Smoothing through State-Space Models for Stream Networks

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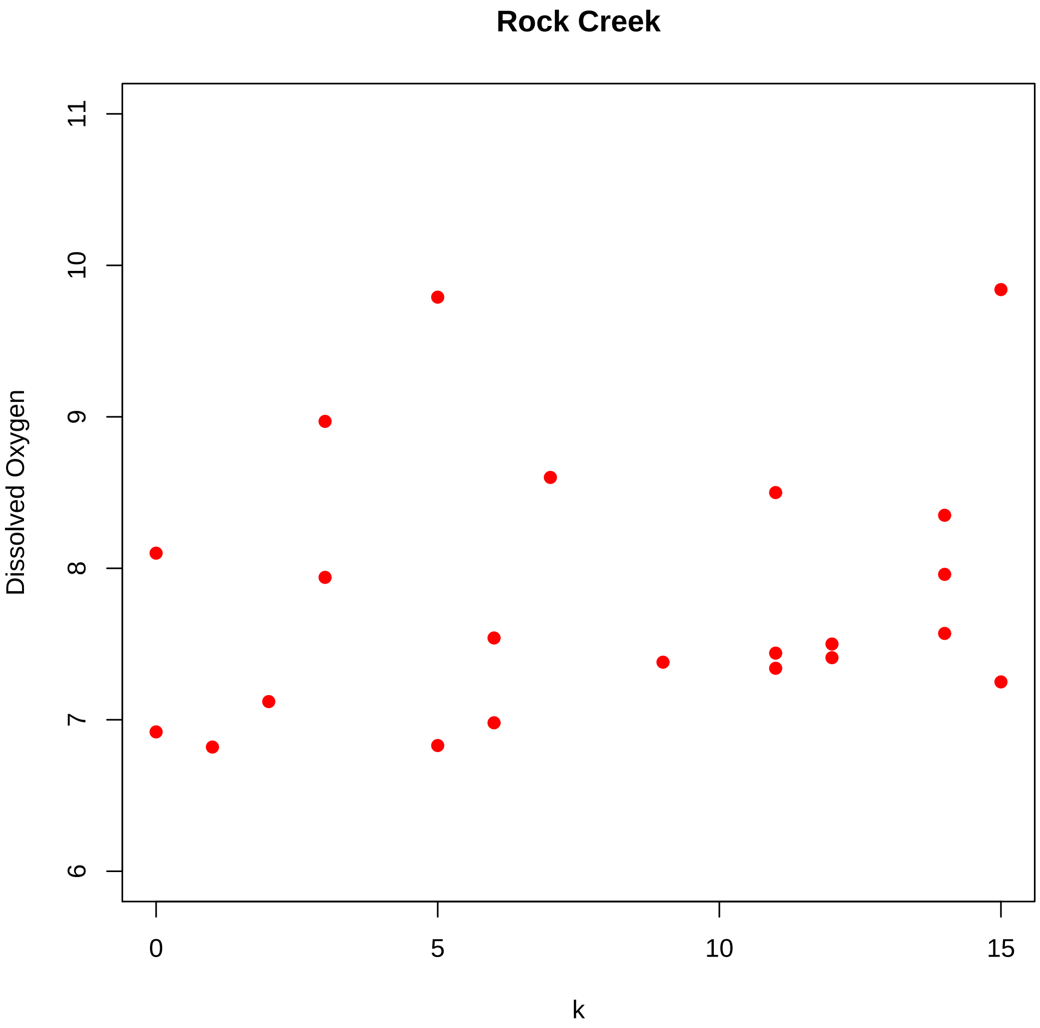
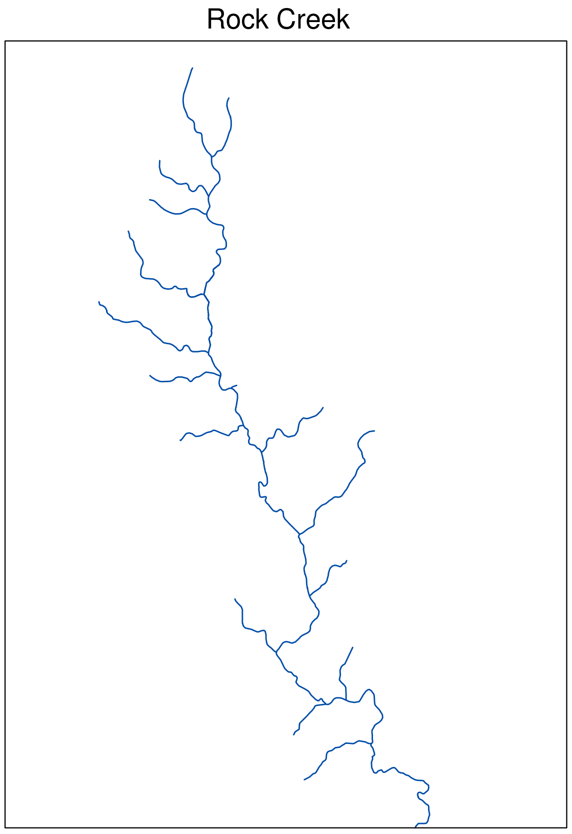
Outline

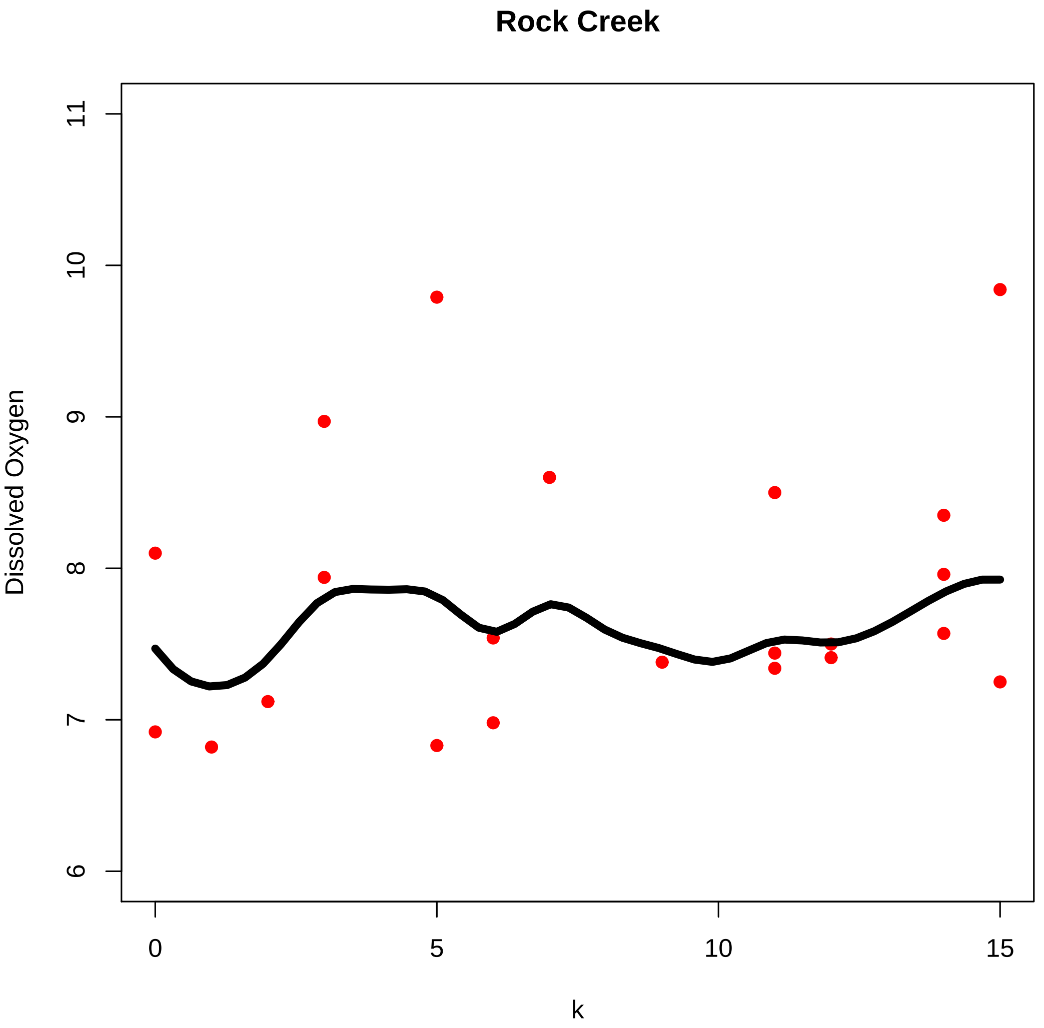
1. A smoothing problem $\longrightarrow$ traditional spline smoother
2. Our goal
3. Stream networks
   (a) Local linear trend
   (b) State-space representation
4. Kalman recursions
5. Connection to a discrete spline smoother
6. Numerical example

One path on a stream network

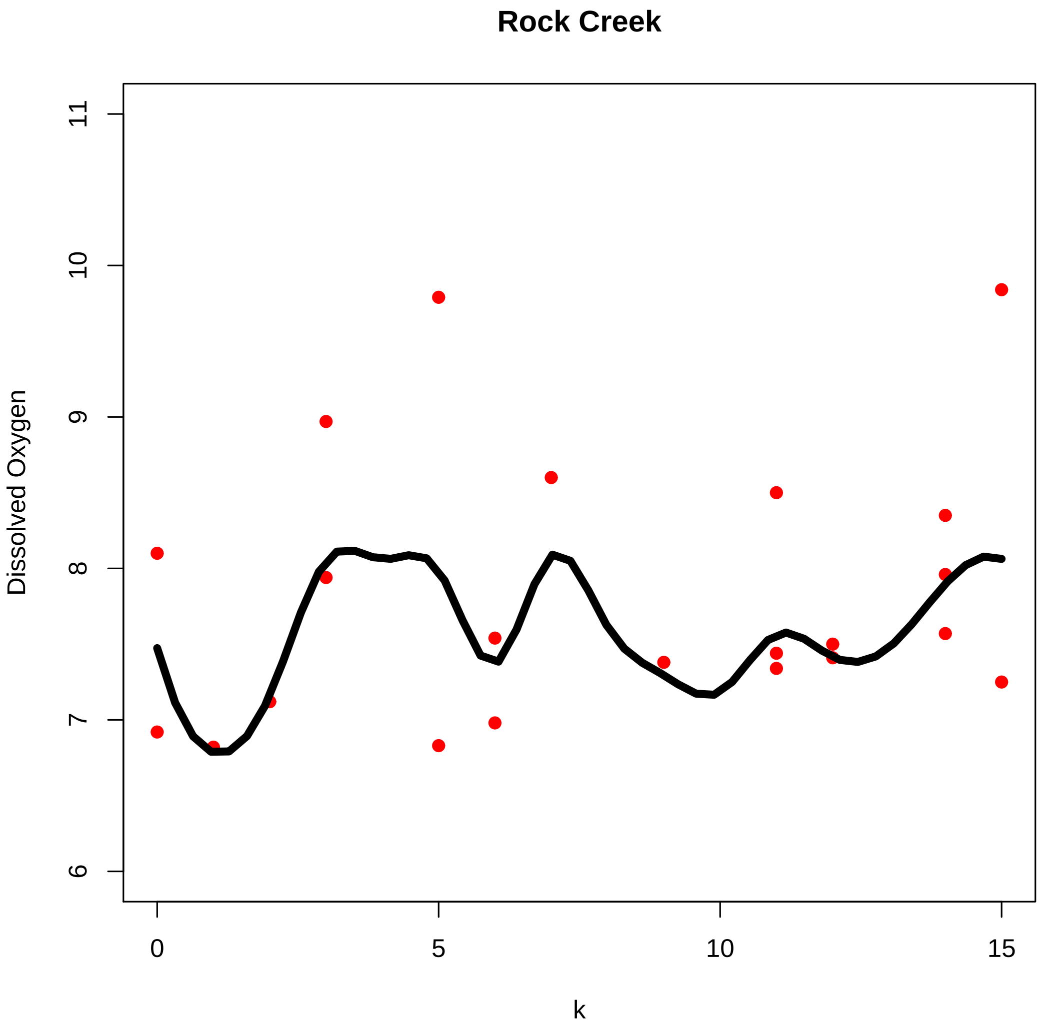




How much to smooth?



Maybe a *better* smooth



Traditional spline smoother in discrete time

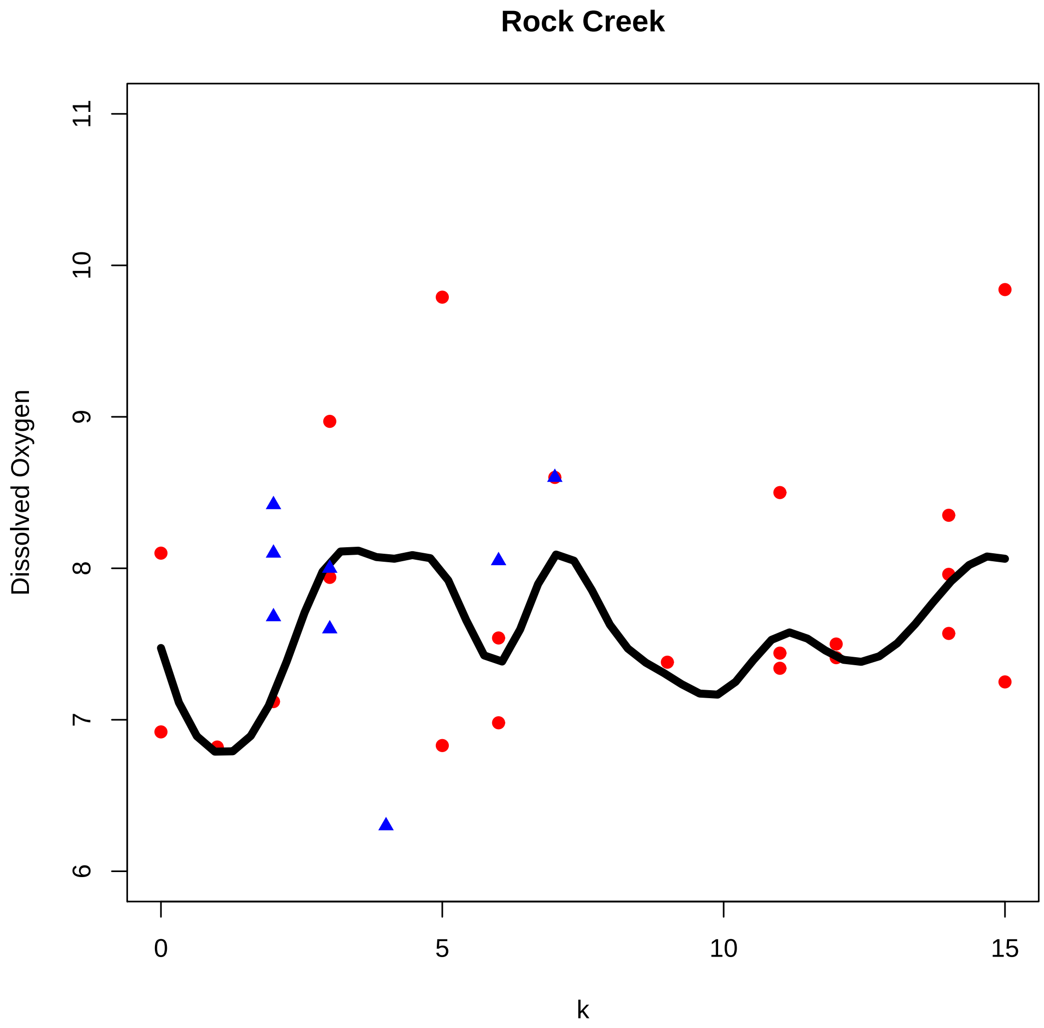
Smooth $\mu(t)$ that minimizes a penalized least squares criterion function

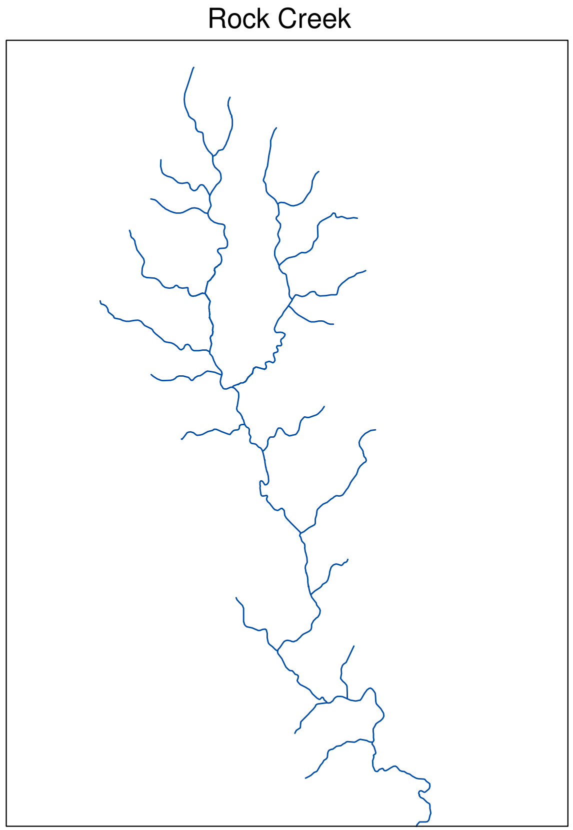
$$\sum_{t=1}^{n} (y(t) - \mu(t))^2 + \lambda \sum_{t=1}^{n} \left(\nabla^2 \mu(t)\right)^2$$

where $\nabla^2 \mu(t)$ is twice differenced $\mu(t)$.

- Trade off between goodness-of-fit and smoothness
- Smoothness determined by λ
  1. Cross-validation
  2. Function of variance components in Local Linear Trend
- Local Linear Trend (LLT) is a state-space model
- Spline obtained as the Kalman smooth using this state-space representation

A new problem → two paths merge



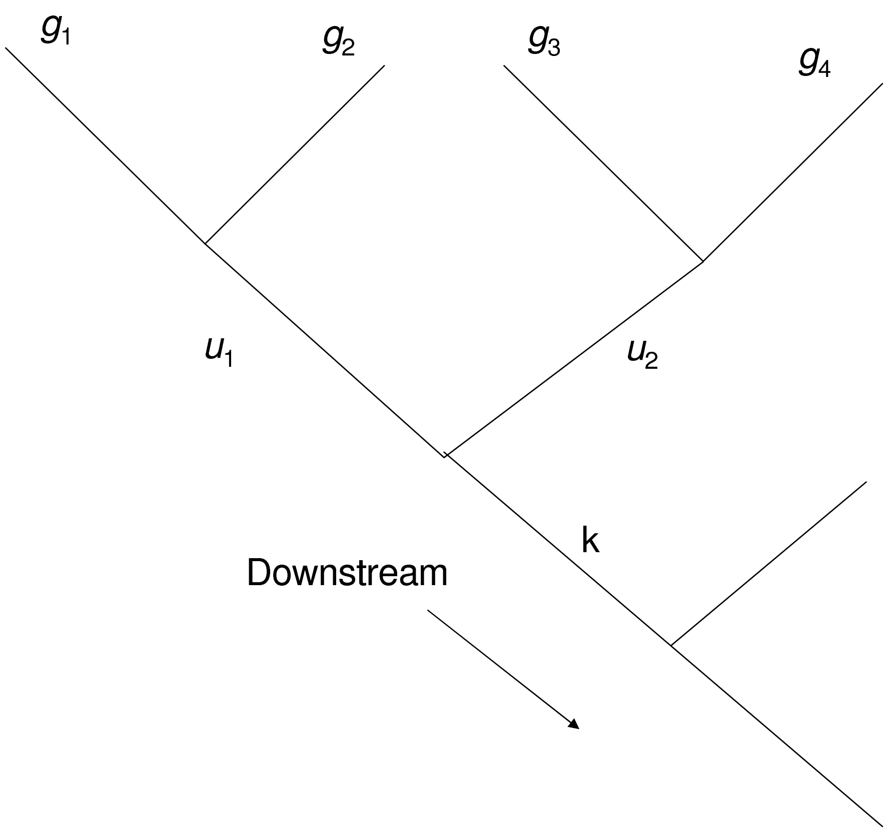


Our Goals

Adapt time series methods to smooth the network

- Define a Local Linear Trend model
- Determine its state-space representation
- Implement Kalman recursions
- Construct a “spline” smoother on the network

Diagram of a stream network



- Reach characterized by (Strahler) order
- Except for first order reaches, each reach k has two parents u_1 and u_2
- Some reaches have grandparents
- Process on reach k depends on the states at each parent
- Natural time-like ordering $\rightarrow$ downstream flow
- Merging with each step downstream
- For simplicity, assume equally spaced discrete locations

State-space model and Local Linear Trend

State-space model on network:

Observation equation $Y(k)$ = Linear function of (unobservable) state + noise
Process equation $\mathbf{X}(k)$ = Linear function of the state at upstream reaches + noise

Local Linear Trend model:

$$\begin{aligned} Y(k) &= \text{Level at reach } k \text{ plus noise} \\ X(k) &= \text{Average levels at parent reaches + slope component} \\ B(k) &= \text{Average slopes at parent reaches + noise} \end{aligned}$$

- Variation associated with measurement error
- Variation due to fluctuation in underlying random process (slope)

State-space model on network:

$$Y(k) = G_k \mathbf{X}(k) + W(k) \qquad (\mathbf{Y}_t = G_t \mathbf{X}_t + \mathbf{W}_t)$$
$$\mathbf{X}(k) = F_{k,u_1} \mathbf{X}(u_1) + F_{k,u_2} \mathbf{X}(u_2) + \mathbf{V}(k) \quad (\mathbf{X}_t = F_t \mathbf{X}_{t-1} + \mathbf{V}_{t-1})$$

Local Linear Trend model:

$$Y(k) = X(k) + W(k) \qquad (\mathbf{Y}_t = \mathbf{X}_t + \mathbf{W}_t)$$
$$X(k) = \tfrac{1}{2}\left(X(u_1) + X(u_2)\right) + B(k) \quad (X_t = X_{t-1} + B_{t-1}$$
$$B(k) = \tfrac{1}{2}\left(B(u_1) + B(u_2)\right) + U(k) \quad (B_t = B_{t-1} + U_{t-1})$$

with state-space components

$$\mathbf{X}(k) = \begin{bmatrix} X(k) \\ B(k) \end{bmatrix} \quad F_{k,u_i} = \begin{bmatrix} 1/2 & 1/2 \\ 0 & 1/2 \end{bmatrix} \quad \mathbf{V}(k) = \begin{bmatrix} U(k) \\ U(k) \end{bmatrix}$$

Smoothing via Kalman recursions

Downstream *predict, filter, predict, filter...*

Given upstream information, predict via

$$\begin{aligned} \mathbf{X}^p(k) &= \text{Prediction based solely on upstream observations} \\ \Omega_k^p &= \text{Variance of this prediction} \end{aligned}$$

Filter once observation is obtained

$$\begin{aligned} \mathbf{X}^f(k) &= \text{Update original prediction with new information from } \mathbf{Y}(k) \\ \Omega_k^f &= \text{Variance of this updated prediction} \end{aligned}$$

Upstream *smooth*

$$\begin{bmatrix} \mathbf{X}^s(u_1) \\ \mathbf{X}^s(u_2) \end{bmatrix} = \text{Update the filtered values with information from downstream reaches}$$

RESULT: Expectation based on all observed information.

Smoothing via Kalman recursions

Downstream *predict, filter, predict, filter...*

Given upstream information, predict via

$$\begin{aligned} \mathbf{X}^p(k) &= F_{k,u_1}\mathbf{X}^f(u_1) + F_{k,u_2}\mathbf{X}^f(u_2) \\ \Omega_k^p &= F_{k,u_1}\Omega_{u_1}^f F_{k,u_1}^T + F_{k,u_2}\Omega_{u_2}^f F_{k,u_2}^T + Q_t, \end{aligned}$$

Filter once observation is obtained

$$\begin{aligned} \mathbf{X}^f(k) &= \mathbf{X}^p(k) + \Omega_k^p G_k^T \Delta_k^{-1}\left(\mathbf{Y}(k) - G_k\mathbf{X}^p(k)\right) \\ \Omega_k^f &= \Omega_k^p - \Omega_k^p G_k^T \Delta_k^{-1} G_k \Omega_k^p. \end{aligned}$$

where $\Delta_k = G_k\Omega_k^p G_k^T + R_k$.

Upstream *smooth*

$$\begin{bmatrix} \mathbf{X}^s(u_1) \\ \mathbf{X}^s(u_2) \end{bmatrix} = \begin{bmatrix} \mathbf{X}^f(u_1) \\ \mathbf{X}^f(u_2) \end{bmatrix} + \begin{bmatrix} \Theta(u_1,k) \\ \Theta(u_2,k) \end{bmatrix} (\mathbf{X}^s(k) - \mathbf{X}^p(k))$$

where $\Theta(u_i,k) = \Omega_{u_i}^f F_{k,u_i}^T (\Omega_k^p)^{-1}$.

RESULT: Smoothed estimates $E(\mathbf{X}|\mathbf{Y})$.

Conditional/Posterior mean

For Gaussian case, conditional/posterior mean is conditional/posterior mode

Conditional/Posterior mode: most probable $\mathbf{X}$ given $\mathbf{Y}$, the mode of $p(\mathbf{X}|\mathbf{Y})$

Another way to get conditional/posterior mode:

- Maximize $p(\mathbf{X}|\mathbf{Y})$ using calculus
- Equivalent to maximizing

$$-\frac{1}{2\sigma_w^2}\sum_{k=1}^{n}(Y(k)-X(k))^2-\frac{1}{2\sigma_u^2}\sum_{k=1}^{n}(\nabla^2 X(k))^2.$$

where $\nabla^2 X(k) = U(k)$

Conditional/Posterior mode is Penalized Least Squares

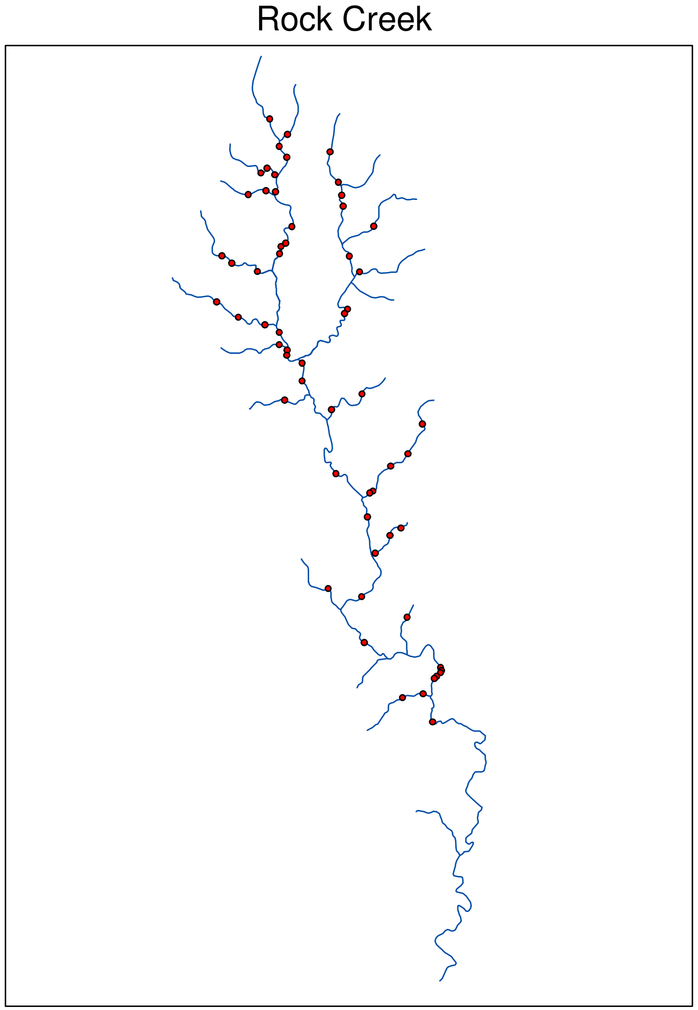
- or equivalently, minimize

$$\sum_{k=1}^{n}(Y(k) - X(k))^2 + \frac{\sigma_w^2}{\sigma_u^2}\sum_{k=1}^{n}(\nabla^2 X(k))^2.$$

  (as was used for traditional spline)

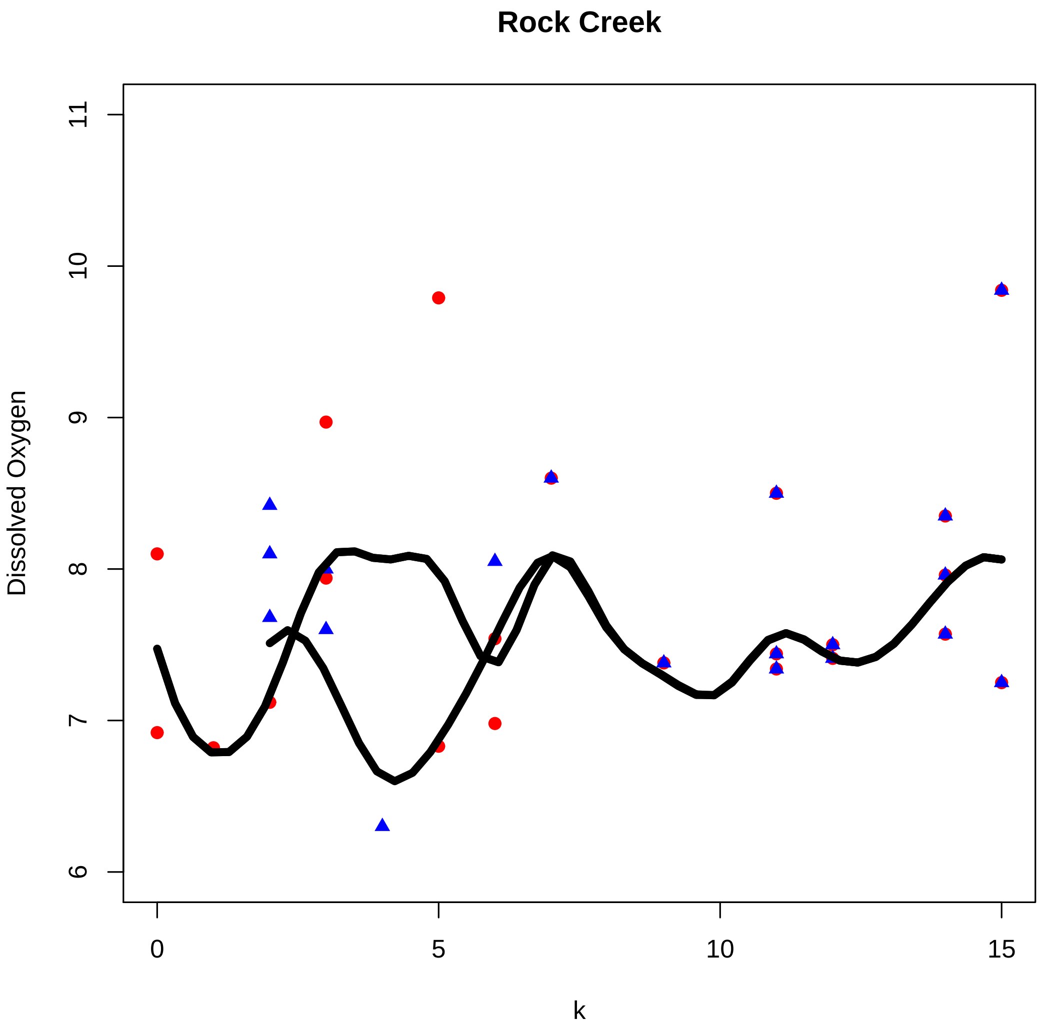
- This defines a *spline smoother* on a stream network through LLT
- Obtain estimate of smoothness parameter $\lambda = \frac{\sigma_w^2}{\sigma_u^2}$ by maximum likelihood
- Obtain $E\left[\mathbf{X}|\mathbf{Y}\right]$ via Kalman smoother

Example - Upper and Lower Rock Creek, MD



- Measure dissolved oxygen
- Summer months
- Some reaches with > 1 station
- Some stations with > 1 observation
- For simplicity, multiple obs/reach treated as independent reps

Example 1: $\hat{\lambda} = 1.312$ with estimated initial conditions



Results

Estimation of initial conditions

- For first order k, $\mathbf{X}(k) \overset{i.i.d}{\sim} N\left(\begin{bmatrix} \mu_0 \\ b_0 \end{bmatrix}, \begin{bmatrix} \sigma_\mu^2 & 0 \\ 0 & \sigma_b^2 \end{bmatrix}\right)$

Mean $\hat{\mu_0} = 7.48$ **Slope** $\hat{b_0} = -2.29$

$\hat{\sigma^2}_\mu = 0.08$ $\hat{\sigma^2}_b = 9.84$

Estimation of smoothing parameter

$\hat{\sigma_w^2} = 4.24$

$\hat{\sigma_u^2} = 3.23$

$\hat{\lambda} = 1.312$

Other considerations

- Addition of seasonal and yearly effects

Further work on State-Space Models

State-space model for stream network:

$$\begin{aligned} Y(k) &= G_k \mathbf{X}(k) + W(k) \\ \mathbf{X}(k) &= F_{k,u_1}\mathbf{X}(u_1) + F_{k,u_2}\mathbf{X}(u_2) + \mathbf{V}(k) \end{aligned}$$

General form is very flexible

- Can be multivariate
- A time component can be added, but process driven by flow
- State matrices are location dependent

Describe a large class of dependencies

- Class of ARMA(p,q) models can be defined
- More general structural models (LLT)

Work in progress

- Adapted state-space to a stream network
- Defined ARMA(p,q) and other structural models on a stream network
- Developed Kalman recursions for this state-space representation
- Likelihood in terms of innovations
- An EM algorithm for missing values
- Application to real data - Montgomery County, MD
  - Network structure from FLoWS
  - Enormous thanks to Stephanie Fitchett, John Norman, and Dave Theobald

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