



Supplement of

Multivariate and long-term time series analysis to assess the effect of nitrogen management policy on groundwater quality in Wallonia, BE

Elise Verstraeten et al.

Correspondence to: Alice Alonso (alice.alonso@uclouvain.be)

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Text S1. Change point detection with linear interpolation method to compute slope indicators.

The method used for slope computation for the pollution indicators I4, I5 and I6 can influence the trend diagnostics.

- I4 – Slope in 2002 (mg/l/year) : Rate of change in nitrate concentration on 01-01-2002. Provides insight into how rapidly nitrate levels were changing at the beginning of the period.
- I5 – Slope in 2020 (mg/l/year): Rate of change in nitrate concentration on 01-01-2020. Useful for understanding recent dynamics and informing current policy decisions.
- I6 - Difference in slope between 2020 and 2002 ($I6 = I5 - I4$) (mg/l/year) : Indicates how the rate of change in nitrate concentration has changed over the study period. A positive value indicates an accelerating increase (or decelerating decrease) in nitrate levels, while a negative value suggests a decelerating increase (or accelerating decrease).

We used two different approaches: (i) local regression and (ii) change point detection with linear interpolation. Since the slope indicators calculated using both approaches were similar, the methodology and results of the local regression approach are presented in the main paper, and the indicators calculated using the method are used later on in the paper. The methodology and results of the change point detection with linear interpolation approach are presented here, in the supplementary materials.

For the change point detection with linear interpolation approach, we determined I4 and I5 as the slopes in 2002 and 2020 of the segments between the change points of the time series. The segments' slopes were calculated using the Theil slope estimator, robust to outliers (Helsel & Hirsch, 2002). The change points were determined by fitting a continuous spline function to the time series, computed using the optimal search algorithm implemented by the Python 'ruptures' package (Truong et al., 2020). We employed an iterative approach to determine the optimal number of change points, increasing from 0 to the maximum feasible while ensuring a minimum five-year interval between the change points. The selection of the optimal number of change points was based on the Bayesian information criterion (BIC, Schwarz, 1978).

For the nine monitoring points whose first measurements were taken after 2002, the slope of the trend in 2002 (I4) was taken as the slope at the first data point, and the mean absolute nitrate concentration in 2002 (I1) was obtained by hindcasting that trend.

References

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- Truong, C., Oudre, L., and Vayatis, N.: Selective review of offline change point detection methods, *Signal Processing*, 167, 107299, <https://doi.org/10.1016/j.sigpro.2019.107299>, 2020.

Figure S1. Illustration of the two alternative methods, the local regression (Lo) and change point detection (CP) methods, used to model the time series and identify the trends in 2002 (I4 indicators) and in 2020 (I5 indicators). Data from one of the monitoring stations of our dataset is used for illustrative purposes.

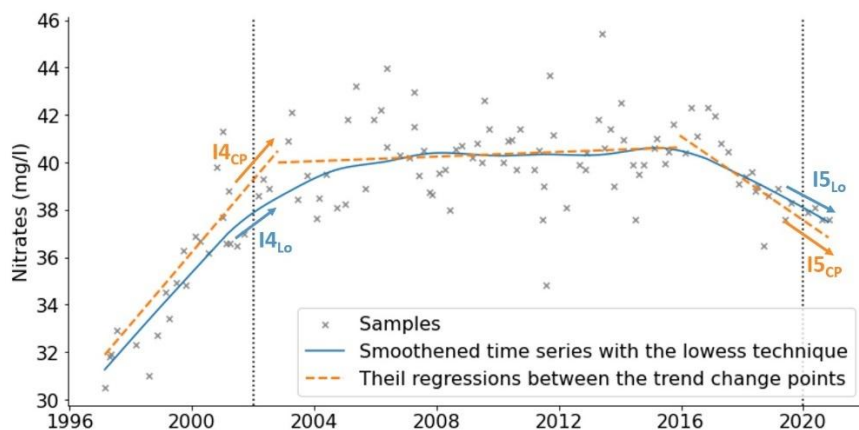


Table S1. Descriptive statistics of slope indicators (I3, I4 and I5) calculated using both computation methods. CP: change point detection method. Lo: local regression method.

Pollution indicator (I)	Unit	Method	Mean \pm standard deviation	Minimum	Percentile 25 (Q1)	Median (Q2)	Percentile 75 (Q3)	Maximum	IQR (Q3-Q1)
I4 – Slope in 2002	mg L ⁻¹ yr ⁻¹	CP	0.0 \pm 1.1	-2.6	-0.4	0.1	0.6	2.2	0.9
		Lo	-0.1 \pm 1.1	-3.1	-0.5	0.1	0.5	2.7	1.1
I5 – Slope in 2020	mg L ⁻¹ yr ⁻¹	CP	-0.5 \pm 1.0	-3.9	-0.9	-0.2	0.2	0.6	1.1
		Lo	-0.5 \pm 1.1	-5.2	-0.7	-0.2	0.1	0.6	0.8
I6 – Slope difference	mg L ⁻¹ yr ⁻¹	CP	-0.5 \pm 1.2	-3.6	-1.1	-0.6	0.0	2.4	1.1
		Lo	-0.4 \pm 1.2	-3.6	-0.8	-0.4	-0.0	2.7	0.7