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

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Outline

- Carbon sequestration in agricultural soils
  - greenhouse gases and carbon credits
  - soil sampling and increment-averaged data
- Semiparametric mixed models
  - integrated cubic splines
  - penalized splines
- Analysis using mixed model formulation
  - fitting with standard software
  - automatic smoothing parameter selection
  - results and extensions

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, CO_2, methane, nitrous oxide, etc.

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

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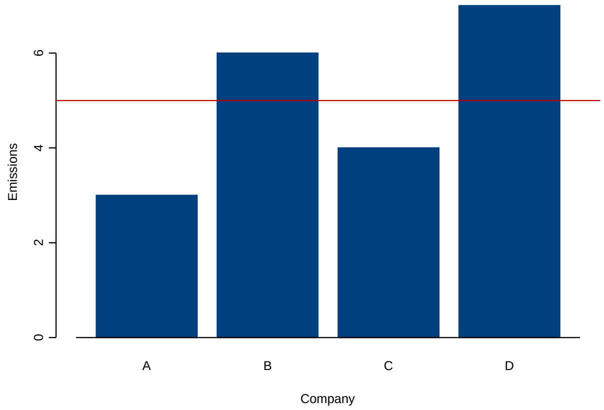
- Participants voluntarily commit to GHG reductions
- Creates a "cap-and-trade" market
  - can make own reductions
  - can buy credits from others with extra reductions to sell



Extra Reductions from No-Till Agriculture

- 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

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** by slowing decomposition

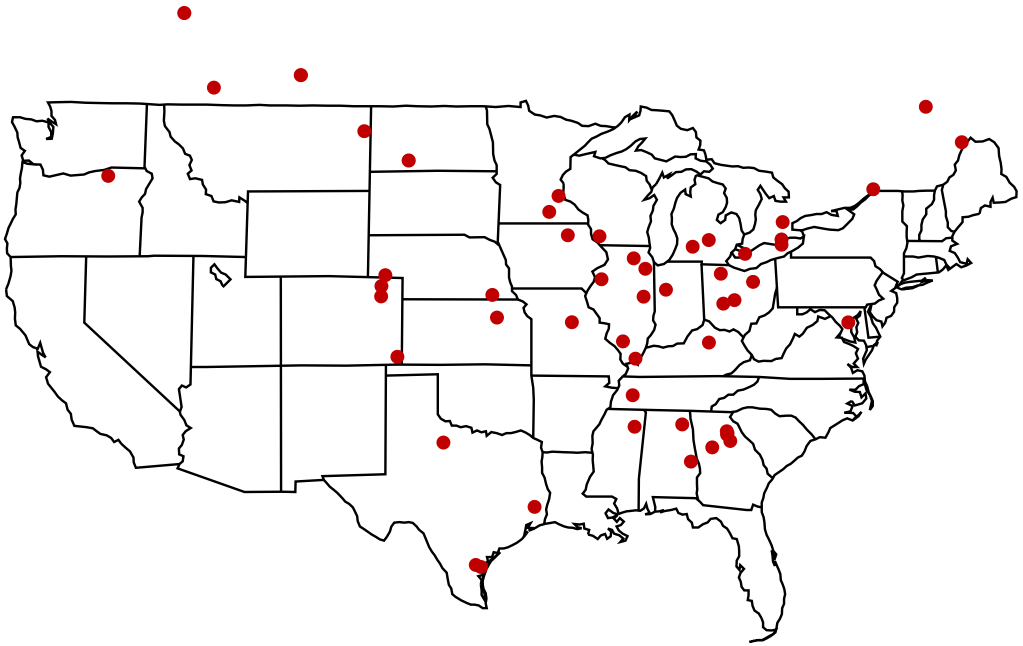
Key Question for Carbon Credits

- Corporations faced with caps on GHG emissions could buy **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

- 211 tillage comparisons on paired fields from 63 studies

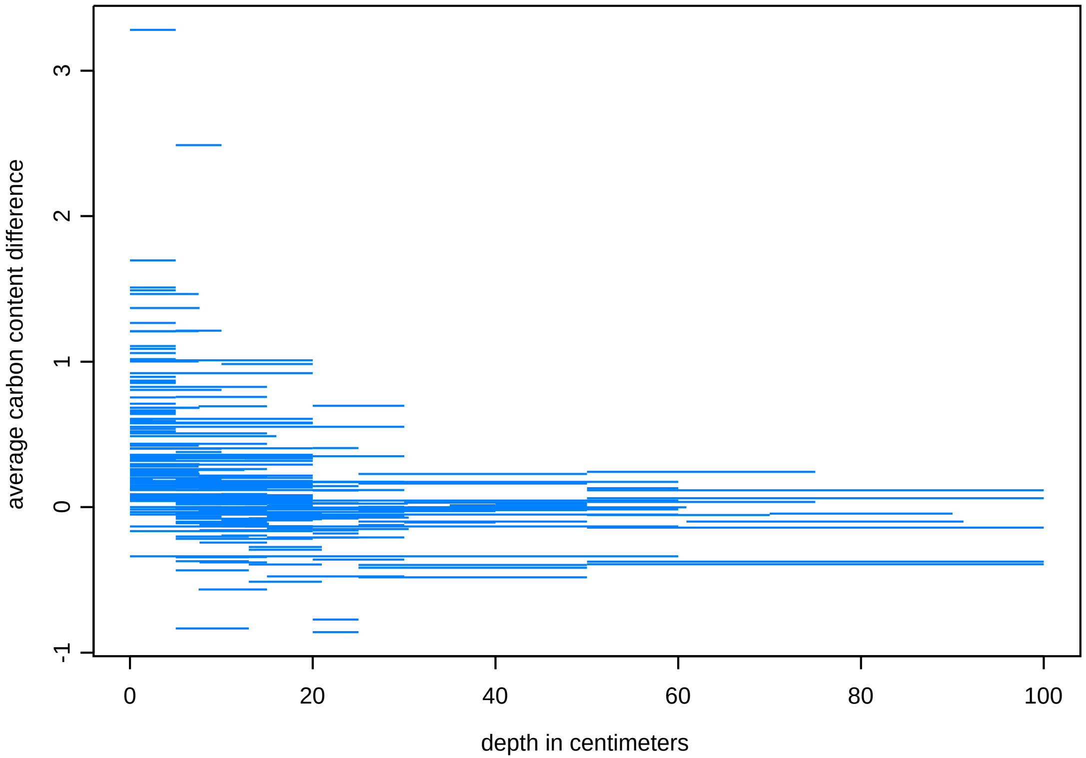


Soil Core Samples

- 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

Increment-Averaged Data

- Difference in metric tons C ha^{-1} vs. depth



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-site dependence
  - increments within same site may be correlated
- Other effects
  - time since change to no-till
  - climate regime
  - soil type

Semiparametric Mixed Model: Longitudinal

- Observation on subject i at jth time point

$$Y_{ij} = \boldsymbol{x}_{ij}^T \boldsymbol{\beta} + g(t_{ij}; \boldsymbol{w}_i) + \boldsymbol{z}_{ij}^T \boldsymbol{b}_i + \epsilon_{ij}$$

  - e.g., Zhang, Lin, Raz, Sowers (1998) *JASA*
  - $\boldsymbol{x}_{ij}, \boldsymbol{w}_i, \boldsymbol{z}_{ij}$: known covariates
  - $g(t; \boldsymbol{w}_i)$: smooth function of time
  - $\boldsymbol{b}_i$: independent q-vectors of random effects
  - ϵ_{ij}: independent errors
- Does not handle increment averages

Semiparametric Stochastic Mixed Model: Increments

- Increment average in ith core, jth increment

$$Y_{ij} = \boldsymbol{x}_{ij}^T \boldsymbol{\beta} + \frac{1}{d_{ij} - d_{i,j-1}} \int_{d_{i,j-1}}^{d_{ij}} g(t; \boldsymbol{w}_i)\, dt + \boldsymbol{z}_{ij}^T \boldsymbol{b}_i + \epsilon_{ij}$$

  - $\boldsymbol{x}_{ij}, \boldsymbol{w}_i, \boldsymbol{z}_{ij}$: known covariates
  - $g(t; \boldsymbol{w}_i)$: smooth function of depth
  - $\boldsymbol{b}_i$: independent q-vectors of random effects
  - ϵ_{ij}: independent errors

Additive Varying Coefficient Models

- Smooth component functions of depth:

$$\alpha_\ell(t) = \alpha_{0\ell} + \alpha_{1\ell} t + \sum_{k=1}^{K} a_{k\ell}(t - \kappa_k)_+$$

  - truncated line basis with knots $\{\kappa_k\}_{k=1}^{K}$
  - penalize unnecessary slope changes via $\lambda_\ell^2 \sum_{k=1}^{K} a_{k\ell}^2$

- Additive depth function with varying coefficients:

$$g(t; \boldsymbol{w}) = \sum_\ell \alpha_\ell(t) w_\ell$$

  - (Hastie and Tibshiranie, 1993; Ruppert, Wand, and Carroll, 2003)

Mixed Model Formulation of Penalized Splines

- Integrated version of varying-coefficient model:

$$Y_{ij} = \boldsymbol{x}_{ij}^T\boldsymbol{\beta} + \sum_{\ell}\left(\alpha_{0\ell} + \alpha_{1\ell}\frac{d_{i,j-1} + d_{ij}}{2}\right) w_{\ell i}$$
$$+ \sum_{\ell}\left(\sum_{k=1}^{K}\frac{a_{k\ell}}{2}\left\{(d_{ij} - \kappa_k)_+^2 - (d_{i,j-1} - \kappa_k)_+^2\right\}\right) w_{\ell i}$$
$$+ \boldsymbol{z}_{ij}^T\boldsymbol{b}_i + \epsilon_{ij}$$

- Regard spline as linear mixed model with $a_{k\ell}$ iid $\mathrm{N}(0, \sigma_{a\ell}^2)$, and $\sigma_{a\ell}^2 = \sigma^2/\lambda_\ell^2$
  - automatic choice of penalty constants λ_ℓ via REML

Back to the Carbon Sequestration Data

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

$$\text{IPCC} = \int_0^{30} \left(\boldsymbol{x}^T \boldsymbol{\beta} + g(t; \boldsymbol{w}) \right) \, dt,$$

$\boldsymbol{x}, \boldsymbol{w} =$ covariates at 20 years after management change

Model Specification

- Available data: 211 paired increments from 63 studies
- Covariates:
  - `study`: study/site identifier
  - `wet`: wet/dry climate
  - `aquic`: aquic/non-aquic soils
  - `years` since management change
- Nonparametric functions:
  - parametric term $\boldsymbol{x}_{ij}^T\boldsymbol{\beta}$ may not be so useful
  - focus on varying coefficient models (parametric-by-nonparametric interactions)

Model Selection: Focus on Interaction Models

depth	aquic*depth	wet*depth	years*depth	AIC	r
	X			323	0.609
	X	X		226	0.797
			X	226	0.789
X	X			218	0.818
X	X	X	X	217	0.854
X				216	0.809
X	X		X	216	0.835
	X	X		216	0.812
		X		214	0.808
X	X	X		212	0.834
X			X	211	0.825
X		X		209	0.828
X		X	X	200	0.846
	X	X	X	193	0.851
		X	X	191	0.846

Final Model

- AIC suggests the following model:

$$
\begin{aligned}
g(t;\boldsymbol{w}_i) &= \Big(\alpha_{01} + \alpha_{11} t + \textstyle\sum_{k=1}^{K} a_{k1}(t-\kappa_k)_+\Big)\,\texttt{wet}_i \\
&\quad + \Big(\alpha_{02} + \alpha_{12} t + \textstyle\sum_{k=1}^{K} a_{k2}(t-\kappa_k)_+\Big)\,\texttt{years}_i \\
Y_{ij} &= \frac{1}{d_{ij} - d_{i,j-1}} \int_{d_{i,j-1}}^{d_{ij}} g(t;\boldsymbol{w}_i)\,dt + b_i + \epsilon_{ij}
\end{aligned}
$$

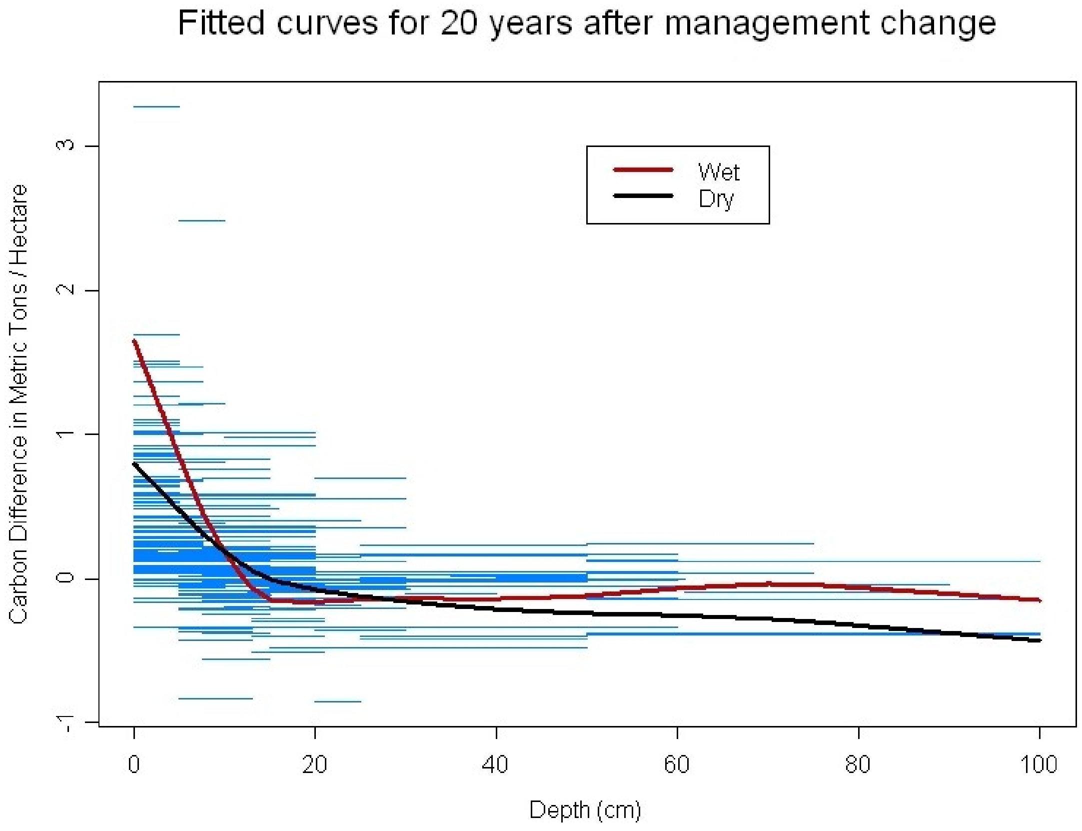
$\{a_{k\ell}\}$ iid $\mathsf{N}(0,\sigma^2_{a\ell})$, $\{b_i\}$ iid $\mathsf{N}(0,\sigma^2_b)$, $\{\epsilon_{ij}\}$ iid $\mathsf{N}(0,\sigma^2)$

S-Plus Code

```
#
# Following Ngo and Wand (2003), Smoothing with mixed model software.
# Set up linear splines, then integrate over increments.
#
Z1 <- outer(d1, knots, "-")
Z1 <- Z1 * (Z1 > 0)
Z2 <- outer(d2, knots, "-")
Z2 <- Z2 * (Z2 > 0)
Z <- 0.5 * diag(1/(d2 - d1)) %*% (Z2^2 - Z1^2)
#
# Create design matrices.
#
X <- cbind(wet, middepth*wet, years, middepth*years)
Z <- cbind(wet*Z, years*Z, study)
re.block.inds <- list(1:K, (K + 1):(2 * K), (2 * K + 1):(2 * K + nstudy))
Z.block <- list()
for(i in 1:length(re.block.inds))
    Z.block[[i]] <- as.formula(paste("~Z[,c(", paste(re.block.inds[[
        i]], collapse = ","), ")]-1"))
#
# Fit the mixed model using lme.
#
fit <- lme(y ~ -1 + X, random = pdBlocked(Z.block, pdClass = "pdIdent"),
    method = "REML")
```

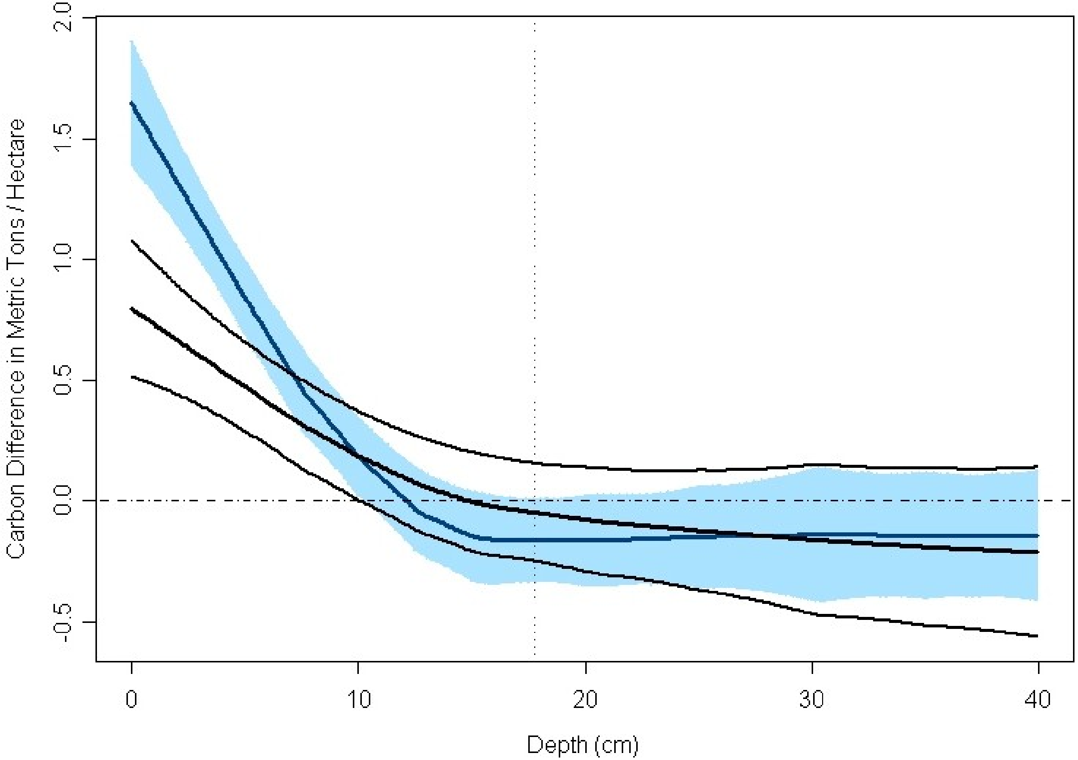
Results: Fitted Curves

- Varying coefficient model fit to no-till data



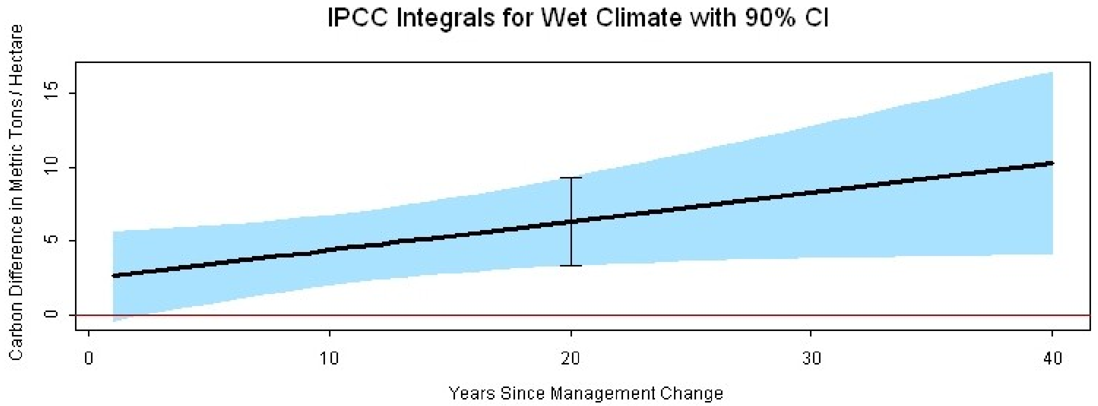
Results: Pointwise Confidence Intervals

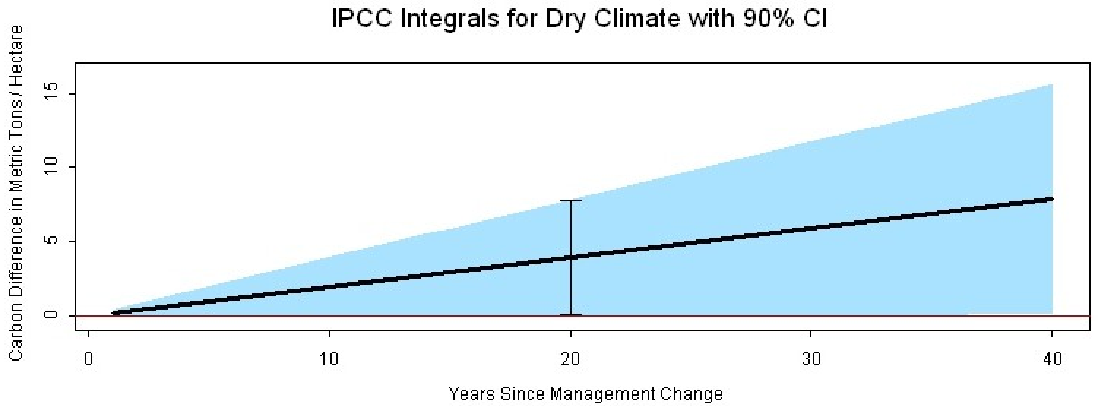
- Fitted curves and confidence intervals



Intergovernmental Panel on Climate Change Integrals

- Cumulative carbon storage versus year in top 30 cm





Summary

- Increment averaging cannot be ignored in core data
- Semiparametric mixed model
  - flexibly models increment averages
  - handles fixed and random effects
  - fits in standard linear mixed model framework
- Further work
  - investigate other dependence structures for noise
  - diagnostics complicated due to increment averaging