

# Going with the flow Regression models for river networks

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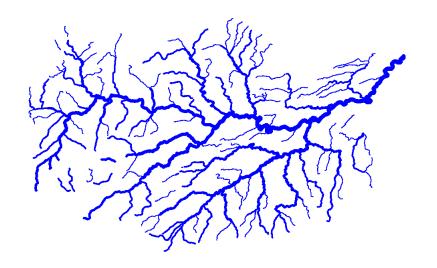


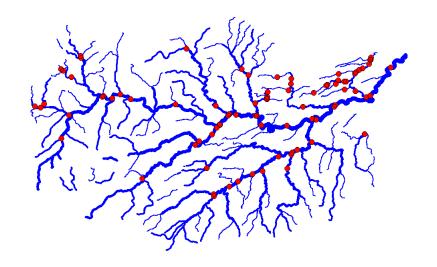


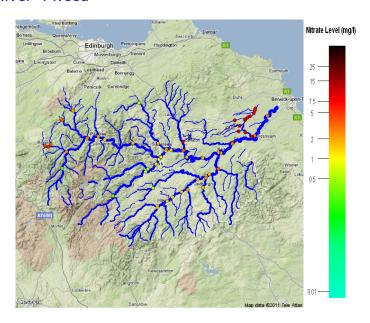
David O'Donnell, Marian Scott, Mark Hallard











# Flow connected



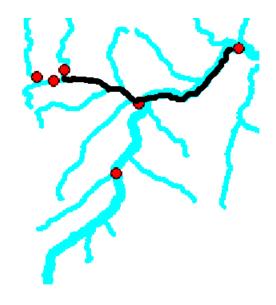
# Not flow connected



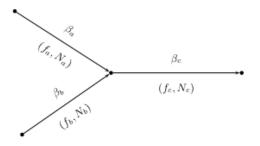
# River distance



# River distance



# Confluences



#### The ver Hoef model

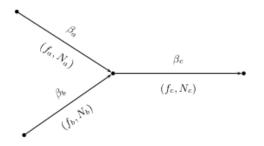
#### Covariance function

$$C(s_i,t_j) = \left\{ egin{array}{ll} 0 & ext{if $s$ and $t$ are not flow connected;} \ c_0+c_1 & ext{if $s=t$;} \ w \ c_1 \exp\left(-rac{d_{s,t}}{c_2}
ight) & ext{otherwise.} \end{array} 
ight.$$

#### where

- $ightharpoonup d_{s,t}$  denotes the river distance between stations s and t;
- $ightharpoonup c_0$ ,  $c_1$ ,  $c_2$  denote the nugget, partial sill and range parameters;
- $\triangleright w = \prod_{k \in B_{s,t}} \sqrt{\omega_k}$
- ▶  $B_{s,t}$  denotes the set of all water stretches between s and t;
- $\blacktriangleright$   $\omega_k$  denotes the proportion of flow contributed by water stretch k to its subsequent confluence.

#### Confluences



The  $\sqrt{\omega}$  ensures that the variance in all water stretches is constant.

$$\operatorname{var}\{\sqrt{\omega_a}N_a + \sqrt{\omega_b}N_b\} = (\omega_a + \omega_b)\sigma^2 = \sigma^2,$$

where  $\sigma^2$  denotes the variance of each measurement.

# Flexible regression - weight functions

Data  $\{(y_i, x_i), i = 1, ..., n\}$  can be modelled by a flexible regression

$$y_i = m(x_i) + \varepsilon_i,$$

where m denotes a smooth function and the  $\varepsilon_i$  denote error terms.

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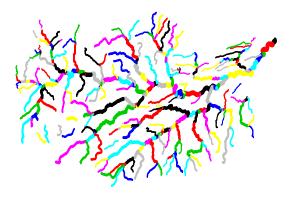
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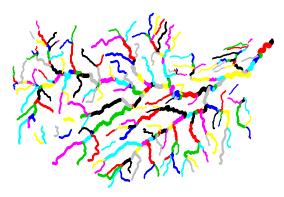
To adapt to a river network, we can use river distance and also incorporate the flow weights  $w=\prod_{k\in B_{s,t}}\sqrt{\omega_k}$  into the weighting scheme.

### Stream segments



An alternative approach to the estimation of smooth functions is to consider the network as a collection of small stream segments.

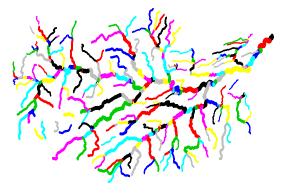
# Stream segments



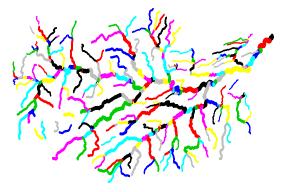
An alternative approach to the estimation of smooth functions is to consider the network as a collection of small stream segments.

An estimator is then available as

 $\hat{m}(x) = \beta_j$ , where x lies in stream segment j

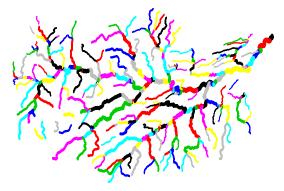


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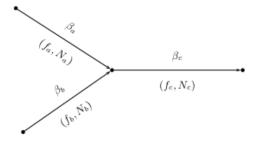
Smoothness is induced by use of a penalty, making this a *p-spline*.



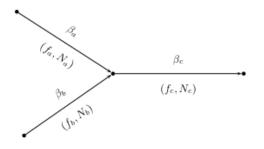
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The 'smoothness' of  $\beta$ -values corresponding to adjacent stream units j and k, with no intervening confluence, can be measured by  $(\beta_i - \beta_k)^2$ .



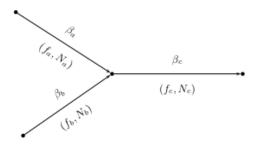
Where a confluence point is involved, the measure of smoothness needs to reflect the relative levels of flow in the contributing streams *a* and *b*.



The relative flows of the inputs are  $\omega_a = f_a/f_c$  and  $\omega_b = f_b/f_c$ .

The combined pollution input  $\omega_a\beta_a + \omega_b\beta_b$  and output  $\beta_c$  are identical, following the principle of mass balance, if

$$\omega_a(\beta_a - \beta_c) + \omega_b(\beta_b - \beta_c) = 0.$$

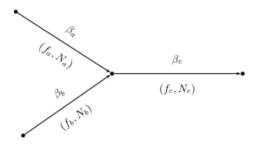


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Smoothness across the confluence can therefore be achieved through the penalty

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This has the attractive form of combining penalties for smoothness across each flow path of the confluence, with weights determined by the relative volumes.

▶ A p-spline model can be formulated as a regression model

$$y = B\beta + \varepsilon$$
,

where the matrix B is simply an indicator matrix whose rows identify the stream unit containing  $y_i$ .

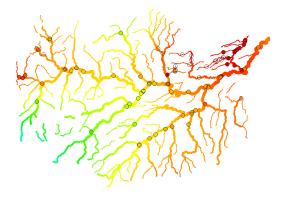
► The model is fitted by minimising the penalised sum-of-squares

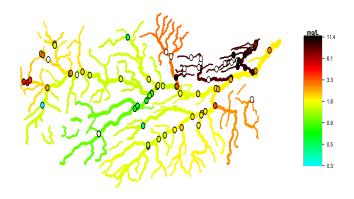
$$(y - B\beta)^T (y - B\beta) + \lambda \beta^T D^T D\beta$$

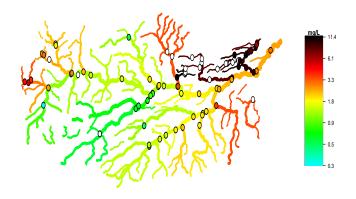
with respect to  $\beta$ . The matrix D generates the penalty.

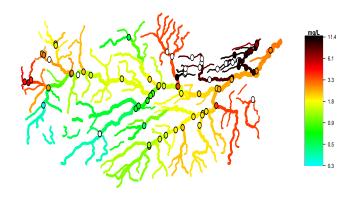
- ightharpoonup The penalty parameter  $\lambda$  controls the degree of smoothing.
- ► The solution to this least squares problem is easily shown to be  $\hat{\beta} = (B^T B + \lambda D^T D)^{-1} B^T y$ .
- The linear form of this expression allows an approximate degrees of freedom to be computed as the trace of the 'hat' matrix.

#### Estimated Euclidean Distance Smooth









In order to incorporate time  $t_i$  and day of the year  $z_i$ ,

$$y_i = \mu + m_s(s_i) + m_t(t_i) + m_z(z_i) + \varepsilon_i$$
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where the three functions  $m_s$ ,  $m_t$ ,  $m_z$  describe spatial, temporal and seasonal trends..

▶ If each each of the trend functions is estimated by b-splines then they can be represented as  $B_s\beta_s$ ,  $B_t\beta_t$ ,  $B_z\beta_z$  where the columns of the design matrices evaluate each basis function at the observed values of the relevant covariate.

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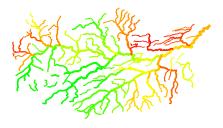
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- In the presence of an overall mean parameter  $\mu$ , identifiability can be achieved simply be requiring the parameter vector for each term to sum to 0.

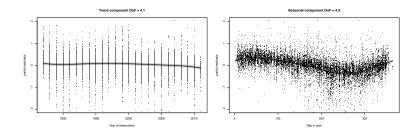
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- ▶ In the presence of an overall mean parameter  $\mu$ , identifiability can be achieved simply be requiring the parameter vector for each term to sum to 0.
- ▶ The full model can be represented as  $y = B\beta + \varepsilon$ , where B combines the columns of the individual design matrices.

#### Spatial component DoF = 55.7





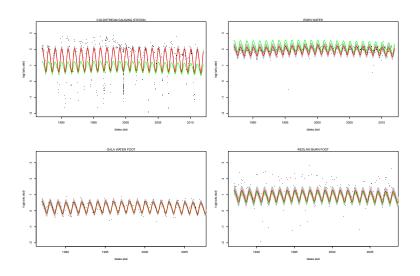
#### Interaction terms

An interaction model has the form

$$y_i = \mu + m_s(s_i) + m_t(t_i) + m_z(z_i) + m_{s,t}(s_i, t_i) + m_{s,z}(s_i, z_i) + \varepsilon_i,$$

where the functions  $m_{s,t}$  and  $m_{s,z}$  encapsulate the adjustments required to capture the changes in time trend and seasonal effects over the river network.

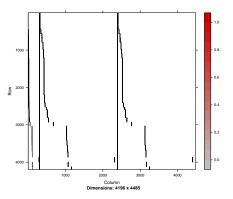
The model can be fitted by exactly the same mechanism described above.



Video

#### Computational issues

Calculations require the tensor product of an  $n \times p$  matrix with n 1's, the rest 0's, which renders all model objects very sparse.



- ► The matrix **X** pictured above is 99.57% sparse.
- ▶ Using the R Matrix package of Bates and Mächler, X takes up only 1Mb of RAM and X<sup>T</sup>X takes 0.03s to calculate (compared to 150Mb and 66s uncompressed).
- ▶ Using a Cholesky factorisation further reduces calculation

#### Further research

- Seasonal-temporal interactions
- Residual autocorrelation
- Use of land-use covariate data
- Flow data (currently modelled values assumed constant)
- Bayesian heirarchical formulation avoids smoothing parameter selection