



## A spatio-temporal statespace model for river network data

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- 1 Introduction
- 2 Methods
- 3 Case Study: Nitrate concentration in the river Yzer
- 4 Conclusions

# Introduction

- Important legislation concerning water quality (WQ):  
Water Framework Directive (WFD)
- Major goal: maintain and improve the aquatic environment
- In Flanders: VMM → develop basin management plans
- Detect impact of previous actions. Assess improvement/trend in WQ

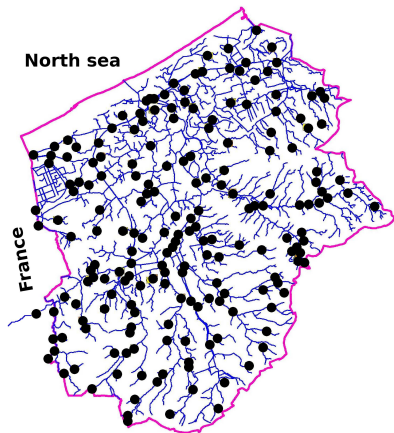
# The Yzer Catchment



## 1 Yzer

- ① length 76 km, 44 km in Belgium
- ② area 1101 km<sup>2</sup>
- ③ mouth Nieuwpoort: complex of sluices.
- ④ Eutrophication due to nutrient pollution: high nitrate

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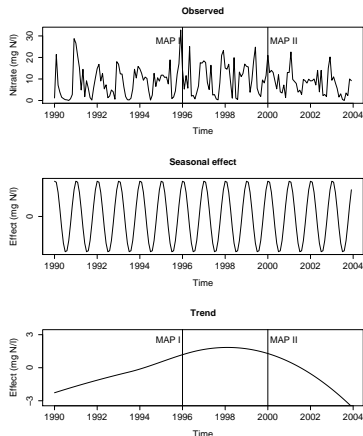
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- 3 1996: MAP I  
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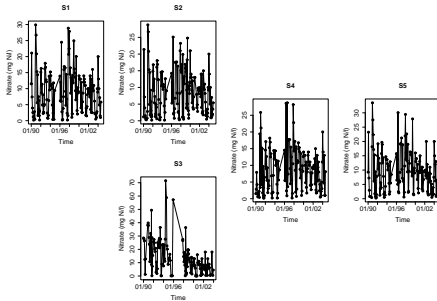
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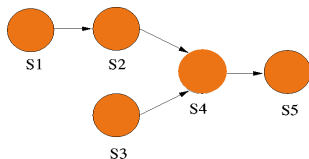
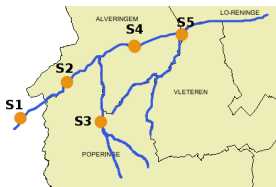
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## Methods: Spatio-Temporal model

- 1 Spatial dependence structure
- 2 Spatio-temporal dependence structure
- 3 Observation model

## Spatial dependence structure (SDP)



$$\mathbf{S} = \mathbf{A}\mathbf{S} + \boldsymbol{\gamma}$$

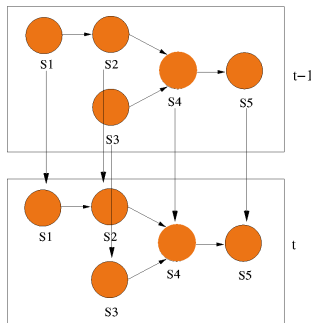
- River networks:
  - The water flows in 1 direction  
→ Causal interpretation of correlations
  - Unidirectional correlation structure
- Isolated river: Directed Acyclic Graph  
→ conditional independence

$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ \rho_{12} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & \rho_{24} & \rho_{34} & 0 & 0 \\ 0 & 0 & 0 & \rho_{45} & 0 \end{bmatrix}$$

- $\boldsymbol{\gamma} \sim MVN(\mathbf{0}, \boldsymbol{\Sigma}_{\boldsymbol{\gamma}})$ ,  $\boldsymbol{\Sigma}_{\boldsymbol{\gamma}}$  diag

## Spatio-temporal dependence structure

$$\mathbf{S}_t = \mathbf{A}\mathbf{S}_t + \mathbf{B}\mathbf{S}_{t-1} + \boldsymbol{\eta}_t$$

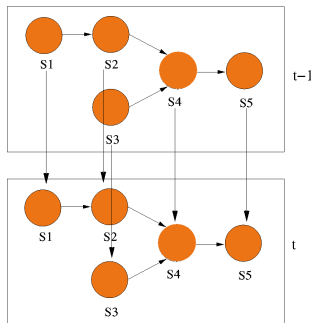


- Unidirectional dependence in time
- Assumption: observation at  $t$  only depends on observation at  $t - 1 \rightarrow$  AR(1) process
- **B** Diagonal matrix with AR coef (only monthly observations)
- $\boldsymbol{\eta}_t \sim MVN(\mathbf{0}, \boldsymbol{\Sigma}_\eta)$  ( $\boldsymbol{\Sigma}_\eta$  diag)

## Spatio-temporal dependence structure

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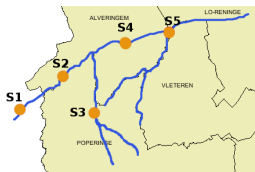
$$\mathbf{S}_t = \boldsymbol{\Phi}\mathbf{S}_{t-1} + \boldsymbol{\delta}_t$$



- Unidirectional dependence in time
- Assumption: observation at  $t$  only depends on observation at  $t - 1 \rightarrow$  AR(1) process
- $\mathbf{B}$  Diagonal matrix with AR coef (only monthly observations)
- $\boldsymbol{\eta}_t \sim MVN(\mathbf{0}, \boldsymbol{\Sigma}_\eta)$  ( $\boldsymbol{\Sigma}_\eta$  diag)
- $\boldsymbol{\Phi} = (\mathbf{I} - \mathbf{A})^{-1} \mathbf{B}$
- $\boldsymbol{\delta}_t \sim MVN(\mathbf{0}, \mathbf{Q})$ ,  
 $\mathbf{Q} = (\mathbf{I} - \mathbf{A})^{-1} \boldsymbol{\Sigma}_\eta (\mathbf{I} - \mathbf{A})^{-T}$

## Observation Model

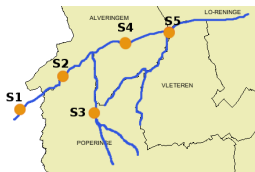
$$\begin{cases} \mathbf{S}_t = \Phi \mathbf{S}_{t-1} + \delta_t \\ \mathbf{Y}_t = \mathbf{S}_t + \epsilon_t \end{cases}$$



- Model of  $\mathbf{S}$  only holds for isolated river model
- Reality: disturbance  
→ put  $\mathbf{S}$  in observation model
- Error term:  $\epsilon_t \sim MVN(\mathbf{0}, \Sigma_\epsilon)$   
→ spatial correlation due to disturbances
- Up to now only covariance structure modelled

## Observation Model

$$\begin{cases} \mathbf{S}_t = \Phi \mathbf{S}_{t-1} + \delta_t \\ \mathbf{Y}_t = \mathbf{X}_t \beta + \mathbf{S}_t + \epsilon_t \end{cases}$$



- Model of  $\mathbf{S}$  only holds for isolated river model
- Reality: disturbance  
→ put  $\mathbf{S}$  in observation model
- Error term:  $\epsilon_t \sim MVN(\mathbf{0}, \Sigma_\epsilon)$   
→ spatial correlation due to disturbances
- Up to now only covariance structure modelled
- Mean model:  
 $E\{\mathbf{Y}_t\} = \mathbf{X}_t \beta$

# Parameter Estimation

- Kalman Filter and Kalman Smoother
- ECM algorithm
  - E step: Calculate expected log likelihood of State Space model
  - CM step1: Parameters dependence structure
  - CM step 2: Parameters of the mean model



# Kalman Filter

State Space model: likelihood can be factorized using the Kalman Filter

$$\begin{aligned}
 E[S_t | t-1] &= \mathbf{a}_{t|t-1} = \Phi \mathbf{a}_{t-1} \\
 E[(\mathbf{S}_t - \mathbf{a}_{t|t-1})(\mathbf{S}_t - \mathbf{a}_{t|t-1})^T] &= \mathbf{P}_{t|t-1} = \Phi \mathbf{P}_{t-1} \Phi^T + \mathbf{Q} \\
 E[S_t] &= \mathbf{a}_t = \mathbf{a}_{t|t-1} + \mathbf{P}_{t|t-1} \mathbf{F}_t^{-1} \mathbf{v}_t \\
 E[(\mathbf{S}_t - \mathbf{a}_t)(\mathbf{S}_t - \mathbf{a}_t)^T] &= \mathbf{P}_t = \mathbf{P}_{t|t-1} - \mathbf{P}_{t|t-1} \mathbf{F}_t^{-1} \mathbf{P}_{t|t-1} \\
 E[\mathbf{v}_t \mathbf{v}_t^T] &= \mathbf{F}_t = \mathbf{P}_{t|t-1} + \Sigma_\epsilon
 \end{aligned}$$

with innovation  $\mathbf{v}_t = (\mathbf{Y}_t - \mathbf{a}_{t|t-1} - \mathbf{X}_t \beta)$

$$\log L_{\mathbf{Y}} = \sum_{t=1}^N \log L_{\mathbf{y}_t | \mathbf{y}_{t-1}} \sim -\frac{1}{2} \sum_{t=1}^N \log |\mathbf{F}_t| - \frac{1}{2} \sum_{t=1}^N \mathbf{v}_t^T \mathbf{F}_t^{-1} \mathbf{v}_t$$

## Kalman Smoother

- Smoothed estimates  $\mathbf{a}_{t|N}$  for  $\mathbf{S}_t$  conditionally on all  $N$   
For  $t = N - 1, \dots, 0$

$$\mathbf{a}_{t|N} = \mathbf{a}_t + \mathbf{P}_t^*(\mathbf{a}_{t+1|N} - \mathbf{a}_{t+1|t})$$

$$\mathbf{P}_{t|N} = \mathbf{P}_t + \mathbf{P}_t^*(\mathbf{P}_{t+1|N} - \mathbf{P}_{t+1|t})\mathbf{P}_t^{*T}$$

$$\mathbf{P}_t^* = \mathbf{P}_t\Phi^T\mathbf{P}_{t+1|t}^{-1}$$

- Lag-one covariance smoothers (Digalakis, Rohlick and Osendorf 1993)  
⇒ Forward recursion:

$$\mathbf{P}_{t,t-1|t} = (\mathbf{I} - \mathbf{P}_{t|t-1}\mathbf{F}_t^{-1})\Phi\mathbf{P}_{t-1}$$

- ⇒ Backward recursion:

$$\mathbf{P}_{t,t-1|N} = \mathbf{P}_{t,t-1|t} + (\mathbf{P}_{t|N} - \mathbf{P}_t)\mathbf{P}_t^{-1}\mathbf{P}_{t,t-1|t}$$

## Using the Kalman filter for GLS

- Apply same Kalman filter to  $\mathbf{Y}_t$  and each of the columns of  $\mathbf{X}_t$
- ⇒ A  $p \times 1$  vector of innovations,  $\mathbf{Y}_t^*$  on  $\mathbf{Y}_t$  and
- ⇒ a  $p \times m$  matrix of innovations,  $\mathbf{X}_t^*$  on  $(\mathbf{X}_{1t}, \dots, \mathbf{X}_{mt})$  are produced.
- ⇒ Run recursions for  $\mathbf{P}_{t|t-1}$ ,  $\mathbf{P}_{t|t}$  and  $\mathbf{F}_t$  only once rather than  $m + 1$  times.
- GLS estimator of  $\beta$  becomes

$$\hat{\beta}_{\text{GLS}} = \left[ \sum_{t=1}^N \mathbf{X}_t^{*T} \mathbf{F}_t^{-1} \mathbf{X}_t^* \right]^{-1} \sum_{t=1}^N \mathbf{X}_t^{*T} \mathbf{F}_t^{-1} \mathbf{y}_t^*. \quad (1)$$

- $\mathbf{v}_t$  become  $\mathbf{v}_t = \mathbf{y}_t^* - \mathbf{x}_t^* \hat{\beta}_{\text{GLS}}$ .
- Maximisation possible by classical numerical algorithms
- Here ECM algorithm

## Existing EM algorithms

- ①  $l_c(\Psi) = \log L_{Y_N, S_N}(\Psi)$  the joint log-likelihood of  $\mathbf{Y}_N$  and  $\mathbf{S}_N$ .
- ② Problem: unobservable state process  $\mathbf{S}$
- ③ Use an EM algorithm (e.g. Shumway and Stoffer 1982)
- ④ RMN topology: restrictions on parametrisation
- ⇒  $\mathbf{Q}$  and  $\Phi$  have some parameters in common
- ⇒ Adapt existing EM algorithm for SS models
- ⑤ Presence of the exogenous variables ⇒ use ECM algorithm.
- ⇒ Split M-step in two CM-steps.
- ⇒ CM step 1: Update the parameters of the dependence structure  $\Psi_\alpha$  given the current values of the mean model  $\beta$ .
- ⇒ CM step 2: estimate of  $\beta$  using the updated values of  $\Psi_\alpha$ .

## ECM algorithm

- 1 Choose initial estimates:  $\Psi^0$
- 2 **E-step**: Calculate  $Q(\Psi, \Psi_\alpha^k, \beta^k) = E \{l_c(\Psi) | \mathbf{Y}_N, \Psi^k\}$
- 3 **CM-step 1**: Find the covariance parameters  $\Psi_\alpha^{k+1}$  that maximise  $Q(\Psi, \Psi_\alpha^k, \beta^k)$
- 4 **CM-step 2**: Find  $\beta^{k+1}$  that maximises  $Q(\Psi, \Psi_\alpha^{k+1}, \beta^k)$
- 5 Repeat steps 2-4 until convergence

## E-step

$$\begin{aligned}
Q(\Psi, \Psi^k) &\sim -\frac{1}{2} E \left\{ \log |\Sigma_{S_0}| + \mathbf{S}_0^T \Sigma_{S_0}^{-1} \mathbf{S}_0 | \mathbf{Y}, \Psi^k, \beta^k \right\} \\
&- \frac{1}{2} E \left\{ N \log |\Sigma_\eta| + \sum_{t=1}^N (\mathbf{S}_t - \mathbf{A}\mathbf{S}_t - \mathbf{B}\mathbf{S}_{t-1})^T \Sigma_\eta^{-1} (\mathbf{S}_t - \mathbf{A}\mathbf{S}_t - \mathbf{B}\mathbf{S}_{t-1}) | \dots \right\} \\
&- \frac{1}{2} E \left\{ N \log |\Sigma_\epsilon| + \sum_{t=1}^N (\mathbf{Y}_t - \mathbf{X}\beta - \mathbf{S}_t)^T \Sigma_\epsilon^{-1} (\mathbf{Y}_t - \mathbf{X}\beta - \mathbf{S}_t) | \dots \right\}.
\end{aligned}$$

Exponential family  $\Rightarrow$  sufficient statistics  $|\mathbf{Y}$

$$E[\mathbf{S}_t | \mathbf{Y}] = \mathbf{a}_{t|N}$$

$$E[\mathbf{S}_t \mathbf{S}_t^T | \mathbf{Y}] = \mathbf{P}_{t|N} + \mathbf{a}_{t|N} \mathbf{a}_{t|N}^T$$

$$E[\mathbf{S}_t \mathbf{S}_{t-1}^T | \mathbf{Y}] = \mathbf{P}_{t,t-1|N} + \mathbf{a}_{t|N} \mathbf{a}_{t-1|N}^T.$$

Maximise the obtained expected likelihood in the CM steps

# CM-step 1: Update parameters of dependence structure given $\beta^k$

$$\begin{aligned}
 Q(\Psi, \Psi^k) &\sim -\frac{1}{2} \mathbb{E} \left\{ \log |\Sigma_{S_0}| + \mathbf{S}_0^T \Sigma_{S_0}^{-1} \mathbf{S}_0 | \mathbf{Y}, \Psi^k, \beta^k \right\} \\
 &- \frac{1}{2} \mathbb{E} \left\{ N \log |\Sigma_\eta| + \sum_{t=1}^N (\mathbf{S}_t - \mathbf{A}\mathbf{S}_t - \mathbf{B}\mathbf{S}_{t-1})^T \Sigma_\eta^{-1} (\mathbf{S}_t - \mathbf{A}\mathbf{S}_t - \mathbf{B}\mathbf{S}_{t-1}) | \dots \right\} \\
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 \end{aligned}$$

$$\hat{\Sigma}_{S_0} = \mathbf{P}_{0|N}$$

Replace all sufficient statistics by their conditional expectations

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 &- \frac{1}{2} E \left\{ N \log |\Sigma_\epsilon| + \sum_{t=1}^N (\mathbf{Y}_t - \mathbf{X}_t \beta - \mathbf{S}_t)^T \Sigma_\epsilon^{-1} (\mathbf{Y}_t - \mathbf{X}_t \beta - \mathbf{S}_t) | \dots \right\}.
 \end{aligned}$$

$$E \{ \log L_S(\Psi) | \dots \} \sim -\frac{1}{2} \sum_{i=1}^p E \left\{ N \log \Delta \sigma_{\eta_i} + \frac{1}{\sigma_{\eta_i}^2} \sum_{t=1}^N (S_t^i - \mathbf{A}^{[i]} S_t^{[i]} - \mathbf{B}^i S_{t-1}^i)^2 | \dots \right\}$$



# CM-step 1: Update parameters of dependence structure given $\beta^k$

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 \end{aligned}$$

$$\left\{ \begin{aligned}
 B_i^{k+1} &= \frac{\sum_{t=1}^N s_t^i s_{t-1}^i - \left( \sum_{t=1}^N s_t^i s_t^{[j]T} \right) \left( \sum_{t=1}^N s_t^{[j]} s_t^{[j]T} \right)^{-1} \left( \sum_{t=1}^N s_{t-1}^i s_t^{[j]} \right)}{\sum_{t=1}^N s_{t-1}^i{}^2 - \left( \sum_{t=1}^N s_{t-1}^i s_{t-1}^{[j]T} \right) \left( \sum_{t=1}^N s_{t-1}^{[j]} s_{t-1}^{[j]T} \right)^{-1} \left( \sum_{t=1}^N s_{t-1}^i s_{t-1}^{[j]} \right)} \\
 \mathbf{A}_i^{k+1} &= \sum_{t=1}^N \left[ \left( s_t^i - B_i^{k+1} s_{t-1}^i \right) s_t^{[j]T} \right] \left( \sum_{t=1}^N s_t^{[j]} s_t^{[j]T} \right)^{-1} \\
 \sigma_{\eta_i}^{2, k+1} &= \frac{\text{RSS}_i^{k+1}}{N}
 \end{aligned} \right.$$

Replace all sufficient statistics by their conditional expectations

## CM-step 1: Update parameters of dependence structure given $\beta^k$

$$\begin{aligned}
 Q(\boldsymbol{\Psi}, \boldsymbol{\Psi}^k) &\sim -\frac{1}{2} \mathbb{E} \left\{ \log |\Sigma_{S_0}| + \mathbf{S}_0^T \Sigma_{S_0}^{-1} \mathbf{S}_0 \mid \mathbf{Y}, \boldsymbol{\Psi}^k, \beta^k \right\} \\
 &- \frac{1}{2} \mathbb{E} \left\{ N \log |\Sigma_\eta| + \sum_{t=1}^N (\mathbf{S}_t - \mathbf{A}\mathbf{S}_t - \mathbf{B}\mathbf{S}_{t-1})^T \Sigma_\eta^{-1} (\mathbf{S}_t - \mathbf{A}\mathbf{S}_t - \mathbf{B}\mathbf{S}_{t-1}) \mid \dots \right\} \\
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 \end{aligned}$$

$$\Sigma_\epsilon^{k+1} = \frac{\sum_{t=1}^N (\mathbf{Y}'_t \mathbf{Y}'_t{}^T) - \sum_{t=1}^N (\mathbf{Y}'_t \mathbf{S}_t^T) - \sum_{t=1}^N (\mathbf{S}_t \mathbf{Y}'_t{}^T) + \sum_{t=1}^N (\mathbf{S}_t \mathbf{S}_t^T)}{N}$$

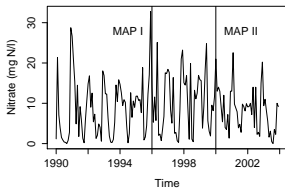
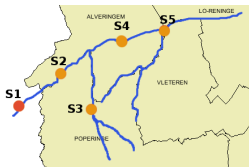
$$\text{with } \mathbf{Y}'_t = \mathbf{Y}_t - \mathbf{X}_t \beta^k$$

Replace all sufficient statistics by their conditional expectations

## CM-step 2: Update $\beta^k$ given $\Psi_{\alpha}^{k+1}$

- $\beta_{k+1}$ : FGLS using Kalman Filter with  $\Psi_{\alpha}^{k+1}$ .
- Kalman filter is already available for next E step.

## Case Study

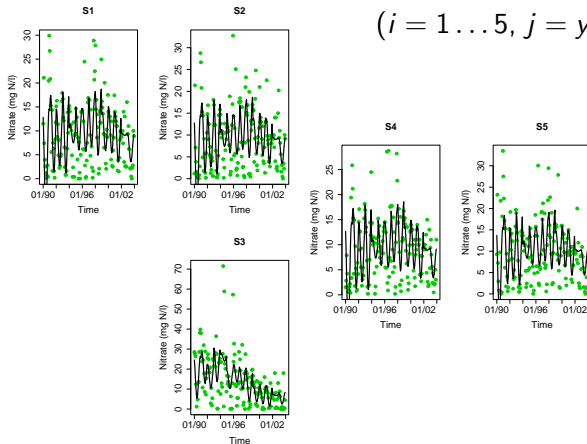


- Has the water quality improved?
- Mean model:  $ST + \text{annual effect}$
- Is mean of 2003 different from
  - ① the general mean
  - ② the mean of 2001-2002

Model for average  $\text{NO}_3^-$  at  $S_i$  on time  $t$

$$E\{y_{i,t}\} = \mu + \alpha_i + \beta_j + (\kappa)_j l(i) + \gamma_1 \sin(2\pi t/12) \\ + \gamma_2 \cos(2\pi t/12) + (\lambda)_{j,1} \sin(2\pi t/12) + (\lambda)_{j,2} \cos(2\pi t/12)$$

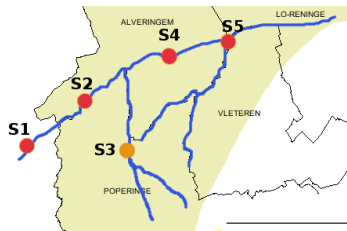
$(i = 1 \dots 5, j = \text{year}_1, \dots, \text{year}_{14})$



## Statistical tests

- $\hat{\beta}(\Psi_\alpha) \xrightarrow{d} MVN(\beta, (\mathbf{X}^T \Sigma_{Y_N}^{-1} \mathbf{X})^{-1})$
- $\hat{\Sigma}_\beta = (\mathbf{X}^T \Sigma_{Y_N}^{-1} (\hat{\Psi}_\alpha) \mathbf{X})^{-1}$ .
- A general linear hypothesis to compare the means:  
 $\mathbf{H}\beta = \mathbf{0}$ , where  $\mathbf{H}$  is the  $r \times q$  hypothesis matrix.
- Test:  $T = (\mathbf{H}\hat{\beta})^T (\mathbf{H}\hat{\Sigma}_\beta \mathbf{H}^T)^{-1} (\mathbf{H}\hat{\beta})$

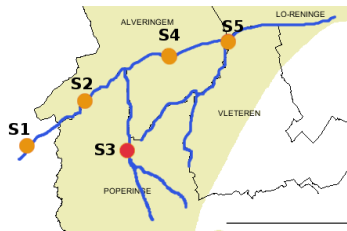
## Statistical tests



- $H_0$ : Mean 2003 equal to Mean 2001-2002
- $H_1$ : Mean 2003 different from Mean 2001-2002

Test	contrast	p-value
	Main river ("Regional")	
2003 ↔ 2001-2002	-2.54	0.016
2003 ↔ general mean	-2.88	0.0005
	Joining creek (S3)	
2003 ↔ 2001-2002	-1.32	0.56
2003 ↔ general mean	-8.40	< 0.0001

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## References

- 1 Clement, L. and Thas, O. (2007). Estimating and modelling spatio-temporal correlation structures for river monitoring networks. *Journal of Agricultural, Biological, and Environmental Statistics*, 12(2), 161-176.
- 2 Clement, L., Thas, O., Vanrolleghem, P.A. and Ottoy, J.P. (2006). Spatio-temporal statistical models for river monitoring networks. *Water, Science and Technology*, 53, 9-15.