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Estimating water quality using linear mixed models with stream discharge and turbidity

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SUMMARY

Most water quality monitoring schemes rely on estimation methods as it is often far too expensive to monitor water quality properties continuously. Estimations are used to evaluate management strategies and long term trends. It is critical that the estimation methods provide accurate estimations and an accurate estimate of the associated uncertainty. Currently the most common estimation methods assume observations are sampled using a probabilistic sampling scheme, however this assumption is often not met. This paper evaluated the ability of a linear mixed model to estimate water quality concentration values based on observations collected using non-probabilistic sampling. The linear mixed models were used to predict total phosphorus and total nitrogen observations from two catchments in south east Australia. A comparison between stream discharge and turbidity as predictors is made to investigate the effectiveness of turbidity to estimate water quality. In addition to stream discharge and turbidity, several covariates were derived from stream discharge in an attempt to account for hydrological processes. To compare models and their covariates leave one out event cross validation was performed. Event cross validation evaluated predictions during periods of high stream discharge. The inclusion of temporal autocorrelation component improved the accuracy of all models for total phosphorus and total nitrogen. For both catchments the use of turbidity instead of stream discharge increased the accuracy of predictions by at least 15% for total phosphorus and total nitrogen. However, event based cross validation indicated that a combination of both turbidity and stream discharge based variables provided more accurate predictions, decreasing the event RMSE by 18% for total phosphorus and 24% for total nitrogen. In catchments characterised by long periods of base-flow and short rainfall events the addition of turbidity measurements provide more accurate predictions during base flow and during events.

1. Introduction

Water quality monitoring provides critical information about the health of a catchment. In many situations catchment managers require accurate information to be able to implement management strategies. In Australia the relationship between stream discharge and other variables is quite complex (Davis and Koop, 2006; Drewry et al., 2009). Total nitrogen and total phosphorus are two key nutrients in Australian catchments, for example in large concentrations these two naturally occurring nutrients can often cause algae blooms (Davis and Koop, 2006; Kristiana et al., 2011). As a result catchment managers require estimates of nutrient fluxes to understand and manage catchment processes.

However environmental sampling is expensive, and water quality is no exception. With large catchments and numerous properties it is unrealistic to expect continuous time series data for all properties at all sampling locations. Combined with large analytical costs larger Australian catchments often have additional expenses due to travel time. The annual expense of water quality monitoring in Australia is estimated to be in excess of $142 M (Bartley et al., 2012; Kristiana et al., 2011). Most monitoring schemes can only afford to continuously monitor stream discharge and rely on sparse water quality sampling. Therefore suitable and reliable methods are required to gain an understanding of the processes within a catchment. Many studies rely on load estimation methods to evaluate water quality over a duration of time (e.g. monthly or annually). Australian catchment managers use the Australian and New Zealand guidelines (ANZECC) to assess water quality (ANZECC, 2000; Bartley et al., 2012). The ANZECC guidelines provide concentration based thresholds for various variables and catchment types. As the guidelines provide threshold values in the form of concentrations, catchment managers require methods to evaluate the observed data in relation to these thresholds. Catchment managers also rely on load estimations to evaluate management practices and perform trend assessments. Regression

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based methods use affordable covariates such as stream discharge to estimate temporal water quality concentrations, which can also provide load estimates, all at the frequency of stream discharge.

The most common water quality sampling scheme is based on approximately sampling at equally spaced intervals in time. In south eastern Australian catchments it is common for catchment managers to use a monthly sampling scheme and in some instances a form of storm based sampling as these events correspond to high nutrient exports (Armstrong and Mackenzie, 2002; Drewry et al., 2009; Bartley et al., 2012). South-east Australian rivers are characterised by short rainfall events. These short rainfall events are often separated by long dry periods, increasing the amount of export in following events (Drewry et al., 2009). Hopmans and Bren (2007) discovered that 70% of 6 years suspended sediments was exported during one rainfall event in a part of the Buffalo River catchment in north eastern Victoria. Increasing complexity is introduced as the relationship between water quality and stream discharge differs within and between events (Drewry et al., 2009). One issue within events is the hysteresis between stream discharge and water quality properties, which is caused by different trends during the rising and falling stages of the hydrograph. In addition, the distance between rainfall events can vary and may effect the amount of nutrients exported during the initial rising stage of the event hydrograph.

The importance of load estimation methods for monitoring water quality is evident by the amount of load estimation methods available. In a single study Marsh and Waters (2009) evaluated 34 different load estimation techniques. More recently artificial neural networks have been shown to provide accurate water quality load estimates (He et al., 2011). However, the majority of load estimation techniques fall into three main categories; average, ratio and regression methods (Cassidy and Jordan, 2011; Marsh and Waters, 2009; Cooper and Watts, 2002; Kronvang and Bruhn, 1996). In the simplest form averaging methods use the product of the mean concentration and the corresponding mean discharge to estimate the average concentration for a given period of time. Ratio based methods extend the averaging methods to include the all observed stream discharge values by including the mean of all discharge observations (Cooper and Watts, 2002). Both averaging and ratio based methods can only provide load estimations for time intervals which have enough observations to calculate a mean. For example, for monthly sampling this would be a 2 monthly average, on the other hand regression methods provide a continuous concentration estimate and the integral of predicted concentration multiplied by observed stream discharge is used to estimate a load. This method often uses log transformed stream discharge to estimate log concentrations. When fitted using ordinary least squares it is assumed that the errors are independent and identically distributed (iid) and have the following distribution; $\epsilon \sim \mathcal{N}(0, \sigma^2)$ (Lark and Cullis, 2004).

The three common load estimation methods have been compared by many studies (Cassidy and Jordan, 2011; Marsh and Waters, 2009; Johnes, 2007; Cooper and Watts, 2002; Kronvang and Bruhn, 1996). These studies often examine the effect of sample size on load estimates. Ratio based methods have been shown to provide the most accurate estimates of the three categories by Cassidy and Jordan (2011) and Johnes (2007). Marsh and Waters (2009) found ratio based methods to provide the most accurate load estimates when water quality sample sizes are smaller then 20 and continuous stream discharge data is available. However, both Marsh and Waters (2009) and Quilbé et al. (2006) proposed the use of a regression method in the presence of a strong correlation between stream discharge and the water quality property.

Sampling schemes that use either routine sampling (e.g. monthly) or a combination of routine and event based sampling are not probabilistic based (i.e the samples times are not selected randomly). By using this type of sampling scheme there is an unknown inclusion probability of collecting a sample at a particular point in time. The three main types of estimation techniques all assume probabilistic sampling. The bias due to these sampling schemes and the assumptions of the load estimation methods has long been acknowledged (Thomas, 1985, 1988; Crawford, 1991; Cohn et al., 1992; Cooper and Watts, 2002; Cohn, 2005). Average and ratio based methods assume the data is sampled using simple random sampling which is rarely the case (Cooper and Watts, 2002). Regularly used regression methods fitted using ordinary least squares will provide unbiased estimates of coefficients, however the variance estimates will be biased when the sampling scheme is not probability based (Lark and Cullis, 2004). This is a problem when both predictions and the prediction variance are required.

Linear mixed models (LMM) provide the ability to handle non-probability based sampling schemes by using a model-based approach (Lark and Cullis, 2004). Lark and Cullis (2004) compared ordinary least squares and LMM methods for estimating soil attributes. Their results indicated that the variance estimates from OLS were biased, as the OLS methods assumed the samples were independent of each other and had equal inclusion probabilities. They found an increase in variance with the use of LMMs as the model accounts for the non-probabilistic sampling scheme. Water quality sampling shares many similarities to systematic soil sampling, as the samples are non-probabilistic and there is auto-correlation between samples. With these similarities, LMM based estimations should provide less biased estimates of the prediction variance, than conventional methods. Furthermore, since LMMs model the auto-correlation in the model residuals, this can also be used to interpolate the model residuals using kriging. The kriged residuals are added to regression predictions at each prediction location to give an improved prediction (Bivand et al., 2008). Another major benefit from using regression based methods is due to the ability to include covariates other then stream discharge e.g. rising and falling limbs and time since the last rainfall event. In addition to these covariates Wang et al. (2011) also proposed the use of a discounted flow covariate which uses a weighting function to account for stream discharge prior to events. Turbidity has also been used in regression based models to estimate TP as it directly relates to the water quality of the stream. Jones et al. (2011) found in situ measurements of turbidity were significant covariates for estimating TP in a catchment in Utah. With the existence of relative low cost reliable turbidity sensors it is now feasible for catchment managers to use these sensors for continuous monitoring.

Therefore the aims of this paper are to

- present the use of LMMs for predicting water quality,
- compare the use of discharge-related predictor variables proposed by Wang et al. (2011) with turbidity measurements,
- focus the comparison on the prediction quality for flow events as these are when most export of nutrients and sediments occurs under Australian conditions.

This will be illustrated with a dataset of TP and TN for 2 sub-catchments draining into Lake Burragorang, the main reservoir for supplying Sydney's drinking water.

2. Materials and methods

2.1. Catchment description

This study involves the analysis of two sub-catchments within the greater Lake Burragorang catchment. Lake Burragorang is