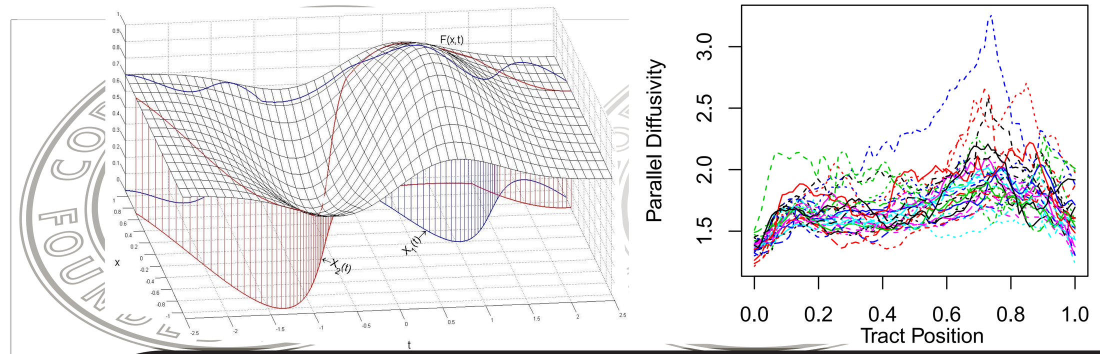

Functional Generalized Additive Models

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Motivating Dataset

- Diffusion Tensor Imaging (DTI) study comparing the white matter tracts of Multiple Sclerosis (MS) patients with healthy controls
- Each scan produces a signal/function $X(t)$ of tract position t
- Goal: use $X(t)$ to predict (scalar) health outcome Y and identify which portions of the tract are most important for the prediction

Standard Model: FLM

- Assume that the predictor, $X(\cdot)$, is observed at a dense grid of points on closed interval $\mathcal{T}$.
- Most commonly used model is

$$E(Y_i|X_i) = \theta_0 + \int_{\mathcal{T}} \beta(t)X_i(t)dt,$$

where $\beta(\cdot)$ is an unknown smooth regression function and $X(t)$ is a functional covariate.
- For each t effect of $X_i(t)$ on Y_i is linear.

New Model: FGAM

- Linearity assumption of FLM is often too strong
- We desire a more flexible model that remains easy to understand and estimate
- We propose the model

$$E(Y_i|X_i) = \theta_0 + \int_{\mathcal{T}} F\{X_i(t), t\}\, dt,$$

where $F(x,t)$ is an unknown, smooth function
- Two tuning parameters control complexity of F
- Need identifiability constraints

Intuition From Multivariate Data

- Let $x_{ij} = X_i(t_j)$; $\quad \beta_j = \beta(t_j)$; $\quad j = 1, \ldots, J$
- Thinking of a Riemann sum, consider

$$E(Y_i|\mathbf{X}_i) = \sum_{j=1}^{p} \beta_j x_{ij} = \sum_{j=1} \frac{\beta_j(t_j)}{J} X_i(t_j) J^{-1}$$

- FLM obtained as limit of this LM as $J \to \infty$.
- Now define $f_j(\cdot) = F(\cdot, t_j)J^{-1}$ and consider AM

$$E(Y_i|\mathbf{X}_i) \sum_{j=1}^{J} f_j\{x_{ij}\} = \sum_{j=1}^{J} F\{x_{ij}, t_j\}J^{-1}$$

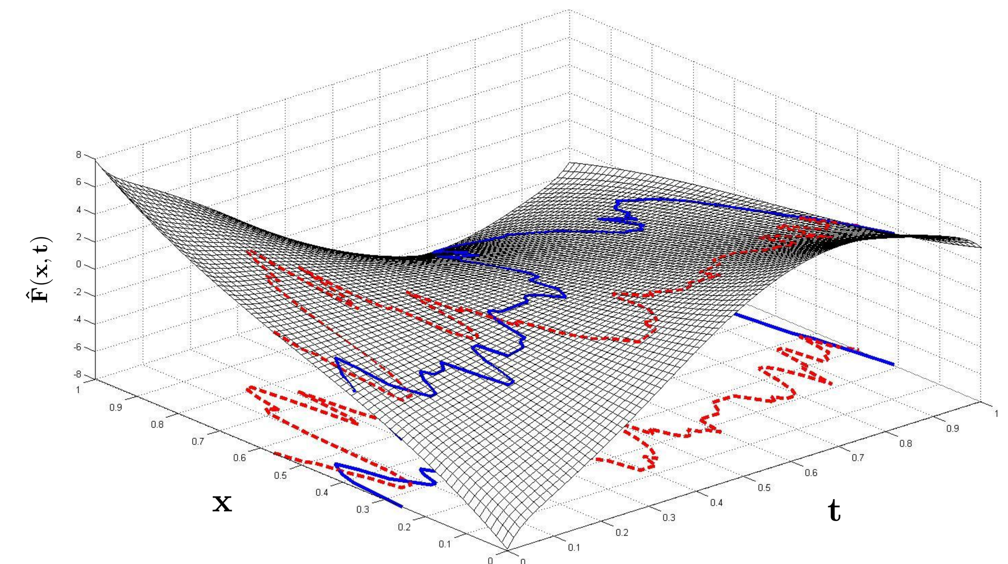
- FGAM is limit of this AM as $J \to \infty$.

Contributions

FGAM: A novel regression model for association studies between a scalar response and a functional predictor that can model complex response-predictor relationships while remaining interpretable.

Our model
- is highly flexible (low bias)
- avoids curse of dimensionality (low variance)
- is easy to interpret (not a "black box")
- Easily fit using fast, polished R package mgcv
- has FLM as a special case ($F(x,t) = \beta(t)x$)

Example Estimated Surface



- Interpretation: Small t values appear most influential; subject with red predictor curve gets higher predicted response
- Nonlinearity in x suggests that an FLM may be inadequate

R Implementation

- FGAM implemented in R package `refund`
- Function `fgam` acts as a wrapper for `gam` in `mgcv`
- E.g. $g(Y_i) = \theta_0 + f(z_1) + \int_{\mathcal{T}_1} F(X_{i1}(t),t)dt + \int_{\mathcal{T}_2} \beta(t)X_{i2}(t)dt$ can be fit by specifying

```
fgam(y~s(z1)+af(X1)+lf(X2),...)
```

- Extends `mgcv`; therefore, it can handle alternative penalties and bases, generalized responses, random effects, automatic model selection, multivariate smooth terms, etc.

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Estimation

- The surface $F(\cdot,\cdot)$ is parameterized using tensor products of B-splines:

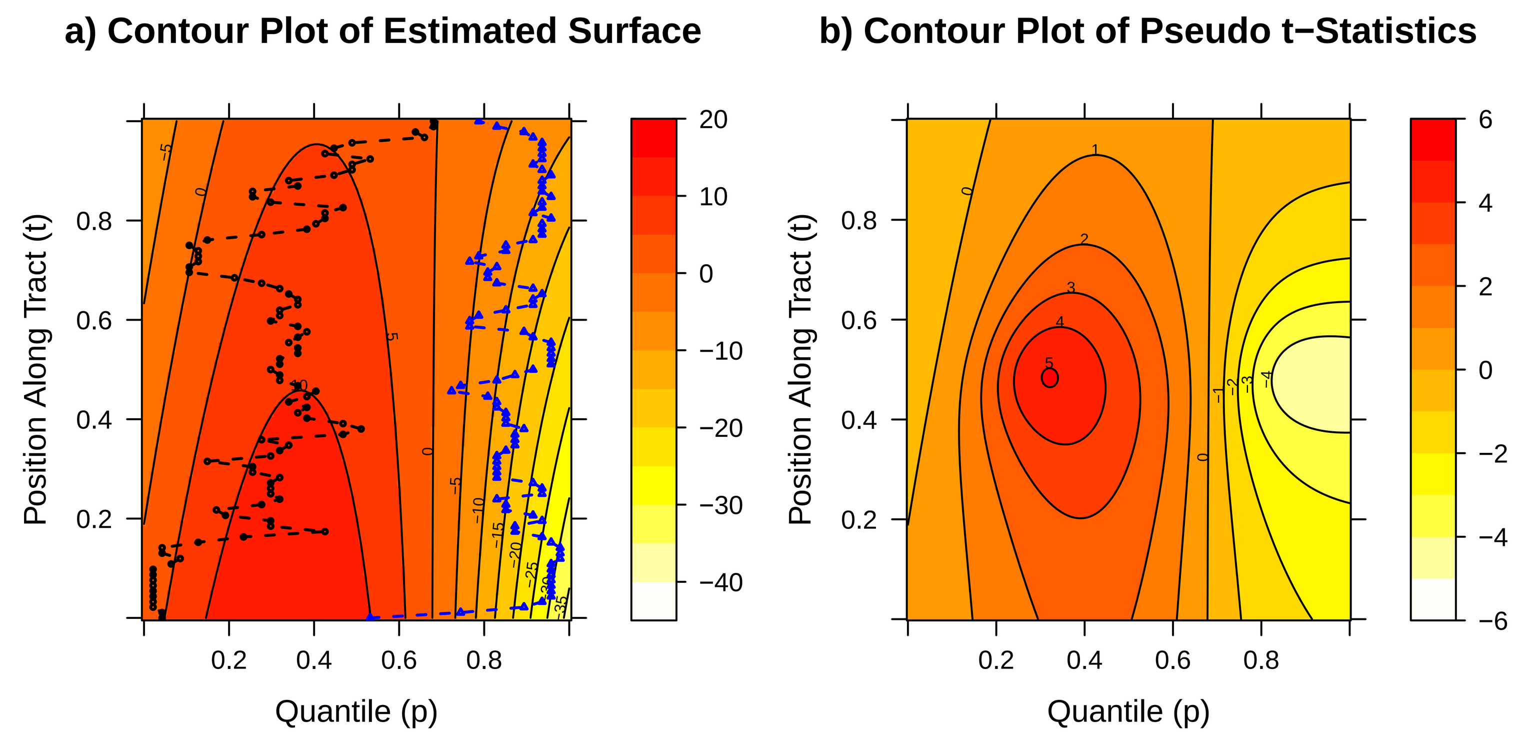
$$F(x,t) = \sum_{j=1}^{K_x}\sum_{k=1}^{K_t} \theta_{j,k} B_j^X(x) B_k^T(t)$$

- We use the P-splines of Eilers & Marx (1996)
- $\{B_j^X(x) : j = 1, \ldots, K_x\}$ and $\{B_k^T(x) : k = 1, \ldots, K_t\}$ are spline bases.
- Y can be from any exponential family distribution
- Smoothing parameters are chosen using generalized cross validation
- Modularity of P-splines: including multiple functional or scalar predictors in the model is simple
- Use generalization of Bayesian confidence bands of Wahba (1983) to construct approximate confidence bands for the true surface to account for bias due to smoothing
- Also obtain confidence bands for the estimated second derivative surface w.r.t. x:

  Significant differences from $\partial^2/\partial x^2 F(x,t) = 0$ at a particular (x,t) suggests FLM does not hold there
- Can transform functional predictor to possibly improve predictions or numerical stability

Results

- Outcome variable is score on a cognitive test called PASAT, which takes integer values between $0-60$
- Predictor is transformed parallel diffusivity: largest eigenvalue summarizing the diffusion at position t
  - Transformation used is the empirical cdf: $\widehat{F}(p,t)$ is effect of $X(t)$ being at its pth quantile
- a) Plot of $\widehat{F}(p,t)$ including two subjects' transformed predictor curves
- Black curve in a) will have higher predicted response than the blue
- b) is contour plot of $\widehat{F}(p,t)$ divided by its estimated standard error
- Middle values of t appear to be very influential on PASAT score
- Good out-of-sample RMSE performance compared with other popular scalar on function regression models



- Simulation studies show
  - FGAM performs nearly as well at out-of sample prediction as FLM when the true model is an FLM
  - FGAM offers substantial gains in predictive performance when FLM is not the true model
  - FGAM is very competitive with other non-FLM scalar on function regression models
  - The proposed Bayesian confidence intervals have good average coverage probabilities

Current Work

- Developing formal test of H_0:FLM vs. H_1:FGAM
  - Use mixed model representation and test particular variance components
- Extending to sparsely observed predictor curves
  - Bayesian MM - estimation via MCMC or VB

For Further Details

- McLean et al. (2012), Functional Generalized Additive Models, *Journal of Computational and Graphical Statistics*, to appear.
- Visit `courses2.cit.cornell.edu/mwmclean`
- R code available in `refund` package on CRAN