Comparison of Methods for Normalisation and Trend Testing of Water Quality Data

Claudia Libiseller
Department of Mathematics, Division of Statistics
Linköping University
SE-58183 Linköping, Sweden
E-mail: cllib@mai.liu.se

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Abstract
To correctly assess trends in water quality data, influencing variables such as discharge or temperature must be taken into account. This can be done by using (i) one-step procedures like the Partial Mann-Kendall (PMK) test or multiple regression, or (ii) two-step techniques that include a normalisation followed by a trend test on the residuals. Which approach is most appropriate depends strongly on the relationship between the response variable under consideration and the influencing variables. For example, PMK tests can be superior if there are long and varying time lags in the water quality response. Two-step procedures are particularly useful when the shape of the temporal trend is the primary interest, but they can be misleading if one of the influencing variables itself exhibits a trend or long-term tendency. The present study discusses the advantages and disadvantages of some trend testing techniques, using Swedish water quality data to illustrate the properties of the methods.

1. Introduction
Time series of environmental data are collected to monitor the state of the environment and how it changes over time. Unfortunately, the measured values are often affected by the weather conditions that prevail before and during sample collection. Therefore, scientists have begun to pay more attention to the impact these natural phenomena have on the time series of interest, and an increasing number of methods have emerged to take meteorological and hydrological variables into account in the assessment of trends.

In general, there are two kinds of trend tests that can include auxiliary information about natural fluctuations: (i) one-step procedures, which simultaneously test for trend and adjust for a covariate; (ii) two-step procedures, which include a normalisation step and a subsequent trend test applied to the residuals. The most common members of these groups are multivariate regression and stagewise regression, both of which entail regression on the covariate(s) and on a time variable.

Nevertheless, in the context of environmental quality, the general requirements for parametric regression procedures are rarely fulfilled. Accordingly, a number of regression-based alternatives have evolved, including non-parametric regression (Hussian et al., 2004a), semi-parametric regression (Stålnacke and Grimvall, 2001; Shively and Sager, 1999), regression trees (Huang and Smith, 1999), and artificial neural networks (Gardner and Dorling, 2000a,b). Also, analysis for trends is normally done using a non-parametric test such as the Mann-Kendall (MK) test for monotone trends (Mann, 1940; Kendall, 1975, Hirsch and Slack, 1984). Moreover, the non-parametric, one-step procedure called the partial Mann-Kendall (PMK) test was recently proposed (Libiseller and Grimvall, 2002).

This paper discusses the ways that particular features of water quality and discharge data can influence assessments of temporal trends. In particular, attempts are made to highlight situations that are difficult to analyse, such as (i) long time delays between a rainfall event and the response in the water chemistry variable; (ii) gradual changes in the covariates that range over a long time period and induce or conceal a trend in the response; (iii) large seasonal variation. The properties of some normalisation and trend testing techniques when analysing such situations are examined.

2. Normalisation techniques and one-step procedures
This study compares the results obtained using three different methods to investigate trends (Table 1): two normalisation techniques (linear regression and semi-parametric regression) and a one-step procedure (the PMK

test) that simultaneously adjusts for covariates and tests for trend. Those results are subsequently compared with the results of seasonal Mann-Kendall tests, in which the covariate is not taken into account.

Table 1. Three different approaches to trend testing

Approach	Robustness	Trend	Method
Normalisation followed by trend test on residuals	Parametric	Monotonic	Linear regression on discharge + Mann-Kendall test
	Semi-parametric	Monotonic	Semi-parametric regression on discharge + Mann-Kendall test
Multivariate trend test	Non-parametric	Monotonic	Partial Mann-Kendall test

2.1. Linear regression model

The linear normalisation model has the general form

$$y_{ij} = a + b_j x_{ij} + e_{ij}, \quad i = 1,\dots,n \quad j = 1,\dots,m$$

where y_{ij} is the observed response for the jth month of the ith year, x_{ij} represents the values of the explanatory variable (water discharge), and e_{ij} is a random error term with mean zero. The slope parameters (b_j) are permitted to vary with the season under consideration (j), and the intercept (a) is constant throughout the year.

2.2. Semi-parametric regression model

The semiparametric normalisation model has the general form

$$y_{ij} = a_{ij} + b_j x_{ij} + e_{ij}, \quad i = 1,\dots,n \quad j = 1,\dots,m$$

where y_{ij} is again the observed response, x_{ij} represents the covariate, and e_{ij} is a random error term. The slope parameters (b_j) are permitted to vary with the season under consideration (j), and the intercept (a_{ij}) is permitted to vary with both season (j) and year (i). However, rapid changes in the intercept are controlled by so-called roughness penalty factors (l_1 and l_2), and the intercept and slope parameters are estimated by minimising the expression

$$S(a, b) = \sum_{i,j} (y_{ij} - a_{ij} - b_j x_{ij})^2 + l_1 \sum_{i,j} (a_{ij} - \frac{a_{i+1,j} + a_{i-1,j}}{2})^2 + l_2 \sum_{i,j} (a_{ij} - \frac{a_{i,j-1} + a_{i,j+1}}{2})^2$$

where the first sum ranges over all values of i and j for which both the response variable and the explanatory variables have been observed. Detailed information about algorithms for parameter estimation has been published by Stålnacke and Grimvall (2001). The penalty factors l_1 and l_2 are determined by minimising the root mean prediction error sum of squares (RMPRESS) using cross-validation with one-year-long blocks (Hussian et al., 2004b).

2.3. Partial Mann-Kendall tests

The univariate MK statistic for a time series $\{y_i, i = 1,2,\dots, n\}$ of data is computed as

$$T = \sum_{k<l} \text{sgn}(y_l - y_k) \quad \text{, where} \quad \text{sgn}(x) = \begin{cases} 1, & if \;\; x > 0 \\ 0, & if \;\; x = 0 \\ -1, & if \;\; x < 0 \end{cases}$$

The test statistic T is asymptotically normally distributed with mean 0 and a variance proportional to n. If the response variable is measured over several (m) seasons, the seasonal MK test is determined by the following: separating the data into m subseries, each representing one season; computing the MK statistic (T_j) for each series; and summing the individual MK statistics. The resulting test statistic S has a normal distribution with mean 0, and the formula for the variance is given in Hirsch and Slack (1984).

The PMK test can account for the influence of one or several explanatory variables and is computed using the conditional mean and the conditional variance of the response variable, given the MK statistics of the explanatory variable (S_x), as follows:

$$PMK = \frac{S_y - \hat{r}\, S_x}{\sqrt{\left(1-\hat{r}^2\right) n(n-1)(2n+5)/18}}$$

where $\hat{r}$ denotes the correlation between the MK statistics S_x and S_y. The PMK statistic is normally distributed with mean 0 and standard deviation 1. (For details, see Libiseller and Grimvall, 2002.)

3. Data

Water quality data for Swedish rivers were retrieved from a database maintained by the Department of Environmental Assessment at the Swedish University of Agricultural Sciences, and the discharge measurements were provided by the Swedish Meteorological and Hydrological Institute.

4. Characteristics of data sets and selection of trend tests

4.1. Long-term delay in relationships

A rainfall event does not necessarily have an immediate impact on water quality. Sometimes part of the effect can be measured over a period of several days or months, depending on the properties of the soil and the size of the drainage area. Figure 1 shows monthly total nitrogen concentrations and discharge measured in the Enningdal River at Norra Bullaren. Visual inspection suggests that the correlation between observations made at the same time point is not very strong, but the two series do change jointly in the long run. Computing the Pearson rank correlation, the values vary between –0.13 and 0.59 for different seasons. If a PMK test is used and the correlations between the MK test statistics are estimated for each month, they are generally larger than the correlations between observations. In the results of the trend tests (given in Table 2), the p-value of the PMK test is slightly smaller than that from the univariate MK test and much smaller than the p-values provided by the normalisation procedures. It should be noted that the normalised total nitrogen loads from the semi-parametric regression in Figure 2 still display some of the the gradual change observed in discharge, indicating that not the entire effect was removed.

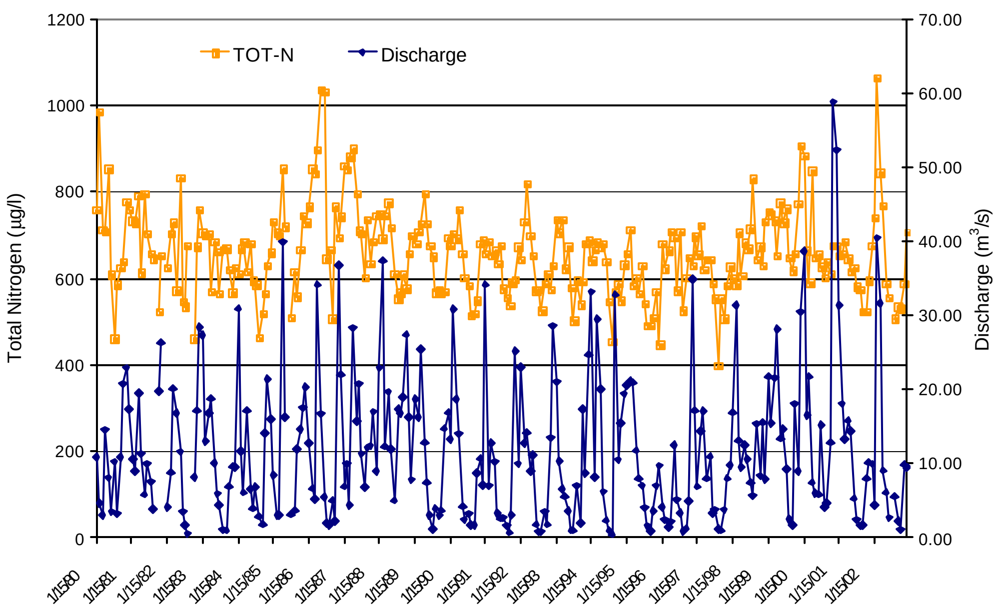

Figure 1. Monthly total nitrogen concentrations and discharge in the Enningdal River from 1980 to 2002.

Many flow adjustment techniques do not consider long memory effects, because they only include simultaneously measured values of discharge. Of the methods applied here, only the PMK test can (indirectly) include time-lagged values (if data are available for several seasons), which means that the covariance between the MK test statistics is estimated, not merely for data from the same season, but also across seasons. Consequently, all these covariances are used to compute the correlation between the test statistics of the response and the covariate.

Table 2. Results provided by the three different trend test procedures

	SP-norm + MK	Reg-norm + MK	PMK	MK
Test statistic	–1.111	–1.052	–1.604	–1.479
p-value	0.266	0.293	0.1086	0.139

Abbreviations: SP-norm, normalised using semi-parametric regression; Reg-norm, normalised by linear regression; MK, univariate Mann-Kendall test; PMK, partial Mann-Kendall test.

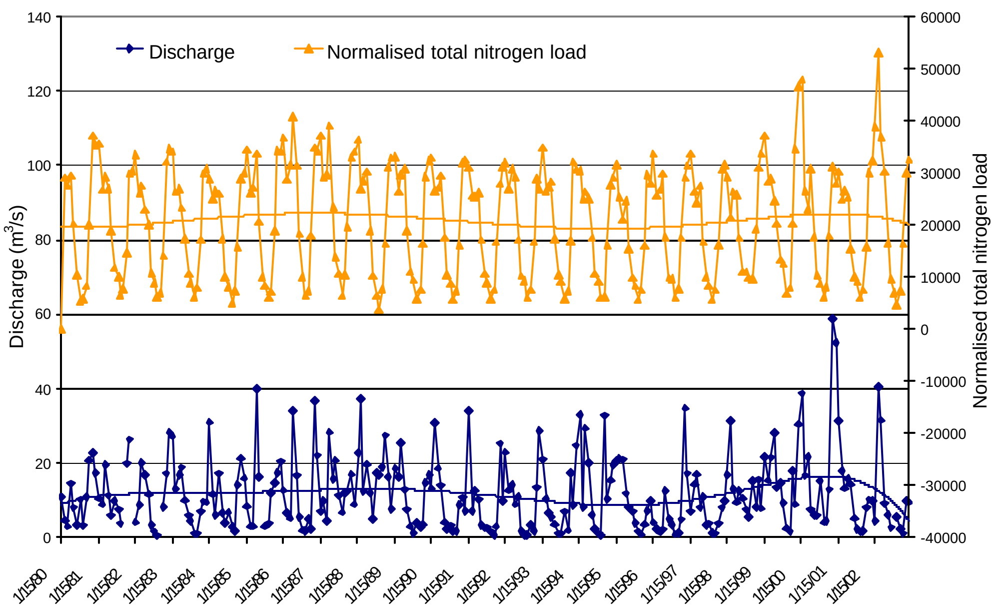

Figure 2. (SP-)normalised total nitrogen load and discharge in the Enningdal River.

4.2. Non-monotonic change in the covariate

Measurements of alkalinity/acidity and discharge in the Dalälven River at Älvkarleby are shown in Figure 3. Clearly, both variables exhibit a long-wave component, more precisely, drier years and wet years occurred intermittently, leading to changes in the level of the water quality variable. The results of the trend tests (given in Table 3) indicate a significant upward trend, but if the years 2001–2002 are included in the analysis (Table 4), only the PMK test yields significant results.

The covariate can easily impose a gradual, long-term change on the response variable (see section 4.3). If the covariate regains its average levels after such a period, the changes in the response variable display a long-wave component. This kind of influence is easier to handle with two-step procedures, since such methods first remove the non-monotonic change and thereby allow a standard trend test to be used on the residuals. Techniques like the PMK test, on the other hand, might be misleading, because univariate MK tests are computed for the covariate and the response variable, even though both exhibit a non-monotonic change. However, the difference between the PMK test and the normalisation procedure in the present example is not very large and may be partly explained by long memory effects (see section 4.1).

Table 3. Results provided by the three different trend test procedures for the period 1986–2000

	SP-norm + MK	Reg-norm + MK	PMK	MK
Test statistics	2.843	2.408	2.631	2.042
p-value	0.013	0.016	0.009	0.041

Abbreviations: SP-norm, normalised using semi-parametric regression; Reg-norm, normalised by linear regression; MK, univariate Mann-Kendall test; PMK, partial Mann-Kendall test.

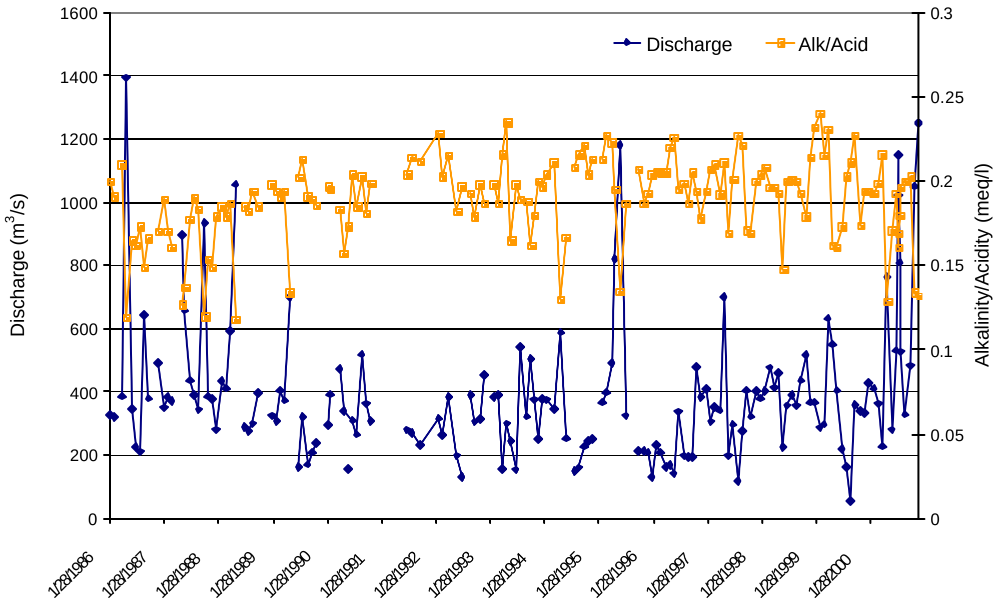

Figure 3. Measurements of alkalinity/acidity and discharge in the Dalälven River from 1986 to 2000.

Table 4. Results provided by the three different trend test procedures for the period 1986–2002

	SP-norm + MK	Reg-norm + MK	PMK	MK
Test-statistics	1.820	1.863	2.310	1.247
p-value	0.069	0.063	0.021	0.212

Abbreviations: SP-norm, normalised using semi-parametric regression; Reg-norm, normalised by linear regression; MK, univariate Mann-Kendall test; PMK, partial Mann-Kendall test.

4.3. Long-term gradual changes in the covariate

Even if it is assumed that the levels of the covariate (e.g., water discharge) do not change in the long run, it is still possible that they can increase or decrease in certain time periods. Figure 4 depicts the time series of total nitrogen concentrations and discharge measured in the Motala River at Norrköping. An upward trend can be seen in both series in the diagram. After correcting for the covariate the trend tests produce *p*-values that are considerably larger than those obtained with the univariate MK test (Table 5). The adjusting effect of the PMK test is somewhat larger than that of the normalisation procedures, which, even in this case, is partly due to time-lagged effects.

In a simulation study conducted by Smith and Rose (1991), it was found that stagewise regression is misleading and less powerful compared to multivariate regression, if the covariate is linearly dependent on time. More precisely, when using normalisation procedures, there is a risk that part of the human-induced trend in the response variable can be attributed to the changes in the covariate. This risk is smaller when both the temporal trend and the dependence on the covariate are handled simultaneously, for example by applying a multiple regression. The PMK test is such a procedure, but it is not known how well it can manage the mentioned situation, since estimation of the correlation between two MK statistics is based on a rather simple correspondence measure for ranks. Clear trends in both series would lead to substantial correlation, even if the correlation between simultaneously measured values (or values with a reasonable time-lag) is small.

Table 5. Results provided by the three different trend test procedures

	SP-norm + MK	Reg-norm + MK	PMK	MK
Test-statistics	–0.264	–0.482	–0.920	1.409
p-value	0.791	0.630	0.927	0.159

Abbreviations: SP-norm, normalised using semi-parametric regression; Reg-norm, normalised by linear regression; MK, univariate Mann-Kendall test; PMK, partial Mann-Kendall test.

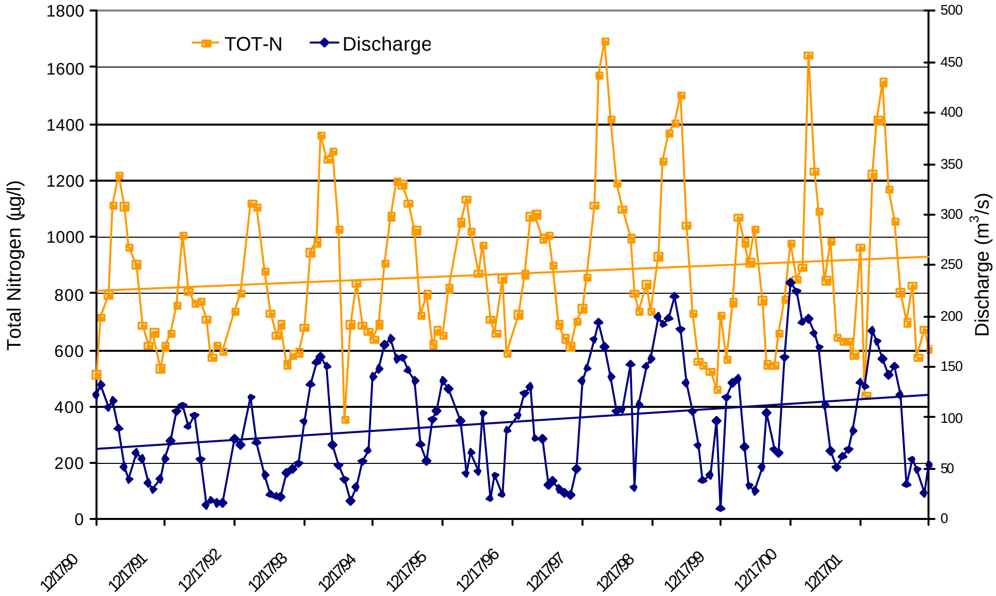

Figure 4. Measurements of total nitrogen concentrations and discharge in the Motala River from 1990 to 2002.

4.4. Changes in concentration-runoff relationships

Figure 5 illustrates measurements of total nitrogen and water discharge in the Pite River, and Table 6 gives the results of the trend tests. Clearly the PMK test does not correct for much of the variation in discharge, and the results of this test are quite similar to those provided by the univariate MK test. This finding can be explained by the fact that, in the analysed data set, total nitrogen shows negative dependence on discharge during spring and early summer (March–July) and positive dependence during late summer and autumn (August–November). The simplest version of the PMK test estimates the correlation between the MK test statistic for nitrogen and that for discharge to be the mean value of all individual correlations (in this case about zero).

If the sign and the magnitude of dependencies between the response and the covariate vary strongly over the year, it can influence the outcome of different trend tests. The trend test must account for any such variation, which is easily done with the present normalisation procedures, since they allow independent estimation of the slope for each month. The PMK test, on the other hand, only computes a mean correlation for all months, hence it is of no use in this situation. Libiseller and Grimvall (2002) have proposed a more elaborate PMK test for such situations.

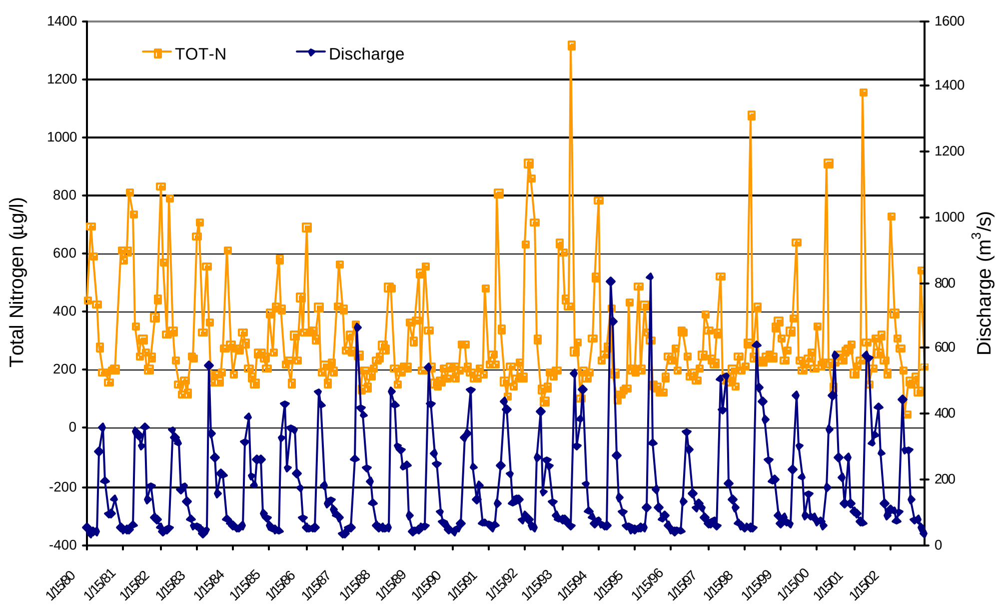

Figure 5. Measurements of total nitrogen concentrations and discharge in the Pite River from 1980 to 2002.

Table 6. Results provided by the three different trend test procedures

	SP-norm + MK	Reg-norm + MK	PMK	MK
Test-statistics	0.469	–0.997	–1.966	–1.725
p-value	0.639	0.319	0.049	0.085

Abbreviations: SP-norm, normalised using semi-parametric regression; Reg-norm, normalised by linear regression; MK, univariate Mann-Kendall test; PMK, partial Mann-Kendall test.

4.5. Large seasonal variation in point sources

The values in Figure 6 represent the sum of nitrite and nitrate concentrations and discharge in the Kalix River, and it is apparent that the seasonal variation is very strong in both series. As can be seen in Table 7, using linear regression for normalisation gives results that differ substantially from those provided by the other trend tests. The reason for this is that the regression model in question assumes a constant intercept throughout the year. However, to achieve a reasonable normalisation model for the current data set, not only the slope , but also the intercept, must change from month to month.

In many cases, the results of the linear regression and those obtained by the semi-parametric regression are very similar, which indicates that the changing intercept is often not essential. Nevertheless, there are also circumstances when the seasonal variation in both slope and intercept are important, for example if point sources vary over the year. The PMK test is not affected by this, because it is not possible to distinguish between point and diffuse sources with that method.

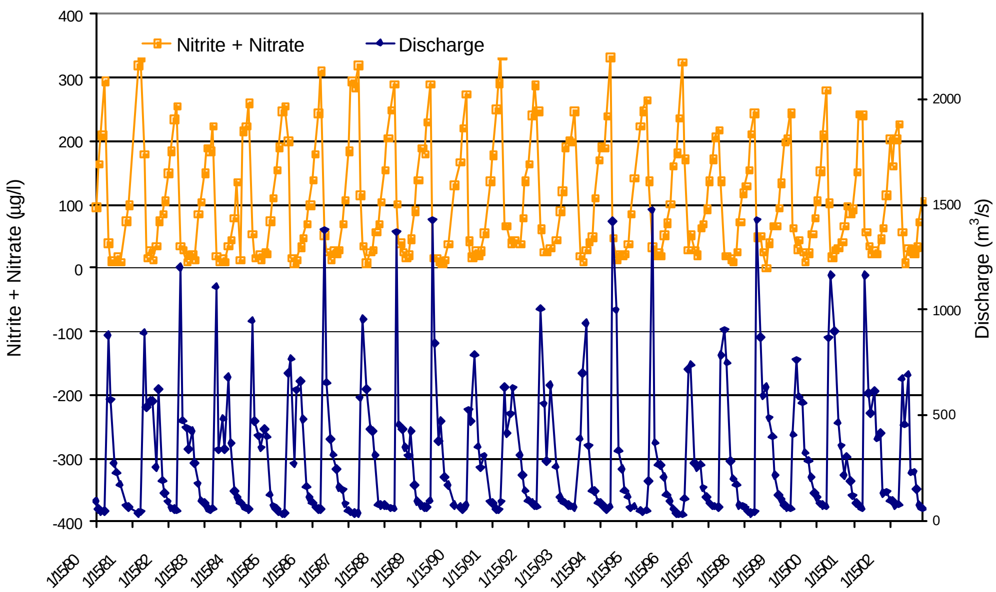

Figure 6. The sum of nitrite and nitrate concentrations and data on the water discharge in the Kalix River from 1980 to 2002.

Table 7. Results provided by the three different trend test procedures

	SP-norm + MK	Reg-norm + MK	PMK	MK
Test statistics	0.043	2.144	–0.058	0.108
p-value	0.986	0.032	0.954	0.914

Abbreviations: SP-norm, normalised using semi-parametric regression; Reg-norm, normalised by linear regression; MK, univariate Mann-Kendall test; PMK, partial Mann-Kendall test.

5. Discussion

Three trend tests that account for a covariate were applied to data on several different variables in a large number of rivers in Sweden. The differences between the results provided by the three procedures are in many cases small. However, the focus was on situations for which it is essential to choose the appropriate method. Accordingly, the time series analysed had at least one of the following characteristics: (i) the covariate had long memory effects on the response variable; (ii) the covariate itself exhibited a gradual long-term change, either a monotonic trend or a long-wave component; (iii) the seasonal variation was strong and the relationship between covariate and response changed over the year.

The PMK proved to be useful in most cases, especially since it could correct for time-delayed effects, which is not possible with the normalisation methods under consideration. However, the PMK test did not perform well when the concentration-runoff relationships varied strongly over seasons, because it estimates an average correlation, which is particularly undesirable if the relationship is positive for some months and negative for others. The two normalisation techniques used here often gave similar results, although in some situations the linear regression was impeded by the assumption of a constant intercept throughout the year.

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