Method for trend analysis

Trend analysis of time series of nutrient concentrations and runoff at river stations in catchments was undertaken using Kendall's seasonal trend test with correction for serial correlation. This test is robust non-parametric site-specific statistical tests for monotone trends. It is robust towards missing values, values reported as "< detection limit", seasonal effects, autocorrelated measurements and non-normality (i.e. non-Gaussian data). The test was introduced in the papers Hirsch et al. (1982) and Hirsch and Slack (1984) and has become a very popular and effective method for trend analysis of water quality data. The statistical trend method can analyse both seasonal and annual data and provide a trend statistic, *P*-value and an estimate of the annual increase or decrease in nutrient concentrations.

A trend analysis starts out with a time series plot (a graph showing observed concentrations versus time of observation) and a Box-Whisker plot (a graph showing the distribution of data for each calendar month). Such plots can give hints on possible trends, seasonality and extreme values.

Both total nitrogen and total phosphorus concentrations are highly depending on runoff. This substance-specific relationship can be modelled by the non-parametric and robust curve fitting method LOWESS (Locally Weighted Scatterplot Smoothing, Cleveland, 1979). The nutrient concentrations must be adjusted for runoff in order to minimise the impact from climate and to prevent a deterioration of the trend detection thereby increasing the power of the test. To remove the effects of runoff calculate residuals, i.e.

$$r = x - \hat{x}_{(LOWESS)},$$

where $\hat{x}_{(LOWESS)}$ is the estimated concentration from LOWESS and x is the observed concentration. A time series plot of the residuals will reveal if the trend is still present in the adjusted values (residuals).

The trend method only operates with one value for each combination of season and year. Therefore an average value for the seasons with more than one observation is used. Let r_{ij} denote the average value of all adjusted measurements in year *i* and season *j*. It is assumed that there have been measurement in *n* years and *p* seasons, i.e. $i = 1,2\ldots,n$ and $j = 1,2,\ldots,p$. In normal applications the number of seasons *p* per year was set to 12 one for each month of the year. Some of the r_{ij}'s can be missing if no measurement have been done in the relevant month and year.

The null hypothesis of the trend analysis is: for each of the *p* seasons the *n* data values are randomly ordered. The null hypothesis is tested against the alternative hypothesis: one or more of the seasons have a monotone trend. The trend test is done by calculating

$$S_g = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \operatorname{sgn}\left(r_{jg} - r_{ig}\right),$$

for $g = 1,2\ldots,p$, and where

$$\operatorname{sgn}(x) = \begin{cases} 1, & x > 0 \\ 0, & x = 0 \\ -1, & x < 0 \end{cases}.$$

If r_{jg} and/or r_{ig} is a missing value, then $\operatorname{sgn}(r_{jg} - r_{ig}) = 0$ per definition.

A combined test for all seasons (months) is done by first calculating

$$S = \sum_{g=1}^{p} S_g ,$$

and

$$\operatorname{var}(S) = \sum_{g=1}^{p} \operatorname{var}(S_g) + \sum_{g,h:g \neq h} \operatorname{cov}(S_g, S_h).$$

The variance for S_g under the null hypothesis can be calculated exactly by

$$\operatorname{var}(S_g) = \frac{n_g(n_g - 1)(2n_g + 5) - \sum_{j=1}^{m} t_j(t_j - 1)(2t_j + 5)}{18},$$

where n_g is the number of non-missing observations in season g. In the formula for the variance of S_g it is assumed that there are groups of observations with completely equal values, m groups in total and in the j'th group there is t_j equal values.

It is not possible under the null hypothesis to calculate the covariance between S_g and S_h exactly, but it can be estimated by (Hirsch and Slack, 1984)

$$\operatorname{cov}(S_g, S_h) = \frac{K_{gh} + 4\sum_{i=1}^{n} R_{ig} R_{ih} - n(n_g + 1)(n_h + 1)}{3},$$

where

$$K_{gh} = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \operatorname{sgn}[(r_{jg} - r_{ig})(r_{jh} - r_{ih})],$$

and

$$R_{ig} = \frac{n_g + 1 + \sum_{j=1}^{n} \operatorname{sgn}(r_{ig} - r_{jg})}{2}.$$

The term R_{ig} is the ranking of x_{ig} amongst all observations in season g, and all the missing values get the value $(n_g + 1)/2$ as ranking.

The test statistic for the aggregate test is

$$Z = \begin{cases} \dfrac{S-1}{(\mathrm{var}(S))^{\frac{1}{2}}}, & S > 0 \\ 0, & S = 0 \\ \dfrac{S+1}{(\mathrm{var}(S))^{\frac{1}{2}}}, & S < 0 \end{cases}.$$

The sign of Z indicates an increasing (+) or decreasing (-) trend. Both increasing and decreasing trends are interesting. The null hypothesis must be rejected if the numerical value of Z is greater than the $(\alpha/2)$ -percentile in the Gaussian distribution with mean 0 and variance 1. Here α stands for the significance level, which typically is 5%. At the 5%-level all Z-values numerically greater than 1.96 are significant. The reason for evaluating Z in a Gaussian distribution is that under the null hypothesis, S has a Gaussian distribution with mean 0 and variance $\mathrm{var}(S)$ for $n \to \infty$. The Gaussian approximation is good if $n \geq 10$ (Hirsch and Slack, 1984). This means 10 years of data with one concentration measurement for each month.

The trend in each season can be tested by calculating

$$Z_g = \begin{cases} \dfrac{S_g-1}{(\mathrm{var}(S_g))^{\frac{1}{2}}}, & S_g > 0 \\ 0, & S_g = 0 \\ \dfrac{S_g+1}{(\mathrm{var}(S_g))^{\frac{1}{2}}}, & S_g < 0 \end{cases}.$$

The null hypothesis of no trend is rejected if the numerical value of Z_g is greater than the $(\alpha/2)$ -percentile in the Gaussian distribution with mean 0 and variance 1.

It is possible to calculate an estimate for the trend (a slope estimate) if one assumes that the trend is constant (linear) during the period and the estimate is given as change per unit time (year). Hirsch et al. (1982) introduced Kendall's seasonal slope estimator, which can be computed in the following way. For all pair of residuals (r_{ij}, r_{kj}) with $j = 1,2\ldots, p$ and $1 \leq k < i \leq n$ calculate

$$d_{ijk} = \frac{r_{ij} - r_{kj}}{i-k}.$$

The slope estimator is then the median of all d_{ijk} -values and is robust, if the time series has serial correlation, seasonality and non-Gaussian data (Hirsch et al., 1982). A slope estimate for each season can be calculated in the same way.

A $100(1-\alpha)$ % confidence interval for the slope can be obtained by the following calculations

- Choose the wanted confidence level α (1, 5 or 10%) and use

$$Z_{1-\alpha/2} = \begin{cases} 2{,}576, & \alpha = 0{,}01 \\ 1{,}960, & \alpha = 0{,}05 \\ 1{,}645, & \alpha = 0{,}10 \end{cases}$$

in the following calculations. For a normal application we use a confidence level of 5%.

- Calculate

$$C_\alpha = Z_{1-\alpha/2} \cdot \left(\mathrm{var}(S)\right)^{\frac{1}{2}}.$$

- Calculate

$$M_1 = \frac{N - C_\alpha}{2},$$
$$M_2 = \frac{N + C_\alpha}{2},$$

where

$$N = \frac{1}{2}\sum_{g=1}^{p} n_g\left(n_g - 1\right).$$

- Lower and upper confidence limits are the M_1th largest and $\left(M_2 + 1\right)$'th largest value of the N ranked slope estimates d_{ijk}.

Using the modified Van Belle and Hughes test for homogeneity (1984) one can test the homogeneity of the separate season trend test. This homogeneity test must be non-significant in order to use the combined trend test.

Time series of daily runoff values also has to be tested for trends. The same trend test as described above can be used on the measured runoff values. Slope estimates and confidence intervals are computed following the methods described above. If no significant trends are detected in the runoff time series, any significant trend in the concentration time series is said to be anthropogenic in origin.

References

Cleveland, W.S. (1979): Robust locally weighted regression and smoothing scatterplots. *Journal of American Statistical Association*, 74, 829-836.

Hirsch, R. M. and Slack, J. R. (1984): A Nonparametric Trend Test for Seasonal Data with Serial Dependence. *Water Resources Research* **20**(6), 727-732.

Hirsch, R. M., Slack, J. R. and Smith, R. A. (1982): Techniques of Trend Analysis for Monthly Water Quality Data. *Water Resources Research* **18**(1), 107-121.

van Belle, G. and Hughes, J. P. (1984): Nonparametric Tests for Trend in Water Quality. *Water Resources Research* **20**(1), 127-136.