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Benchmarking uncertainty quantification of water quality monitoring by high-frequency phosphorus data: comparison of Bayesian inference and bootstrap

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Water quality monitoring enables the evaluation of the ecological status of water bodies and assists in managing them. The European Water Framework Directive, for example, requires member states to regularly feed monitoring results into river basin management plans. However, water quality is monitored at low frequencies because resources are limited. Infrequent monitoring leads to sampling error when estimating water quality statistics and may subsequently lead to false grading, which impedes water quality management. Quantifying the uncertainty caused by low-frequency sampling is therefore important for assisting decision making.

In the present contribution, we approach sampling uncertainty through a subsampling study using total reactive phosphorus (TRP) concentration measured on a sub-hourly basis at three monitoring sites in Ireland for four hydrological years. These high-frequency TRP data were considered the “true” populations of TRP concentration in any given year and location. Sampling distributions of mean and 95th percentile (Q95) were simulated by resampling fortnightly monitoring subsamples from the populations. The sampling error caused by low-frequency monitoring was quantified using Bayesian parametric models, Bayesian bootstrap and frequentist bootstrap; and the performances of the different methods were subsequently compared.

According to the central limit theorem, the variance of the sampling distribution of a statistic is proportional to the variance of its population. In the Irish dataset, flashy flow and low flow increase the variance of the population, thus increasing sampling uncertainty. The increase in variance occurs because TRP concentration increases at flashy flow when TRP is flushed from, in this case, non-point sources by rainfall and overland runoff, and when TRP is highly concentrated during low flow. In addition, the TRP statistics are more uncertain in highly polluted catchments, because the tails of the populations are more pronounced at high pollution load.

Although the lognormal distribution is generally the best-fitting parametric model of the population of TRP concentration in the cases studied, the resultant uncertainty estimates of the TRP statistics are largely inaccurate, especially when the population follows a shape that defies any parametric model, which is frequently the case. Uncertainty quantification for the Q95 is less accurate compared to that for the mean and the probability distribution of the Q95 is not smooth. The Bayesian and frequentist bootstraps estimate the sampling distributions of mean and Q95 more accurately. The probability distribution of Q95 computed by the frequentist bootstrap is more accurate and smoother than that obtained by the Bayesian bootstrap, despite a small bin size used in the Bayesian bootstrap.

The results of this study demonstrate the limits of parametric models for modelling TRP concentration and advocate the use of quasi non-parametric models. Using these, in line with previous studies, the estimation of the Q95 is more uncertain than the estimation of the mean. Even though the mean is frequently used for determining ecological status, the Q95 is entirely more meaningful in describing the actual impacts of pollution on aquatic ecology. Open questions include the specification of prior assumptions about sampling bias, a discussion of which will conclude this contribution.