Computational Strategies in Lévy Adative Regression Kernels

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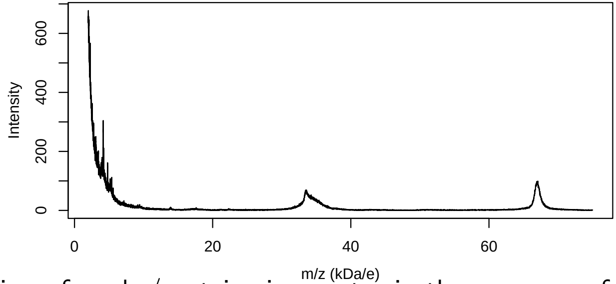
Outline

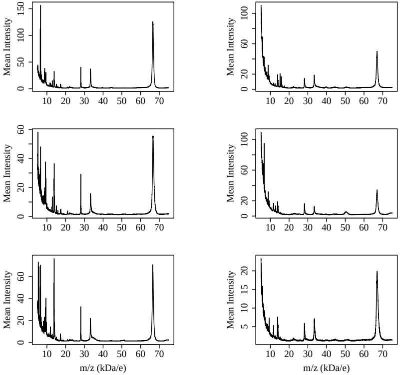
MALDI-TOF Mass Spectroscopy



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

Predict Ovarian Cancer Risk

- age
- family history of ovarian and breast cancer
- oral contraceptive use (duration)
- hormone replacement therapy
- hysterectomy
- number of pregnancies
- breastfeeding
- genetic single nucleotide polymorphisms (SNPs)

potential nonlinear functions and interactions?

Problem Setting

Regression problem

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

with unknown function $f(\boldsymbol{x}) : \mathcal{X} \to \mathbb{R}$
Nonparametric Bayesian would place prior distribution on functions

- Gaussian Process Priors
- Dirichlet Process priors
- Lévy Processes

latter related to GP & DP and completely randomized measures

Expansions

Expand

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

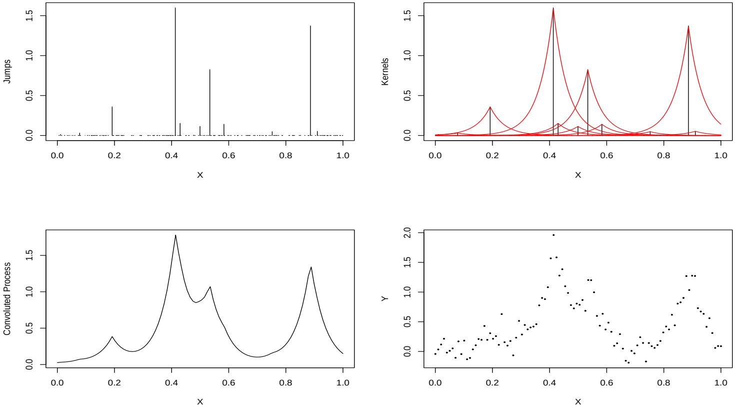
in terms of an (over-complete) dictionary where

- $\{\beta_j\}$: unknown coefficients
- J: number of terms in expansion (finite and infinite)
- $\psi(\boldsymbol{x}, \boldsymbol{\omega}_j)$ Dictionary elements from a "generator function g
  - translation and scaling wavelet families
  - multivariate kernels (Gaussian, Cauchy, Exponential, e.g.)

$$g(\boldsymbol{\Lambda}_j(\boldsymbol{x} - \chi_j)) = \exp\left\{-\frac{1}{2}(\boldsymbol{x} - \chi_j)^T \boldsymbol{\Lambda}_j(\boldsymbol{x} - \chi_j)\right\}$$

  - Problem driven choices - Naulet, Barat & Rousseau
  - Need not be symmetric!

Kernel Convolution



Easy to generate non-stationarity processes

Stochastic Integral Representation

$$f(x) = \sum_{j \le J} \psi(\boldsymbol{x}; \boldsymbol{\omega}_j)\beta_j \equiv \int_{\boldsymbol{\Omega}} \psi(x; \boldsymbol{\omega})\mathcal{L}(d\omega)$$

$$\psi(\boldsymbol{x}, \boldsymbol{\omega}_j) \equiv g(\boldsymbol{\Lambda}_j(\boldsymbol{x} - \boldsymbol{\chi}_j)) \quad \text{"generator"}$$

$\mathcal{L}$ is a Signed Measure (generalization of Completely Random Measures):

$$\mathcal{L}(d\omega) = \sum_{j \le J} \beta_j \delta_{\boldsymbol{\omega}_j}(d\omega)$$

- support points of measure $\mathcal{L}$: $\{\boldsymbol{\omega}_j\} = \{\boldsymbol{\chi}_j, \boldsymbol{\lambda}_j\}$
  - "location" parameters: $\boldsymbol{\chi}_j \in \mathcal{X}$
  - "scaling" parameters: $\boldsymbol{\lambda}_j \in \mathbb{R}^+$
- measure: β_j
- number of support points J

Lévy Random Fields

- $\mathcal{L}(d\omega)$ is a random (signed) measure on $\mathbf{\Omega}$
- Convenient to think of a random measure as stochastic process where $\mathcal{L}$ assigns random variables to sets $A \in \mathbf{\Omega}$
- Take

$$\mathcal{L} \sim \mathrm{Lv}(\nu) \text{ with Lévy measure } \nu(d\beta, d\omega)$$

where ν satisfies integrability condition:

$$\int_{\mathbb{R}\times\Omega} \min(1, \beta^2)\, \nu(d\beta, d\omega) < \infty \tag{1}$$

Choose ν so the resulting f is well defined with desired smoothness properties or covariance function inherited from g (Wolpert, Clyde and Tu - 2011)

Poisson Representation of Lévy Random Fields

$$
\begin{aligned}
f(x) &= \int_\Omega \psi(x;\omega)\mathcal{L}(d\omega) \\
&= \int_{\mathbb{R}\times\Omega} \beta\,\psi(x;\omega)\,N(d\beta d\omega), \\
N(d\beta d\omega) &\sim \mathsf{P}(\nu)
\end{aligned}
$$

when

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

is satisfied and no need for "drift" term that arises with compensation under (1).

If $\nu_+ \equiv \nu(\mathbb{R}\times\Theta) = \infty$, must approximate to implement.

Lévy- Khinchine Poisson Representation

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

Sufficient condition for bounded g:

$$\int_{\mathbb{R}\times\Omega} \min(1, |\beta|)\nu(d\beta, d\boldsymbol{\omega}) < \infty \tag{2}$$

$\Rightarrow$ $J \sim \mathsf{P}(\nu_+), \qquad \nu_+ \equiv \nu(\mathbb{R} \times \boldsymbol{\Omega})$

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

- Finite number of "big" coefficients $|\beta_j|$
- Possibly infinite number of $\beta \in [-\epsilon, \epsilon]$
- Coefficients $|\beta_j|$ are absolutely summable[1]

[1] need to add a deterministic drift term to "compensate" for the infinite number of tiny jumps that are not absolutely summable under the more general integrability condition Equation (1)

Existence Theorem

Theorem

Let ν be a Lévy measure on $\mathbb{R} \times \Omega$ satisfying (1). Then $f(\boldsymbol{x})$ is well-defined if $\psi(\omega) \equiv g(\boldsymbol{\Lambda}(\cdot - \chi))$ satisfies

$$\iint_{[-1,1]^c \times \Omega} (1 \wedge |\beta\psi(\omega)|)\, \nu(d\beta\ d\omega) < \infty \tag{3a}$$

$$\iint_{[-1,1] \times \Omega} (|\beta\psi(\omega)| \wedge |\beta\psi(\omega)|^2)\, \nu(d\beta\ d\omega) < \infty. \tag{3b}$$

For ν satisfying Equation (2) the condition simplifies

$$\iint_{\mathbb{R} \times \Omega} (1 \wedge |\beta\phi(\omega)|)\, \nu(d\beta\ d\omega) < \infty \tag{3c}$$

g is in a "Musielak-Orlicz space"

α-Stable Lévy Measures

Lévy measure: $\nu(d\beta, d\boldsymbol{\omega}) = c_\alpha |\beta|^{-(\alpha+1)} \, \gamma(d\boldsymbol{\omega}) \qquad 0 < \alpha < 2$
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 $\nu_\epsilon(d\beta, d\boldsymbol{\omega}) \equiv \nu(d\beta, d\boldsymbol{\omega})\mathbf{1}(|\beta| > \epsilon)$

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

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

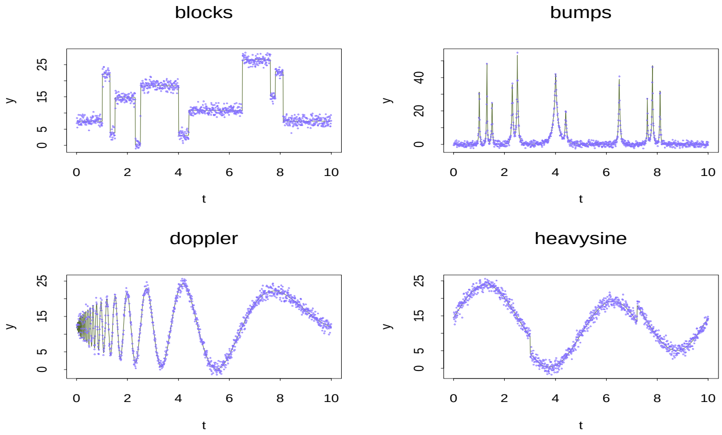
- need term for compensation for $\alpha \geq 1$ for non-symmetric kernels

Computation - Reversible Jump MCMC

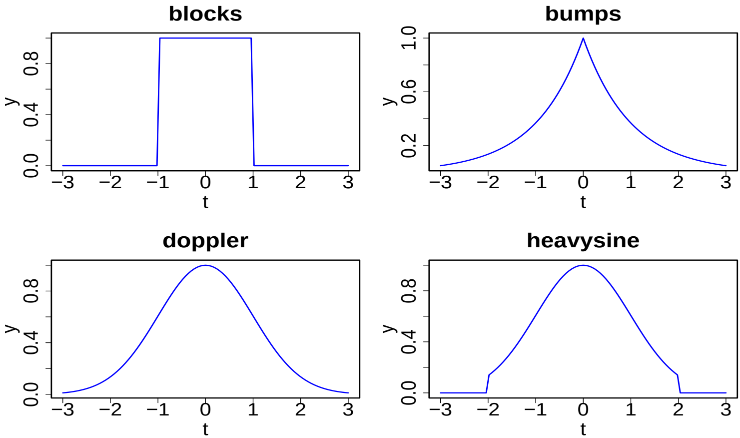
- Birth: generate coefficients β_j near ϵ in absolute value and generate kernel parameters $\boldsymbol{\omega}_j$ given increase in $J \to J + 1$
- Death: $\beta_j = 0$ drop dictionary element when J decrements by 1.
- Update: Random-Walk update, but also leads to deaths with coefficients that wander out of bounds and cross ϵ 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



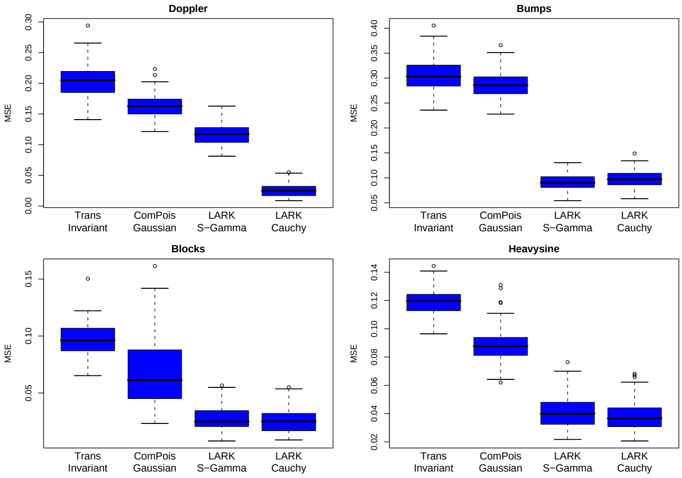
Comparisons of OCD Methods

- 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

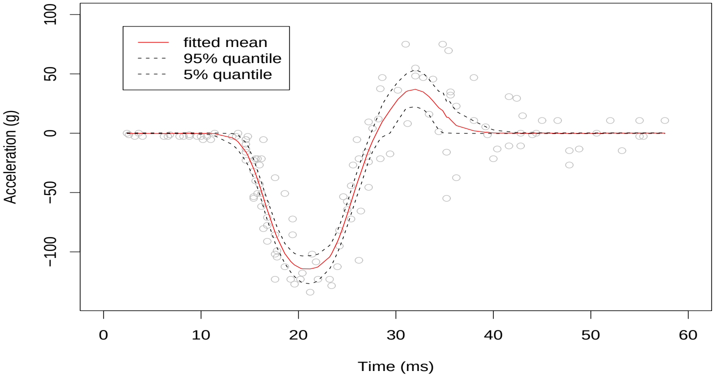
Comparison of Mean Square Error w/ OCDs

100 realizations of each function



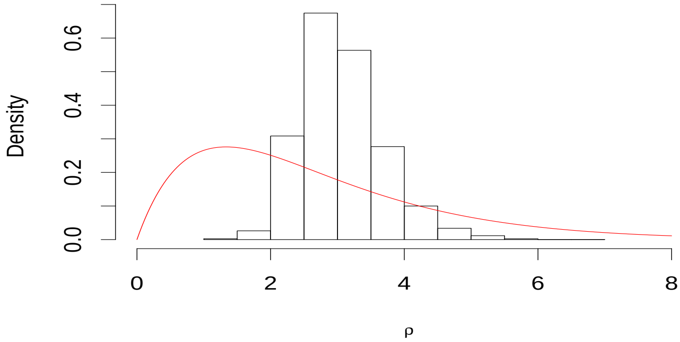
Motorcycle Crash Data: A Real Example

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 $\mathcal{X}$

R-MCMC is too slow in higher dimensional space to allow

- $\boldsymbol{\chi}$ to be completely arbitrary; restrict support to observed $\{\boldsymbol{x}_i\}$
- 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 $\nu_\epsilon^+ = \nu_\epsilon(\mathbb{R}, \boldsymbol{\Omega}) = \frac{\alpha^{1-\alpha/2}\Gamma(\alpha)\Gamma(\alpha/2)}{\epsilon^\alpha \pi^{1/2}\Gamma(\frac{\alpha+1}{2})} \sin(\frac{\pi\alpha}{2})\gamma(\boldsymbol{\Omega})$

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 $0 < \alpha < 2$ for characteristic function for $\mathcal{L}$ and functionals to exist. Additional restrictions on ω
- Cauchy process corresponds to $\alpha = 1$
- Tipping's choice corresponds to $\alpha = 0$
- Provides an extension of Generalized Ridge Priors to infinite dimensional
- 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

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

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!

Collapsed Sampler

Advantage: Gaussian prior so β can be integrated out for MCMC under Gaussian error model in the n dimensional problem

- Integrate out β vector in Normal regression leaving kernel parameters $\mathbf{\Lambda}$ and φ with multinomial weights n_i
- n_i may be 0 which drops dictionary elements from representation in finite representation for fixed ϵ - Holmes approximate models?
- still trans-dimensional in φ 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

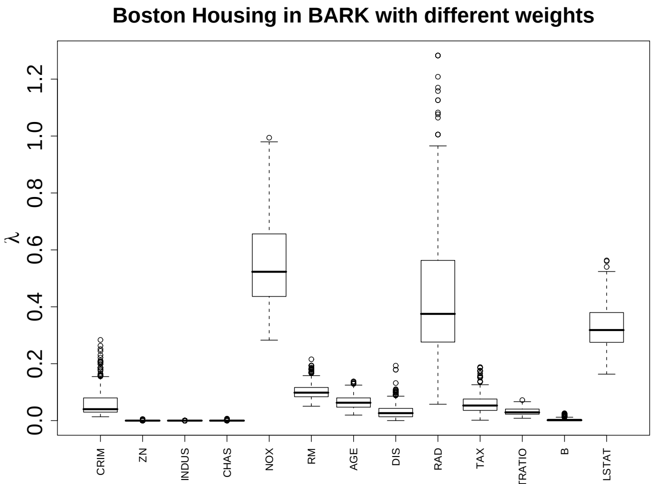
Data Sets	BARK			SVM	BART
	D	S + E	S + D		
Friedman1	1.22	2.26	1.93	5.36	1.97
Friedman2	1.07	1.09	1.04	4.36	3.64
Friedman3	1.46	2.30	1.44	2.70	1.00
Boston Housing	1.09	1.23	1.20	1.56	1.01
Body Fat	1.81	1.01	2.19	4.04	1.68
Basketball	1.01	1.01	1.02	1.16	1.10

D: dimension specific scale λ_d

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

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

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 (LARK, BART, Treed GP, more)
- Hyper-parameter specification - theory & computational approximation
- need faster code that is easier for users (BART & TGP are great!)
- 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)

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- Chong Tu
- Zhi Ouyang

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For papers see `http://stat.duke.edu/ clyde`