Variance Reduction for Trend Analysis of Hydrochemical Data in Brackish Waters

Claudia Libiseller¹ and Anders Nordgaard¹

Abstract
We propose one parametric and one nonparametric method for conducting trend tests on nutrient concentrations in brackish waters taking into account that the temporal variation in both nitrogen and phosphorus records can be strongly influenced by the mixing of sea water and fresh water. Both methods utilise salinity as a covariate in the trend analysis. Data on total phosphorus in the Baltic Sea showed that there was a downward trend, although it was very weak when the natural fluctuations in salinity had been taken into account.

1. Introduction
Cultural eutrophication of water bodies has become an important topic during the last decades. Its adverse effects are typically found in areas of reduced water exchange, such as semi-enclosed seas like the Baltic Sea (Richardson/Jørgensen 1996). Since eutrophication can seriously affect the whole marine food web, the Helsinki Commission (HELCOM) recommended a 50% reduction of nutrient emissions from industrial and municipal point sources and diffuse sources such as agriculture, and established a common monitoring and assessment group.

The concentrations of nutrients in a water body like the Baltic Sea are, however, strongly influenced by the mixing of waters of different origin, which makes detection of a decrease due to the adoption of some policy measures quite difficult. In this paper, we examine how the human impact on nutrient concentrations in such water bodies can be clarified by replacing conventional time series or geostatistical approaches by trend detection techniques in which we analyse the variation in nutrient concentrations with salinity and time. In particular, we examine how data collected at different depths at a single station or a network of stations can be simultaneously analysed for temporal trends in the concentrations of different forms of nitrogen and phosphorus.

¹ Department of Mathematics / Division of Statistics, Linköping University, SE-58183 Linköping, Sweden
2. **Natural variation in the Baltic Sea**

In the Baltic Sea the brackish surface layer is well mixed due to wind and the time series of concentrations exhibit a clear seasonal variation. Below this layer a strong halocline is formed. The deep waters are a mixture of saline Kattegat water and entrained surface water and the predominant natural fluctuation is caused by the rare saltwater inflow from the North Sea (Fig 1). Such so-called major inflows happen only about nine times per century, which makes the bottom waters stagnant for long time periods and allows hypoxic or anoxic conditions to develop (Stigebrandt 2001).

![Fig. 1: The inflow of saline Kattegat water induces an undulatory fluctuation in the time series of total phosphorus in the Western Gotland Basin. The graph shows data recorded at a depth of at least 80 m.](image)

3. **Data**

The data considered in this paper consists of monthly measurements of different nutrients as well as other hydrological parameters at a number of sampling sites in the Baltic Sea during the period 1989-1998. At each sampling site observations are taken at different depths with a resolution of 5-10 metres.
4. Trend testing of total phosphorus in the Baltic Sea

The inflowing saltwater induces an undulatory fluctuation with a period of about a decade to the time series of nutrients. Since the actual trend, which normally is much smaller than the natural fluctuation, can be masked by this phenomenon, a conventional univariate trend test is not appropriate.

A considerable variance reduction can be achieved by plotting the concentration values against salinity (see figure 2) or salinity and time. Therefore we divided the time series of nutrient concentrations representing different salinity levels.

![Figure 2: Total phosphorus concentrations in the Western Gotland Basin plotted against depth (left) and against salinity (right).](image)

We propose two different methods for trend testing, a non-parametric test and a test based on a linear model. Both alternatives are applied to observations of total phosphorus in the Western Gotland Basin.

4.1 A non-parametric trend test

The Mann-Kendall test is a non-parametric test for randomness against trend, and the test statistic for a time series \( y_t, t = 1, \ldots, n \), is computed as follows:

\[
K = \sum_{j<k} \text{sign}(y_k - y_j)
\]

Under the null hypothesis of no trend, the test statistic is asymptotically normally distributed with mean 0 and variance \( n(n-1)(2n+5)/18 \). Different versions of Mann-Kendall tests have been developed to accommodate missing values, ties and seasonality (Hirsch/Slack 1984).
We propose a procedure in which Mann-Kendall statistics are computed for different seasons and salinity levels. If multiple observations are present for a given combination of time and salinity the median of these observations is computed. Furthermore all covariances between test statistics are calculated. To perform an overall trend test for all seasons and salinity levels a test statistic is calculated as

$$z = \mathbf{1}' K / \sqrt{\mathbf{1}' \Gamma \mathbf{1}}$$

where \( K \) is the vector of the Mann-Kendall statistics and \( \Gamma \) is the variance-covariance matrix of these test statistics. \( \mathbf{1} \) is a vector with all elements equal to 1. Under the null hypothesis of no trend, \( z \) is asymptotically standard normally distributed.

To illustrate the proposed test we divided the previously illustrated total phosphorus data (Fig. 2) into three salinity levels and four seasons (Dec-Feb, Mar-May, Jun-Aug, Sep-Nov). Although the dependence between total phosphorus and salinity was not fully removed, the overall test statistics suggested a significant downward trend (Table 1). Closer examination of the different salinity levels indicated that the downward trend in total phosphorus primarily emerged for low salinity levels. At the highest salinity level, where only few observations were available, there was even an upward tendency in the phosphorus data.

Further studies showed that similar results were obtained for other stratification into salinity levels and seasons. However, in general the detected trends were not significant at the 5% level (Table 1).

Since for this test observations of the uppermost 20 m in the water column were omitted, the seasonal variation of the time series was not very strong and a part of this seasonality could be explained by varying salinity. Therefore in the last approach no seasons were assumed and salinity was divided into 14 levels. The result was again a non-significant downward trend (Table 1). The time series that were examined are seen in figure 3. Even here it can be clearly seen that phosphorus time series for the levels with high salinity show an upward trend during the last two years. For these series, however, hardly any observations were available at the beginning of the observation period and phosphorus levels cannot be compared to earlier conditions. In all of the time series with lower salinity a slight downward trend can be seen.
Table 1: Overall trends in total phosphorus obtained by performing Mann-Kendall tests with different stratification into salinity levels and seasons.

<table>
<thead>
<tr>
<th>Stratification</th>
<th>Test statistic</th>
<th>p-value</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 salinity levels / 4 seasons</td>
<td>-2.05</td>
<td>0.0201</td>
</tr>
<tr>
<td>5 salinity levels / 4 seasons</td>
<td>-1.35</td>
<td>0.0885</td>
</tr>
<tr>
<td>14 salinity levels / no seasons</td>
<td>-1.35</td>
<td>0.0885</td>
</tr>
</tbody>
</table>

4.2 A parametric approach

If we assume that within salinity class \( i (i=1,\ldots,K) \) the time series of nutrient concentration data contains a possible linear trend and a deterministic seasonal pattern, a time series regression model can be applied

\[
y^{(i)}_t = \beta_0^{(i)} + \beta_1^{(i)} t + \sum_{j=1}^{S-1} \beta_j^{(i)} x_j + \varepsilon^{(i)}
\]  

(4.2.1)
where $S$ is the number of seasons, $x_{1i},...,x_{Si}$ are seasonal dummies ($=1$ for season $j$ and 0 otherwise) and $\varepsilon^{(i)}_t$ are random errors possibly correlated. We propose the following overall trend parameter:

$$\beta = \sum_{i=1}^{K} w(i) \hat{\beta}^{(i)}_1$$  \hspace{1cm} (4.2.2)

where $w(i),...,w(K)$ are weights proportional to sizes of the $K$ salinity classes. An unbiased estimator of $\beta$ is

$$\hat{\beta} = \sum_{i=1}^{K} w(i) \hat{\beta}^{(i)}_1$$  \hspace{1cm} (4.2.3)

where $\hat{\beta}^{(i)}_1$ is the Ordinary Least Squares (OLS) estimate of $\beta^{(i)}_1$. If we ignore any correlation structure between observations in different salinity classes a studentised version of (4.2.3) becomes

$$t = \frac{\hat{\beta} - \beta}{\sqrt{\sum_{i=1}^{K} w(i)^2 s(i)^2 \left(X^TX\right)^{-1}_{i11}}}$$  \hspace{1cm} (4.2.4)

where $s(i)^2$ is the mean square error and $\left(X^TX\right)^{-1}_{i11}$ is the diagonal element corresponding with $\hat{\beta}^{(i)}_1$ in the information matrix from the OLS estimation in salinity class $i$.

The statistic $t$ can be used to construct a confidence interval for $\beta$ provided we have some information about the underlying probability distribution of data. However, to avoid making any assumptions about this distribution we will compute confidence intervals for $\beta$ using a bootstrap approach.

The bootstrap in its original form (Efron 1979) does not allow for any dependencies among the observations. However, different ways to apply the bootstrap idea to such cases have been proposed by several authors. We shall here use the method of ARMA bootstrap (Kreiss/Franke 1992).

Applying OLS to the regression model (4.2.1) will give a set of residuals $\tilde{\varepsilon}^{(i)}_1,...,\tilde{\varepsilon}^{(i)}_n$ where $n$ is the number of observations in the corresponding salinity class. From descriptive studies of such residuals an auto-regressive model of order 2 is proposed: $\tilde{\varepsilon}^{(i)}_t = \varphi_{1,1} \tilde{\varepsilon}^{(i)}_{t-1} + \varphi_{1,2} \tilde{\varepsilon}^{(i)}_{t-2} + a^{(i)}_t$ where the $\varphi$-coefficients are estimated by OLS and subsequently residuals are calculated as

$$\tilde{a}_t = \varepsilon_t - \hat{\varphi}_1 \varepsilon_{t-1} + \hat{\varphi}_2 \varepsilon_{t-2}, t \geq 2$$  \hspace{1cm} (4.2.5)
These residuals are standardised to zero mean and then resampled by ordinary bootstrap. From the resampled residuals $\hat{\epsilon}_1, \ldots, \hat{\epsilon}_n$, resampled versions of $\hat{\epsilon}_t$ are calculated using equation (4.2.5) with suitable initial values. Finally, resampled versions of $\gamma$, are calculated according to

$$y_{i(t)} = \hat{\beta}_0^{(i)} + \hat{\beta}_1^{(i)} t + \sum_{j=1}^{S} \hat{\beta}_{j}^{(i)} x_j + \hat{\epsilon}_i^{(t)}, t \geq 2$$

and resampled OLS estimates of the $\beta$-parameters can be obtained.

It is now possible to calculate a resampling distribution for the statistic $t$, i.e. we compute resampled versions of $t$:

$$t^* = \frac{\hat{\beta}^* - \hat{\beta}}{\sqrt{\sum_{i=1}^{K} W_{i(t)}^2 s_{(t)}^2 (X^T X)^{-1}}};$$

by repeating the bootstrap procedure a large number of times. The quantities $\hat{\beta}$ and $s_{(t)}^2$, are the counterparts of $\hat{\beta}$ and $s_{(t)}^2$ from the OLS estimation on $\{y_{i(t)}\}$.

We apply this method with the same number of seasons ($S=4$) as in the non-parametric approach. Fig. 4 shows the histogram of 200 values of $t^*$ for trends in total phosphorus in the Western Gotland Basin.

![Histogram of 200 values of $t^*$ for trends in total phosphorus in the Western Gotland Basin.](image)

Fig.4: Histogram of 200 values of $t^*$ for trends in total phosphorus in the Western Gotland Basin.

The bootstrap principle now says that this distribution is a good estimate of the true distribution of $t$. We therefore compute the 2.5 and 97.5 percentiles and use these to
construct a 95% confidence interval for $\beta$ through equation (4.2.4). The resulting interval becomes

$$(-0.00094, -0.00013)$$

and thus demonstrates negative significant downward trend.

5. Conclusions

We have shown that by taking into account that the temporal variation of nutrients in the Baltic Sea strongly depends on water changes (measured as salinity), we can conduct a test for trend both with a non-parametric and a parametric approach. The results from the different approaches are consistent and show that the reduction of variance obtained by the normalisation for salinity can clarify the presence of anthropogenic trends. However, we also note that the stratification of data into different salinity classes combined with seasonal adjustment is somewhat crucial for the results. We therefore suggest that further work on this subject is needed in which the seasonal-salinity variation must be taken care of more comprehensively.

6. Acknowledgements

This work is part of the project IMPACT (EC-IST-1999-11313) financed by the IST programme of the European Community.

Bibliography


Stigebrandt A., Physical oceanography of the Baltic Sea, in F. Wulff et al. (eds.): A Systems Analysis of the Baltic Sea, Ecological Studies 148