Lecture 22: Nonparametric Regression

STA702

Merlise Clyde
Duke University

Semi-parametric Regression

- Consider model

$$Y_1, \ldots, Y_n \sim \mathsf{N}\left(\mu(\mathbf{x}_i, \boldsymbol{\theta}), \sigma\right)$$

- Mean function $\mathsf{E}[Y_i \mid \boldsymbol{\theta}] = \mu(\mathbf{x}_i, \boldsymbol{\theta})$ falls in some class of nonlinear functions
- Basis Function Expansion

$$\mu(\mathbf{x}, \boldsymbol{\theta}) = \sum_{j=1}^{J} \beta_j b_j(\mathbf{x})$$

- $b_j(\mathbf{x})$ is a pre-specified set of *basis functions* and $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_J)^T$ is a vector of coefficients or coordinates wrt to the basis

Examples

- Taylor Series expansion of $\mu(\mathbf{x})$ about point χ

$$\begin{aligned}\mu(x) &= \sum_k \frac{\mu^{(k)}(\chi)}{k!}(x-\chi)^k \\ &= \sum_k \beta_k (x-\chi)^k\end{aligned}$$

- polynomial basis
- can require a large number of terms to model globally
- can have really poor behavior in regions without data
- each basis function has a "global" impact

Other Basis Functions

- cubic splines

$$b_j(x, \chi_j) = (x - \chi_j)^3_+$$

- Gaussian Radial Basis

$$b_j(x, \chi_j) = \exp\left(\frac{(x - \chi_j)^2}{l^2}\right)$$

- centers of basis functions χ_j
- width parameter l controls the scale at which the mean function dies out as a function of $\mathbf{x}$ from the center
- localized basis elements

Local Models

- Multivariate Gaussian Kernel g with parameters $\boldsymbol{\omega} = (\boldsymbol{\chi}, \boldsymbol{\Lambda})$

$$b_j(\mathbf{x}, \boldsymbol{\omega}_j) = g(\boldsymbol{\Lambda}_j^{1/2}(\mathbf{x} - \boldsymbol{\chi}_j)) = \exp\left\{-\frac{1}{2}(\mathbf{x} - \boldsymbol{\chi}_j)^T \boldsymbol{\Lambda}_j (\mathbf{x} - \boldsymbol{\chi}_j)\right\}$$

- Gaussian, Cauchy, Exponential, Double Exponential kernels (can be asymmetric)
- translation and scaling of wavelet families
- basis functions formed from a generator function g with location and scaling parameters

Bayesian Nonparametric Model

Mean function

$$\mu(\mathbf{x}_i) = \sum_j^J b_j(\mathbf{x}_i, \boldsymbol{\omega}_j)\beta_j$$

- conditional on the basis elements back to our Bayesian regression model
- usually uncertainty about number of basis elements needed
- could use BMA or other shrinkage priors
- how should coefficients scale as J increases?
- choice of J?
- what about uncertainty in $\boldsymbol{\omega}$ (locations and scales)?
- priors on unknowns (J, $\{\beta_j\}$, $\{\boldsymbol{\omega}_j\}$) induces a prior on functions!

Stochastic Expansions

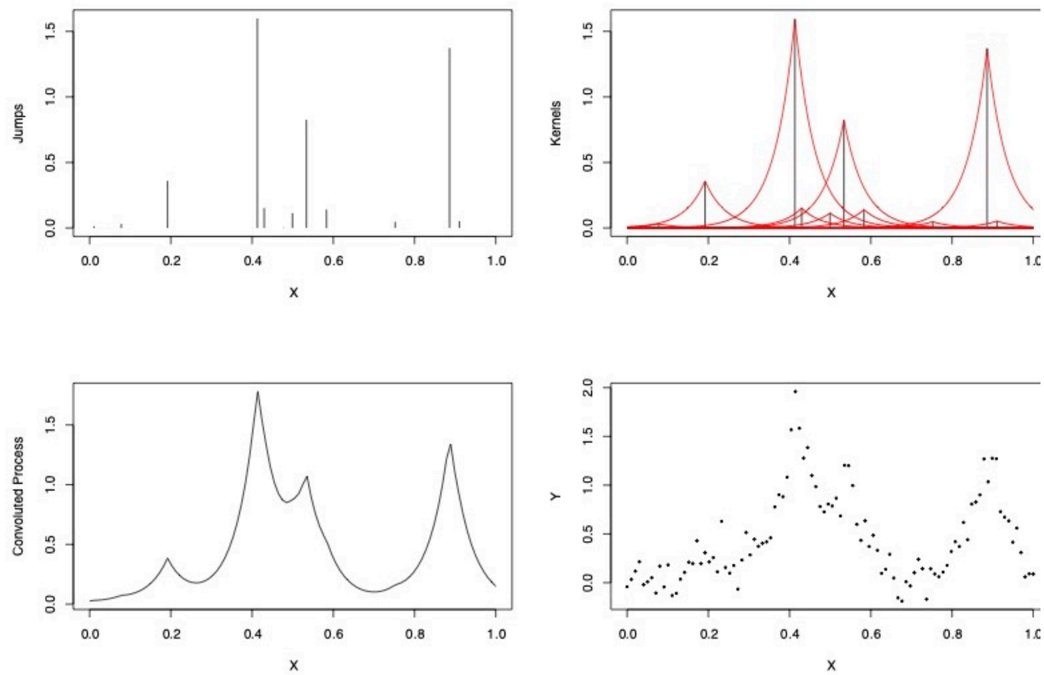
$$\mu(\mathbf{x}) = \sum_{j=0}^{J} b_j(\mathbf{x}, \boldsymbol{\omega}_j)\beta_j = \sum_{j=0}^{J} g(\boldsymbol{\Lambda}^{1/2}(\mathbf{x} - \boldsymbol{\omega}_j))\beta_j$$

- introduce a Lévy measure $\nu(d\beta, d\boldsymbol{\omega})$
- Poisson distribution $J \sim \textsf{Poi}(\nu_+)$ where $\nu_+ \equiv \nu(\mathbb{R} \times \boldsymbol{\Omega}) = \iint \nu(\beta, \boldsymbol{\omega}) d\beta\, d\boldsymbol{\omega}$
- conditional prior on $\beta_j, \boldsymbol{\omega}_j \mid J \overset{\text{iid}}{\sim} \pi(\beta, \boldsymbol{\omega}) \propto \nu(\beta, \boldsymbol{\omega})$
- Conditions on ν (and g)
  - need to have that $|\beta_j|$ are absolutely summable
  - finite number of large coefficients (in absolute value)
  - allows an infinite number of small $\beta_j \in [-\epsilon, \epsilon]$

See Wolpert, Clyde and Tu (2011) AoS

Gamma Process Example

$$\nu(\beta, \chi) = \beta^{-1} e^{-\beta\eta} \gamma(\chi) d\beta\, d\chi$$



Stochastic Integral Representation

$$\mu(\mathbf{x}) = \sum_{j=0}^{J} b_j(\mathbf{x}, \boldsymbol{\omega}_j)\beta_j = \sum_{j=0}^{J} g(\boldsymbol{\Lambda}^{1/2}(\mathbf{x} - \boldsymbol{\omega}_j))\beta_j = \int_{\boldsymbol{\Omega}} b(\mathbf{x}, \boldsymbol{\omega})\mathcal{L}(d\boldsymbol{\omega})$$

- $\mathcal{L}$ is a **random signed measure** (generalization of Completely Random Measures)

$$\mathcal{L} \sim \textsf{Lévy}(\nu) \qquad\qquad \mathcal{L}(d\boldsymbol{\omega}) = \sum_{j \le J} \beta_j \delta_{\boldsymbol{\omega}_j}(d\boldsymbol{\omega})$$

- Lévy-Khinchine Poisson Representation of $\mathcal{L}$
- Poisson number of support points (possibly infinite!)
- random support points of discrete measure $\{\boldsymbol{\omega}_j\}$
- random "jumps" β_j
- Convenient to think of a random measure as stochastic process where $\mathcal{L}$ assigns random variables to sets $A \in \boldsymbol{\Omega}$

Examples

- gamma process

$$\nu(\beta, \boldsymbol{\omega}) = \beta^{-1} e^{-\beta\eta} \pi(\boldsymbol{\omega}) d\beta\, d\boldsymbol{\omega}$$
$$\mathcal{L}(A) \sim \mathsf{Gamma}(\pi(A), \eta)$$

- non-negative coefficients plus non-negative basis functions allows priors on non-negative functions without transformations
- α-Stable process (Cauchy process is $\alpha = 1$)

$$\nu(\beta, \boldsymbol{\omega}) = c_\alpha |\beta|^{-(\alpha+1)}\, \pi(\boldsymbol{\omega}) \qquad 0 < \alpha < 2$$

- $\nu^+(\mathbb{R}, \boldsymbol{\Omega}) = \infty$ for both the Gamma and α-Stable processes
- Fine in theory, but problematic for MCMC!

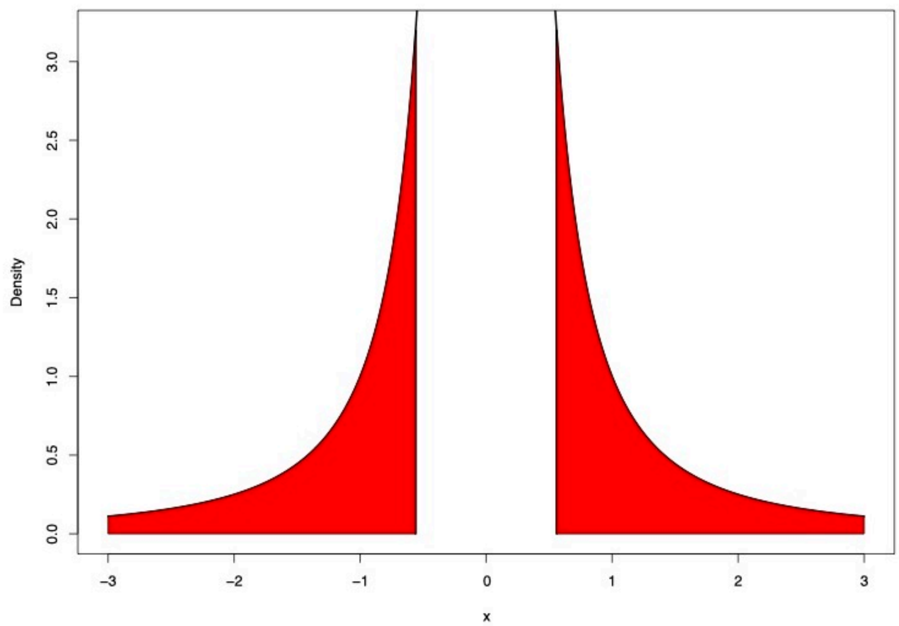
Prior Approximation I

Truncate measure ν to obtain a finite expansion:

- Finite number of support points $\boldsymbol{\omega}$ with β in $[-\epsilon, \epsilon]^c$
- Fix ϵ (for given prior approximation error)
- Use approximate Lévy measure $\nu_\epsilon(\beta, \boldsymbol{\omega}) \equiv \nu(\beta, \boldsymbol{\omega}) \mathbf{1}(|\beta| > \epsilon)$
- $\Rightarrow J \sim \textsf{Poi}(\nu_\epsilon^+)$ where $\nu_\epsilon^+ = \nu([-\epsilon, \epsilon]^c, \boldsymbol{\Omega})$
- $\Rightarrow \beta_j, \boldsymbol{\omega}_j \overset{\text{iid}}{\sim} \pi(d\beta, d\boldsymbol{\omega}) \equiv \nu_\epsilon(d\beta, d\boldsymbol{\omega}) / \nu_\epsilon^+$
- for α-Stable, the approximation leads to double Pareto distributions for β

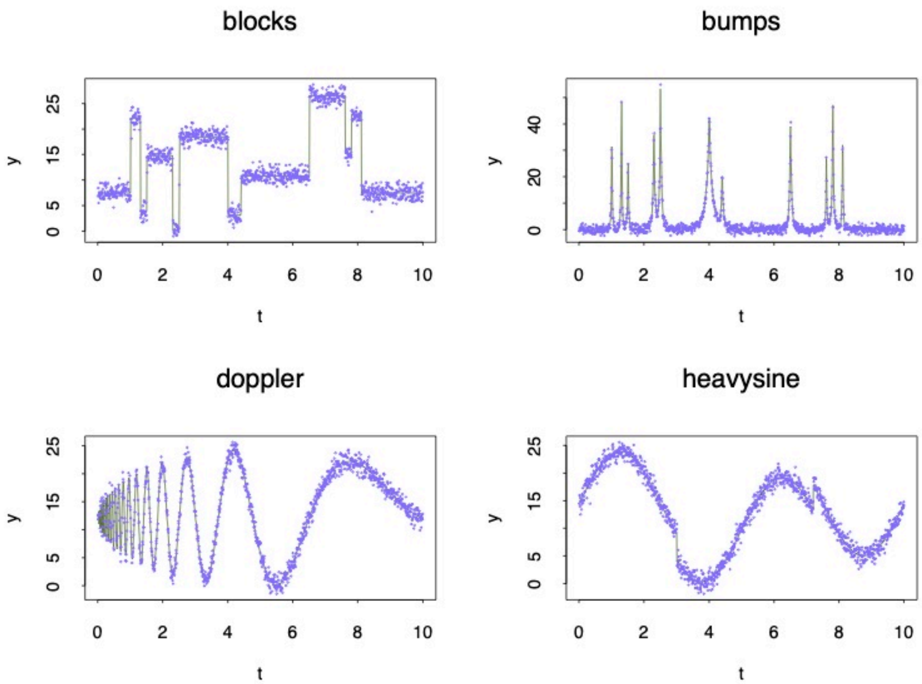
$$\pi(\beta_j) = \frac{\epsilon}{2\eta} |\beta|^{-\alpha - 1} \mathbf{1}_{|\beta| > \frac{\epsilon}{\eta}}$$

Truncated Cauchy Process Prior

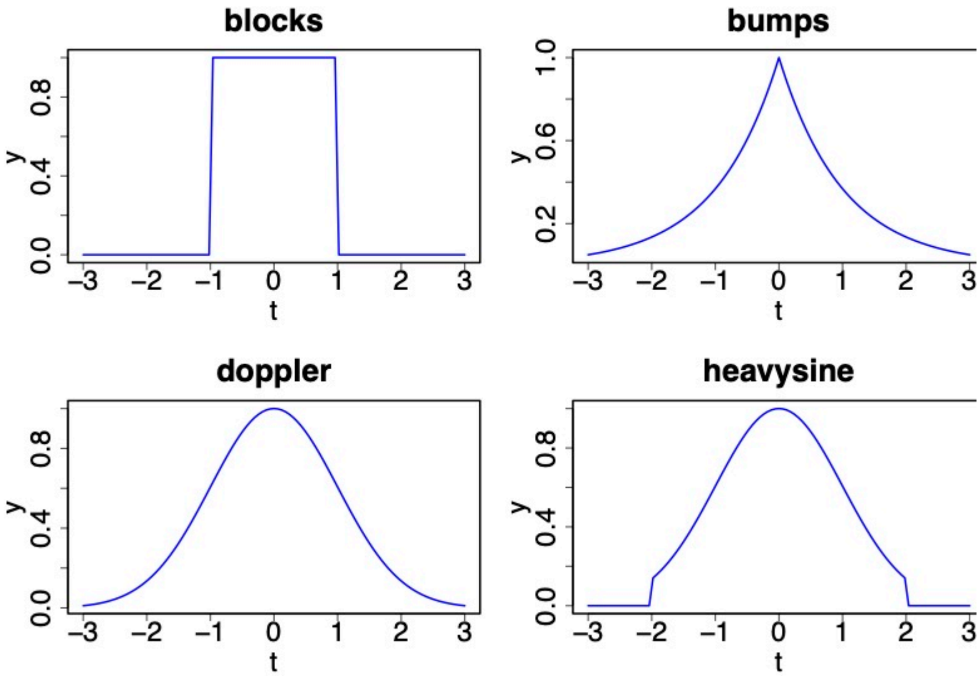


Truncated Cauchy

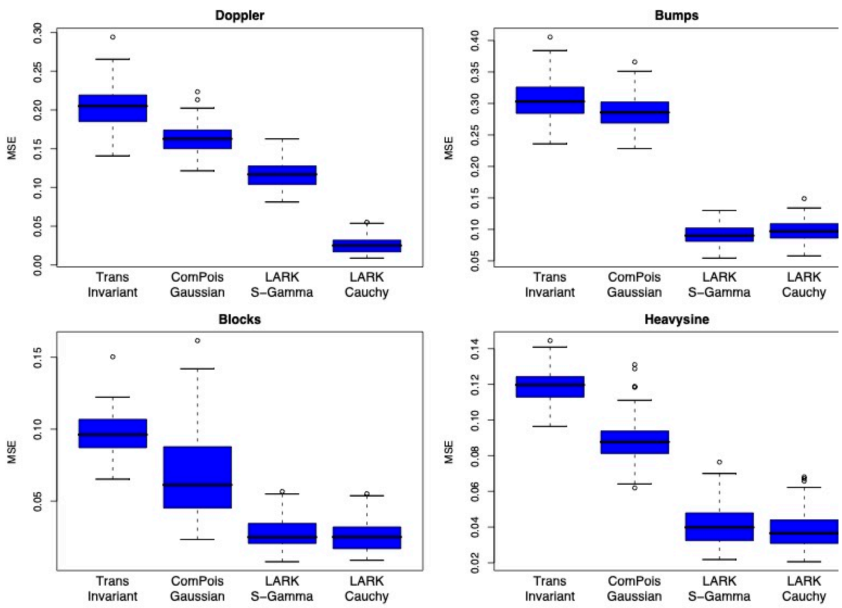
Simulation



Kernels



Comparison of Lévy Adaptive Regression Kernels

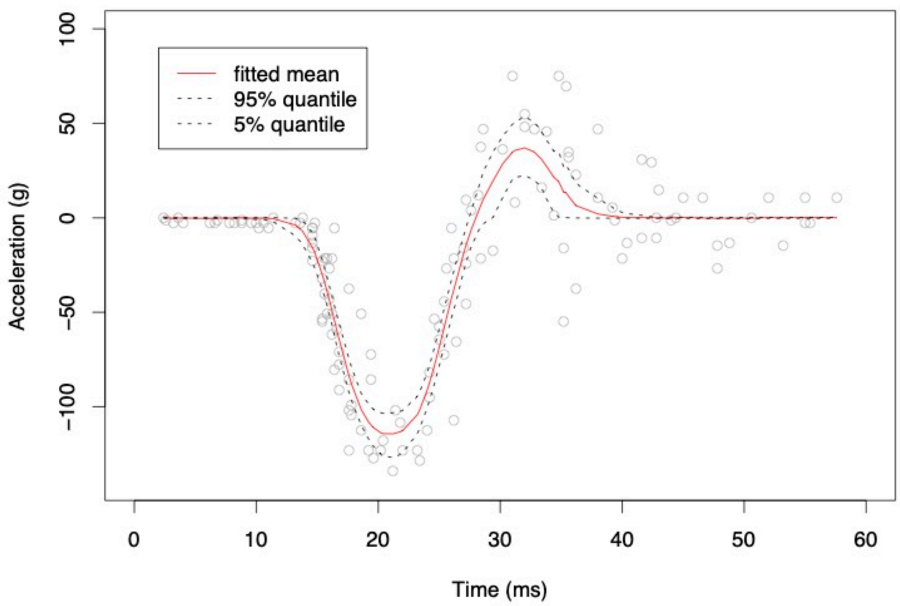


Inference via Reversible Jump MCMC

trans-dimensional MCMC

- number of support points J varies from iteration to iteration
  - add a new point (birth)
  - delete an existing point (death)
  - combine two points (merge)
  - split a point into two
- update existing point(s)

MotorCycle Acceleration



Summary

- more parsimonious than "shrinkage" priors or SVM
- allows for increasing number of support points as n increases
- control MSE *a priori* through choice of ϵ
- no problem with non-normal data, non-negative functions or even discontinuous functions
- credible and prediction intervals
- robust alternative to Gaussian Process Priors
- hard to scale up random scales, locations as dimension of $\mathbf{x}$ increases
- next - Prior Approximation II