Smoothing through State-Space Models for Stream Networks

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Outline

1. A smoothing problem → 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?

\[ Y(k) \]
Maybe a better smooth
Traditional spline smoother in discrete time

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

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

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

- Smoothness determined by $\lambda$
- Choice of $\lambda$?
  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
• 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 state 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:

\[ Y(k) = G_k X(k) + W(k) \]
\[ X(k) = F_{k,u_1} X(u_1) + F_{k,u_2} X(u_2) + V(k) \]
\[ (X_t = F_t X_{t-1} + V_{t-1}) \]

Local Linear Trend model:

\[ Y(k) = X(k) + W(k) \]
\[ X(k) = \frac{1}{2} (X(u_1) + X(u_2)) + B(k) + V(k) \]
\[ (X_t = X_{t-1} + B_{t-1} + V_{t-1}) \]
\[ B(k) = \frac{1}{2} (B(u_1) + B(u_2)) + U(k) \]
\[ (B_t = B_{t-1} + U_{t-1}) \]

with state-space components

\[ X(k) = \begin{bmatrix} X(k) \\ B(k) \end{bmatrix} \]
\[ F_{k,u_i} = \begin{bmatrix} 1/2 & 1/2 \\ 0 & 1/2 \end{bmatrix} \]
\[ V(k) = \begin{bmatrix} V(k) + U(k) \\ U(k) \end{bmatrix} \]

**SPECIAL CASE:** \( V(k) = 0, \sigma^2_v = 0 \)
Smoothing via Kalman recursions

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

Given upstream information, predict via

\[
X^p(k) = F_{k,u_1}X^f(u_1) + F_{k,u_2}X^f(u_2)
\]

\[
\Omega^p_k = F_{k,u_1}\Omega^f_{u_1}F_{k,u_1}^T + F_{k,u_2}\Omega^f_{u_2}F_{k,u_2}^T + Q_t,
\]

Filter once observation is obtained

\[
X^f(k) = X^p(k) + \Omega^p_{k}G_{k}^T\Delta^{-1}_k (Y(k) - G_kX^p(k))
\]

\[
\Omega^f_k = \Omega^p_{k} - \Omega^p_{k}G_{k}^T\Delta^{-1}_k G_k\Omega^p_{k}.
\]

where \(\Delta_k = G_k\Omega^p_{k}G_{k}^T + R_k\).

Upstream *smooth*

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

where \(\Theta(u_i, k) = \Omega^f_{u_i}F_{k,u_i}^T(\Omega^p_{k})^{-1}\).

**RESULT: Smoothed estimates** \(E(X|Y)\).
Conditional mean

Is conditional mode for Gaussian

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

Maximize $\log p(\mathbf{X}|\mathbf{Y})$ with respect to $\mathbf{X}$

- Equivalent to maximizing $\log p(\mathbf{Y}, \mathbf{X})$ with respect to $\mathbf{X}$

- Maximize

$$-\frac{1}{2\sigma^2_w} \sum_{k=1}^{n} (Y(k) - X(k))^2 - \frac{1}{2\sigma^2_u} \sum_{k=1}^{n} (\nabla^2 X(k))^2.$$ 

where $\nabla^2 X(k) = U(k)$
Conditional mode is Penalized Least Squares

- or equivalently,

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

(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 MLE \( \hat{\lambda} \)
- Obtain \( E[X|Y] \) via Kalman smoother
Series of first order reaches keep merging - random inputs with every step.

For first order reaches,

- \( X(k) = m_0 + B(k), B(k) = b_0 + U(k) \)

Unknown initial conditions

- Moment estimators for \( m_0 \) and \( b_0 \)
- Naive estimators for initial prediction error variance
Example - The data
Example 1: \( \hat{\lambda} = 1.18 \) - estimated initial conditions
Results

Estimation of initial conditions
• Moment type estimators
• ML estimators?
• Try 0 with diffuse prior
• Sensitivity to initial prediction error variances

Impact of initial conditions
• With larger initial prediction error variance, more weight on observed $Y(k)$
Further work on State-Space Models

State-space model for stream network:

\[ Y(k) = G_k X(k) + W(k) \]
\[ X(k) = F_{k,u_1} X(u_1) + F_{k,u_2} X(u_2) + V(k) \]

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)
• Adapted state-space to a stream network
• Defined ARMA(p,q) and other structural models on a stream network
• Developed of Kalman recursions for this state-space representation
• Likelihood in terms of innovations
• An EM algorithm for missing values
• Starting to look at real data
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