event ground cover condition, we averaged all available NDVI measurements for 3 months prior to an event. The runoff after the event (7 d) was also included as an indicator of catchment wetness at the end of the event to assess if the hydrologic condition towards the end of an event influences the temporal variation in water quality.

Similar to the EMCs, all the explanatory variables were Box-Cox transformed, following the procedure described in Sect. 2.2.2. In addition, prior to the analyses, both transformed EMCs and explanatory variables were standardised to a mean of 0 and standard deviation of 1. As such, the magnitude of a coefficient indicates the effect of each predictor relative to other predictors (Wan et al., 2014). The cross-correlation (non-parametric Spearman's rank correlation coefficient) of all transformed predictors is provided in Fig. S2 in the Supplement. Some of the variables are proxies for the same process, and thus, some paired predictors are highly correlated (e.g. pre-event NDVI and during-event NDVI with Spearman's  $\rho = 0.97$ ). Freckleton (2011) highlighted that, when applying the model averaging approach, it is not safe to simply exclude correlated variables without due consideration of their likely independent effects. In our case, the high correlation among predictors mainly comes from time lag effects between predictors (e.g. pre-event, during event and post-event). The relative importance of these predictors provides a strong management indication for future water quality management strategies. Therefore, we have not removed any correlated predictors in this analysis. It is likely that different model structures result in similar predictive performance (discussed in the analysis of the results, i.e. Sect. 3.1).

Group	Explanatory variable	Abbreviation used in figures and tables in the paper	Calculation method
During event	Average runoff	Event_ave_Q	Average of daily runoff during the event
	Maximum runoff	Event_max_Q	Maximum of daily runoff during the event
	Average rainfall	Event_ave_P	Average of daily rainfall during the event
	Maximum rainfall	Event_max_P	Maximum of daily rainfall during the event
	Average temperature	Event_T	Average of daily temperature during the event
	Average NDVI	Event_NDVI	Average of NDVI during the event
	Average soil moisture	Event_SM	Average of daily soil moisture during the event
	Average actual ET	Event_AET	Average of daily actual ET during the event
Pre-event	Average runoff	Ante_Q	Average of daily runoff for 7 d prior to the event
	Average rainfall	Ante_P	Average of daily rainfall for 7 d prior to the event
	Average NDVI	Ante_NDVI	Average of NDVI for 3 months prior to the event
	Average soil moisture	Ante_SM	Average of daily soil moisture for 7 d prior to the event
	Average actual ET	Ante_AET	Average of actual ET for 7 d prior to the event
Post-event	Average runoff	Post_Q	Average of daily runoff for 7 d after the event

Table 3. The three groups of event characteristics and the averaging method.

Note: Q - runoff; P - rainfall; T - temperature; NDVI - normalised difference vegetation index; SM - root zone soil moisture; ET - evapotranspiration.



Figure 3. Analyses steps – the detailed methods used in the hierarchical modelling framework and model prediction and evaluation are in the following sections.

# 2.3 Modelling – driver identification and water quality prediction using multi-model inference

The statistical analysis and modelling followed several steps (Fig. 3). The Bayesian modelling framework was applied to catchments in clusters 1 and 2 separately. There are strong practical merits in handling the clusters separately. Previous results from clustering analyses on spatial patterns of water quality and catchment characteristics were highly correlated and the two clusters had quite different key explanatory variables (Liu et al., 2018). If all the sites were pooled into the same analysis, it would make it more difficult to identify a universal set of key explanatory variables that represent both clusters and likely increase the uncertainty of the coefficients too. The analysis would identify the same key factors identified for the two different clusters. It is important to consider and model these clusters separately so that we can better inform how water quality can be managed in these separate environmental conditions.

#### 2.3.1 Bayesian variable selection

To investigate the relative importance of individual predictors, an indicator Bayesian variable selection method was used, and it is called the Gibbs variable selection (GVS; George and McCulloch, 1993). An auxiliary inclusion variable  $I_n$  (Eq. 2) for each predictor was introduced to indicate whether that predictor was in or out of an individual iteration of the hierarchical modelling structure.

$$I_n \left\{ \begin{array}{ll} 1, & n \text{th predictor present} \\ 0, & n \text{th predictor absent} \end{array} \right\}.$$
(2)

 $I_n$  was modelled at the top level of the hierarchy, which enabled the use of identical model structures (i.e. combination of predictors) across different sites. The overarching hierarchical modelling framework was defined as follows:

$$y_{i,j} \sim N(\mu_{i,j}\sigma) \tag{3}$$

$$\mu_{i,j} = \overline{\mathrm{mean}}_j + \overline{\mathrm{SD}}_j \cdot \Delta_{i,j} \tag{4}$$

$$\Delta_{i,j} = \sum_{n=1}^{N} \theta_{n,j} \cdot x_{n,i,j} \tag{5}$$

$$\theta_{n,j} = I_n \cdot \beta_{n,j}. \tag{6}$$

The data-level model (Eq. 3) assumed that the EMC of a particular constituent (e.g. one of TSS,  $NO_x$ , EC, etc.) at *i*th time step in the *j*th subcatchment,  $y_{i,j}$ , followed a normal distribution (denoted as  $N(\bullet)$ ), with mean  $\mu_{i,i}$  and a global standard deviation  $\sigma$ . The mean value,  $\mu_{i,j}$  was modelled as the observed site-level-averaged EMC  $\overline{\text{mean}}_i$  plus  $SD_i \cdot \Delta_{i,i}$ , with the latter term being defined as the deviation from this averaged value (Eq. 4; Guo et al., 2019). The deviation term incorporated the site-level-observed standard deviation SD<sub>i</sub>, making  $\Delta_{i,i}$  a standardised measure that could be compared across sites.  $\Delta_{i,i}$  was further modelled as a linear additive function (Eq. 5) of all candidate predictors  $x_n$  in  $n = 1, 2, \dots, N = 14$  (e.g. event average runoff, rainfall and NDVI). Consequently,  $\Delta_{i, i}$  was defined as the temporal variability in water quality and was the quantity of interest. The effect size  $(\theta_{n,i})$  of individual predictors was another latent variable used in the GVS and was estimated as the product of  $I_n$  and the regression coefficient  $\beta_{n,i}$  (Eq. 6), such that  $\theta_{n,i}$ was either  $\beta_{n,i}$  ( $I_n = 1$ ) or 0 ( $I_n = 0$ ).

# 2.3.2 Hierarchical prior specification and Bayesian inference of key drivers

Bayesian inference required specification of prior distributions for each model parameter. We used a hierarchical conditional prior specification for predictor coefficients, allowing the site-specific parameter values that describe the effects of each of the temporal predictors  $(\beta_{1,j}, \beta_{2,j...}, \beta_{n,j})$ to be exchangeable between sites (O'Hara and Sillanpää, 2009; Webb and King, 2009). The detail specification of priors for each model parameter can be found in the Supplement. In addition, to identify key drivers affecting temporal changes in water quality, the posterior inclusion probability (PIP –  $P(I_n = 1|y)$ ; Eq. A8 in the Supplement) of each predictor was used to compare the relative importance of individual predictors (i.e. how often the *n*th predictor was in the model).

#### 2.3.3 Prediction from multi-model inference

We used Bayesian model averaging to generate an ensemble of predictions of temporal variation in EMC for individual constituents (Eq. 7). The average posterior distribution of a quantity of interest (i.e. temporal variability in EMC) was generated using the parameters (e.g.  $\beta_{1,j}$ ,  $\beta_{2,j...}$ ,  $\beta_{n,j}$ ) sampled from the posterior distribution to simulate EMC values using the specific model, which is defined as follows:

$$\left[\hat{\boldsymbol{y}}|\boldsymbol{y}\right] = \sum_{x=1}^{L} \left[\hat{\boldsymbol{y}}|\boldsymbol{y}, \boldsymbol{M}_{x}\right] \boldsymbol{P}(\boldsymbol{M}_{x}|\boldsymbol{y}), \tag{7}$$

where  $[\hat{y}|y, M_x]$  is the posterior distribution of a vector  $\hat{y}$  of (prediction) derived from model  $M_x$ , and  $P(M_k|y)$  is the posterior model probability (PMP; Eq. A8 in the Supplement; O'Hara and Sillanpää, 2009).

#### 2.3.4 Model evaluation and implementation

The proposed modelling framework was applied to the two clusters of sites independently. This allowed an investigation of whether the spatial heterogeneity in catchment landscapes led to differences in the key factors controlling temporal variation in water quality. The key drivers were determined as the predictors with a PIP above 0.8 (i.e. over 80 % of the models included these predictors).

To further understand the reliability and robustness of the BMA framework, the consistency of the posterior inclusion probability of individual predictors was investigated by resampling subsets of the observations multiple times (Kohavi, 1995). For each cluster, 80 % of events within one site were first randomly selected, and the posterior inclusion probability for this subset of observations was estimated. This was repeated 1000 times to produce a distribution of posterior inclusion probabilities for individual predictors, which was then used to assess the uncertainty in the posterior inclusion probability.

An ensemble of the averaged prediction in temporal variability of each event was obtained from each iteration of parameter updating, using Markov chain Monte Carlo (MCMC). The model fit was evaluated using the Nash–Sutcliffe efficiency (NSE; Nash and Sutcliffe, 1970) between the observed temporal variability and the median of ensemble predictions  $\hat{y}$  derived from the BMA (Eq. 7). The NSE was calculated at both the cluster levels and site levels. The model residuals were also checked for normality and heteroscedasticity (i.e. relationship between the residual and predictors). In addition, model performance was evaluated by providing the 50 % and 95 % credible interval (CI) of each prediction.

To compare the relative importance of the predictors that have been widely used in the existing literature (i.e. runoff and rainfall) and other predictors (e.g. soil moisture, temperature, evapotranspiration and vegetation cover), the modelling framework was recalibrated using only the rainfalland/or runoff-related predictors (including all pre-, duringand post-event predictors). This estimated the degree of improvement in the model's explanatory power with the inclusion of environmental variables, such as catchment wetness and ground vegetation cover conditions.

The hierarchical modelling framework was implemented in *JAGS* (Plummer, 2013a), using the package *rjags* in R (Plummer, 2013b; R Core Team, 2013), which enabled both the estimation of parameter values from prior distributions with MCMC and the generation of model-averaged predictions. The MCMC sampling had three parallel chains with 25 000 iterations for each chain. The first 5000 iterations were discarded as a burn-in period to allow convergence of the Markov chains, resulting in 60 000 values to estimate the posterior distribution for each model parameter and make model predictions.

#### **3** Results

#### 3.1 Key drivers of temporal variability in water quality

The three key measures that were used to quantify the effect of individual predictors are (1) estimates of posterior inclusion probability (PIP), which quantifies relative importance of individual predictors; (2) posterior model probability (PMP), which estimates differences in plausible model structures; and (3) posterior distributions of coefficients for the key drivers (i.e. effect size; e.g.  $\theta_{1,j}, \theta_{2,j...}, \theta_{n,j}$  in Eq. 6), which measures direction and magnitude of the effect of key predictors on water quality temporal variability.

Posterior inclusion probability (Fig. 4 and Table S3 in Supplement) from the Bayesian modelling results indicated that, in general, antecedent vegetation condition and antecedent soil moisture were key factors in explaining temporal variation in water quality, especially for cluster 2 (warmer and drier) sites. Catchment runoff and rainfall were the second most important group of factors, especially for particulate pollutants (TSS, PN and PP; clusters 1 and 2) and salinity. In addition, the three groups of predictors (pre-, during and post-event) showed varying effects among the constituents. With regard to during-event conditions, event average runoff (Event\_ave\_Q), event maximum runoff (Event\_max\_Q) and event average rainfall (Event\_ave\_P) were three important factors with relatively high PIP. In contrast, among pre-event conditions, antecedent NDVI (Ante NDVI) and antecedent soil moisture (Ante SM) were driving factors for the majority of the constituents. Post-event runoff (Post\_Q) only affected a few constituents (e.g. on  $NO_x$  and FRP for cluster 2) compared with the other two groups of predictors. Overall, there were notable differences in the important predictors for clusters 1 and 2, and more important predictors were found for the cluster 2 sites.

It is also worth noting that strong correlations between predictors does not necessary mean that the posterior inclusion probability of these factors is similar (e.g. 1.00 and 0.34 for pre-event NDVI and event NDVI, respectively, for DON in cluster 2). The BMA can handle the collinearity by shrinking the posterior distribution of inclusion probability of one of the correlated variables towards zero (Nakagawa and Freckleton, 2011; Posch et al., 2020; Walker, 2019). This shrinkage effect leads to a lower posterior probability of a more complex model that includes correlated variables because each extra predictor dilutes the prior density of the existing predictor that it correlates with. Such a complex model is unlikely to be selected unless the loss in posterior probability can be outweighed by the gain in achieving a higher likelihood (Daoud, 2017; Hinne et al., 2020; Kruschke, 2014).

Results from here on will focus mainly on TSS,  $NO_x$  and FRP due to their impacts on the marine receiving environment. Results for the other six constituents are in the Supplement. Figure 5 shows the posterior model probabilities for TSS,  $NO_x$  and FRP for the 100 models with highest PMP (Figs. S3 and S4 in the Supplement show other constituents). Red indicates a negative influence and blue a positive influence. The difference in PIP between the two clusters resulted in quite different plausible model structures (models with relatively high posterior model probability). A stand-out difference between the results for the two clusters was antecedent vegetation cover condition (Ante NDVI), which tended to be a more important predictor of TSS for cluster 2 than for cluster 1 (Fig. 5a). In addition, the plausible models for cluster 2 were generally more complex (with a larger number of predictors), except for DOP and EC (Figs. B3 and B4).

The distribution of posterior model coefficients for the key predictors (Figs. 6, B5 and B6) further demonstrated that the key drivers of temporal variability in water quality vary between catchments and between constituents. During-event runoff and rainfall tended to have a positive effect on sediment and particulate constituents and a negative effect on  $NO_x$  and EC. In addition, there was strong negative effect of antecedent vegetation condition on the majority of the constituents.

The uncertainty in PIP, derived from 1000 subsampled BMA runs (Figs. 7, B7 and B8) highlighted that the BMA results were robust for most constituents, except for EC (Fig. S7c in the Supplement). BMA tends to identify important predictors and is less sensitive to the input data, which is evidenced by the relatively narrow range of interquartile ranges (IQRs), when PIP for a specific predictor is large (e.g. antecedent soil moisture for FRP in Fig. 7). It is also worth noting that large uncertainty in the PIP for EC was observed, indicating the BMA results were sensitive to the observations of EC. This might be related to data availability, which is further discussed in Sect. 4.2.

#### 3.2 Predictive performance

Moderate levels of temporal variability were explained by the BMA framework for the two independent clusters of sites (Figs. 8, S9 and S10 in the Supplement). At the cluster level, the NSE ranged from 0.04 (DOP) to 0.68 (EC) and from 0.34 (NH<sub>4</sub>) to 0.64 (NO<sub>x</sub>) for clusters 1 and 2 (full model columns in Table S6 in the Supplement), respectively. The comparison of the modelling performance (posterior median of BMA prediction) showed that the modelling framework performed better on the cluster 2 sites than cluster 1 (Fig. 8; red; 50 % prediction CI – cluster 2), except for NH<sub>4</sub> and EC (not shown). This was reflected in a better match to the 1 : 1 line within the 90 % prediction CI for cluster 2 catchments. According to model performance criteria recommended by



**Figure 4.** Posterior inclusion probability (PIP) of each candidate predictor for (**a**) cluster 1 (wet) catchments and (**b**) cluster 2 (dry) catchments. Dark blue refers to high PIP, and light blue refers to low PIP. The definitions of the abbreviations of each predictor on the *y* axes are given in Table 3.

Moriasi et al. (2015), model performance is satisfactory (Table S7 in the Supplement), especially for the cluster 2 models. Generally, low NSE is acceptable for modelling nutrients and sediment compared to hydrology. It is also worth noting that, in contrast to the models developed here, most of the water quality models evaluated in Moriasi et al. (2015) are process-based models and focus on individual catchments.

It is also worth noting that the prediction interval for EC (Fig. S10c) was much wider than the rest of the constituents. Similar results were found in the site-level performance, with the average site-level NSE (Fig. S11 in the Supplement) for cluster 2 models typically higher than for cluster 1. The site-specific performance varied across sites, with the largest variation in EC (NSE for the cluster 2 result ranged from approximately 0.20 to 0.90). The modelling performance of DOP in the cluster 1 sites was poor (NSE = 0.04); all candidate covariates had low predictive power, resulting in the poor mixing of chains of the inclusion variable  $I_n$  (i.e. posterior  $I_n$  was around 0.5). The model residuals were normally distributed (Fig. S12 in the Supplement), and there was no clear heteroscedasticity within the residuals (Figs. S13 to S21 in the Supplement).

Table S6 (Supplement) compares the model performance using rainfall- and/or runoff-related predictors only and all candidate predictors (full model). A large increase in NSE was found for most dissolved nutrient species (e.g.  $NO_x$ , NH<sub>4</sub>, DON, FRP and DOP) for the full model. Notably, for NH<sub>4</sub> in cluster 1, factors other than rainfall and runoff explained almost all the variability that could be captured by the BMA.

#### 4 Discussion

# 4.1 Factors influencing temporal variability in stream water quality

#### 4.1.1 Runoff and rainfall

Our results demonstrated that runoff and rainfall were important factors in explaining the temporal dynamics of particulate pollutants (i.e. TSS, PN and PP) and dissolved species (e.g.  $NO_x$ , DOP and EC) in the GBR catchments. These results align with the findings of previous studies that have used these variables to understand changes in water quality over time (Beiter et al., 2020; McKergow et al., 2003; Schwarz et al., 2006).

Hydrologic and climatic variables (i.e. rainfall and runoff) showed distinct effects on different constituents and different groups of catchments. The positive effect of event runoff and rainfall on sediment and particulate nutrients (i.e. PN and PP) revealed their underlying impacts on pollutant mobilisation and transport processes in catchments (Hirsch et al., 2010; Lintern et al., 2018b; Musolff et al., 2015). In contrast, there were negative effects of during-event runoff on  $NO_x$  (cluster 1), DOP (cluster 2) and EC (both clusters). For  $NO_x$  and EC, this was most likely caused by hydrological transport processes; these constituents tend to be transported to receiving rivers via subsurface flows (Kratz et al., 1997; McKergow et al., 2003). For events with relatively low surface runoff, higher  $NO_x$  and EC event concentrations could be expected in these catchments (Clow and Sueker, 2000; Skoulikidis et al., 2006). In addition, for DOP, in-stream bio-



Cumulative Model Probabilities

Cumulative Model Probabilities

**Figure 5.** Comparison of BMA model coefficients and cumulative model probabilities (only the first 100 models ranked according to the highest probability are shown) between cluster 1 (wet – **a**, **c**, **e**) and cluster 2 (dry – **b**, **d**, **f**) sites for (**a**) TSS, (**b**) NO<sub>x</sub> and (**c**) FRP. Each column in the heat map represents the one specific model (ranked from the highest model probability from left to right), and the width of the column is normalised by the posterior model probability (i.e. the widest columns indicate models with the largest increase in probability compared to the next most probable model). The colour indicates the direction of the coefficients; red is negative, and blue is positive. The coefficient value was averaged across the posterior median value of the site-specific coefficient within each cluster (effect size,  $\theta_{n,j}$ , in Eq. 6). The definitions of the abbreviations of each predictor on the *y* axes are given in Table 3.



**Figure 6.** Distribution of median of site-level coefficients for all plausible models in BMA between cluster 1 (wet – **a**, **c**, **e**) and cluster 2 (dry – **b**, **d**, **f**) sites for (**a**) TSS, (**b**) NO<sub>*x*</sub> and (**c**) FRP. Only predictors with PIP >0.8 are included. For each specific model structure, the coefficient value of a predictor was the median of the site-specific coefficient across all sites (effect size,  $\theta_{n,j}$ , in Eq. 6). The distribution of this value thus represents the probability of the model (PMP) and the variability in the same predictor across different sites. Black dots show the median, grey vertical lines show the 95 % CI, and blue coloured vertical lines show the 50 % CI. The definitions of the abbreviations of each predictor on *x* axes are given in Table 3.

geochemical cycling was likely to have caused the negative effect of event runoff. The events with low runoff, coupled with high temperatures (positive effect of event temperature for DOP cluster 2; Fig. S4a) may relate to increases in the rate of P releases from organic forms at higher temperatures (Verheyen et al., 2015).

Post-event runoff ( $Post_Q$ ) showed effects on specific constituents (e.g. NO<sub>x</sub>, FRP and EC). There are two alternative reasons that might explain this. First, high post-event runoff may be an indicator of large baseflow contribution during the events (Cuomo and Guida, 2016). Therefore, as discussed in the above paragraph, constituents that can be transported through subsurface flows tend to be influenced by amount of runoff post-event. Alternatively, it was significantly and positively correlated with other event characteristics and catchment biophysical conditions (e.g. vegetation cover; Fig. S2).



**Figure 7.** The comparisons of the distribution of posterior inclusion probabilities of the individual predictors derived from 1000 subsampled BMA runs. The boxes are the interquartile ranges (IQRs; 25th to 75th percentile), and the whiskers are the ranges between the 1.5 IQR of the lower quartile and 1.5 IQR of the higher quartile. The vertical bar is the median. Blue shows cluster 1 (wet) catchments, and red shows cluster 2 (dry) catchments. The definitions of the abbreviations of each predictor on *y* axes are given in Table 3.

Together, these intercorrelated factors could have influenced pollutant source, mobilisation and delivery (see discussions below; Granger et al., 2010; Lintern et al., 2018a).

#### 4.1.2 Vegetation cover

Vegetation cover was another driving factor that was found to have influenced water quality dynamics; antecedent NDVI (*Ante\_NDVI*) was included in the plausible models more frequently than event NDVI. The negative effect of antecedent NDVI on particulate and dissolved nutrients (except for DOP) was in line with previous studies that have found that NDVI was negatively correlated with these constituent concentrations in streams (Griffith et al., 2002; Masocha et al., 2017). An explanation for these results could be that high vegetation groundcover tended to stabilise the surface soil and reduce sediment losses by erosion (Meyer et al., 1997; Singh et al., 2008). In addition, vegetation nutrient assimilation and retention processes consumed nutrients in sediment and waterbodies, and these processes peaked in spring and early summer, typically before the wet season in the GBR catchments (Tabacchi et al., 2000; Vymazal, 2007).

The effect of antecedent NDVI varied among groups of constituents in clusters 1 and 2. Specifically, it was a key predictor for  $NO_x$ ,  $NH_4$  and FRP for cluster 1 and almost all constituents for cluster 2. This can be explained by the contrasting landscapes and climate of these two regions (Liu



**Figure 8.** Performance of the BMA models of the temporal variability of three constituents across 32 sites, represented by prediction intervals from BMA and observed Box–Cox EMC across two clusters of sites for (**a**, **b**) TSS, (**c**, **d**)  $NO_x$  and (**e**, **f**) FRP. Each bar shows a single event, and all events at all sites in the cluster are included. The NSE values were calculated based on median predictions. Black dots show prediction median, and grey vertical lines show the 95 % CI. Coloured vertical lines show the 50 % CI, and blue is cluster 1 (wet) catchments, and red is cluster 2 (dry) catchments. Dashed black lines are the 1 : 1 relationship.

et al., 2018). In the dense, vegetation-covered catchments in cluster 1 (i.e. the sites in the wet tropics), dissolved inorganic nutrient losses were likely due to more fertile soils (e.g. application of fertiliser on sugarcane) during the growing season (McKergow et al., 2005a). Furthermore, denser natural vegetation cover (e.g. riparian vegetation and forest) could increase plant uptake and assimilation of dissolved nutrients compared to the sparse vegetation cover in the dry tropics (cluster 2) region. Conversely, among cluster 2 sites, vege-

tation coverage showed clear seasonal variation, which was linked closely to the seasonality in rainfall and grazing activity. Sediments and particulate pollutants were likely to be mobilised in grazed catchments (high rate of soil erosion) and delivered to streams via surface runoff (Neil et al., 2002; Turner et al., 2012). More importantly, high vegetation cover tended to mitigate mobilisation of pollutants through stabilising the surface soil and reducing sediment losses from erosion (Meyer et al., 1997; Singh et al., 2008).

#### 4.1.3 Soil moisture and evapotranspiration

The results showed that soil moisture (SM) and actual evapotranspiration (AET) had a high impact on different constituents, particularly in the cluster 2 catchments (e.g. antecedent soil moisture - DON and EC; antecedent AET -TSS and EC). These two variables were intercorrelated and affect the hydrological cycle and vegetation cover (Correll, 1996). The results indicated that antecedent soil moisture had a negative effect on PN, NO<sub>x</sub>, NH<sub>4</sub>, DON, DOP and FRP. On one hand, this was expected as antecedent soil moisture was positively correlated with vegetation cover, and high soil moisture tends to reduce soil erosion and increase plant nutrient uptake. It may also be that soil water content affected soil microbial activity, influencing the biogeochemical processes in catchments, such as denitrification (Doran et al., 1988; Weier et al., 1993). The rate of denitrification was also enhanced under anoxic conditions, when soil moisture was high (Zhu et al., 2019). On the other hand, higher soil water can be associated with increased shallow subsurface flow and leaching of some constituents such as  $NO_x$  (Zhu et al., 2018). This appears not to occur to a sufficient extent for it to override other impacts of soil moisture.

#### 4.1.4 Temperature

Our results suggested that average event temperature (*Event*\_*T*) had a positive effect on  $NO_x$ , FRP and DOP. This may be attributed to the strong negative cross-correlation between temperature and event runoff and antecedent vegetation condition (Fig. S2). Rainfall during a warmer period might have been associated with less event runoff, resulting in higher event mean concentrations (Sect. 4.1.1). The effect of event temperature can be also attributed to the fact that the higher temperatures could lead to more recent mineralisation of nutrients, increasing readily transportable dissolved nutrient sources (Liu et al., 2017; Wang et al., 2020). Temperature is one controlling factor that affects pollution transformation (Barnard et al., 2005). For instance, temperature has a direct impact on the activity of microorganisms, which affects the intensity of biological processes such as denitrification (Wakelin et al., 2011). In addition, higher event temperature might be associated with higher pre-event temperature, resulting in poor groundcover, potentially lowering the dissolved nutrients losses through plant assimilation and/or uptake (Sect. 4.1.2; Muro et al., 2018).

#### 4.2 Predicting temporal variations in water quality

The Bayesian modelling framework in this study provided a useful tool to assess in-stream water quality dynamics. The models were able to explain more temporal variation in  $NO_x$  and EC than in other constituents. This is related to the sources and delivery processes of these two constituents. Anthropogenic inputs (e.g. agriculture) for  $NO_x$  and large stores in groundwater together with limited geochemical transformation for EC (salts) suggested that temporal changes in event concentration could be well captured by the changes in catchment hydroclimatic and vegetation conditions. In addition,  $NO_x$  and EC tend to be transported in subsurface flow pathways. The dynamics of catchment soil wetness and vegetation cover have been previously linked to hydrological interactions between surface and subsurface flows (Ursino et al., 2004). The incorporation of soil moisture and vegetation cover into the Bayesian modelling framework more readily allowed the description of the main ecohydrological processes of these two constituents.

In contrast, model performance for DOP was poor in cluster 1 catchments, which can be explained by two reasons. First, in the wet tropics catchments, DOP concentrations were generally stable, regardless of changes in flow, which can be explained by chemical exchange processes between water and sediment in stream (White et al., 1998). This means that the variability in DOP cannot be captured by the environmental variables considered here. Second, the poor performance might be attributed to the data set having fewer observations of DOP EMCs among cluster 1 sites. There were only 66 observations, compared to the next lowest number of 167 (EC) among other constituents in the cluster 1 catchments, which may not be sufficient to fully inform the model. This small sample size could have led to (1) poor mixing of MCMC chains for inclusion variables (Fig. S8a in the Supplement), where no predictors showed predictive power, and (2) the BMA failed to identify the plausible models, since none of the candidate models had enough predictive power to fit the data well (Guthke, 2017; Höge et al., 2019). Continuous DOP monitoring would be required to achieve a better understanding of the factors driving temporal variation in this constituent. Therefore, we did not infer any conclusions from the modelling results of DOP in cluster 1 due to the poor modelling performance.

The modelling performance in this study is generally higher than our previous studies (i.e. Guo et al. (2019, 2020)). This improved performance can be attributed to the following:

#### 1. Differences in water quality monitoring data.

Rivers in Queensland are more event dominated; thus, we used event-based water quality data compared to our

previous studies, which used monthly water quality data in Victoria. The uncertainty in event-based water quality samples has less impact on modelling performance because we considered the variability in streamflow when developing EMCs in this study (Chen et al., 2017; Lessels and Bishop, 2015; Letcher et al., 2002).

#### 2. Differences in modelling methods.

Here, we used a model-averaging approach that considered model predictions from multiple candidate models, rather than a single model approach that was used our previous studies (Guo et al., 2020, 2019). This approach is a more robust approach to providing predictions because the predictions consider the model selection uncertainty (Höge et al., 2019; Raftery et al., 1997).

Statistical modelling in hydrology or water quality is affected by uncertainty, only some of which can be characterised within any particular modelling framework (Kavetski et al., 2006; Mantovan and Todini, 2006; Renard et al., 2010). The Bayesian modelling framework used in this study incorporated the uncertainties in model selection (between model), observations and model parameters (within model) directly into the model predictions (Steel, 2019). This is a more comprehensive characterisation than in studies where model structures are assumed a priori. Reporting of predictive uncertainty of temporal variations in water quality also provided valuable information on the confidence in the averaged predictions. In addition, as discussed in Sect. 2.3, due to strong practical and conceptual reasons, our modelling framework was applied to two clusters of sites separately. However, this method can be used anywhere, e.g. a single modelling framework for all sites. Thus, we are not making claims that there are always variables that will be important in such catchments. Our method is universal, but our results are not.

Nevertheless, limitations remain in the BMA approach which are important to understand. For example, for EC, there was a larger predictive uncertainty and larger uncertainty in posterior inclusion probability for each predictor from the robustness assessment than estimated in the fit to the complete data set. A limitation of BMA is that the posterior model probability could be sensitive to the specification of the parameter prior distribution (Fernandez et al., 2001). Specifying more informative priors on model parameters (i.e. inclusion variable  $I_n$ ) would have the effect of restricting the set of candidate models (Rockey and Temple, 2016). Indeed, several studies have compared different predictive performances of different prior specification of BMA coefficients and found that the choice of prior matters (Bavarri et al., 2012; Liang et al., 2008). Future investigation of the sensitivity of prior distributions for BMA coefficients might achieve a reduction in predictive uncertainty and instability in posterior inclusion probabilities.

#### 4.3 Management implications

The identification of key drivers of temporal variation in water quality can inform catchment water quality management. The results of this study showed that the effects of hydro-climatic drivers (e.g. rainfall and runoff) and vegetation cover varied among constituents and regions. This may allow funding bodies, such as government and regional natural resource management groups, to identify regions where land management and restoration would have a greater effect on mitigating sediments and nutrients export. The results suggested that, compared to wet catchments, maintaining vegetation ground cover in large dry grazed catchments (e.g. the Burdekin and Fitzroy catchments in cluster 2) before the wet seasons could be an effective way of reducing sediment losses via erosion processes. These results are consistent with current, improved land management practices across the GBR catchments (Brodie et al., 2012; Queensland Government, 2017). Management measures (e.g. establishment of wetlands, revegetation and/or rehabilitation of gullies and stabilisation of river banks) can reduce sediment losses from hillslope and gully erosions (Koci et al., 2020; Sherriff et al., 2016). In addition, catchment-specific management that accounts for temporal variation in catchment hydrological connectivity is required for the control of dissolved nutrients. Dominant flow pathways for dissolved nutrients can vary spatially and temporally. For example, subsurface flow in the wet tropics region have tended to transmit more dissolved nutrients because prolonged wet conditions lead to this region being more likely to be connected via lateral subsurface flow (Geng et al., 2017). The enhanced mobilisation of leached dissolved nutrients from intensive cropping (e.g. sugarcane) from perched groundwater should be targeted in these catchments (Melland et al., 2012). Management practices, such as conservation tillage, and adaptation of the 4R concept (right source, right rate, right time and right place) for fertiliser application may help to minimise dissolved nitrogen losses (Lintern et al., 2020; Snyder, 2017).

### 5 Conclusions

This study provides a data-driven understanding of key drivers influencing the temporal variation in water quality. A hierarchical Bayesian model averaging framework was used to identify the key environmental drivers and predict the water quality dynamics at multiple catchments. Results showed that the temporal dynamics of water quality can be predicted well using models considering the combined effects of hydroclimate and vegetation groundcover. The effects of key hydro-climatic and vegetation conditions varied among different constituents and across regions. This study reinforces the importance of vegetation cover management as one key management response, especially for large grazed catchments. Future investigation could involve the development of a spatio-temporal modelling framework to fully capture the water quality dynamics. More importantly, it has continued to be challenging to prioritise management practices and evaluate the effectiveness of the improved management interventions. Consequently, with more land management surveys and continuous water quality monitoring data available, an extended temporal or spatio-temporal modelling framework could potentially be used to assess if the success of the restoration measures.

*Data availability.* Water quality data that supported this study are available upon request from the Great Barrier Reef Catchment loads monitoring programme (gbrevents@dsiti.qld.gov.au). Sources of explanatory variables are listed in Table 2.

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*Author contributions.* SL carried out data collation, performed the simulations and took the lead in writing the paper. DR, AWW, JAW, AL and DG contributed to the design of the research, interpretation of the results and supervision of the project. DW assisted with the data collation and provided critical feedback and helped shape the research, analysis and paper.

*Competing interests.* The authors declare that they have no conflict of interest.

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