# Bayesian Adpative Regression Kernels & SVM

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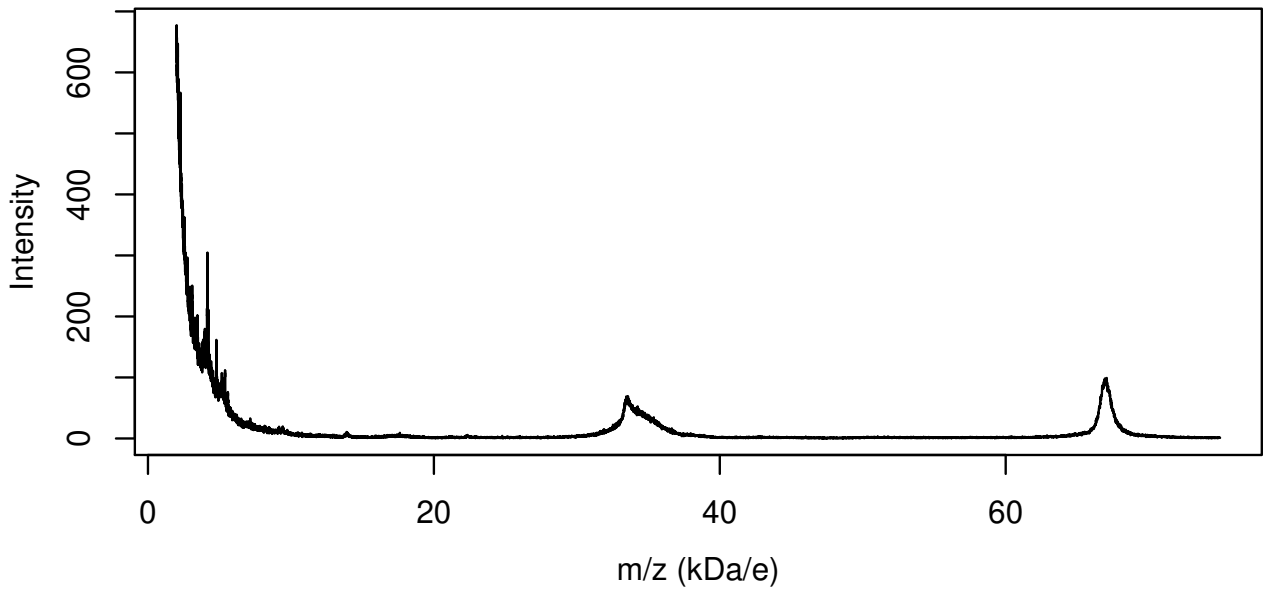
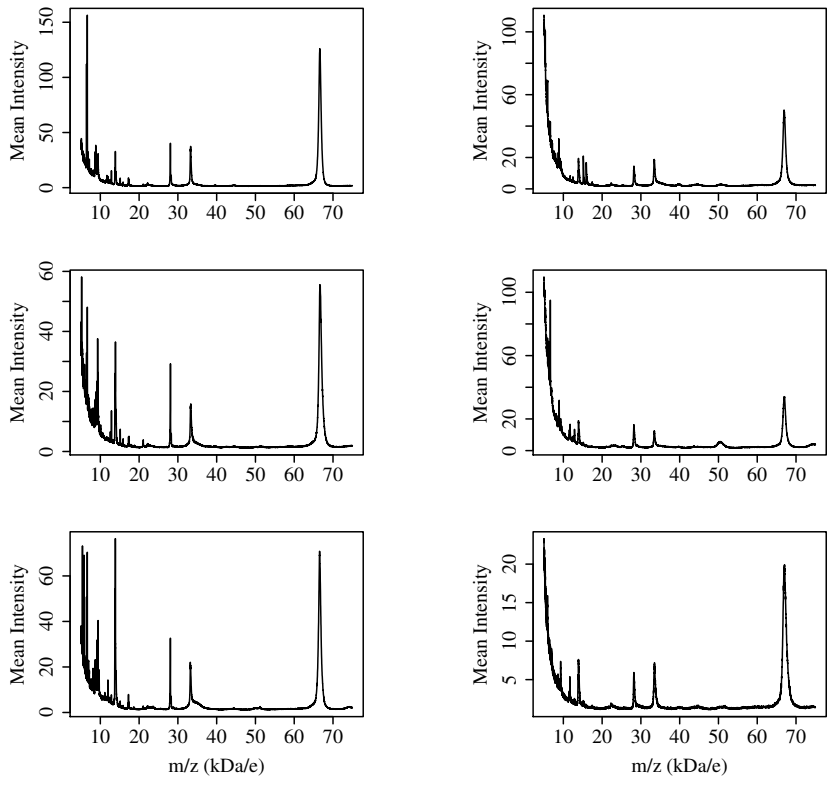
# MALDI-TOF Mass Spectroscopy




Location of peaks/proteins in spectra in the presence of noise
Non-Gaussian Noise

# Multiple Spectra




Learning “features” that are common versus those that separate groups of spectra but do not know a prior the number of ions

# Problem Setting

Regression problem

$$\mathsf{E}[Y \mid \boldsymbol{x}] = f(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathcal{X}$$

with unknown function $f(\boldsymbol{x}) : \mathcal{X} \to \mathbb{R}$

Nonparametric Bayesian would place prior distribution on functions

# Expansions

Write function as

$$f(\boldsymbol{x}_i) = \sum_{j=0}^{J} \psi(\boldsymbol{x}_i, \boldsymbol{\omega}_j)\beta_j$$

in terms of an (over-complete) dictionary where

- $\{\beta_j\}$: unknown coefficients
- $J$: number of terms in expansion (finite or infinite)
- $\psi(\boldsymbol{x}, \boldsymbol{\omega}_j)$ Dictionary elements from a "generator function" $g$
  - cubic splines

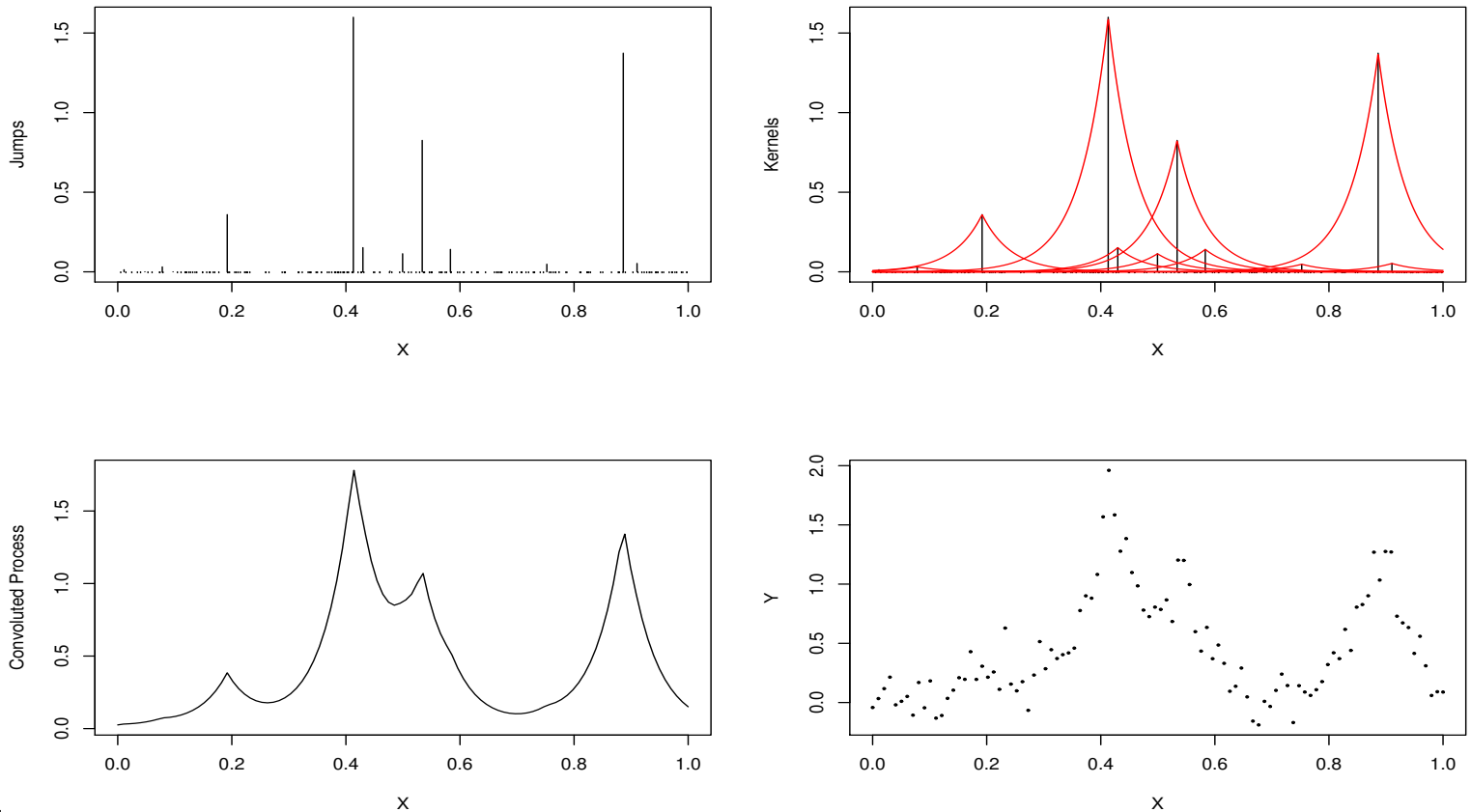
    $$\psi(x_i, \omega_j) = (x_i - \omega_j)_+^3$$

  - multivariate kernels (Gaussian, Cauchy, Exponential, e.g.)

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

  - translation and scaling wavelet families
  - Need not be symmetric!

# Kernel Convolution




Easy to generate non-stationarity processes

# Bayesian NonParametrics

Goal: $f(x) = \sum_{j<J} \psi(\boldsymbol{x}, \boldsymbol{\omega}_j)\beta_j = \sum_{j<J} g(\boldsymbol{\Lambda}_j(\boldsymbol{x} - \boldsymbol{\chi}_j))\beta_j$

- Poisson prior on $J$ (could be infinite!)

$\Rightarrow$ $J \sim \mathrm{P}(\nu_+)$, $\qquad \nu_+ \equiv \nu(\mathbb{R} \times \boldsymbol{\Omega}) = \iint \nu(\beta, \boldsymbol{\omega}) d\beta \, d\boldsymbol{\omega}$

$\Rightarrow$ $\beta_j, \boldsymbol{\omega}_j \mid J \overset{iid}{\sim} \pi(\beta, \boldsymbol{\omega}) \propto \nu(\beta, \boldsymbol{\omega})$.

- Finite number of "big" coefficients $|\beta_j|$
- Possibly infinite number of $\beta \in [-\epsilon, \epsilon]$
- Coefficients $|\beta_j|$ are absolutely summable

Sufficient condition for bounded $g$:

$$\int_{\mathbb{R}\times\Omega} \min(1, |\beta|)\nu(\beta, \boldsymbol{\omega}) d\beta \, d\boldsymbol{\omega} < \infty \tag{1}$$

# $\alpha$-Stable Lévy Measures

Lévy measure: $\nu(\beta, \boldsymbol{\omega}) = c_\alpha |\beta|^{-(\alpha+1)}\ \pi(\boldsymbol{\omega}) \qquad 0 < \alpha < 2$
For $\alpha$- Stable $\nu^+(\mathbb{R}, \boldsymbol{\Omega}) = \infty$
Fine in theory, but not in practice for MCMC!

Truncate measure to obtain a finite expansion:

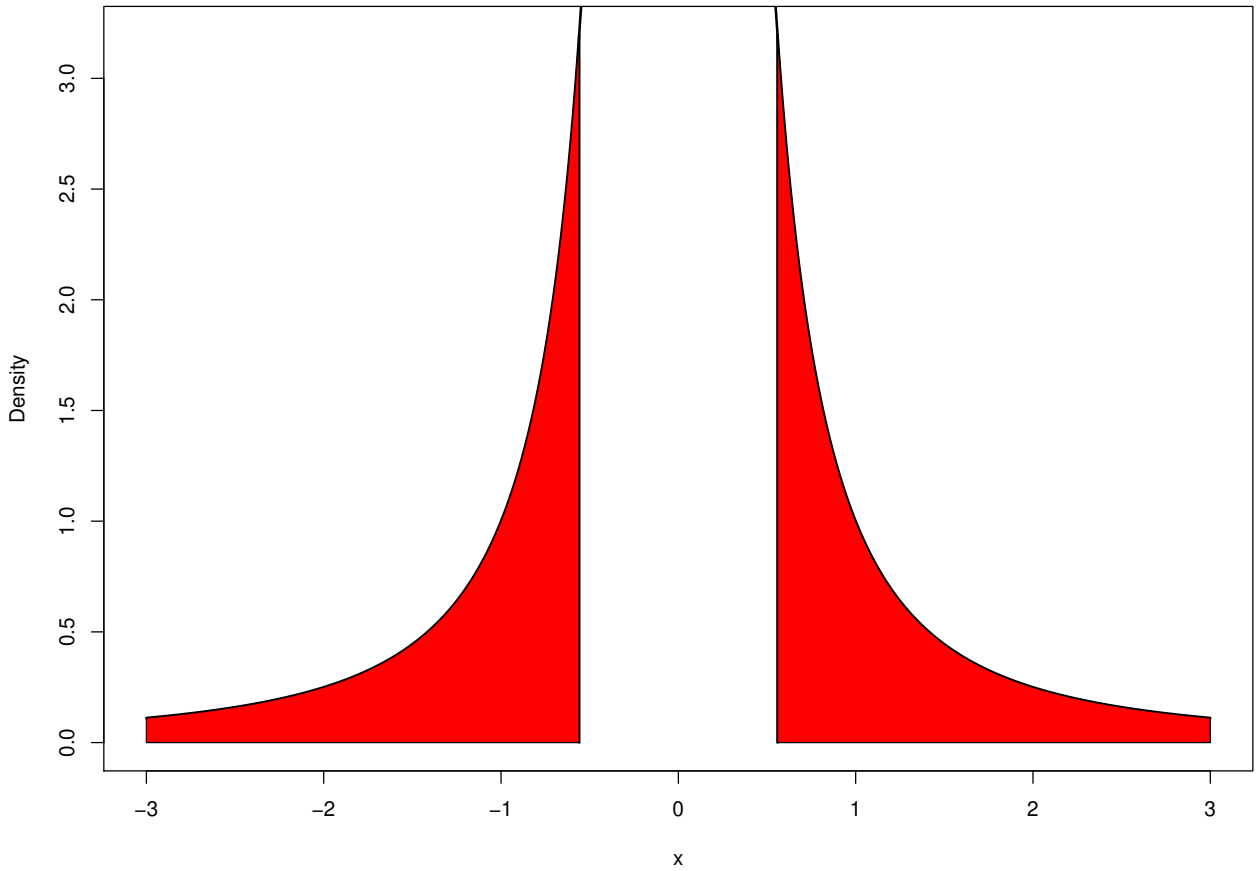
- Finite number of support points $\boldsymbol{\omega}$ with $\beta$ in $[-\epsilon, \epsilon]^c$
- Fix $\epsilon$ (for given prior approximation error)
- Use approximate Lévy measure $\nu_\epsilon(\beta, \boldsymbol{\omega}) \equiv \nu(\beta, \boldsymbol{\omega})\mathbf{1}(|\beta| > \epsilon)$

$\Rightarrow$ $J \sim \mathrm{P}(\nu_\epsilon^+)$ where $\nu_\epsilon^+ = \nu([-\epsilon, \epsilon]^c, \boldsymbol{\Omega})$

$\Rightarrow$ $\beta_j, \boldsymbol{\omega}_j \overset{iid}{\sim} \pi(d\beta, d\boldsymbol{\omega}) \equiv \nu_\epsilon(d\beta, d\boldsymbol{\omega})/\nu_\epsilon^+$ ($\beta_j$ distributed as Pareto)

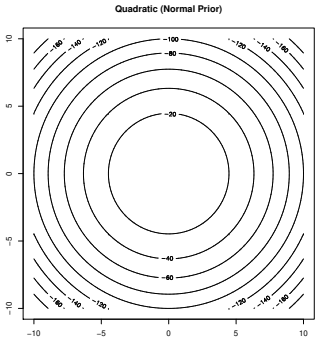
# Truncated Cauchy Process

Restriction $|\beta| > \epsilon$

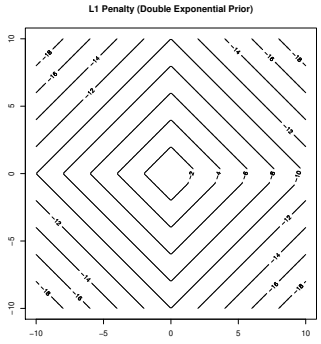


# Contours of Log Prior (in $\mathbb{R}^2$) – Penalties

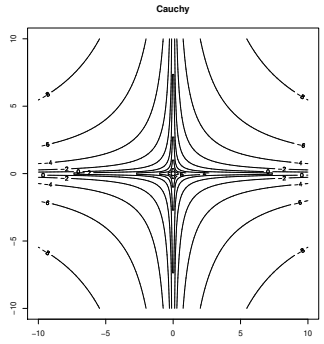
Normal




DE




Cauchy




Penalized Likelihood:

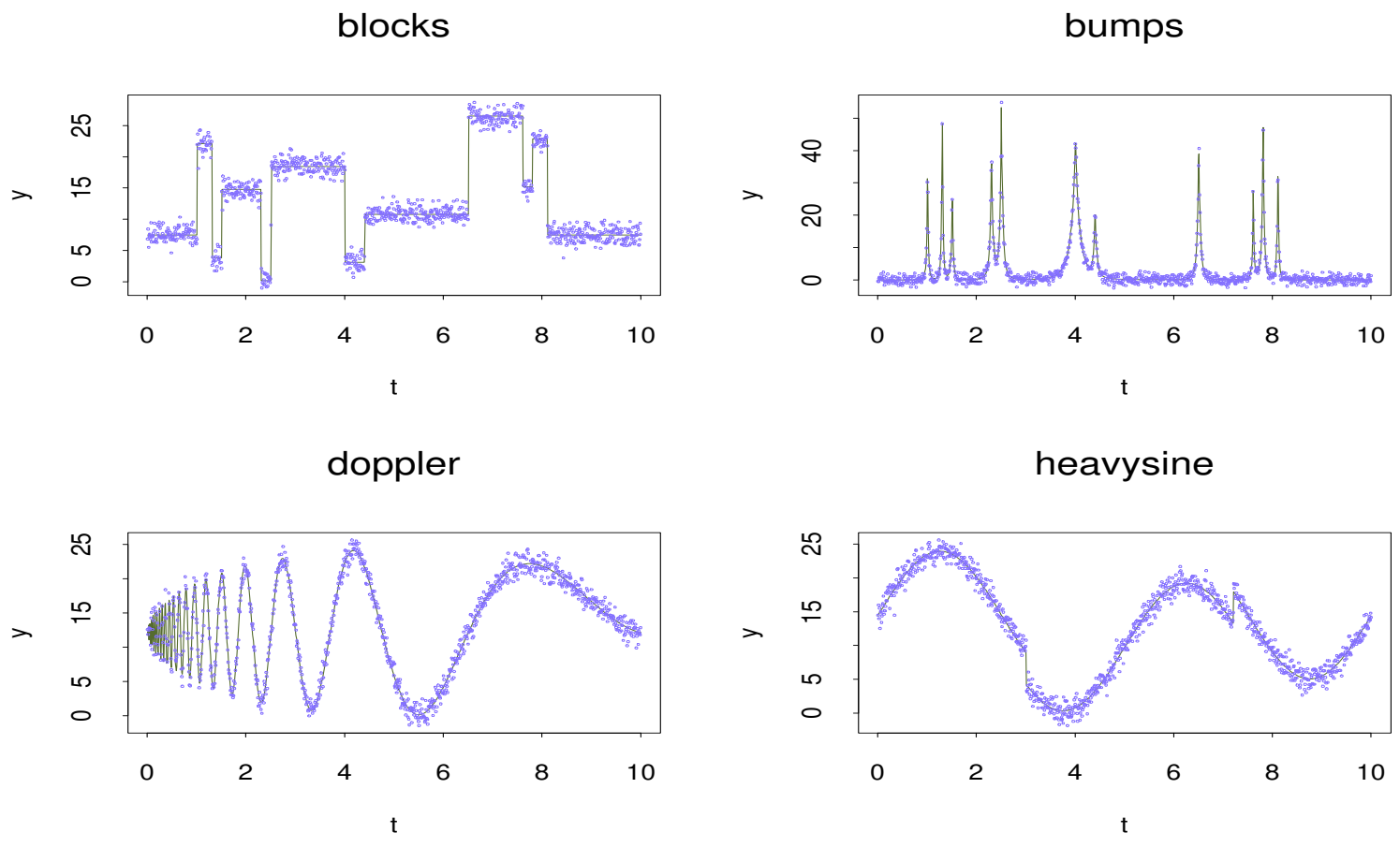
$$-\frac{1}{2\sigma^2}\sum_i (Y_i - f(\boldsymbol{x}_i))^2 - (\alpha+1)\sum_j \log(|\beta_j|) - \nu_\epsilon^+ \ldots$$

# Computation - Reversible Jump MCMC

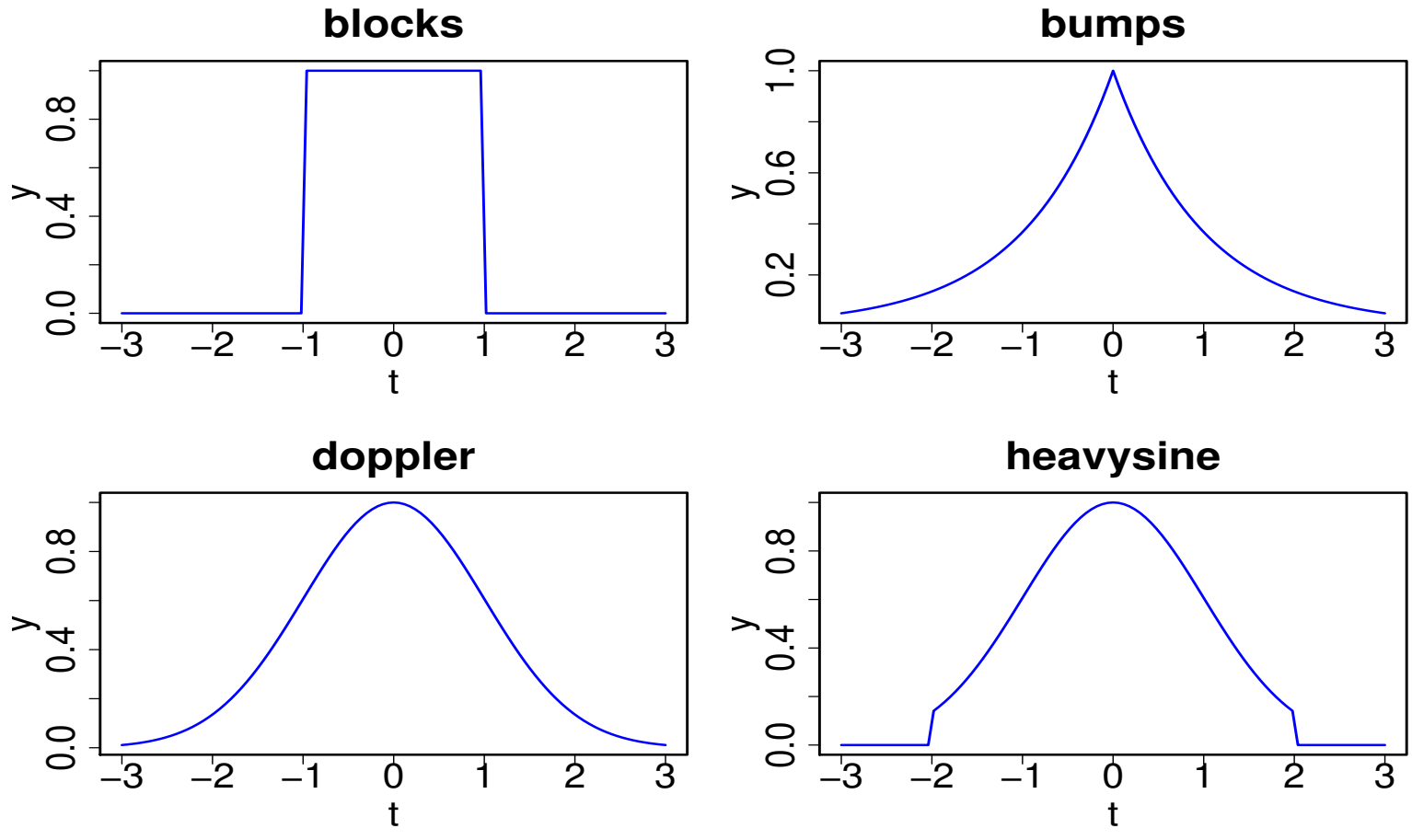
- Birth: generate coefficients $\beta_j$ near $\epsilon$ in absolute value and generate kernel parameters $\boldsymbol{\omega}_j$ given increase in $J \to J+1$
- Death: $\beta_j = 0$ drop dictionary element when $J$ decrements by 1.
- Update: Random-Walk update, but also leads to deaths with coefficients that wander out of bounds and cross $\epsilon$ boundary!
- Merge-Split: allow "neighboring points" to merge into one dictionary element (an alternative death) or a split into new dictionary elements

Advantage over fixed dimensional over-complete methods (frames)

# Wavelet Test Functions (SNR = 7)



# Kernel Functions



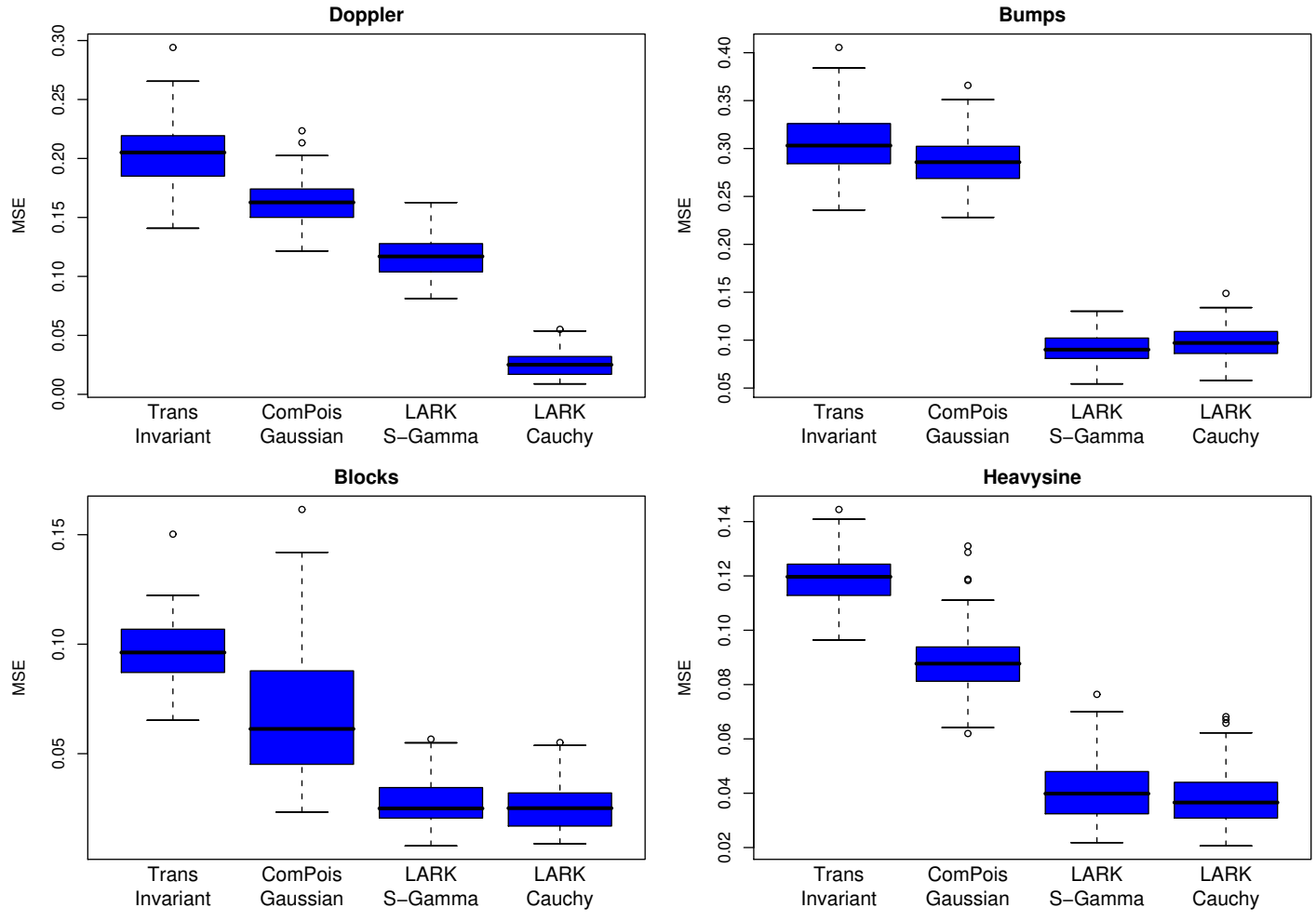
# Comparisons of OCD Methods

- Translational Invariant Wavelets – Laplace Priors (Johnstone & Silverman 2005)
- Continuous Wavelet Dictionary – Compound Poisson with Gaussian Priors (Chu, Clyde, Liang 2007)
- LARK Symmetric Gamma
- LARK Cauchy

Range of Over-complete Dictionaries and Priors

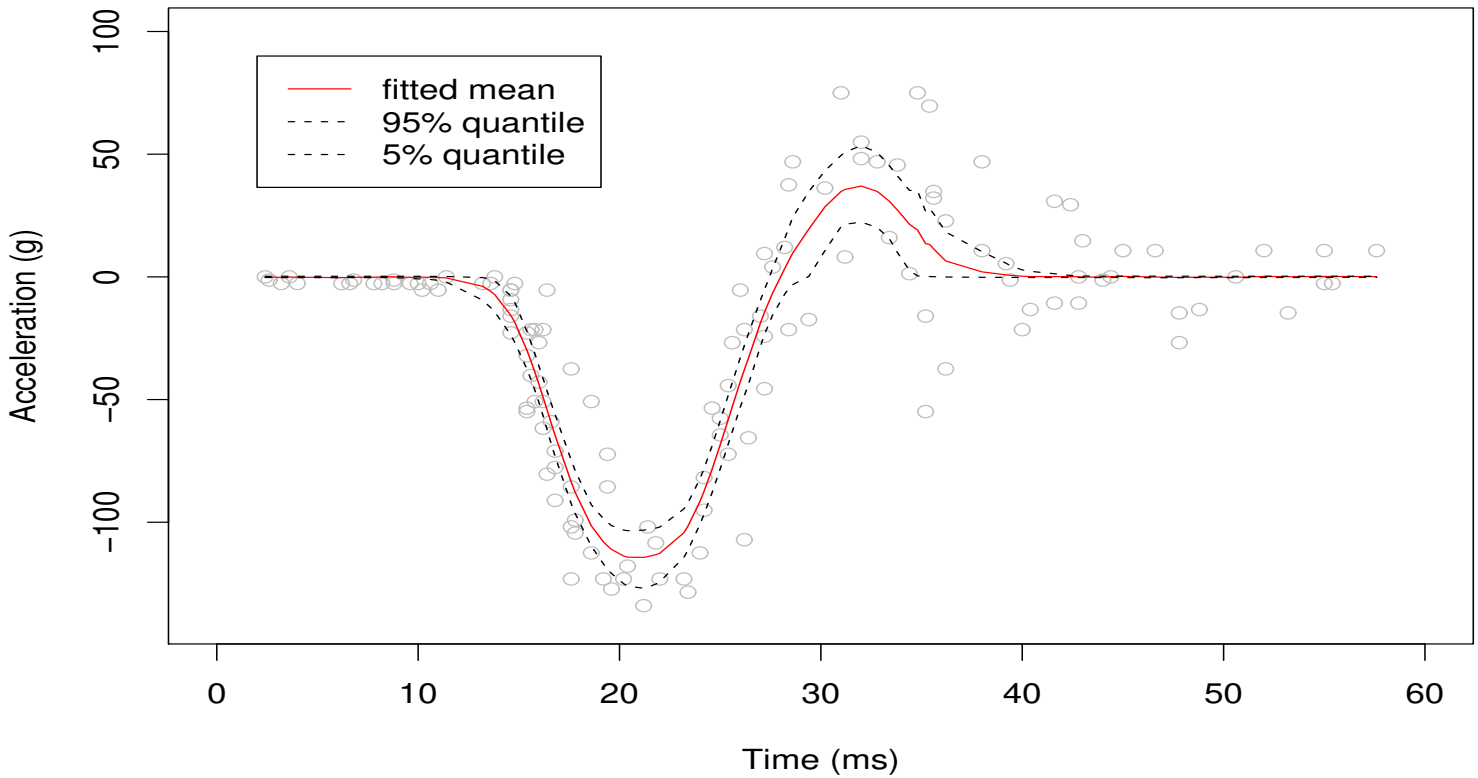
# Comparison of Mean Square Error w/ OCDs

100 realizations of each function



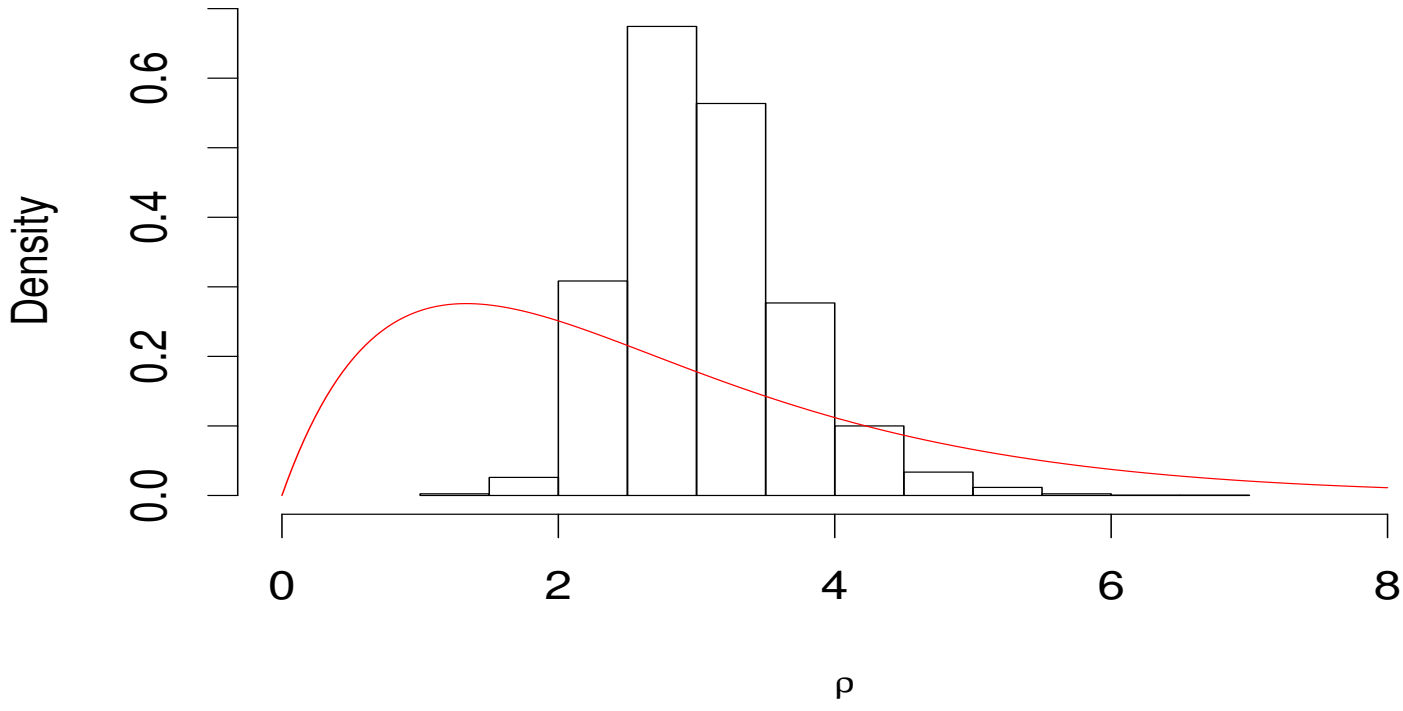
# Motorcycle Crash Data: A Real Example

On average, only $\mathrm{E}[J \mid Y] \approx 4$ jumps are needed for fit:



# Form of Kernel

$$k(t_i; \tau_j, \lambda_j) = e^{-\lambda_j |t_i - \tau_j|^\rho}$$



# Higher Dimensional $\mathcal{X}$

RJ-MCMC is (currently) too slow in higher dimensional space to allow

- $\chi$ to be completely arbitrary; restrict support to observed $\{\boldsymbol{x}_i\}$ like in SVM
- use diagonal $\boldsymbol{\Lambda}$

Kernels take form:

$$\begin{aligned} \psi(\boldsymbol{x}, \boldsymbol{\omega}_j) &= \prod_d \exp\{-\frac{1}{2}\lambda_d(x_d - \chi_d)^2\} \\ f(\boldsymbol{x}) &= \sum_j \psi(\boldsymbol{x}, \boldsymbol{\omega}_j)\beta_j \end{aligned}$$

# Approximate Lévy Prior II

Continuous Approximation Student $t(\alpha, 0, \epsilon)$ approximation:

$$\nu_\epsilon(d\beta, d\boldsymbol{\omega}) = c_\alpha(\beta^2 + \alpha\epsilon^2)^{-(\alpha+1)/2} d\beta \; \gamma(d\boldsymbol{\omega})$$

Based on the following hierarchical prior

$$\begin{aligned} \beta_j \mid \phi_j &\overset{ind}{\sim} \mathsf{N}(0, \varphi_j^{-1}) \\ \phi_j &\overset{ind}{\sim} \mathsf{G}\left(\frac{\alpha}{2}, \frac{\alpha\epsilon^2}{2}\right) \\ J &\sim \mathsf{P}(\nu_\epsilon^+) \end{aligned}$$

where $\nu_\epsilon^+ = \nu_\epsilon(\mathbb{R}, \boldsymbol{\Omega}) = \frac{\alpha^{1-\alpha/2}\Gamma(\alpha)\Gamma(\alpha/2)}{\epsilon^\alpha \pi^{1/2}\Gamma(\frac{\alpha+1}{2})} \sin(\frac{\pi\alpha}{2})\gamma(\boldsymbol{\Omega})$

Key: need to have variance of coefficients decrease as $J$ increases

# Limiting Case

$$\begin{aligned} \beta_j \mid \varphi_j &\overset{ind}{\sim} \mathrm{N}(0, 1/\varphi_j) \\ \varphi_j &\overset{iid}{\sim} \mathrm{G}(\alpha/2, "0") \end{aligned}$$

Notes:

- Require $0 < \alpha < 2$ Additional restrictions on $\omega$
- Cauchy process corresponds to $\alpha = 1$
- Tipping's "Relevance Vector Machine" corresponds to $\alpha = 0$ (improper posterior!)
- Provides an extension of **Generalized Ridge Priors** to infinite dimensional case
- Infinite dimensional analog of Cauchy priors

# Further Simplification in Case with $\alpha = 1$

- Poisson number of points $J_\epsilon \sim \mathrm{P}\big(\nu_\epsilon^+(\alpha,\gamma)\big)$ with $\nu_\epsilon^+(\alpha,\gamma) = \frac{\gamma\alpha^{1-\alpha/2}}{2^{1-\alpha}\epsilon^\alpha}\frac{\Gamma(\alpha/2)}{\Gamma(1-\alpha/2)}$
- Given $J$, $[n_1 : n_n] \sim MN(J, 1/(n+1))$ points supported at each kernel located at $\boldsymbol{x}_j$

The regression mean function can be rewritten as

$$f(\boldsymbol{x}) = \sum_{i=0}^{n} \tilde{\beta}_i \psi(\boldsymbol{x}, \boldsymbol{\omega}_i), \quad \tilde{\beta}_i = \sum_{\{j\,|\boldsymbol{\chi}_j = \boldsymbol{x}_i\}} \beta_j.$$

In particular, if $\alpha = 1$, not only the Cauchy process is infinitely divisible, the approximated Cauchy prior distributions on the regression coefficients are also infinitely divisible:

$$\tilde{\beta}_i \overset{ind}{\sim} \mathrm{N}(0, n_i^2\tilde{\varphi}_i^{-1}), \qquad \tilde{\varphi}_i \overset{iid}{\sim} \mathrm{G}(1/2, \epsilon^2/2)$$

At most $n$ non-zero coefficients! (JAGS is possible now?)

# Collapsed Sampler

**Advantage**: Gaussian prior so $\beta$ can be integrated out for MCMC under Gaussian error model in the $n$ dimensional problem

- Integrate out $\beta$ vector in Normal regression leaving kernel parameters $\mathbf{\Lambda}$ and $\varphi$ with multinomial weights $n_i$
- $n_i$ may be 0 which drops dictionary elements from representation in finite representation for fixed $\epsilon$
- still trans-dimensional in $\varphi$ but much simpler RJMCMC now

# Feature Selection in Kernel

- Product structure allows interactions between variables
- Many input variables may be irrelevant
- Feature selection; if $\lambda_d = 0$ variable $x_d$ is removed from all kernels
- Allow point mass on $\lambda_h = 0$ with probability $p_\lambda \sim B(a, b)$ (in practice have used $a = b = 1$

Consider 3 Scenarios

- $D$ Different $\lambda - D$ parameters in each dimension
- $S + D$ Different $\lambda_d$ parameters + Selection
- $S + E$ Selection + Equal for Remaining $\lambda_d = \lambda$

# Regression Out of Sample Prediction

Average Relative MSE to best procedure

| Data Sets | BARK | | | SVM | BART |
|---|---|---|---|---|---|
| | D | S + E | S + D | | |
| Friedman1 | 1.22 | 2.26 | 1.93 | 5.36 | 1.97 |
| Friedman2 | 1.07 | 1.09 | 1.04 | 4.36 | 3.64 |
| Friedman3 | 1.46 | 2.30 | 1.44 | 2.70 | 1.00 |
| Boston Housing | 1.09 | 1.23 | 1.20 | 1.56 | 1.01 |
| Body Fat | 1.81 | 1.01 | 2.19 | 4.04 | 1.68 |
| Basketball | 1.01 | 1.01 | 1.02 | 1.16 | 1.10 |

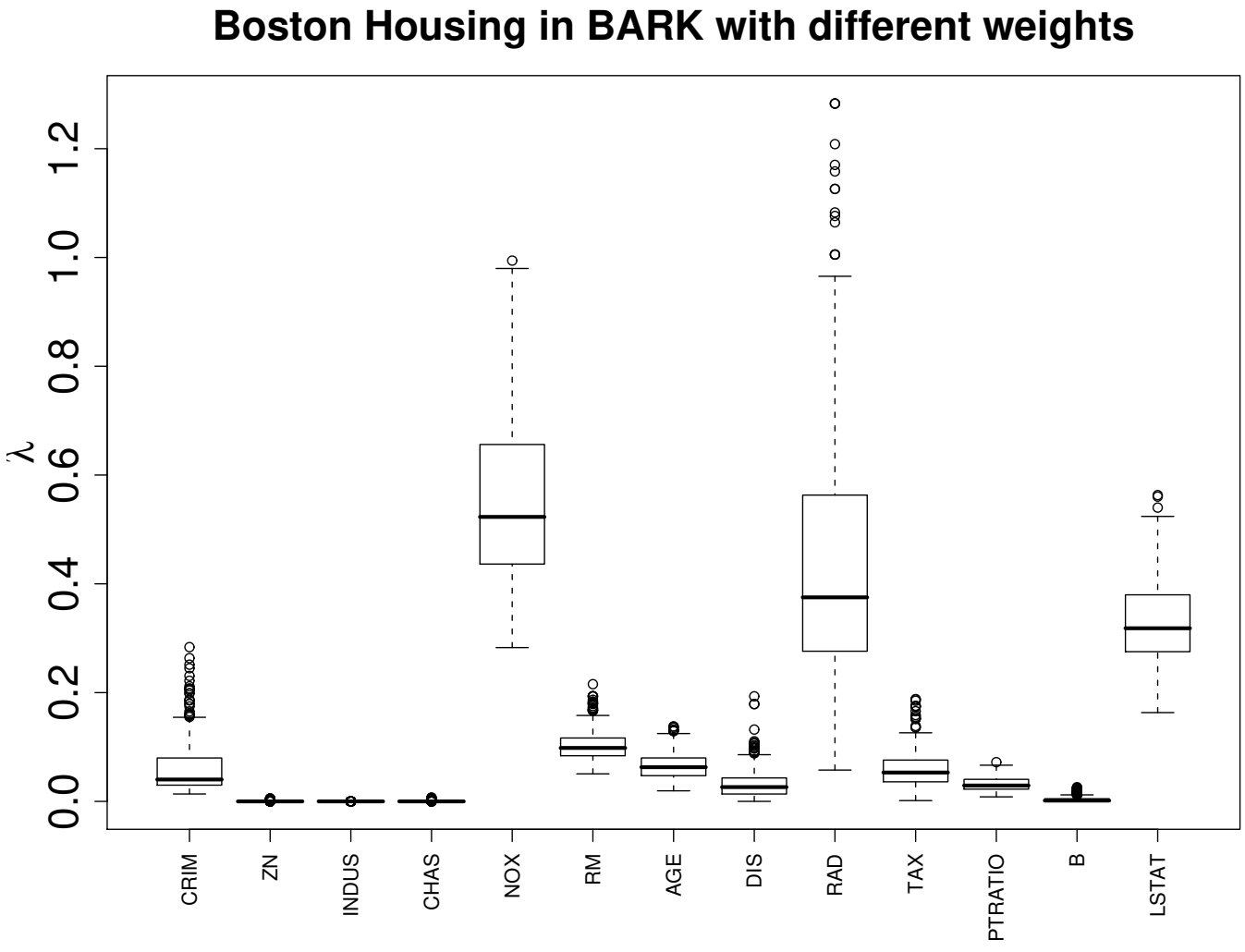
D: dimension specific scale $\lambda_d$

E: equal scales $\lambda_d = \lambda \, \forall \, d$

S: selection $\lambda_d = 0$ with probability $\rho$

# Feature Selection in Boston Housing Data

Posterior Distribution of $\lambda_d$



# Classification Examples

| Name | $d$ | data type | $n$ (train/test) |
|---|---|---|---|
| Circle | 2 | simulation | 200/1000 |
| Circle (3 null) | 5 | simulation | 200/1000 |
| Circle (18 null) | 20 | simulation | 200/1000 |
| Swiss Bank Notes | 6 | real data | 200 (5 $cv$) |
| Breast Cancer | 30 | real data | 569 (5 $cv$) |
| Ionosphere | 33 | real data | 351 (5 $cv$) |

- Add latent Gaussian $Z_i$ for probit regression (as in Albert & Chib)
- Same model as before conditional on $\boldsymbol{Z}$
- Advantage: Draw $\boldsymbol{\beta}$ in a block from full conditional
- Can extend to Logistic

# Predictive Error Rate for Classification

| Data Sets | BARK | | | SVM | BART |
|---|---|---|---|---|---|
| | D | S + E | S + D | | |
| Circle 2 | 4.91% | 1.88% | 1.93% | 5.03% | 3.97% |
| Circle 5 | 4.70% | 1.47% | 1.65% | 10.99% | 6.51% |
| Circle 20 | 4.84% | 2.09% | 3.69% | 44.10% | 15.10% |
| Bank | 1.25% | 0.55% | 0.88% | 1.12% | 0.50% |
| BC | 4.02% | 2.49% | 6.09% | 2.70% | 3.36% |
| Ionosphere | 8.59% | 5.78% | 10.87% | 5.17% | 7.34% |

D: dimension specific scale $\lambda_d$

E: equal scales $\lambda_d = \lambda \forall d$

S: selection $\lambda_d = 0$ with probability $\rho$

# Needs & Limitations

- NP Bayes of many flavors often does better than frequentist methods (BARK, BART, Treed GP, more)
- Hyper-parameter specification - theory & computational approximation
- need faster code for BARK that is easier for users (BART & TGP are great!) (`library(bark)` or github
- Can these models be added to JAGS, STAN, etc instead of stand-alone R packages
- With availability of code what are caveats for users?

# Summary

Lévy Random Field Priors & LARK models:

- Provide limit of finite dimensional priors (GRP & SVSS) to infinite dimensional setting
- Adaptive bandwidth for kernel regression
- Allow flexible generating functions
- Provide sparser representations compared to SVM & RVM, with coherent Bayesian interpretation
- Incorporation of prior knowledge if available
- Relax assumptions of equally spaced data and Gaussian likelihood
- Hierarchical Extensions
- Formulation allows one to define stochastic processes on arbitrary spaces (spheres, manifolds)