

# GEOSTATISTICAL INDICATORS OF WATERWAY QUALITY FOR NUTRIENTS

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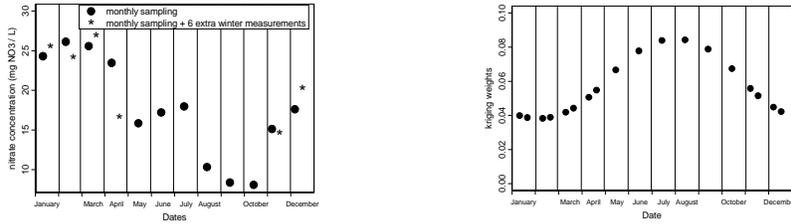
**Abstract.** This paper aims at constructing geostatistical indicators to quantify water quality for nutrients. It presents a method to estimate the yearly mean and the 90th percentile of concentrations, taking into account temporal correlation, irregularity of sampling and seasonal variations of concentrations. On simulations, segment of influence declustering, kriging weighting and a linear interpolation of empirical quantiles are calculated and compared to the currently used statistical inference, based on the independence of random variables. These methods make it possible to correct the bias of the yearly mean and the quantile, and to improve their precision, giving a better prediction of the estimation variance. The study focuses on nitrates, in the Loire-Bretagne basin (France).

## 1 Introduction

In order to assess river water quality, nitrate concentrations are measured in different monitoring stations and summarized in a few synthetic quantitative indicators such as the 90% quantile of yearly concentrations or the annual mean, making it possible to compare water quality in different stations, and its yearly evolution. The current French recommendations are based on the water quality's evaluation system (SEQ EAU) and the water framework directive in Europe, which aims at achieving good water status for all waters by 2015. These calculations, however, use classical statistical inference, essentially based on a hypothesis proved to be incorrect for many parameters: time correlation is not taken into account. Moreover, the seasonal variations of concentrations and the monitoring strategy are ignored. Because of the streaming, nitrate concentrations are high in winter and low in summer (Payne, 1993), and then if sampling frequency is increased in time in winter out of precaution, the annual mean and the quantile are falsely increased. It is therefore necessary that the estimation takes into account both time correlations and irregularity of the measurements. We show that kriging or segment weights facilitate correction of the bias and improved assessment of the yearly temporal mean, as well as the quantile. For quantile estimation, the known bias of classical empirical calculations can be reduced using a linear interpolation of the empirical quantile function. Methods are presented and compared for simulations of nutrients.

## 2 Annual concentrations at one station on the river Cher

Classical statistical inference consists of estimating the annual mean of nitrate concentrations by the sample mean and the 90% quantile by the empirical quantile. Figure 1 (left) and table 1 give an example of nitrate concentration measurements from the river Cher in 1985 in France. The annual mean and the 90th percentile have been estimated first with the totality of measurements (6 in summer, 12 in winter), then with an extracted sample of one regular measurement a month.



**Figure 1.** Preferential sampling of nitrates concentration during one year at one monitoring station (70300). Left: concentrations as a function of dates. Note that the frequency of measurements is doubled in winter. Right: associated kriging weights.

**Table 1.** Statistical yearly mean and quantile estimations corresponding to nitrates concentrations of Figure 2.

Sample size	Sample mean	90% quantile
12	17.49	25.56
18	18.75	26.12

Note that the sample mean is increased by 7% and quantile is increased by 3% when sampling is increased in winter. This difference, which can be much more important (up to 15 %) depending on the monitoring station, is a consequence of the temporal correlation (Figure 2, left). Because of this correlation, better methods are needed to assess the yearly temporal mean and the quantiles.

## 3 Methodology

### 3.1 THE YEARLY MEAN

For most of the monitoring stations, experimental temporal variograms calculated on nitrates concentrations show the evidence of a time correlation. For independent data, the sample mean (i.e., the arithmetic mean of the experimental data) is known to be an unbiased estimator; but in the presence of a time correlation, the sample mean is no longer unbiased, particularly when sampling is preferential. To correct this bias, two methods are studied:

- Kriging with an unknown mean (ordinary kriging, or OK), which takes into account correlation in the estimation of the annual mean and in the calculation of the estimation variance;

- A geometrical declustering, the only objective of which is to correct the irregularity of sampling.

These methods, detailed below, will be compared with simulations (Section 4):

a) In classical statistics (Saporta, 1990; Gaudoin, 2002): sample values  $z_1, z_2, \dots, z_n$  are interpreted as realizations of independent and identically distributed random variables  $Z_1, Z_2, \dots, Z_n$  with expectation  $m$ . The yearly mean is estimated by the sample mean,

denoted  $m^* = \frac{1}{n} \sum_{i=1}^n Z_i$ . The estimation variance  $Var(m^* - m) = \sigma^2/n$  is deduced from

the experimental variance  $\sigma^2$ :

b) With temporal kriging (Matheron, 1970; Chilès and Delfiner, 1999): sample values are interpreted as a realization of a random correlated function  $Z(t)$  at dates  $t_1, t_2, \dots, t_n$ .

In this situation the usual parameter of a distribution is not estimated, but rather the

temporal,  $Z_T = \frac{1}{T} \int_T Z(t) dt$ , which is defined even in the absence of stationarity.

Estimation proceeds using ordinary block kriging, as follows,  $Z_T^* = \sum_{i=1}^n \lambda_i Z_i$  where  $\lambda_i$

are the kriging weights and the kriging variance is given by  $Var(Z_T^* - Z_T)$

Analytical expressions necessary to calculate the kriging weights are easy to calculate in 1D, even without discretization. Figure 1 (right) gives an example of the kriging weights, assigning lower weights to winter values, which corrects the bias. The estimation variance and confidence interval, overestimated by classical statistics, are reduced by kriging taking into account the temporal correlation (figure 2, left) and the annual periodicity of the concentration.

c) Segment declustering, corresponding to 1D polygonal declustering (Chilès and Delfiner, 1999).

### 3.2 THE 90% QUANTILE OF NUTRIENTS CONCENTRATIONS

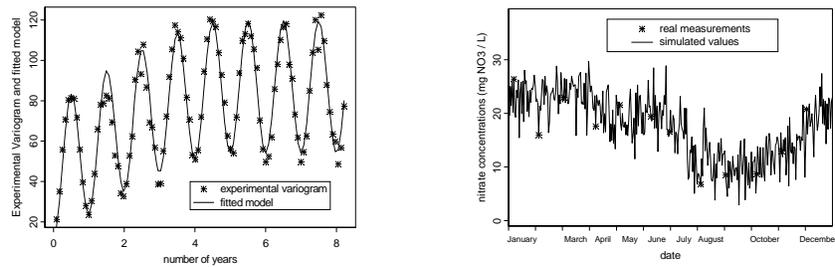
The 90% quantile is used to characterize high concentrations but the empirical quantile has proven to be biased even for independent realizations of the same random variable (Gaudoin, 2002). Moreover, it does not take into account temporal correlation and sample irregularity. In the literature there are many references pertaining to percentile estimation, especially with regard to statistical modelling of extreme values. However, many measurements are needed because of the appeal to asymptotic theorems. For an average of 12 measurements a year, classical non-parametric statistics will be used here, applying a linear interpolation of the empirical quantile. Then, to take temporal correlation into account, the data will be weighted using kriging or segment weights

## 4 Testing methods on simulations

### 4.1 CHOICE OF THE MONITORING STATION AND SIMULATION

Because complete time series for one year are not available, we use simulations for which the annual mean and the 90% quantile are known. Assuming that measurement per day corresponds to the daily concentration, we construct conditional simulations of “daily” concentrations with respect to the experimental data of real monitoring stations. Thus, we are able to compare the different estimations to the real yearly mean and quantile values. Different samplings schemes will be used: preferential, regular and irregular sampling.

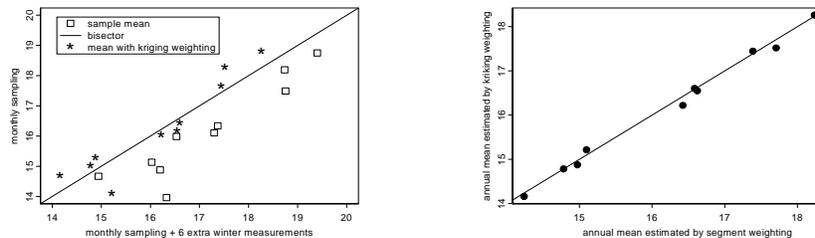
The presentation is here restricted to station number 70300, on the river Cher, sampled monthly. One thousand of conditional simulations of 365 days conditioned by real measurements in 1985 were constructed (one simulation example is given on figure 2 (right)), using the fitted variogram presented on figure 2 (left). This experimental variogram calculated over several years reflects the annual periodicity of nitrate concentrations. Variograms calculated for each season would differ, but as we are interested in the global annual statistics, the averaged variogram on one year is sufficient (Matheron, 1970).



**Figure 2.** Monitoring station on the river Cher, nitrate concentration. Left: experimental variogram and fitted model, with a lag of 30 days. Right: one conditional simulation.

#### 4.2 ESTIMATION OF THE YEARLY MEAN ON PREFERENTIAL SAMPLING

The results of the estimation of the yearly mean are presented In Figure 3 using 10 simulations. Estimations are compared on preferential sampling which comprises 18 measurements a year (6 values in summer and 12 values in winter) using monthly sampling (as in figure 1).



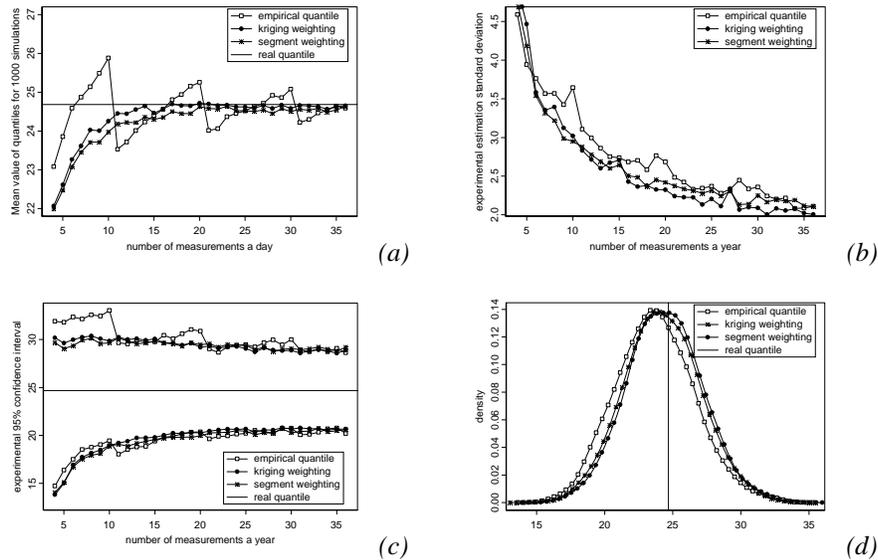
**Figure 3.** A comparison between the kriging and sample mean for the estimation of the yearly mean. On the left, scatter diagram between monthly sampling and preferential sampling estimations by kriging and statistics. On the right, scatter diagram between the yearly mean estimated with kriging weights and segment weights.

Figure 3 (left) shows that kriging rectifies the bias of the sample mean in the case of preferential sampling. Moreover, the kriging variance is lower than the predicted statistical variance of the mean of independent variables, namely because of the yearly periodic component of the variogram. Here, the calculation of the estimation variance obtained with classical statistics is on average 70 % higher than that obtained with kriging. Figure 3 (right) shows the equivalence of segment and kriging weighting in the estimation of the yearly mean.

It can be concluded that kriging corrects the bias in case of preferential sampling, that it yields a better assessment of the yearly mean, and improved precision. However, if we are only interest in the value of the annual mean, segment declustering can be used because of its simplicity. If precision is needed, then kriging should be preferred.

#### 4.3 QUANTILE ESTIMATION ON IRREGULAR SAMPLING

In this example, samples of different sizes have been extracted from each of the 1000 simulations, for 4 to 36 measurements a year, irregularly spaced in time. Thus we obtain 1000 samples of size 4, 1000 of size 5 etc... We estimate the 90% quantile for each sample using classical statistics and kriging or segment declustering on a linearly interpolated empirical quantile (Bernard-Michel and de Fouquet, 2004). Results are given in average for each different sample size and shown in Figure 4. They are compared to quantiles calculated in average on the 1000 simulations of 365 days.



**Figure 4.** Average of the quantile estimation for temporal correlated concentrations, compared with the empirical quantity, for 1000 simulations. This empirical quantity corresponds to the mean, calculated on all the simulations, of the 90% quantiles of 365 values. All calculations are made by linear interpolation of quantiles. Upper left figure (a): average of quantiles estimation. Upper right figure (b): experimental estimation standard error. Lower left figure (c): experimental 95% confidence interval. Lower right figure (d): histogram of quantile errors for samples of size 12.

Figure 4 (a) shows that the linear interpolation of the empirical quantile corrects the bias very well. Kriging or segment of influence weighting takes into account the sampling irregularity. However, the estimation variance (figure 8 (b)) remains large. Actually, for 36 measurements a year, errors still represent approximately 8% of the real quantile which gives an approximate 95% confidence interval (figure 8. (c)) of  $\pm 20\%$  around the real quantile because of the quasi normality distribution of errors (figure 8 (d)). For 12 measurements a year, they reach 11% of the real quantile, and 18% for 4 measurements a year. In the presence of time correlation, the theoretical estimator of a confidence interval would be difficult to construct. Even when random variables are independent, the theoretical interval (Gaudoin, 2002) is not satisfactory because it is limited by the higher order statistics. Simulations can be used to evaluate errors made in estimations and to determine the required sample size to achieve a desired precision.

## 5 Conclusions

Results are similar for other stations. Kriging the annual mean allows the bias induced by a preferential sampling of high concentration periods to be corrected. Associated with linear interpolation of the experimental quantile function, the kriging weights give an empirical estimation of quantiles that is practically unbiased. The segment of influence weighting can be used to simplify the calculations. In all cases, one or two measurements a month are not sufficient for a precise estimation of the yearly 90% quantile.

## Acknowledgements

Thanks to the French Ministry of Environment (MEDD) for financing this study and L-C. Oudin and D. Maupas of the Agence de l'Eau Loire-Bretagne for their help.

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