

A Semiparametric Stochastic Mixed Model for Increment-Averaged Data with Application to Carbon Sequestration in Agricultural Soils

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Space-Time Aquatic Resources Modeling & Analysis Program

- **STARMAP:** EPA-funded STAR grant
 - study probability surveys of aquatic resources
 - CSU focuses on modeling side
 - partners with sister program at OSU (design side)
- Um, agricultural soils \neq aquatic resources?
 - spin-off from other work on nonparametric survey regression estimation

Greenhouse Effect

- Solar energy transmitted to earth as visible and ultraviolet radiation

	Atmosphere	Surface
Reflected	25%	5%
Absorbed	25%	45%

- Radiation absorbed by surface gets re-radiated as infrared
- **Greenhouse Gases (GHGs)**
 - pass visible and UV, but trap infrared
 - include water vapor, CO₂, methane, nitrous oxide, others

Kyoto Protocol

- December 1997 meeting in Kyoto, Japan
- Resulted in Kyoto Protocol
 - signed by over 170 nations, including US
- Binding commitment for US to reduce emissions of six GHGs
 - reduce 7% from 1990 levels during 2008–2012
- US never ratified Kyoto
 - no commitment by developing nations
 - potentially large economic impact

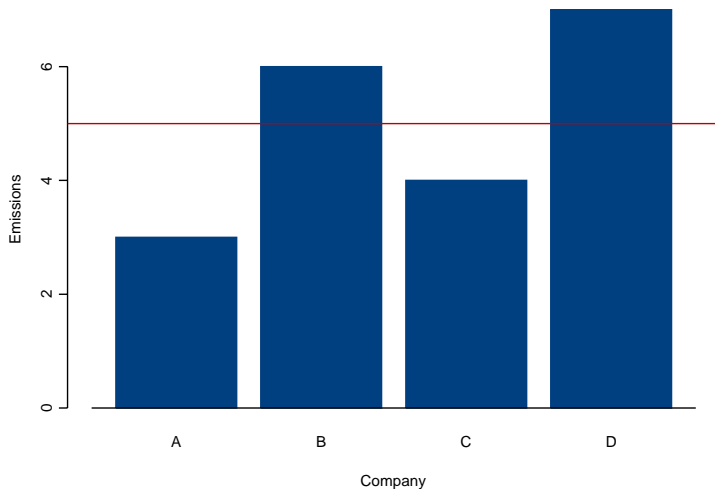
Chicago Climate Exchange

- www.chicagoclimatex.com
- Participants set voluntary limits on GHG emissions
 - legally binding commitments for reductions

	Commitments			
Baseline	2003	2004	2005	2006
avg. 1998–2001	-1%	-2%	-3%	-4%

Why Submit to Binding Commitments?

- Creates a “cap-and-trade” market
 - can make own reductions
 - can buy credits from others that have extra reductions to sell



Why Participate?

- Participants include Ford, Motorola, DuPont, City of Chicago, Waste Management, ...
- Reduce long-term costs of carbon reduction
- Get financial benefits (e.g., reduced energy costs)
- Enhance environmental leadership reputation
- Build trading skills / help create market rules

Examples of GHG Mitigation and Offset Projects

- Renewal energy systems
 - wind power, solar power
- Energy efficient process innovations
- Recovery / use of landfill and agricultural methane
- Carbon sequestration
 - tree biomass
 - agricultural soils: **no-till agriculture**

Agriculture 001: Tillage

- Traditional Tillage:
 - after harvest, field contains crop residues
 - tillage turns over the soil to bury residues
 - often repeated several times prior to planting
- Conservation Tillage:
 - Reduced-Till: limited tillage; substantial crop residues on surface
 - No-Till (**NT**): doesn't use tillage; all crop residues left on surface
 - Economically feasible due to new technology

Advantages of No-Till Management

- NT results in lower production costs
 - fewer management steps
 - cheaper, lower horsepower tractors
- NT leaves crop residue on soil surface
 - reduces soil loss due to wind and water erosion
 - reduces flow of sediments, nutrients, and pesticides into surface waters
 - improves soil fertility; enhances soil organic matter
 - **sequesters carbon**

Carbon Sequestration via No-Till

- Original soil carbon content has been reduced 50% since invention of the steel plow
 - aeration due to tillage leads to faster decomposition
 - decomposition releases CO₂ to atmosphere
- No-till significantly slows decomposition
 - widespread adoption could restore original carbon within 40 years
 - could cut projected growth in US CO₂ emissions by 20%

Show Me the Money

- Carbon as a cash crop?
- Government could subsidize switch to no-till
- Corporations faced with caps on GHG emissions could buy **carbon credits**
 - some Canadian companies have already paid Iowa farmers for carbon credits
- Estimates of value range from \$4–\$40 per acre

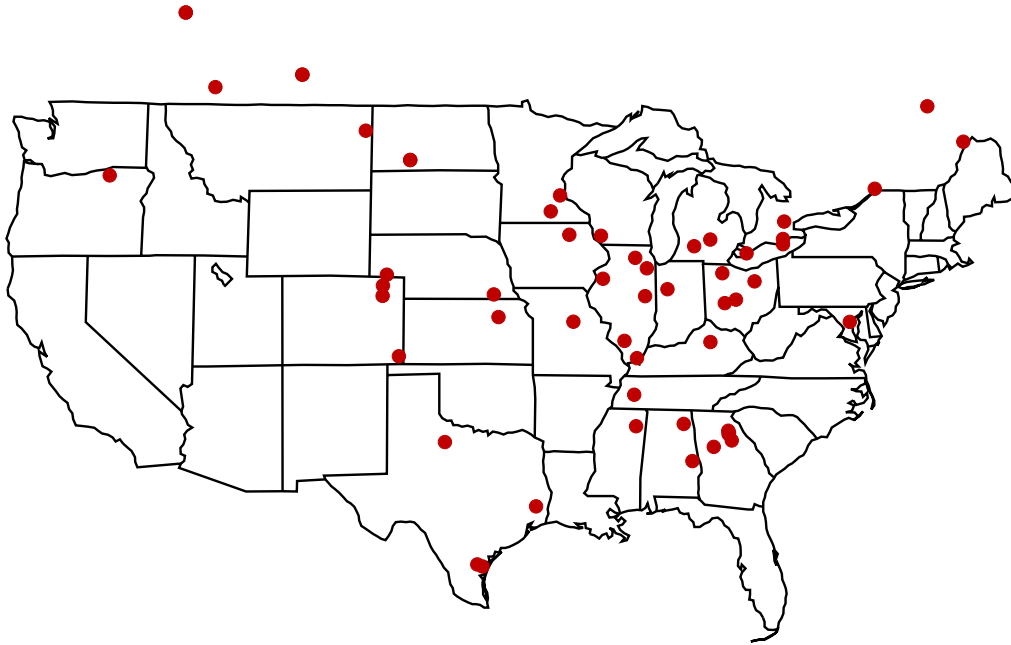
Key Question for Carbon Credits

- How much carbon is sequestered in switching to no-till?
- Several studies have compared no-till with traditional tillage on paired fields
- Measure carbon difference after one or more years since management change:

$$Y = (\text{no-till carbon}) - (\text{traditional tillage carbon})$$

Available North American Studies

- 63 studies compare tillage types on paired fields



Soil Core Samples

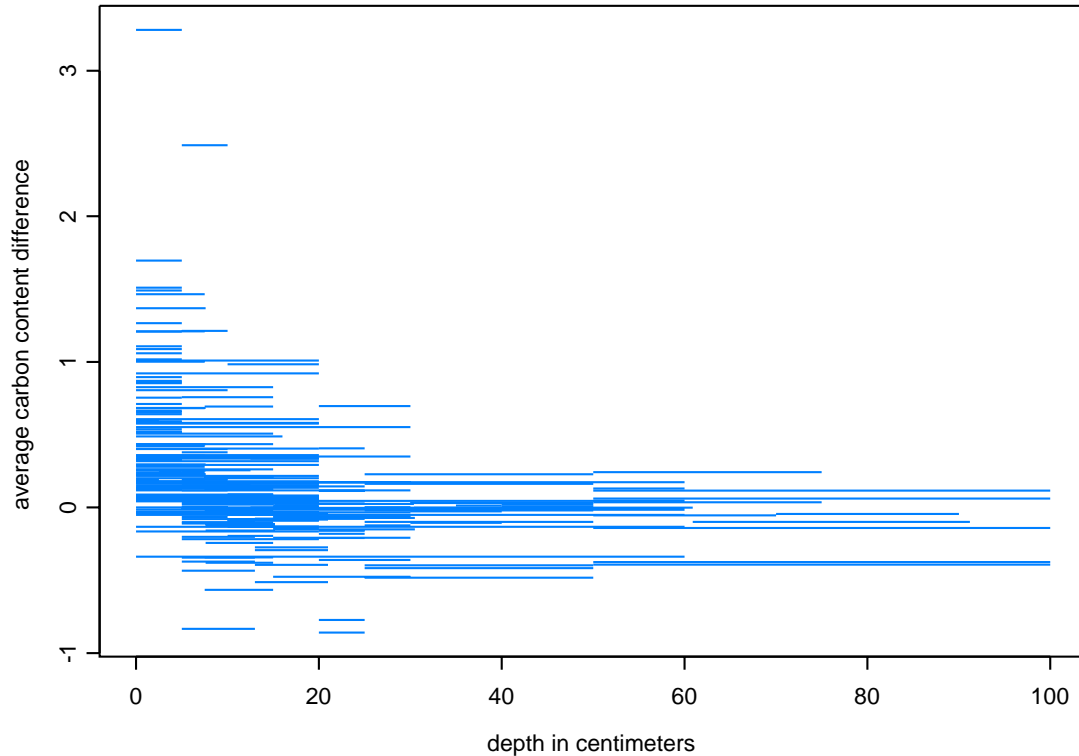
- Use probe to select one or more cores
- Separate cores into increments
 - may be fixed increments (e.g., 0–15 cm, 15–30 cm)
 - may be determined by soil profile (e.g., plow layer, A horizon, B horizon, C horizon)
- Mix matching increments in a bucket
- Bag a subsample and send to the lab

Aside on Core Data

- Like a time series, with depth replacing time
 - specifically, a **flow**: defined on interval (income, expenditure, precipitation)
 - not a **stock**: instantaneous (interest rate, temp)
- Other “cores”:
 - ice cores: increment represents one year of snowfall
 - vertical ozone profiles
 - like time series, tend to be many, regularly spaced, relatively narrow increments
- Not true for soil cores!

Increment-Averaged Data

- Difference in metric tons C ha⁻¹ vs. depth



Ad Hoc Methods: Midpoint Assignment

- True model is

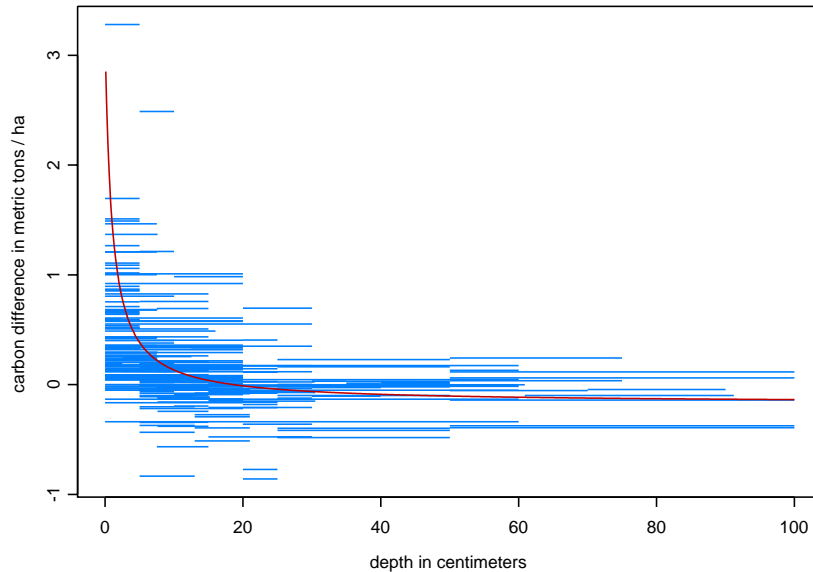
$$\begin{aligned} Y_{ij} &= \frac{1}{d_{ij} - d_{i,j-1}} \int_{d_{i,j-1}}^{d_{ij}} \sum_k \alpha_k g_k(t) dt + \epsilon_{ij} \\ &= \sum_k \alpha_k \frac{1}{d_{ij} - d_{i,j-1}} \int_{d_{i,j-1}}^{d_{ij}} g_k(t) dt + \epsilon_{ij} \\ &= \sum_k \alpha_k g_k(t_{ijk}^*) + \epsilon_{ij} \text{ where } t_{ijk}^* \in (d_{i,j-1}, d_{ij}) \end{aligned}$$

- But we regress on $g_k(m_{ij}) \neq g_k(t_{ijk}^*)$: measurement error problem
- Least squares estimators are biased and inconsistent

Do We Need to Worry?

- Simulate from the fitted model

$$Y_{ij} = \frac{1}{d_{ij} - d_{i,j-1}} \int_{d_{i,j-1}}^{d_{ij}} (\alpha_0 + \alpha_1/(1+t)) dt + \epsilon_{ij}$$



Simulation Results

- Simulate from true model, then estimate with midpoint assignment
 - use actual increments from data set
 - resample if necessary

sample size	reps	$\alpha_0 = -0.17$	$\alpha_1 = 3.32$
218	10,000	$E[\hat{\alpha}_0] = -0.17$	$E[\hat{\alpha}_1] = 4.21$
10,000	1	$\hat{\alpha}_0 = -0.17$	$\hat{\alpha}_1 = 4.18$

- Over 25% relative bias in slope estimate

Ad Hoc Methods: Adjustment of Increments

- Study 1 measures

Y_{11} = carbon stock change over increment 0–15 cm

Y_{12} = carbon stock change over increment 15–30 cm

- Study 2 measures

Y_{21} = carbon stock change over increment 0–50 cm

- “Adjustment” of Y -values

$Y_1^* := Y_{11} + Y_{12}$ represents 0–30 cm

$Y_2^* := \frac{30}{50}Y_{21}$ represents 0–30 cm

Ad Hoc Methods for Increments

- Midpoint assignment leads to bias, inconsistency
- “Adjustment” leads to loss of information, likely bias
- One final method: simply drop studies with non-matching increments
 - obvious loss of information
- Need to recognize the increment nature of the data

Key Data Features

- Increment averaging
 - irregular, wide
 - difficult to specify parametric model
- Within-core dependence
 - increments within same core may be correlated
- Other effects
 - time since change to no-till
 - climate regime
 - soil type

Semiparametric Stochastic Mixed Model: Longitudinal

- Zhang, Lin, Raz, Sowers (1998) *JASA*:

$$Y_{ij} = \mathbf{X}_{ij}^T \boldsymbol{\beta} + g(t_{ij}) + \mathbf{Z}_{ij}^T \mathbf{b}_i + U_i(t_{ij}) + \epsilon_{ij}$$

- $\boldsymbol{\beta}$: p unknown regression coefficients
 - $\mathbf{X}_{ij}, \mathbf{Z}_{ij}$: known covariates
 - $g(t)$: twice-differentiable function of time
 - \mathbf{b}_i : independent q -vectors of random effects
 - $U_i(t)$: independent stochastic processes
 - ϵ_{ij} : independent errors
- Does not handle increment averages

Semiparametric Stochastic Mixed Model: Increments

- Increment average in i th core, j th increment

$$Y_{ij} = \mathbf{X}_{ij}^T \boldsymbol{\beta} + \frac{1}{d_{ij} - d_{i,j-1}} \int_{d_{i,j-1}}^{d_{ij}} g(t) dt + \mathbf{Z}_{ij}^T \mathbf{b}_i + U_{ij} + \epsilon_{ij}$$

- $\boldsymbol{\beta}$: p unknown regression coefficients
- $\mathbf{X}_{ij}, \mathbf{Z}_{ij}$: known covariates
- $g(t)$: twice-differentiable function of depth
- \mathbf{b}_i : independent q -vectors of random effects
- U_{ij} : increment-averaged stochastic process
- ϵ_{ij} : independent errors

Assumptions for Semiparametric Stochastic Mixed Model

- Define

$$\mathbf{U}_i = (U_{i1}, U_{i2}, \dots, U_{in_i})^T$$

- Assume

- \mathbf{U}_i are independent normal($\mathbf{0}, \mathbf{\Gamma}_i$) where $\mathbf{\Gamma}_i = \text{cov}(\mathbf{U}_i, \mathbf{U}_i; \boldsymbol{\xi})$
- \mathbf{b}_i are independent normal($\mathbf{0}, \mathbf{D}(\phi)$) where \mathbf{D} is a positive definite matrix
- ϵ_{ij} are independent normal($0, \sigma^2$)
- $\mathbf{b}_i, \mathbf{U}_i$, and ϵ_{ij} are mutually independent

Integrated Stochastic Process Specification

- Increment-averaged form:

$$U_{ij} = \frac{1}{d_{ij} - d_{i,j-1}} \int_{d_{i,j-1}}^{d_{ij}} U_i(t) dt,$$

where $U_i(t)$ are independent, mean zero, Gaussian stochastic processes

- Choices for instantaneous process:
 - Wiener process
 - integrated Wiener process
 - non-homogeneous Ornstein-Uhlenbeck process

Nonhomogeneous Ornstein-Uhlenbeck Process

- Covariance structure for instantaneous process:

$$\begin{aligned}\text{var}(U_i(t)) &= \xi(t) = \exp\{\xi_0 + \xi_1 t\} \\ \text{corr}(U_i(s), U_i(t)) &= \exp\{-\alpha|s - t|\}\end{aligned}$$

- Covariances for increment-averaged process:

$$\begin{aligned}\text{cov}(U_{ij}, U_{ik}) &= \frac{e^{\xi_0}}{(d_{ij} - d_{i,j-1})(d_{ik} - d_{i,k-1})} \\ &\times \frac{e^{d_{ij}(\frac{\xi_1}{2} + \alpha)} - e^{d_{i,j-1}(\frac{\xi_1}{2} + \alpha)}}{\frac{\xi_1}{2} + \alpha} \frac{e^{d_{ik}(\frac{\xi_1}{2} - \alpha)} - e^{d_{i,k-1}(\frac{\xi_1}{2} - \alpha)}}{\frac{\xi_1}{2} - \alpha}\end{aligned}$$

Integrated Nonparametric Function Specification

- “Parameter” $g(t)$ is infinite-dimensional
- Assume $g(t)$ is **natural cubic spline**
 - knots at distinct right-hand endpoints
 - cubic polynomial between knots
 - g, g', g'' continuous at knots (hence everywhere)
 - linear before first knot, after last knot

Splitting Up the Integral

- Distinct right-hand endpoints = $\mathbf{t} = (t_1, t_2, \dots, t_r)^T$
- Increment total:

$$\begin{aligned} & \int_{d_1}^{d_2} g(t) dt \\ &= \int_{t_k=d_1}^{t_{k+1}} g(t) dt + \int_{t_{k+1}}^{t_{k+2}} g(t) dt + \dots + \int_{t_{k+p-1}}^{t_{k+p}=d_2} g(t) dt \\ &= (0, \dots, 0, 1, \dots, 1, 0, \dots, 0) \mathbf{G} \end{aligned}$$

for some non-negative integer k and some positive integer p , where

$$\mathbf{G} = \left(\int_{t_0}^{t_1} g(t) dt, \int_{t_1}^{t_2} g(t) dt, \dots, \int_{t_{r-1}}^{t_r} g(t) dt \right)^T$$

Value-Second Derivative Representation

- Define $g_i = g(t_i)$ and $\gamma_i = g''(t_i)$ for $i = 1, 2, \dots, r$
($\gamma_1 = \gamma_r = 0$)
- For $h_i = t_{i+1} - t_i$, we have

$$G_1 = \int_0^{t_1} g(t) dt = \left(t_1 + \frac{t_1^2}{2h_1} \right) g_1 - \frac{t_1^2}{2h_1} g_2 + \frac{h_1 t_1^2}{6 \cdot 2} \gamma_2$$

and

$$G_{i+1} = \int_{t_i}^{t_{i+1}} g(t) dt = \frac{h_i}{2} (g_i + g_{i+1}) - \frac{h_i^3}{24} (\gamma_i + \gamma_{i+1})$$

for $i = 1, 2, \dots, r - 1$

Ah, Linear

- So \mathbf{G} is a linear function of $\mathbf{g} = (g_1, \dots, g_r)^T$ and $\boldsymbol{\gamma} = (\gamma_2, \dots, \gamma_{r-1})^T$:

$$\mathbf{G} = [\mathbf{A}_1, \mathbf{A}_2] \begin{bmatrix} \mathbf{g} \\ \boldsymbol{\gamma} \end{bmatrix} = [\mathbf{A}_1, \mathbf{A}_2] \begin{bmatrix} \mathbf{I} \\ \mathbf{R}^{-1} \mathbf{Q}^T \end{bmatrix} \mathbf{g},$$

where \mathbf{A}_1 , \mathbf{A}_2 , \mathbf{R} and \mathbf{Q} are known matrices (depending only on $\{h_i\}$)

- In fact, \mathbf{G} is linear function of \mathbf{g} alone

Finite-Dimensional Model

- Integrals of infinite-dimensional parameter now reduced to r unknown constants:

$$\begin{aligned} \mathbf{Y}_i &= \mathbf{X}_i \boldsymbol{\beta} + \left[\frac{\int_{d_{i,j-1}}^{d_{ij}} g(t) dt}{d_{ij} - d_{i,j-1}} \right]_{j=1}^{n_i} + \mathbf{Z}_i \mathbf{b}_i + \mathbf{U}_i + \boldsymbol{\epsilon}_i \\ &= \mathbf{X}_i \boldsymbol{\beta} + \begin{bmatrix} \mathbf{c}_{i1}^T \\ \vdots \\ \mathbf{c}_{in_i}^T \end{bmatrix} \mathbf{G} + \mathbf{Z}_i \mathbf{b}_i + \mathbf{U}_i + \boldsymbol{\epsilon}_i \\ &= \mathbf{X}_i \boldsymbol{\beta} + \mathbf{N}_i \mathbf{g} + \mathbf{Z}_i \mathbf{b}_i + \mathbf{U}_i + \boldsymbol{\epsilon}_i \end{aligned}$$

Likelihood

- Log-likelihood given covariance parameters $\boldsymbol{\phi}$, $\boldsymbol{\xi}$, and σ^2

$$\begin{aligned} \ell(\boldsymbol{\beta}, \mathbf{g}; \mathbf{Y}) &= -\frac{1}{2} \log |\mathbf{V}| \\ &\quad -\frac{1}{2} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{N}\mathbf{g})^T \mathbf{V}^{-1} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{N}\mathbf{g}) \end{aligned}$$

where

$$\begin{aligned} -\mathbf{V} &= \text{diag}\{\mathbf{V}_1, \mathbf{V}_2, \dots, \mathbf{V}_m\} \\ -\mathbf{V}_i &= \mathbf{Z}_i \mathbf{D}(\boldsymbol{\phi}) \mathbf{Z}_i^T + \boldsymbol{\Gamma}_i + \sigma^2 \mathbf{I} \end{aligned}$$

Penalized Likelihood

- Log-likelihood given covariance parameters ϕ , ξ , and σ^2

$$\begin{aligned} \ell(\boldsymbol{\beta}, \mathbf{g}; \mathbf{Y}) &= -\frac{1}{2} \log |\mathbf{V}| \\ &\quad -\frac{1}{2} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{N}\mathbf{g})^T \mathbf{V}^{-1} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{N}\mathbf{g}) \end{aligned}$$

- Penalized likelihood:

$$\ell(\boldsymbol{\beta}, \mathbf{g}; \mathbf{Y}) - \frac{\lambda}{2} \int_0^{tr} [g''(t)]^2 dt$$

where $\lambda > 0$ controls smoothness

- $\lambda \rightarrow 0$ implies interpolating
- $\lambda \rightarrow \infty$ implies global regression

Penalized Likelihood, Continued

- Penalized likelihood can be rewritten:

$$\ell(\boldsymbol{\beta}, \mathbf{g}; \mathbf{Y}) - \frac{\lambda}{2} \int_0^{t_r} [g''(t)]^2 dt = \ell(\boldsymbol{\beta}, \mathbf{g}; \mathbf{Y}) - \frac{\lambda}{2} \mathbf{g}^T \mathbf{K} \mathbf{g},$$

where $\mathbf{K} = \mathbf{Q}\mathbf{R}^{-1}\mathbf{Q}^T$ is known

- Now differentiate with respect to $\boldsymbol{\beta}$ and \mathbf{g}

Maximum Penalized Likelihood Estimators

- Assume λ as well as ϕ , ξ , and σ^2 are given
- MPLEs solve the following linear equations:

$$\begin{bmatrix} \mathbf{X}^T \mathbf{V}^{-1} \mathbf{X} & \mathbf{X}^T \mathbf{V}^{-1} \mathbf{N} \\ \mathbf{N}^T \mathbf{V}^{-1} \mathbf{X} & \mathbf{N}^T \mathbf{V}^{-1} \mathbf{N} + \lambda \mathbf{K} \end{bmatrix} \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{g} \end{bmatrix} = \begin{bmatrix} \mathbf{X}^T \mathbf{V}^{-1} \mathbf{Y} \\ \mathbf{N}^T \mathbf{V}^{-1} \mathbf{Y} \end{bmatrix}$$

- Unique solution?

Uniqueness of MPLEs

- By Theorem 4.1 of Green and Silverman (1994), unique solution if $[\mathbf{X}, \mathbf{N}\mathbf{1}, \mathbf{N}\mathbf{t}]$ has full column rank
- **Result:** If $\theta_0\mathbf{1} + \theta_1\mathbf{m} \notin \text{Col}(\mathbf{X})$, where \mathbf{m} is vector of increment midpoints, then

$$\begin{bmatrix} \mathbf{X}^T \mathbf{V}^{-1} \mathbf{X} & \mathbf{X}^T \mathbf{V}^{-1} \mathbf{N} \\ \mathbf{N}^T \mathbf{V}^{-1} \mathbf{X} & \mathbf{N}^T \mathbf{V}^{-1} \mathbf{N} + \lambda \mathbf{K} \end{bmatrix} \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{g} \end{bmatrix} = \begin{bmatrix} \mathbf{X}^T \mathbf{V}^{-1} \mathbf{Y} \\ \mathbf{N}^T \mathbf{V}^{-1} \mathbf{Y} \end{bmatrix}$$

has a unique solution $(\hat{\boldsymbol{\beta}}, \hat{\mathbf{g}}) = \text{MPLE}$

Yet Another Representation: Linear Mixed Model

- From Green (1987) *ISR*, it turns out that

$$\mathbf{g} = (\mathbf{1}, \mathbf{t})\boldsymbol{\delta}_{2 \times 1} + \mathbf{B}\mathbf{a}_{(r-2) \times 1},$$

where \mathbf{B} is a known matrix derived from \mathbf{K}

- Linear mixed model representation:

$$\begin{aligned} \mathbf{Y} &= [\mathbf{X}, \mathbf{NT}] \begin{bmatrix} \boldsymbol{\beta} \\ \boldsymbol{\delta} \end{bmatrix} + \mathbf{NB}\mathbf{a} + \mathbf{Z}\mathbf{b} + \mathbf{U} + \boldsymbol{\epsilon} \\ &= \mathbf{X}_*\boldsymbol{\beta}_* + \mathbf{NB}\mathbf{a} + \mathbf{Z}\mathbf{b} + \mathbf{U} + \boldsymbol{\epsilon}, \end{aligned}$$

where \mathbf{a} is normal($\mathbf{0}, \tau\mathbf{I}$) and $\tau = 1/\lambda$

– Tricky: *not* the data-generating mechanism

- “BLUE” of $\boldsymbol{\beta}$ and “BLUP” of \mathbf{g} from mixed model = MPLEs

Estimation of Covariance and Smoothing Parameters

- Use REML = Restricted Maximum Likelihood
 - standard method for linear mixed models

- Define $\mathbf{V}_* = \tau(\mathbf{N}\mathbf{B})(\mathbf{N}\mathbf{B})^T + \mathbf{V}$

- REML criterion for $(\boldsymbol{\phi}^T, \boldsymbol{\xi}^T, \sigma^2, \tau)$ is

$$\begin{aligned} \ell_R((\boldsymbol{\phi}^T, \boldsymbol{\xi}^T, \sigma^2, \tau); \mathbf{Y}) \\ &= -\frac{1}{2} \log |\mathbf{V}_*| - \frac{1}{2} \log |\mathbf{X}_*^T \mathbf{V}_*^{-1} \mathbf{X}_*| \\ &\quad - \frac{1}{2} (\mathbf{Y} - \mathbf{X}_* \hat{\boldsymbol{\beta}}_*)^T \mathbf{V}_*^{-1} (\mathbf{Y} - \mathbf{X}_* \hat{\boldsymbol{\beta}}_*) \end{aligned}$$

- Given REML estimates, MPLEs are immediate

Back to the Carbon Sequestration Data

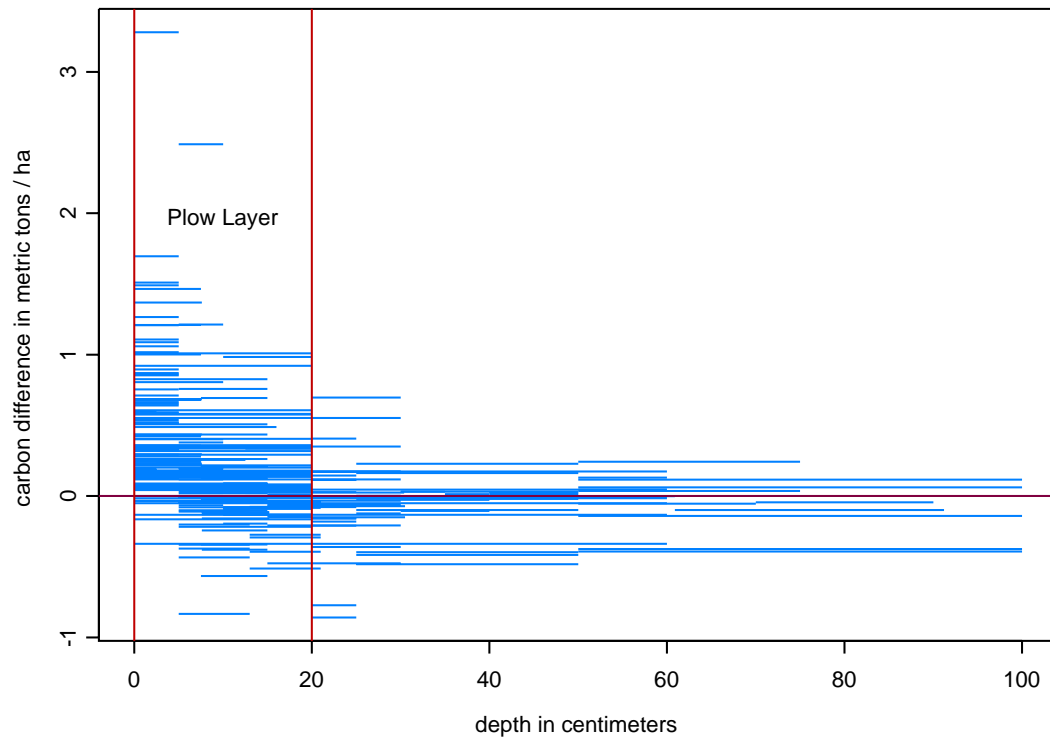
- Now have all the tools needed for inference in the carbon data set
- **Goals:**
 - identify important fixed effects
 - identify important sources of variation and correlation
 - estimate depth function
 - estimate expected carbon sequestered due to no-till:

$$\text{IPCC} = \int_0^{30} (\mathbf{X}_{00}^T \boldsymbol{\beta} + g(t)) dt,$$

where \mathbf{X}_{00} = covariates at 20 years after management change

The Plow Layer

- Top 15–20 cm of agricultural soil



Model Specification

- Fixed effects:
 - wet/dry climate
 - aquic/non-aquic soils
 - years since management change
 - parametric or nonparametric year*depth interactions
- Random effect: soil core
- Stochastic process: non-homogeneous OU

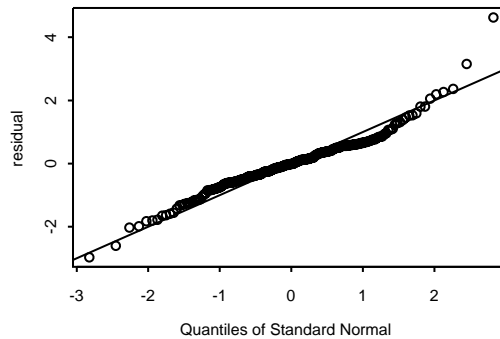
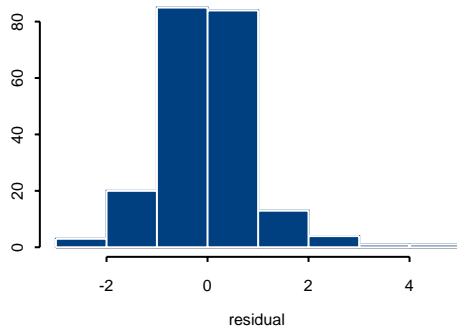
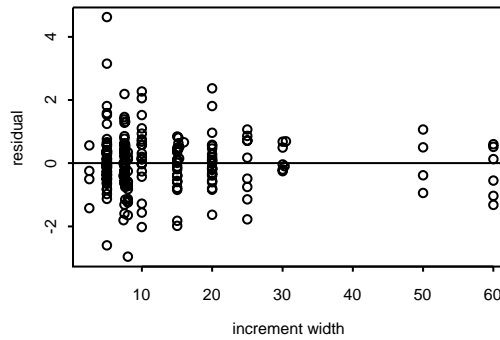
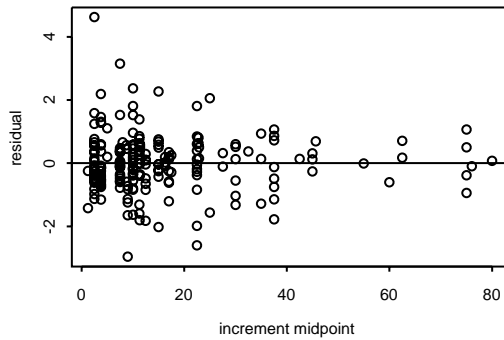
Some Results

- Estimation results from REML and MPLE:

Parameter	Model 1		Model 2	
	Estimate	Standard Error	Estimate	Standard Error
aquic	-0.1383	0.0587	-0.1371	0.0592
wet	0.1725	0.0593	0.1720	0.0596
years	0.0157	0.0047	0.0031	0.0032
year*depth	-0.0003	0.0001		
ϕ	0.0078	0.0077	0.0094	0.0093
σ^2	0.0073	0.0091	0.0064	0.0102
ξ_0	-0.8260	0.2368	-0.7911	0.2463
ξ_1	-0.0601	0.0205	-0.0643	0.0219
α	0.2607	0.0447	0.2693	0.0490
$\tau = \lambda^{-1}$	0.0326	0.0046	0.0189	0.0026
$\tau_x = \lambda_x^{-1}$			0.00005	0.000008

Residual Diagnostics

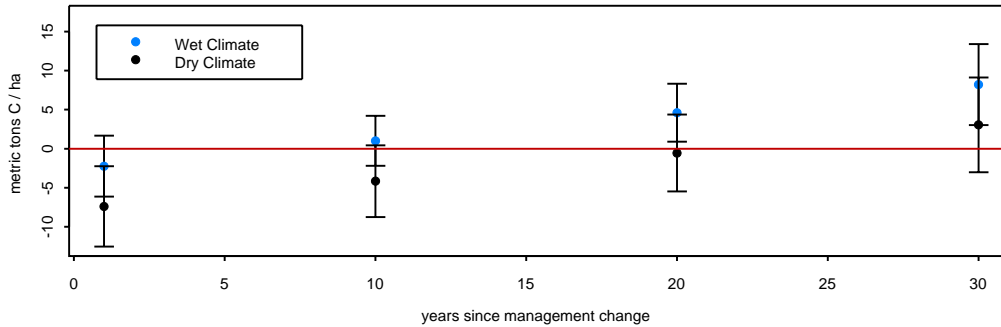
- Accounting for OU dependence structure



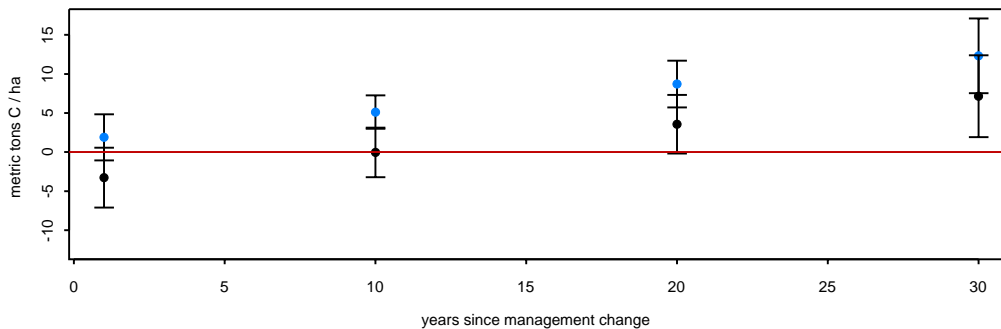
Intergovernmental Panel on Climate Change Integrals

- Estimated IPCC integrals

Carbon Change in Aquic Soils



Carbon Change in Non-Aquic Soils



Summary and Future Research

- Increment averaging cannot be ignored in soil core data
- Semiparametric stochastic mixed model
 - flexibly models increment averages
 - handles fixed and random effects
 - fits in standard linear mixed model framework
- Further work:
 - more modeling and diagnostics for carbon data
 - extension to generalized linear mixed models