Bayesian Adpative Regression Kernels

November 17, 2021

Problem Setting

Regression problem

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

with unknown function $f(\boldsymbol{x})R$
Write

$$f(\boldsymbol{x}_i) = \beta_0 + \sum_{j=1}^{n} \beta_j k(x_i, x_j)$$

where $k(x_i, x_j)$ is a kernel function

- Linear Kernel

$$k(x_i, x_j) = x_i^T x_j$$

- Radial or Gaussian Kernel

$$k(x_i, x_j) = \exp(-\frac{\lambda}{2}((x_i - x_j)^T(x_i - x_j))$$

"support vectors"

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

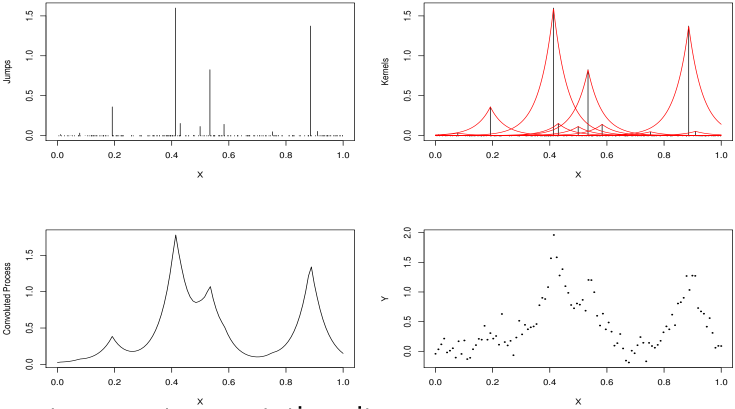
    $$\psi(x_i, \omega_j) = (x_i - \omega_j)_+^3$$

  - 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 (BNP)

Goal

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

- Poisson prior on J (could be infinite!)

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

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

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

α-Stable Lévy Measures

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

Truncate measure to obtain a finite expansion:

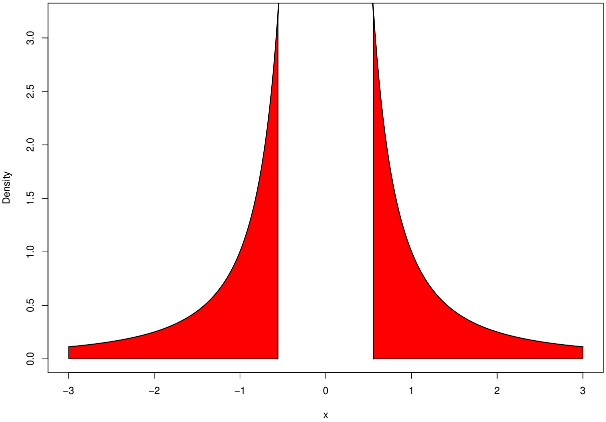
- Finite number of support points $\boldsymbol{\omega}$ with β in $[-\epsilon, \epsilon]^c$
- Fix ϵ (for given prior approximation error)
- Use approximate Lévy measure $\nu_\epsilon(\beta, \boldsymbol{\omega}) \equiv \nu(\beta, \boldsymbol{\omega})\mathbf{1}(|\beta| > \epsilon)$

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

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

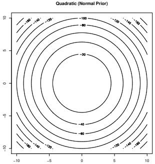
Truncated Cauchy Process

Restriction $|\beta| > \epsilon$

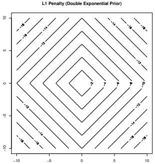


Contours of Log Prior (in $\mathbb{R}^2$) – Penalties

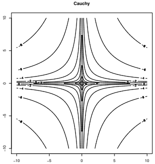
Normal



DE



Cauchy



Penalized Likelihood:

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

Higher Dimensional $\mathcal{X}$

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

- $\boldsymbol{\chi}$ 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

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

Notes:

- Require $0 < \alpha < 2$ Additional restrictions on ω
- 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 $J_\epsilon \sim \mathsf{P}\big(\nu_\epsilon^+(\alpha,\gamma)\big)$ 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

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

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:

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

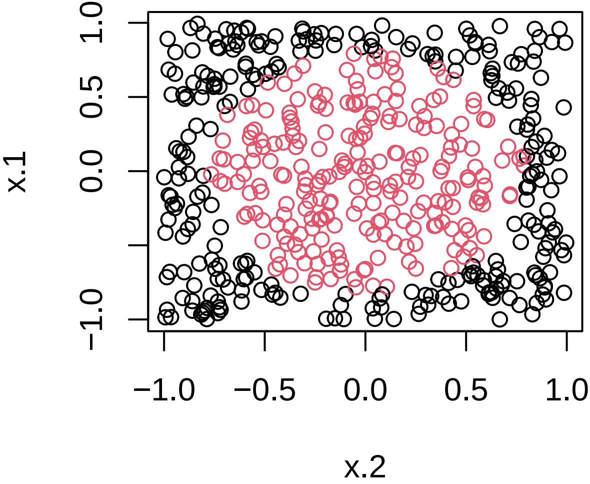
At most n non-zero coefficients!

BARK: Bayesian Additive Regression Kernels

```
#library(devtools)
#suppressMessages(install_github("merliseclyde/bark"))
library(bark)

set.seed(42)
n = 500
circle2 = as.data.frame(sim_circle(n, dim = 2))
```

Circle

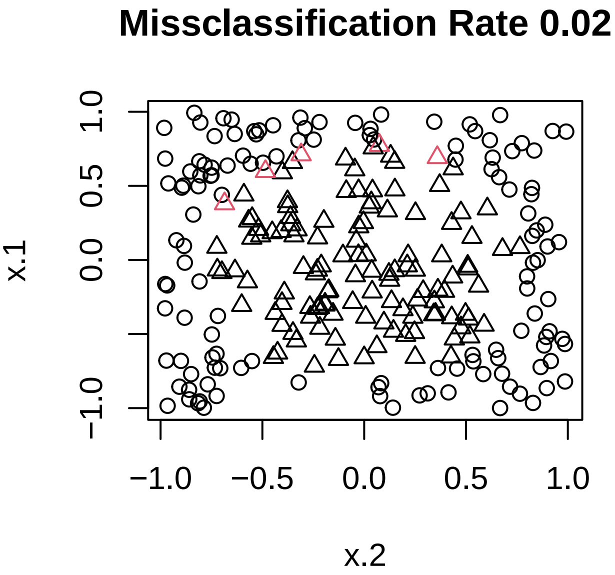


Circle Example

```
set.seed(42)
train = sample(1:n, size = floor(n/2), rep=FALSE)
circle2.bark = bark(as.matrix(circle2[train, 1:2]),
                    circle2[train, 3],
                    x.test = as.matrix(circle2[-train, 1:2]
                    classification = TRUE,
                    printevery = 10000,
                    type="se")

## [1] "Starting BARK-se for this classification problem"
## [1] "burning iteration 10000, J=5, max(nj)=2"
## [1] "posterior mcmc iteration 10000, J=4, max(nj)=1"
```

Missclassification



SVM

```
library(e1071)
circle2.svm = svm(y ~ x.1 + x.2, data=circle2[train,],
                  type="C")
pred.svm = predict(circle2.svm, circle2[-train,])
mean(pred.svm != circle2[-train, "y"])

## [1] 0.048
```

BART

```
suppressMessages(library(BART))
circle.bart = pbart(x.train = circle2[train, 1:2],
                    y.train = circle2[train, "y"])
pred.bart = predict(circle.bart, circle2[-train, 1:2])
mean((pred.bart$prob.test.mean > .5) !=
      circle2[-train, "y"])
```

```
## [1] 0.036
```

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 λ_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

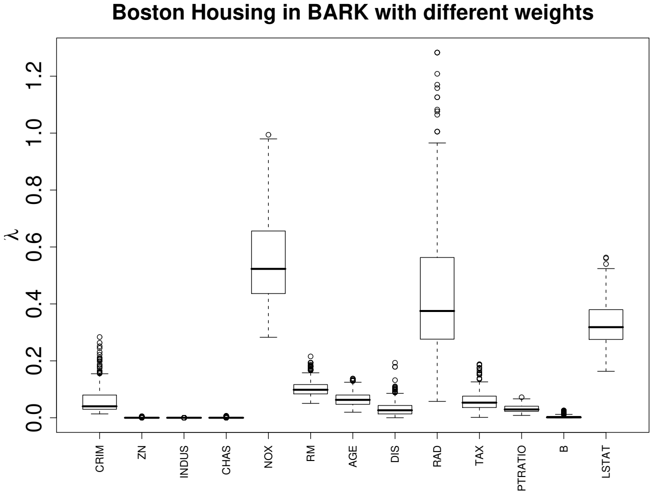
D: dimension specific scale λ_d

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

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

Feature Selection in Boston Housing Data

Posterior Distribution of λ_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 λ_d

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

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

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)