Spatial Ensemble Estimates of Temporal Trends in Acid Neutralizing Capacity

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PRogram for **I**nterdisciplinary **M**athematics, **E**cology, & **S**tatistics

- **PRIMES:** NSF-funded IGERT program
  - degree-plus program in quantitative ecology
  - generous fellowships for students ($27,500 for 03–04)
  - workshops, short courses, etc. encouraging team research
  - internship support by CDC, US Forest Service, and NCAR
- Five research focus groups:
  - Dynamics of Introduced Disease
  - Evolution in Structured Populations
  - Ecology of Managed Ecosystems
  - Ecology of Global Change
  - Aquatic Resources Modeling (STARMAP)

Preliminary Work on Temporal Trends in ANC

- Acid Neutralizing Capacity (ANC)
  - surface waters are acidic if ANC < 0
  - supply of acids from atmospheric deposition and watershed processes exceeds buffering capacity
- Temporal trends in ANC within watersheds (8-digit HUC's)
  - characterize the spatial **ensemble** of trends
  - make a map, construct a histogram, plot an empirical distribution function

Data Set

- 88 HUC's in Mid-Atlantic Highlands
- ANC in at least two years from 1993–1998
- HUC-level covariates:
  - area
  - average elevation
  - average slope, max slope
  - percents agriculture, urban, and forest
  - spatial coordinates

Small Area Estimation

- Probability sample across region
  - regional-level inferences are model-free
  - sample sizes too small to support HUC-level inferences
  - need to construct statistical model to borrow strength across areas
- Two standard types of small area models (Rao, 2003)
  - **area-level**: watersheds
  - **unit-level**: site within watershed

Basic Area-Level Model

- Temporal trend estimates:

$$\begin{aligned}\hat{\beta}_h &= \text{within-HUC WLS slope} \\ &= \beta_h + e_h \\ \beta_h &= \mathbf{x}_h^T \boldsymbol{\theta} + \omega_h\end{aligned}$$

- Design properties:

$$\mathrm{E}_p[e_h \,|\, \beta_h] = 0 \text{ and } \mathrm{Var}_p(e_h \,|\, \beta_h) = \psi_h$$

– design variances assumed known

- Model properties:

$$\mathrm{E}_m[\omega_h] = 0 \text{ and } \mathrm{Var}_m(\omega_h) = \sigma_\omega^2 \geq 0$$

Two Inferential Goals

- Interested in estimating **individual** HUC-specific slopes
- Also interested in **ensemble**:
  spatially-indexed true values: $\{\beta_h\}_{h=1}^m$
  spatially-indexed estimates: $\{\beta_h^{\text{est}}\}_{h=1}^m$
  - **subgroup analysis**: what proportion of HUC's have ANC decreasing over time?
  - "empirical" distribution function (**edf**):

$$F_\beta(z) = \frac{1}{m} \sum_{h=1}^m I_{\{\beta_h \le z\}}$$

Deconvolution Approach

- Treat this as measurement error problem

$$\hat{\beta}_h = \beta_h + e_h$$
$$\{e_h\} \sim \mathrm{N}(0, \psi_h)$$

- Deconvolve:
  - *parametric:* assume F_β in parametric class
  - *semi-parametric:* assume F_β well-approximated within class (like splines, normal mixtures)
  - *non-parametric:* assume $\mathrm{E}_{F_\beta}[e^{i\lambda\beta}]$ is smooth
- Not so appropriate for heteroskedastic measurements, explanatory variables, two inferential goals

Hierarchical Area-Level Model

- Extend model specification by describing parameter uncertainty:

$$
\begin{aligned}
\hat{\beta}_h &= \beta_h + e_h,\ \{e_h\}\ \mathrm{NID}(0, \psi_h) \\
\beta_h &= \mathbf{x}_h^T \boldsymbol{\theta} + \omega_h,\ \{\omega_h\}\ \mathrm{NID}(0, \sigma_\omega^2)
\end{aligned}
$$

- Prior specification:

$$
f(\boldsymbol{\theta}, \sigma_\omega^2) = f(\boldsymbol{\theta}) f(\sigma_\omega^2) \propto f(\sigma_\omega^2)
$$

Bayesian Inference

- **Individual** estimates: use posterior means

$$\beta_h^B = \mathrm{E}[\beta_h \mid \hat{\boldsymbol{\beta}}] = \mathrm{E}\left[\gamma_h \hat{\beta}_h + (1-\gamma_h)\mathbf{x}_h^T \boldsymbol{\theta} \mid \hat{\boldsymbol{\beta}}\right]$$

where $\gamma_h = \sigma_\omega^2/(\psi_h + \sigma_\omega^2)$

- Do Bayes estimates yield a good **ensemble** estimate?
  – use edf of Bayes estimates to estimate F_β?
- **No!** Bayes estimates are "over-shrunk"
  – too little variability to give good representation of edf (Louis 1984, Ghosh 1992)

$$\sum_{h=1}^{m} (\beta_h^B - \bar{\beta}^B)^2 < \mathrm{E}\left[\sum_{h=1}^{m} (\beta_h - \bar{\beta})^2 \mid \hat{\boldsymbol{\beta}}\right]$$

Adjusted Shrinkage

- Posterior means not good for *both* individual and ensemble estimates
- Improve by reducing shrinkage
  - sample mean of Bayes estimates already matches posterior mean of $\{\beta_h\}$
  - adjust shrinkage so that sample variance of estimates matches posterior variance of true values
- Louis (1984), Ghosh (1992)

Constrained Bayes Estimates

- Compute the scalars

$$H_1(\hat{\boldsymbol{\beta}}) = \operatorname{tr}\left\{\operatorname{Var}\left(\boldsymbol{\beta} - \bar{\beta}\mathbf{1} \mid \hat{\boldsymbol{\beta}}\right)\right\}$$

$$H_2(\hat{\boldsymbol{\beta}}) = \sum_{h=1}^{m} \left(\beta_h^B - \bar{\beta}^B\right)^2$$

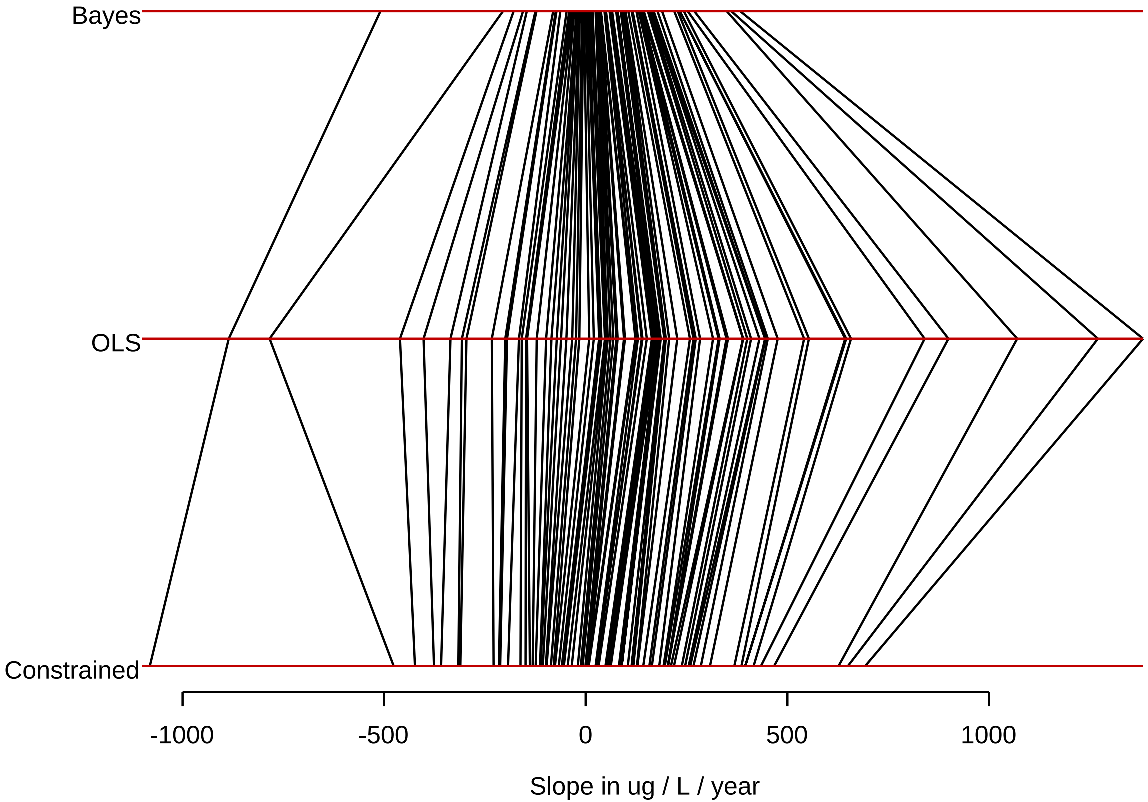
- Form the **constrained Bayes** (CB) estimates as

$$\beta_h^{CB} = a\beta_h^B + (1-a)\bar{\beta}^B$$

where

$$a = \left(1 + \frac{H_1(\hat{\boldsymbol{\beta}})}{H_2(\hat{\boldsymbol{\beta}})}\right)^{1/2} > 1$$

Shrinkage Comparisons for the Slope Ensemble



Numerical Illustration

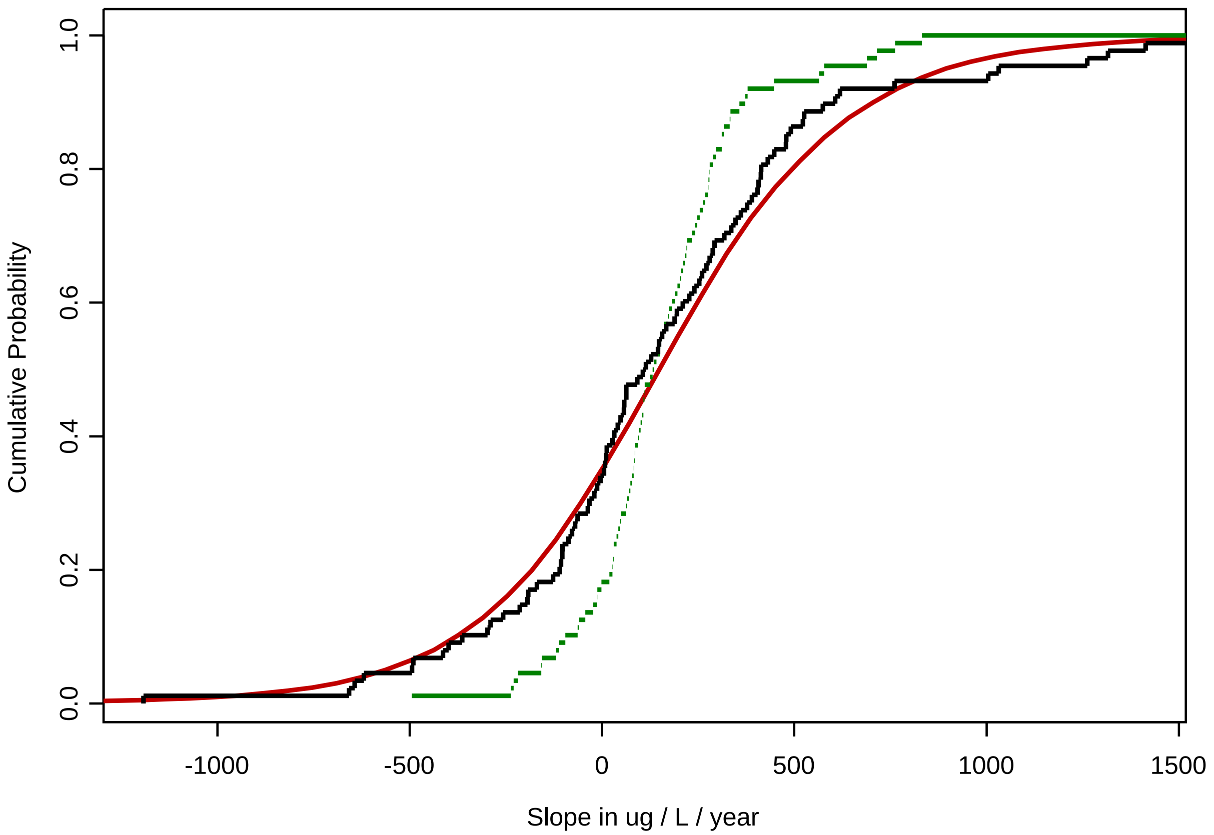
- Compare edf's of estimates to posterior mean of F_β:

$$F_\beta^B(z) = \frac{1}{m} \sum_{h=1}^{m} \mathrm{E}\left[I_{\{\beta_h \le z\}} \,|\, \hat{\boldsymbol{\beta}} \right]$$

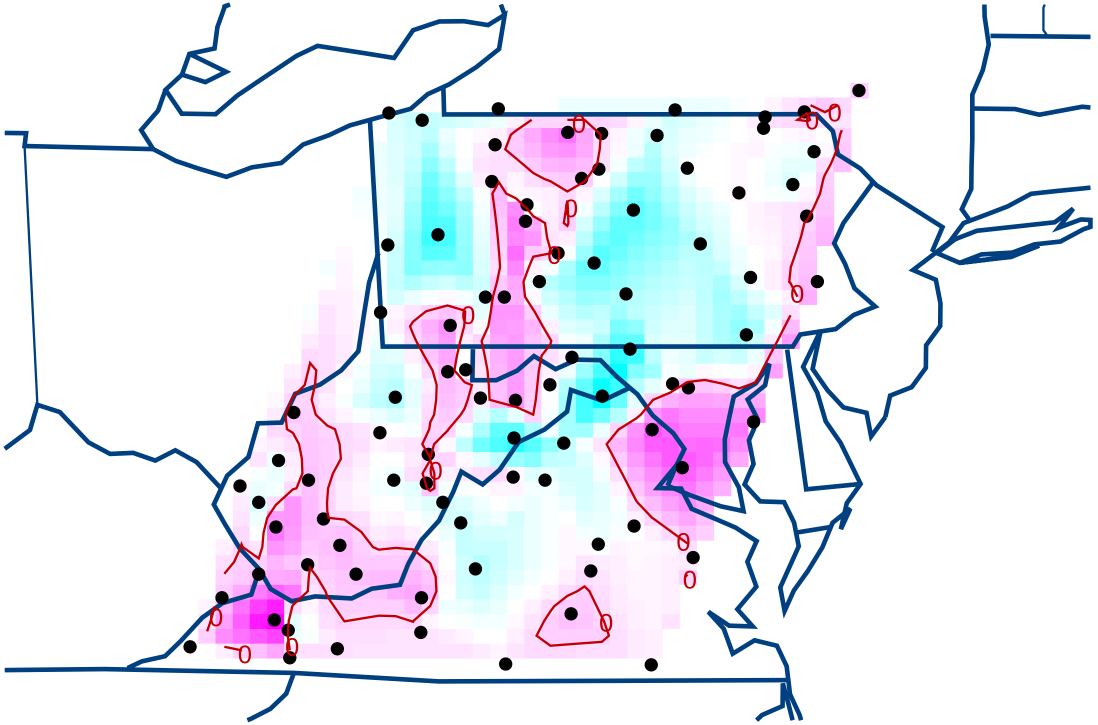
- Comparison of ensemble estimates at selected quantiles:

Estimate	$F_\beta(0)$	$F_\beta(400)$
edf of $\{\beta_h^B\}$	0.205	0.932
posterior mean	0.356	0.743
edf of $\{\beta_h^{CB}\}$	0.352	0.739

Estimated EDF's of the Slope Ensemble



Spatial Structure for the Slope Ensemble



Further Work: Spatial Model

- Let A_h denote set of neighboring HUC's for HUC h
- Conditional autoregression (CAR) model:

$$\begin{aligned}\hat{\beta}_h &= \beta_h + e_h \\ \beta_h &= \mathbf{x}_h^T \boldsymbol{\theta} + \omega_h \\ \omega_h \,|\, \{\omega_k, k \neq h\} &\sim \mathrm{N}\left(\rho \sum_{k \in A_h} q_{hk}\omega_k, \sigma_\omega^2\right)\end{aligned}$$

- Adjacency matrix $[q_{hk}]$ can reflect watershed structure

Further Work

- Restrict to acid-sensitive waters
- Combine probability and convenience samples
  - weights from selection functions to get $E_p[e_h \mid \beta_h] = 0$
- Other covariates?
  - deposition maps/trends from CASTNet?
- Other trend summaries?
- Site-level model?
  - useful sub-watershed covariates?
  - spatial scales: HUC to HUC, site to site
  - more concern with design, normality assumptions