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Linking CWA Sections 305(b)/303(d): Small Area Estimation

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Outline

- Primer on small area estimation
  - direct and indirect estimation
  - synthetic and composite estimation
  - borrowing strength and shrinkage
  - simultaneous and ensemble estimation
- Small area estimation examples
  - semi-parametric small area estimation
  - constrained estimation for ensembles

Domains

- $Domain =$ subpopulation of interest in a survey
  - geographic domains = areas (EPA region, state, county, HUC)
- Major domains: addressed by CWA 305(b)
  - sufficient sample size allocated at the design stage
  - standard survey estimation procedures yields estimates of adequate precision

Major Domains: Use Direct Estimation

- Direct estimators:
  - use data only from the study units in the domain and time period of interest
  - include standard weighted survey estimators
  - good design properties: unbiased estimator and valid confidence intervals *without any statistical model!*
- Direct estimation is not reliable if sample size is extremely small

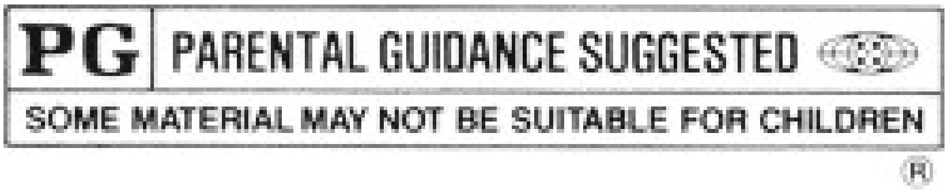
Small Domains: Direct Estimates Not Reliable

- Small domains/Small areas
  - sample size is small and may be zero in some domains
  - model-based inference is necessary to yield estimates of adequate precision
  - (definition depends on sampling resources and precision requirements)
- Might consider small area estimates for CWA 303(d)
  - rare to have adequate sample size everywhere

Indirect Estimation: Borrowing Strength

- Indirect estimators:
  - use data from outside the domain and/or time period of interest
  - (time indirect, domain indirect, domain and time indirect)
  - explicitly use statistical model to "borrow strength" across time or space
  - include various small area estimators

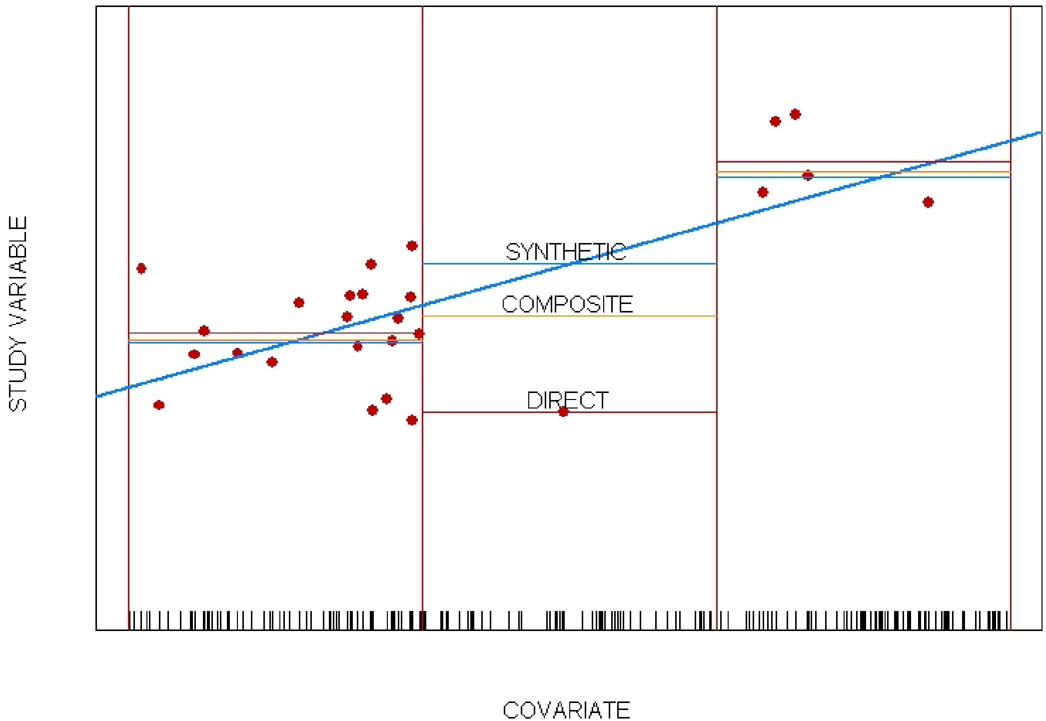
Indirect Estimation: Synthetic Estimator



- Have: study variables for sample, covariates for entire landscape
- Fit "global" model relating study variable to covariates
- Predict study variable at unobserved locations using available covariates and fitted model
  - works even if no samples in the area
  - may be poor if model is incorrectly specified

Direct, Synthetic and Composite Estimators

- One covariate, three small areas



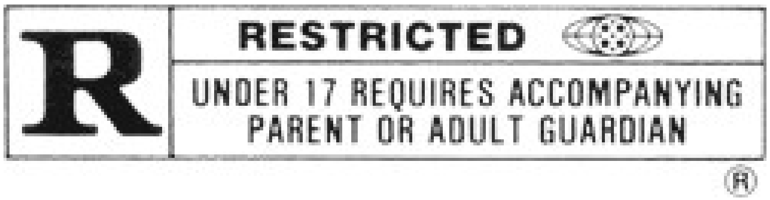
Shrinkage in the Composite Estimator

- Direct is moved toward synthetic to get composite estimator
  - equivalently, small-area specific effect "shrinks toward zero"
- Much of small area estimation involves choosing the shrinkage factor
- *Ad hoc* composite estimator

$$\text{composite} = w_h(\text{direct}) + (1 - w_h)(\text{synthetic})$$

  - still rated $\mathbf{PG}$

Formal Composite Estimation



- $w_h =$ function of parameters from a fitted mixed model
- Mature audiences only:
  - good auxiliary information
  - correctly-specified global regression structure
  - correctly-specified local correlation structure
  - (may require violence or coarse language)
  - sexy models and methods: EBLUP/EB, HB

Basic Small Area Models

- Model for direct estimates:

$$
\begin{aligned}
\hat{\theta}_h &= \text{direct estimate for small area } h \\
&= \theta_h + e_h \\
&= \text{truth+sampling error} \\
\theta_h &= \mathbf{x}_h^T \boldsymbol{\beta} + \omega_h \\
&= \text{regression + area-specific deviation}
\end{aligned}
$$

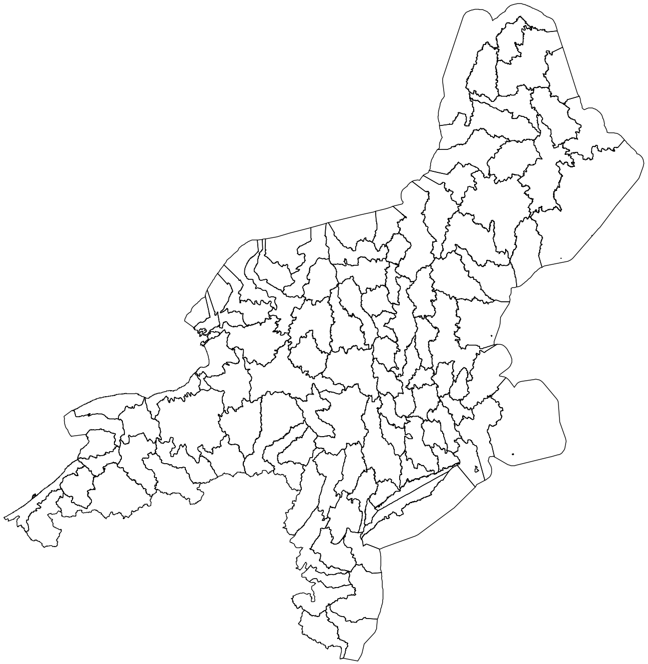
- Two ways to borrow strength:
  - globally, through regression fitted to all data
  - locally, through spatially (or temporally) correlated random effects

Two Small Area Estimation Problems

- Acid Neutralizing Capacity (ANC)
  - surface waters are acidic if ANC < 0
  - supply of acids from atmospheric deposition and watershed processes exceeds buffering capacity
- ANC level: Semiparametric small area estimation
  - HUCs in Northeast
- ANC trend: Constrained ensemble estimates
  - HUCs in mid-Atlantic highlands

Semiparametric Small Area Estimation of ANC Level

- Joint work with J. Opsomer, G. Ranalli, G. Claeskens, G. Kauermann
- 557 observations over 113 HUCs



HUCs as Small Areas

- Few sample observations available in most HUCs
  - Average sample size/HUC: 4.9
  - 64 HUCs contain less than 5 observations
  - 27 out of 113 HUCs contain no sample observations
- Site-specific covariates: lake location and elevation
  - need to account for spatial structure
  - worry about spatial model misspecification
- Simpler way to capture spatial effects?

Semiparametric Small Area Model

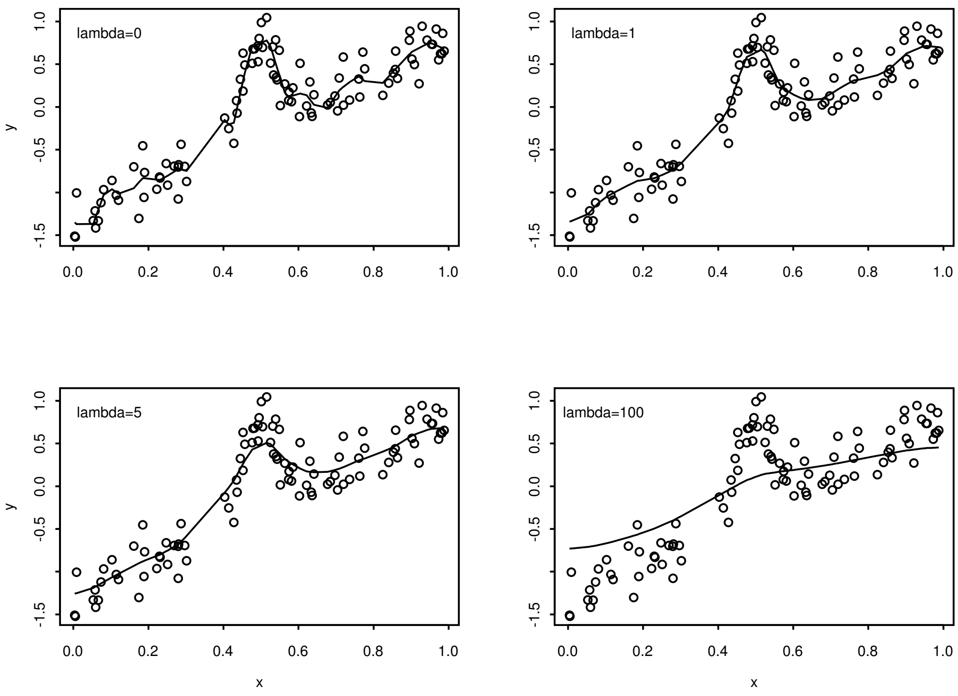
- Replace linear function of covariates by more general model:

$$\begin{aligned}
\text{direct} &= \text{truth}+\text{sampling error} \\
\text{truth} &= m(\mathbf{x}_h;\boldsymbol{\gamma}) + \omega_h \\
&= \text{semiparametric regression} + \text{area-specific deviation} \\
&= \mathbf{x}_h^T\boldsymbol{\beta} + \mathbf{z}_h^T\boldsymbol{\alpha} + \omega_h
\end{aligned}$$

- Semiparametric regression expressed as mixed linear model
  - penalized splines (P-splines)
  - thin plate splines
  - kriging
- EBLUP easily handled with standard software (SAS, SPlus)

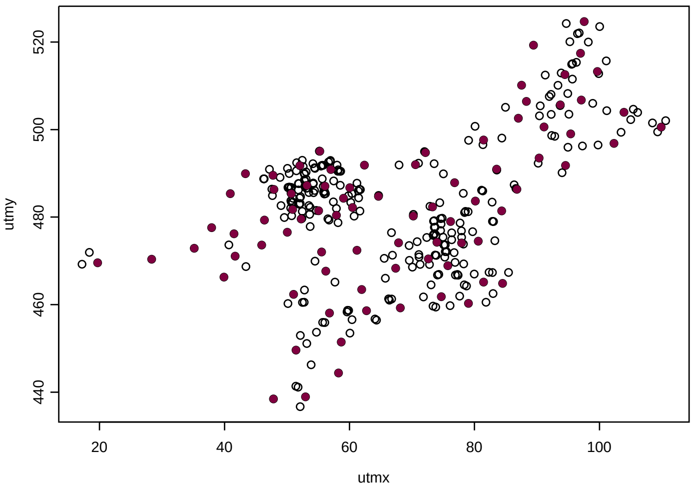
Fitting by Penalized Splines Regression

- Allow slope changes at each of many knots
  - penalize excessive slope changes via λ



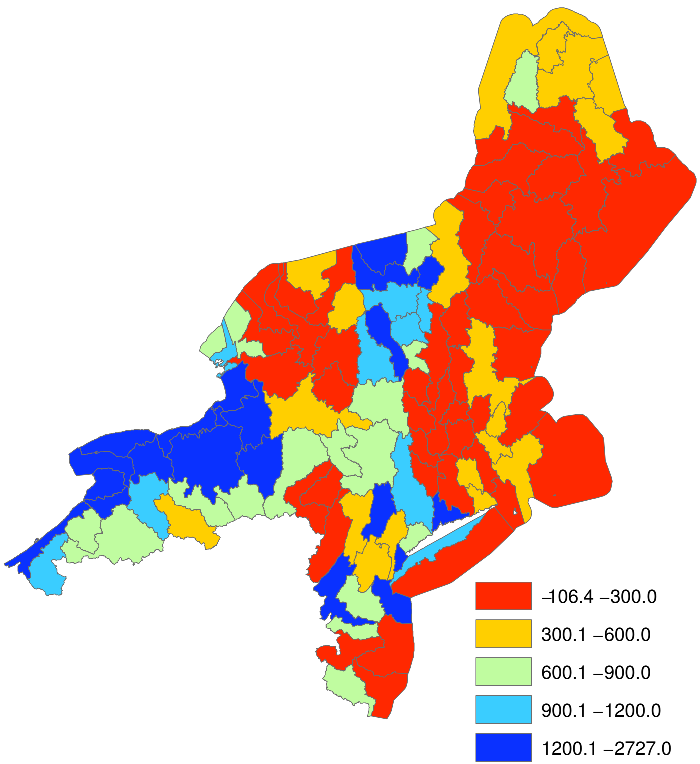
Spatial Smoothing Using P-Splines

- NE Lakes data require bivariate (spatial) smoothing $\approx$ thin-plate spline (Ruppert *et al.* 2003)
- Knot selection: space-filling algorithm



NE Lakes HUC Predictions

- Correlation between ANC and model prediction: 0.96



Constrained Bayes Estimation for ANC Trend

- Joint work with M. Delorey
- 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 Model for Trend Estimates

- Temporal trend estimates:

$$\begin{aligned}\hat{\tau}_h &= \text{within-HUC estimated slope} = \tau_h + e_h \\ &= \text{truth} + \text{sampling error} \\ \tau_h &= \mathbf{x}_h^T \boldsymbol{\beta} + \omega_h \\ &= \text{regression} + \text{area-specific effect}\end{aligned}$$

- Spatial correlation in $\{\omega_h\}$ modeled by conditional autoregression (CAR)

Two Inferential Goals

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

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

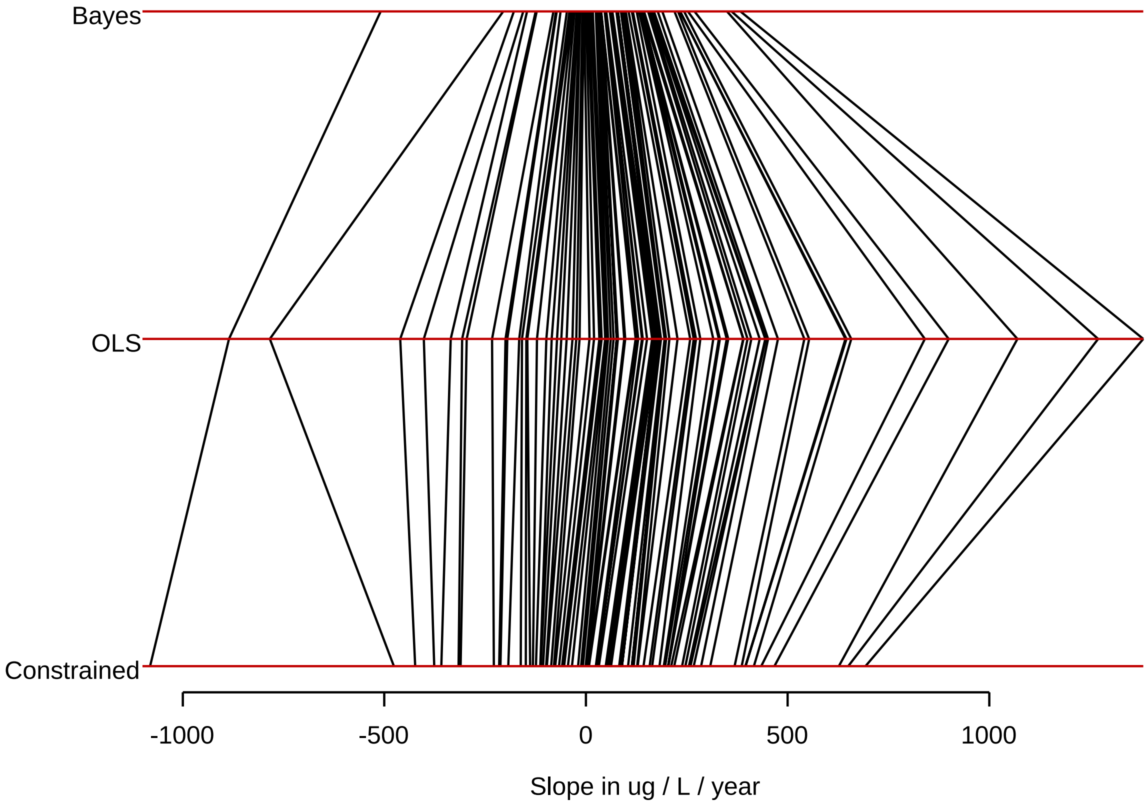
Bayesian Inference

- **Individual** estimates: use posterior means
  - pretty much sophisticated composite estimators
- Do Bayes estimates yield a good **ensemble** estimate?
  - use edf of Bayes estimates to estimate $F_{\mathcal{T}}$?
- **No!** Bayes estimates are "over-shrunk"
  - too little variability to give good representation of edf (Louis 1984, Ghosh 1992)

Constrained Bayes Adjusts the 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 $\{\tau_h\}$
  - adjust shrinkage so that sample variance of estimates matches posterior variance of true values
- Resulting estimates are called **Constrained Bayes**
  - Louis (1984), Ghosh (1992)
  - require posterior analysis

Shrinkage Comparisons for the Slope Ensemble



Numerical Implementation of Hierarchical Bayes

- Markov chain Monte Carlo (MCMC): often necessary to approximate posterior distribution of unknowns given data
- Idea: any distribution can be studied provided we can simulate from it
  - iid draws from distribution would be ideal
  - dependent, identically distributed draws would be fine if dependence is not too strong (ergodic theorem)
  - dependent, nearly identically distributed draws might be OK

Markov Chain Monte Carlo (MCMC)

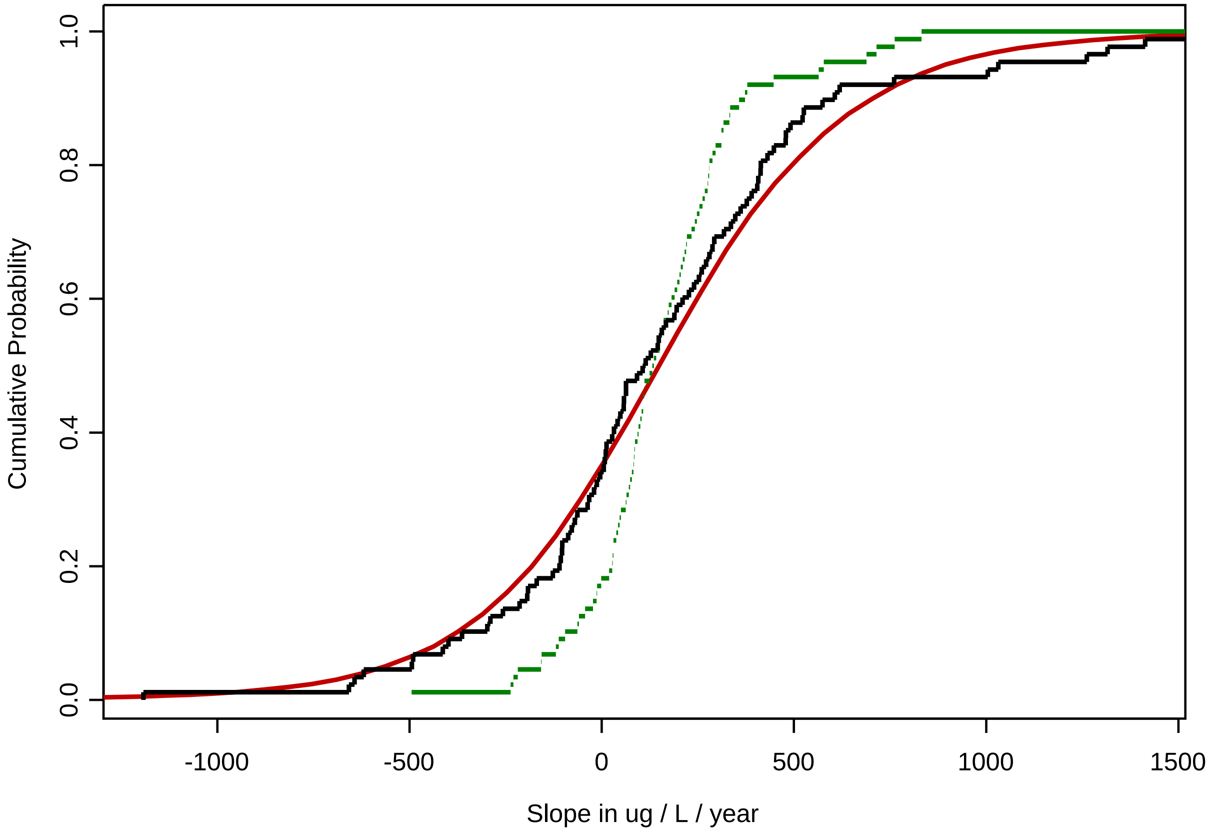
- MCMC generates Markov chain with invariant distribution equal to posterior distribution of interest
  - not independent due to Markov structure
  - not identically distributed except asymptotically, due to initialization problem
  - assessing convergence is critical
- MCMC recipes for constructing suitable Markov chains include
  - Gibbs sampler
  - Metropolis-Hastings algorithm

Gibbs Sampler: DISCO

- Derive full set of conditionals
- Initialize unknowns
- Sample sequentially from conditionals many times
- Check convergence, discarding a large number of "burn-in" draws
- Ordinary data analysis on remaining data set

$$\text{posterior mean of } \tau_h \simeq \text{sample mean of draws}$$
$$\text{posterior variance of } \tau_h \simeq \text{sample variance of draws}$$
$$\text{posterior median of } \tau_h \simeq \text{sample median of draws}$$

Estimated EDF's of the Slope Ensemble



Small Area Estimation Needed to Link 305(b) and 303(d)

- $\mathbf{G}$-rated direct estimates: no shrinkage
- Indirect estimates: $\mathbf{PG}$ or $\mathbf{R}$
  - need good covariates and/or useful correlations
  - rare in aquatic resources
- Shrinkage:
  - none = direct: $\mathbf{G}$-rated
  - total = synthetic: $\mathbf{PG}$-rated
  - ad hoc composite: $\mathbf{PG}$-rated
  - formal composite: $\mathbf{R}$-rated
- Two examples: semiparametric and constrained