Finding religion: kernels and the Bayesian persuasion

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Not a Bayesian



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What makes someone Bayesian

Is it Bayes rule ?

$$\mathsf{P}\mathsf{rob}(\mathsf{parameters}|\mathsf{data}) = rac{\mathsf{Lik}(\mathsf{data}|\mathsf{paramaters})\cdot \pi(\mathsf{parameters})}{\mathsf{P}\mathsf{rob}(\mathsf{data})}$$

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What makes someone Bayesian

Is it Bayes rule ?

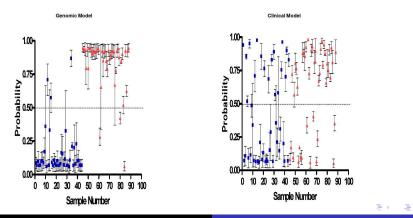
$$\mathsf{P}\mathsf{rob}(\mathsf{parameters}|\mathsf{data}) = rac{\mathsf{Lik}(\mathsf{data}|\mathsf{paramaters})\cdot\pi(\mathsf{parameters})}{\mathsf{P}\mathsf{rob}(\mathsf{data})}.$$

NO!!!!!!!!!!!!!!!! Necessary but no where near sufficient.

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Why I am a Bayesian

Bayesian statistics is about embracing and formally modelling uncertainty.



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A simple example

I draw points $x_1, ..., x_n$ from iid from a normal distribution and I want to know the mean and I know $\sigma = 1$. My likelihood and prior are

$$\mathsf{Lik}(x_1,...,x_n|\mu) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi}} exp(-|x_i - \mu|^2/2)$$
$$\pi(\mu) = \frac{1}{\sqrt{2\pi}} exp(-|\mu - 5|^2/2).$$

The posterior can be computed closed form and it is a product of normals

$$p(\mu|x_1,...,x_n) = \frac{\text{Lik}(x_1,...,x_n|\mu)\pi(\mu)}{\int_{-\infty}^{\infty}\text{Lik}(x_1,...,x_n|\mu)\pi(\mu)d\mu}.$$

Relevant papers

- Characterizing the function space for Bayesian kernel models. Natesh Pillai, Qiang Wu, Feng Liang, Sayan Mukherjee, Robert L. Wolpert. Journal Machine Learning Research, in press.
- Understanding the use of unlabelled data in predictive modelling. Feng Liang, Sayan Mukherjee, and Mike West. Statistical Science, in press.
- Non-parametric Bayesian kernel models. Feng Liang, Kai Mao, Ming Liao, Sayan Mukherjee and Mike West. Biometrika, submitted.

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Table of contents

- Kernel models and penalized loss
- 2 Bayesian kernel model
 - Direct prior elicitation
 - Priors and integral operators
- Option Priors on measures
 - Lévy processes
 - Gaussian processes
 - Bayesian representer theorem
- 4 Estimation and inference
 - Likelihood and prior specification
 - Variable selection
 - Semi-supervised learning
 - Results on data
 - Open problems

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Regression

data =
$$\{L_i = (x_i, y_i)\}_{i=1}^n$$
 with $L_i \stackrel{iid}{\sim} \rho(X, Y)$.
 $X \in \mathcal{X} \subset \mathbb{R}^p$ and $Y \subset \mathbb{R}$ and $p \gg n$.
A natural idea

 $f(x) = \mathbb{E}_{Y}[Y|x].$

Kernel models and penalized loss

Bayesian kernel model Priors on measures Estimation and inference Results on data Open problems

An excellent estimator

 $\hat{f}(x) = \arg \min_{f \in bs} [\text{error on data} + \text{smoothness of function}]$

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Kernel models and penalized loss Bayesian kernel model

Bayesian kernel model Priors on measures Estimation and inference Results on data Open problems

An excellent estimator

$$\widehat{f}(x) = rgmin_{f\in \mathsf{bs}} [ext{error on data} + ext{smoothness of function}]$$

error on data =
$$L(f, data) = (f(x) - y)^2$$

smoothness of function = $||f||_{K}^{2} = \int |f'(x)|^2 dx$
big function space = reproducing kernel Hilbert space = \mathcal{H}_{K}

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Kernel models and penalized loss

Bayesian kernel model Priors on measures Estimation and inference Results on data Open problems

An excellent estimator

$$\widehat{f}(x) = rg\min_{f \in \mathcal{H}_K} \left[L(f, \mathsf{data}) + \lambda \| f \|_K^2
ight]$$

The kernel: $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ e.g. $K(u, v) = e^{(-\|u-v\|^2)}$. The RKHS

$$\mathcal{H}_{\mathcal{K}} = \overline{\left\{ f \mid f(x) = \sum_{i=1}^{\ell} \alpha_i \mathcal{K}(x, x_i), \ x_i \in \mathcal{X}, \, \alpha_i \in \mathbb{R}, \, \ell \in \mathbb{N} \right\}}.$$

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Kernel models and penalized loss Bayesian kernel model

Bayesian kernel model Priors on measures Estimation and inference Results on data Open problems

Representer theorem

$$\hat{f}(x) = \arg\min_{f \in \mathcal{H}_{K}} \left[L(f, \mathsf{data}) + \lambda \|f\|_{K}^{2} \right]$$

$$\hat{f}(x) = \sum_{i=1}^{n} a_i K(x, x_i).$$

Great when $p \gg n$.

Very popular and useful

Support vector machines

$$\hat{f}(x) = \arg\min_{f \in \mathcal{H}_K} \left[\sum_{i=1}^n |1 - y_i \cdot f(x_i)|_+ + \lambda \|f\|_K^2 \right],$$

Regularized Kernel regression

$$\hat{f}(x) = \arg\min_{f\in\mathcal{H}_K}\left[\sum_{i=1}^n |y_i - f(x_i)|^2 + \lambda \|f\|_K^2\right],$$

Regularized logistic regression

$$\hat{f}(x) = \arg\min_{f \in \mathcal{H}_K} \left[\sum_{i=1}^n \ln\left(1 + e^{-y_i \cdot f(x_i)}\right) + \lambda \|f\|_K^2 \right].$$

Direct prior elicitation Priors and integral operators

Bayesian interpretation of RBF

$$y_i = f(x_i) + \varepsilon, \quad \varepsilon \stackrel{iid}{\sim} \operatorname{No}(0, \sigma^2).$$

$$\begin{aligned} \mathsf{Lik}(\mathsf{data}|f) \propto \prod_{i=1}^{n} \exp(-(y_i - f(x_i))^2 / 2\sigma^2) & \pi(f) \propto \exp(-\|f\|_{\mathcal{K}}^2). \\ & \mathbf{P}\mathsf{rob}(f|\mathsf{data}) \propto \mathsf{Lik}(\mathsf{data}|f) \cdot \pi(f). \end{aligned}$$

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Direct prior elicitation Priors and integral operators

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Bayesian interpretation of RBF

$$y_i = f(x_i) + \varepsilon, \quad \varepsilon \stackrel{iid}{\sim} \operatorname{No}(0, \sigma^2).$$

Maximum a posteriori (MAP) estimator

$$\hat{f} = rg\max_{f \in \mathcal{H}_{\mathcal{K}}} \mathbf{P} \mathrm{rob}(f|\mathsf{data}).$$

I want the full posterior.

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Direct prior elicitation Priors and integral operators

Priors via spectral expansion

$$\mathcal{H}_{\mathcal{K}} = \left\{ f \mid f(x) = \sum_{i=1}^{\infty} a_i \phi_i(x) \text{ with } \sum_{i=1}^{\infty} a_i^2 / \lambda_i < \infty \right\},$$

 $\phi_i(x)$ and $\lambda_i \ge 0$ are eigenfunctions and eigenvalues of K:

$$\lambda_i\phi_i(x) = \int_{\mathcal{X}} \mathcal{K}(x,u)\phi_i(u)d\gamma(u).$$

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Direct prior elicitation Priors and integral operators

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 $\phi_i(x)$ and $\lambda_i \ge 0$ are eigenfunctions and eigenvalues of K:

$$\lambda_i\phi_i(x) = \int_{\mathcal{X}} K(x,u)\phi_i(u)d\gamma(u).$$

Specify a prior on $\mathcal{H}_{\mathcal{K}}$ via a prior on \mathcal{A}

$$\mathcal{A} = \Big\{ \big(a_k \big)_{k=1}^{\infty} \Big| \sum_k a_k^2 / \lambda_k < \infty \Big\}.$$

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Direct prior elicitation Priors and integral operators

Priors via spectral expansion

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Specify a prior on $\mathcal{H}_{\mathcal{K}}$ via a prior on \mathcal{A}

$$\mathcal{A} = \Big\{ \big(a_k \big)_{k=1}^{\infty} \Big| \sum_k a_k^2 / \lambda_k < \infty \Big\}.$$

Hard to sample and relies on computation of eigenvalues and eigenvectors.

Direct prior elicitation Priors and integral operators

Priors via duality

The duality between Gaussian processes and RKHS implies the following construction $% \left(\mathcal{A}_{n}^{\prime}\right) =\left(\mathcal{A}_{n}^{\prime}\right) \left(\mathcal{A}_{n}^{\prime$

$$f(\cdot) \sim GP(\mu_f, K),$$

where K is given by the kernel.

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Direct prior elicitation Priors and integral operators

Priors via duality

The duality between Gaussian processes and RKHS implies the following construction

$$f(\cdot) \sim GP(\mu_f, K),$$

where K is given by the kernel.

 $f(\cdot) \notin \mathcal{H}_K$ almost surely.

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Direct prior elicitation Priors and integral operators

Integral operators

Integral operator $\mathcal{L}_{\kappa}: \Gamma \rightarrow \mathcal{G}$

$$\mathcal{G} = \left\{ f \mid f(x) := \mathcal{L}_{\kappa}[\gamma](x) = \int_{\mathcal{X}} \mathcal{K}(x, u) \, d\gamma(u), \quad \gamma \in \Gamma \right\},$$

with $\Gamma \subseteq \mathcal{B}(\mathcal{X})$.

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Direct prior elicitation Priors and integral operators

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with $\Gamma \subseteq \mathcal{B}(\mathcal{X})$.

A prior on Γ implies a prior on \mathcal{G} .

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Direct prior elicitation Priors and integral operators

Equivalence with RKHS

For what Γ is $\mathcal{H}_{\mathcal{K}} = \operatorname{span}(\mathcal{G})$?

What is $\mathcal{L}_{\kappa}^{-1}(\mathcal{H}_{\kappa}) = ??$. This is hard to characterize.

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Direct prior elicitation Priors and integral operators

Equivalence with RKHS

For what Γ is $\mathcal{H}_{\mathcal{K}} = \operatorname{span}(\mathcal{G})$?

What is $\mathcal{L}_{\kappa}^{-1}(\mathcal{H}_{\kappa}) = ??$. This is hard to characterize.

- The candidates for Γ will be
 - square integrable functions
 - integrable functions
 - discrete measures
 - the union or integrable functions and discrete measures.

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Direct prior elicitation Priors and integral operators

Square integrable functions are too small

Proposition

For every $\gamma \in L^{2}(\mathcal{X})$, $\mathcal{L}_{K}[\gamma] \in \mathcal{H}_{K}$. Consequently, $L^{2}(\mathcal{X}) \subset \mathcal{L}_{K}^{-1}(\mathcal{H}_{K})$.

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Direct prior elicitation Priors and integral operators

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For every $\gamma \in L^{2}(\mathcal{X})$, $\mathcal{L}_{K}[\gamma] \in \mathcal{H}_{K}$. Consequently, $L^{2}(\mathcal{X}) \subset \mathcal{L}_{K}^{-1}(\mathcal{H}_{K})$.

Corollary

If $\Lambda = \{k : \lambda_k > 0\}$ is a finite set, then $\mathcal{L}_K(L^2(\mathcal{X})) = \mathcal{H}_K$ otherwise $\mathcal{L}_K(L^2(\mathcal{X})) \subsetneq \mathcal{H}_K$. The latter occurs when the kernel K is strictly positive definite, the RKHS is infinite-dimensional.

Direct prior elicitation Priors and integral operators

Signed measures are (almost) just right

Measures: The class of functions $L^1(\mathcal{X})$ are signed measures.

Proposition

For every $\gamma \in L^{1}(\mathcal{X})$, $\mathcal{L}_{K}[\gamma] \in \mathcal{H}_{K}$. Consequently, $L^{1}(\mathcal{X}) \subset \mathcal{L}_{K}^{-1}(\mathcal{H}_{K})$.

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Direct prior elicitation Priors and integral operators

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For every
$$\gamma \in L^{1}(\mathcal{X})$$
, $\mathcal{L}_{K}[\gamma] \in \mathcal{H}_{K}$. Consequently, $L^{1}(\mathcal{X}) \subset \mathcal{L}_{K}^{-1}(\mathcal{H}_{K})$.

Discrete measures:

$$\mathcal{M}_D = \left\{ \mu = \sum_{i=1}^n c_i \delta_{x_i} : \sum_{i=1}^n |c_i| < \infty, x_i \in \mathcal{X}, \ n \in \mathbb{N} \right\}.$$

Proposition

Given the set of finite discrete measures, $\mathcal{M}_D \subset \mathcal{L}_{\mathcal{K}}^{-1}(\mathcal{H}_{\mathcal{K}})$.

Direct prior elicitation Priors and integral operators

Signed measures are (almost) just right

Nonsingular measures: $\mathcal{M} = L^1(\mathcal{X}) \cup \mathcal{M}_D$

Proposition

 $\mathcal{L}_{\mathcal{K}}(\mathcal{M})$ is dense in $\mathcal{H}_{\mathcal{K}}$ with respect to the RKHS norm.

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Direct prior elicitation Priors and integral operators

Signed measures are (almost) just right

Nonsingular measures: $\mathcal{M} = L^1(\mathcal{X}) \cup \mathcal{M}_D$

Proposition

 $\mathcal{L}_{\mathcal{K}}(\mathcal{M})$ is dense in $\mathcal{H}_{\mathcal{K}}$ with respect to the RKHS norm.

Proposition

 $\mathcal{B}(\mathcal{X}) \subseteq \mathcal{L}_{K}^{-1}(\mathcal{H}_{K}(\mathcal{X})).$

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Direct prior elicitation Priors and integral operators

The implication

Take home message - need priors on signed measures.

A function theoretic foundation for random signed measures such as Gaussian, Dirichlet and Lévy process priors.

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Lévy processes Gaussian processes Bayesian representer theorem

Bayesian kernel model

$$y_i = f(x_i) + \varepsilon, \quad \varepsilon \stackrel{iid}{\sim} \operatorname{No}(0, \sigma^2).$$

$$f(x) = \int_{\mathcal{X}} K(x, u) Z(du)$$

where $Z(du) \in \mathcal{M}(\mathcal{X})$ is a signed measure on \mathcal{X} .

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Lévy processes Gaussian processes Bayesian representer theorem

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where $Z(du) \in \mathcal{M}(\mathcal{X})$ is a signed measure on \mathcal{X} .

$$\pi(Z|\mathsf{data}) \propto L(\mathsf{data}|Z) \ \pi(Z),$$

this implies a posterior on f.

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Lévy processes Gaussian processes Bayesian representer theorem

Lévy processes

A stochastic process $Z := \{Z_u \in \mathbb{R} : u \in \mathcal{X}\}$ is called a Lévy process if it satisfies the following conditions:

- $Z_0 = 0$ almost surely.
- ② For any choice of $m \ge 1$ and $0 \le u_0 < u_1 < ... < u_m$, the random variables $Z_{u_0}, Z_{u_1} Z_{u_0}, ..., Z_{u_m} Z_{u_{m-1}}$ are independent. (Independent increments property)
- The distribution of $Z_{s+u} Z_s$ is independent of Z_s (Temporal homogeneity or stationary increments property).
- Z has càdlàg paths almost surely.

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Lévy processes Gaussian processes Bayesian representer theorem

Lévy processes

Theorem (Lévy-Khintchine)

If Z is a Lévy process, then the characteristic function of $Z_u : u \ge 0$ has the following form:

$$\mathbb{E}[e^{i\lambda Z_{u}}] = \exp\left\{u\left[i\lambda a - \frac{1}{2}\sigma^{2}\lambda^{2} + \int_{\mathbb{R}\setminus\{0\}}[e^{i\lambda w} - 1 - i\lambda w1_{\{w:|w| < 1\}}(w)]\nu(dw)\right]\right\},\$$

where $a \in \mathbb{R}, \sigma^2 \ge 0$ and ν is a nonnegative measure on \mathbb{R} with $\int_{\mathbb{R}} (1 \wedge |w|^2) \nu(dw) < \infty$.

Lévy processes Gaussian processes Bayesian representer theorem



- drift term a
- variance of Brownian motion σ^2
- $\nu(dw)$ the jump process or Lévy measure.

$$\exp\left\{u\left[i\lambda a - \frac{1}{2}\sigma^{2}\lambda^{2}\right]\right\}$$
$$\exp\left\{u\int_{\mathbb{R}\setminus\{0\}}\left[e^{i\lambda w} - 1 - i\lambda w \mathbf{1}_{\{w:|w|<1\}}(w)\right]\nu(dw)\right\}$$

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Lévy processes Gaussian processes Bayesian representer theorem

Two approaches to Gaussian processes

Two modelling approaches

- prior directly on the space of functions by sampling from paths of the Gaussian process defined by K;
- **2** Gaussian process prior on Z(du) implies on prior on function space via integral operator.

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Lévy processes Gaussian processes Bayesian representer theorem

Prior on random measure

A Gaussian process prior on Z(du) is a signed measure so span $(\mathcal{G}) \subset \mathcal{H}_{\mathcal{K}}$.

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Lévy processes Gaussian processes Bayesian representer theorem

Direct prior elicitation

Theorem (Kallianpur)

If $\{Z_u, u \in \mathcal{X}\}$ is a Gaussian process with covariance K and mean $m \in \mathcal{H}_K$ and \mathcal{H}_K is infinite dimensional, then

$$\mathbf{P}(Z_{\bullet} \in \mathcal{H}_{K}) = 0.$$

The sample paths are almost surely outside $\mathcal{H}_{\mathcal{K}}$.

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Lévy processes Gaussian processes Bayesian representer theorem

A bigger RKHS

Theorem (Lukić and Beder)

Given two kernel functions R and K, R dominates K $(R \succ K)$ if $\mathcal{H}_K \subseteq \mathcal{H}_R$. Let $R \succ K$. Then

 $\|g\|_R \leq \|g\|_K, \ \forall g \in \mathcal{H}_K.$

There exists a unique linear operator $L: \mathcal{H}_R \to \mathcal{H}_R$ whose range is contained in \mathcal{H}_K such that

 $\langle f, g \rangle_R = \langle Lf, g \rangle_K, \quad \forall f \in \mathcal{H}_R, \, \forall g \in \mathcal{H}_K.$

In particular

 $LR_u = K_u, \quad \forall u \in \mathcal{X}.$

As an operator into \mathcal{H}_R , L is bounded, symmetric, and positive. Conversely, let $L : \mathcal{H}_R \to \mathcal{H}_R$ be a positive, continuous, self-adjoint operator then

 $K(s,t) = \langle LR_s, R_t \rangle_R, s, t \in \mathcal{X}$

defines a reproducing kernel on \mathcal{X} such that $K \leq R$.

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Lévy processes Gaussian processes Bayesian representer theorem

A bigger RKHS

If *L* is nucular (an operator that is compact with finite trace independent of basis choice) then we have nucular dominance $R \succ K$.

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Lévy processes Gaussian processes Bayesian representer theorem

A bigger RKHS

If *L* is nucular (an operator that is compact with finite trace independent of basis choice) then we have nucular dominance $R \succ K$.

Theorem (Lukić and Beder)

Let K and R be two reproducing kernels. Assume that the RKHS \mathcal{H}_R is separable.

A necessary and sufficient condition for the existence of a Gaussian process with covariance K and mean $m \in \mathcal{H}_R$ and with trajectories in \mathcal{H}_R with probability 1 is that $R \gg K$.

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Lévy processes Gaussian processes Bayesian representer theorem

A bigger RKHS

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Theorem (Lukić and Beder)

Let K and R be two reproducing kernels. Assume that the RKHS \mathcal{H}_R is separable.

A necessary and sufficient condition for the existence of a Gaussian process with covariance K and mean $m \in \mathcal{H}_R$ and with trajectories in \mathcal{H}_R with probability 1 is that $R \gg K$.

Characterize \mathcal{H}_R by $\mathcal{L}_K^{-1}(\mathcal{H}_K)$.

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Lévy processes Gaussian processes Bayesian representer theorem

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Dirichlet distribution

Multinomial distribution

$$g(x_1,...,x_k|n,p_1,...,p_k) = \frac{n!}{x_1!\cdots x_n!}p_1^{x_1}\cdots p_k^{x_k}, \quad \sum_{i=1}^k x_i = n, x_i \ge 0.$$

Lévy processes Gaussian processes <mark>Bayesian representer theorem</mark>

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Dirichlet distribution

Multinomial distribution

$$g(x_1,...,x_k|n,p_1,...,p_k) = \frac{n!}{x_1!\cdots x_n!}p_1^{x_1}\cdots p_k^{x_k}, \quad \sum_{i=1}^k x_i = n, x_i \ge 0.$$

Dirichlet distribution

$$f(p_1, \dots, p_k | \alpha_1, \dots, \alpha_k) = \frac{1}{B(\alpha)} \prod_{i=1}^k x_i^{\alpha_i - 1}, \quad \sum_{i=1}^k p_i = 1, p_i \ge 0,$$
$$B(\alpha) = \frac{\prod_{i=1}^k \Gamma(\alpha_i)}{\Gamma(\sum_{i=1}^k \alpha_i)}.$$

Lévy processes Gaussian processes Bayesian representer theorem

Conjugacy

If $\mathbf{P}rob(\theta|data)$ and $\pi(\theta)$ belong to the same family they are conjugate.

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Lévy processes Gaussian processes <mark>Bayesian representer theorem</mark>

Conjugacy

If $\mathbf{P}rob(\theta|data)$ and $\pi(\theta)$ belong to the same family they are conjugate.

Let
$$x = \{x_1, ..., x_k\}$$
 and $p = \{p_1, ..., p_k\}$
 $p \sim \text{Dir}(\alpha)$
 $x|p \sim \text{Mult}(p)$
 $p|x \sim \text{Dir}(p + \alpha).$

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Lévy processes Gaussian processes Bayesian representer theorem

Dirichlet process prior

Given distribution function F and a specified distribution F_0 with the same support on a space \mathcal{X} . Dirichlet process $DP(\alpha, F_0)$ implies that for any partition of the space $B_1, ..., B_K$

 $F(B_1), ..., F(B_k) \sim \mathsf{Dir}(\alpha(F_0(B_1)), ..., \alpha(F_0(B_k))).$

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Lévy processes Gaussian processes Bayesian representer theorem

Dirichlet process prior

$$f(x) = \int_{\mathcal{X}} K(x, u) Z(du) = \int_{\mathcal{X}} K(x, u) w(u) F(du)$$

F(du) is a distribution and w(u) a coefficient function.

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Lévy processes Gaussian processes Bayesian representer theorem

Dirichlet process prior

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F(du) is a distribution and w(u) a coefficient function.

Model F using a Dirichlet process prior: $DP(\alpha, F_0)$

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Lévy processes Gaussian processes <mark>Bayesian representer theorem</mark>

Bayesian representer theorem

Given
$$X_n = (x_1, ..., x_n) \stackrel{n\alpha}{\sim} F$$

 $F \mid X_n \sim \mathsf{DP}(\alpha + n, F_n), \quad F_n = (\alpha F_0 + \sum_{i=1}^n \delta_{x_i})/(\alpha + n).$

$$\mathbb{E}[f \mid X_n] = a_n \int K(x, u) w(u) dF_0(u) + n^{-1}(1-a_n) \sum_{i=1}^n w(x_i) K(x, x_i),$$
$$a_n = \alpha/(\alpha + n).$$

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Lévy processes Gaussian processes <mark>Bayesian representer theorem</mark>

Bayesian representer theorem

Taking $\lim \alpha \to 0$ to represent a non-informative prior:

Theorem (Bayesian representor theorem)

$$\hat{f}_n(x) = \sum_{i=1}^n w_i \, K(x, x_i),$$

 $w_i = w(x_i)/n.$

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Results on data Open problems Likelihood and prior specification Variable selection Semi-supervised learning

Likelihood

$$y_i = f(x_i) + \varepsilon_i = w_0 + \sum_{j=1}^n w_j K(x_i, x_j) + \varepsilon_i, \quad i = 1, ..., n$$

where $\varepsilon_i \sim No(0, \sigma^2)$.

$$Y \sim \operatorname{No}(w_0\iota + Kw, \sigma^2 I).$$

where $\iota = (1, ..., 1)'$.

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Results on data Open problems

Prior specification

Likelihood and prior specification Variable selection Semi-supervised learning

Factor: $K = F\Delta F'$ with $\Delta := \text{diag}(\lambda_1^2, ..., \lambda_n^2)$ and $w = F\Delta^{-1}\beta$.

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Results on data Open problems Likelihood and prior specification Variable selection Semi-supervised learning

Prior specification

Factor: $K = F\Delta F'$ with $\Delta := \text{diag}(\lambda_1^2, ..., \lambda_n^2)$ and $w = F\Delta^{-1}\beta$.

$$\begin{aligned} \pi(w_0,\sigma^2) &\propto 1/\sigma^2 \\ \tau_i^{-1} &\sim \operatorname{Ga}(a_\tau/2,b_\tau/2) \\ T &:= \operatorname{diag}(\tau_1,...,\tau_n) \\ \beta &\sim \operatorname{No}(0,T) \\ w|K,T &\sim \operatorname{No}(0,F\Delta^{-1}T\Delta^{-1}F') \end{aligned}$$

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Results on data Open problems Likelihood and prior specification Variable selection Semi-supervised learning

Prior specification

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Standard Gibbs sampler simulates $p(w, w_0, \sigma^2 | data)$.

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Results on data Open problems Likelihood and prior specification Variable selection Semi-supervised learning

Sampling from posterior

Objective: sample from $p(w, w_0, \sigma^2 | \text{data})$.

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Results on data Open problems Likelihood and prior specification Variable selection Semi-supervised learning

Sampling from posterior

Objective: sample from $p(w, w_0, \sigma^2 | data)$.

Given for $\{w^{(i)}, w_0^{(i)}, p_i(w, w_0)\}_{i=1}^T$ we have T functions can compute Bayes average and variance pointwise

$$\bar{f}(x) = \sum_{i=1}^{T} p_i(w, w_0) \left[w_0^{(j)} + \sum_{j=1}^{n} K(x, x_j) w_j^{(i)} \right]$$
$$var[f(x)] = \sum_{i=1}^{T} p_i(w, w_0) \left[\bar{f}(x) - f_i(x) \right]^2.$$

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Results on data Open problems Likelihood and prior specification Variable selection Semi-supervised learning

Markov chain Monte Carlo

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It may be difficult to sample from $p(w, w_0, \sigma^2 | \text{data})$, for example high dimensions. Also the normalizing constant \mathcal{Z} is unavailable

$$p(w, w_0, \sigma^2 | \mathsf{data}) = rac{\mathsf{Lik}(\mathsf{data} | w, w_0, \sigma^2) \cdot \pi(w, w_0, \sigma^2)}{\mathcal{Z}}$$

$$\mathcal{Z} = \int \mathsf{Lik}(\mathsf{data}|w, w_0, \sigma^2) \cdot \pi(w, w_0, \sigma^2) dw_0 \, dw \, d\sigma.$$

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Results on data Open problems Likelihood and prior specification Variable selection Semi-supervised learning

Markov chain Monte Carlo

Say we want to sample $p(\theta|data)$ but its hard. Say we have a Markov chain (aperiodic, irreducible, detailed balance)

$$q(\theta^*|\theta) = \mathsf{Prob}(\theta^*|\theta)$$

 $\mathsf{Prob}(\theta)q(\theta^*|\theta) = \mathsf{Prob}(\theta^*)q(\theta|\theta^*).$

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Results on data Open problems Likelihood and prior specification Variable selection Semi-supervised learning

Markov chain Monte Carlo

Metropolis-Hastings

- Given $\theta^{(t)}$ sample θ^* from $q(\theta^*|\theta^{(t)})$
- 2 Accept, $\theta^{(t+1)} = \theta^*$ with probability

$$\mathcal{A} = \min\left[1, \frac{p(\theta^*)q(\theta^{(t)}|\theta^*)}{p(\theta^{(t)})q(\theta^*|\theta^{(t)})}\right]$$

otherwise $\theta^{(t+1)} = \theta^{(t)}$.

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Results on data Open problems Likelihood and prior specification Variable selection Semi-supervised learning

Gibbs sampling

Given *d*-dimensional θ with known conditional

$$p(\theta_j| heta_{-j}) = p(heta_j| heta_1,... heta_{j-1}, heta_{j+1},..., heta_d).$$

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Results on data Open problems Likelihood and prior specification Variable selection Semi-supervised learning

Gibbs sampling

Given *d*-dimensional θ with known conditional

$$p(\theta_j|\theta_{-j}) = p(\theta_j|\theta_1,...\theta_{j-1},\theta_{j+1},...,\theta_d).$$

Proposal distribution

$$q(heta^*| heta^{(t)})=p(heta_j^*| heta_{-j}^{(t)}).$$

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Results on data Open problems Likelihood and prior specification Variable selection Semi-supervised learning

Gibbs sampling

Acceptance probability

$$\begin{aligned} \mathcal{A} &= \min\left[1, \frac{p(\theta^*)q(\theta^{(t)}|\theta^*)}{p(\theta^{(t)})q(\theta^*|\theta^{(t)})}\right] \\ &= \min\left[1, \frac{p(\theta^*)p(\theta_j^{(t)}|\theta_{-j}^{(t)})}{p(\theta^{(t)})q(\theta_j^*|\theta_{-j}^*)}\right] \\ &= \min\left[1, \frac{p(\theta_{-j}^*)}{p(\theta_{-j}^{(t)})}\right]. \end{aligned}$$

Results on data Open problems Likelihood and prior specification Variable selection Semi-supervised learning

Gibbs sampling example

We want to sample from x = 1, 2, 3, ..., n and $y \in [0, 1]$

$$p(x, y|n, \alpha, \beta) = \frac{n!}{(n-x)!x!} y^{x+\alpha-1} (1-y)^{n-x+\beta-1}$$

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Results on data Open problems Likelihood and prior specification Variable selection Semi-supervised learning

Gibbs sampling example

We want to sample from x = 1, 2, 3, ..., n and $y \in [0, 1]$

$$p(x, y | n, \alpha, \beta) = \frac{n!}{(n-x)! x!} y^{x+\alpha-1} (1-y)^{n-x+\beta-1}$$

Conditionals

$$\begin{aligned} x|y &\sim & \mathsf{Bin}(n,y) = \frac{n!}{(n-x)!} y^x (1-y)^{(n-x)} \\ y|x &\sim & \mathsf{Be}(x+\alpha, n-x+\beta) \propto y^{x+\alpha} (1-y)^{n-x+\beta} \end{aligned}$$

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> Results on data Open problems

Likelihood and prior specification Variable selection Semi-supervised learning

Gibbs sampling example



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> Results on data Open problems

Likelihood and prior specification Variable selection Semi-supervised learning

Gibbs sampling example



2 draw $x_{t+1} \sim Bin(n, y_t)$

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Likelihood and prior specification Variable selection Semi-supervised learning

Gibbs sampling example

- **1** given y_t
- 2 draw $x_{t+1} \sim Bin(n, y_t)$
- 3 draw $y_{t+1} \sim \text{Be}(x_{t+1} + \alpha, n x_{t+1} + \beta)$

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> Results on data Open problems

Likelihood and prior specification Variable selection Semi-supervised learning

Gibbs sampling example

- **1** given y_t
- 2 draw $x_{t+1} \sim Bin(n, y_t)$
- 3 draw $y_{t+1} \sim \text{Be}(x_{t+1} + \alpha, n x_{t+1} + \beta)$
- return to (2).

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Results on data Open problems Likelihood and prior specification Variable selection Semi-supervised learning

Kernel model extension

$$K_{\nu}(x, u) = K(\sqrt{\nu \otimes x}, \sqrt{\nu \otimes u})$$

with $\nu = \{\nu_1, ..., \nu_p\}$ with $\nu_k \in [0, \infty)$ as a scale parameter

$$k_{\nu}(x, u) = \sum_{k=1}^{p} \nu_{k} x_{k} u_{k},$$

$$k_{\nu}(x, u) = \left(1 + \sum_{k=1}^{p} \nu_{k} x_{k} u_{k}\right)^{d},$$

$$k_{\nu}(x, u) = \exp\left(-\sum_{k=1}^{p} \nu_{k} (x_{k} - u_{k})^{2}\right)$$

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Results on data Open problems

Prior specification

Likelihood and prior specification Variable selection Semi-supervised learning

$$\begin{array}{ll} \nu_k & \sim & (1-\gamma)\delta_0 + \gamma \; \mathsf{Ga}(a_\nu,a_\nu s), & (k=1,\ldots,p), \\ s & \sim \; \mathsf{Exp}(a_s), & \gamma \sim \mathsf{Be}(a_\gamma,b_\gamma) \end{array}$$

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Results on data Open problems

Prior specification

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$$egin{array}{rcl}
u_k &\sim & (1-\gamma)\delta_0+\gamma \; {
m Ga}(a_
u,a_
u s), & (k=1,\ldots,p), \ s &\sim \; {
m Exp}(a_s), & \gamma \sim {
m Be}(a_\gamma,b_\gamma) \end{array}$$

Standard Gibbs sampler does not work: Metropolis-Hastings.

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Likelihood and prior specification Variable selection Semi-supervised learning

Problem setup

Labelled data : $(Y^p, X^p) = \{(y_i^p, x_i^p); i = 1 : n_p\} \stackrel{iid}{\sim} \rho(Y, X | \phi, \theta).$ Unlabelled data: $X^m = \{x_i^m, i = (1) : (n_m)\} \stackrel{iid}{\sim} \rho(X | \theta).$

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Likelihood and prior specification Variable selection Semi-supervised learning

Problem setup

Labelled data :
$$(Y^p, X^p) = \{(y_i^p, x_i^p); i = 1 : n_p\} \stackrel{iid}{\sim} \rho(Y, X | \phi, \theta).$$

Unlabelled data: $X^m = \{x_i^m, i = (1) : (n_m)\} \stackrel{iid}{\sim} \rho(X | \theta).$
How can the unlabelled data help our a predictive model ?
data = $\{Y, X, X^m\}$

 $p(\phi, \theta | \mathsf{data}) \propto \pi(\phi, \theta) p(Y | X, \phi) p(X | \theta) p(X^m | \theta).$

Need very strong dependence between θ and ϕ .

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Results on data Open problems Likelihood and prior specification Variable selection Semi-supervised learning

Bayesian kernel model

Result of DP prior

$$\hat{f}_n(x) = \sum_{i=1}^{n_p+n_m} w_i \, \mathcal{K}(x, x_i).$$

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Results on data Open problems Likelihood and prior specification Variable selection Semi-supervised learning

Bayesian kernel model

Result of DP prior

$$\hat{f}_n(x) = \sum_{i=1}^{n_p+n_m} w_i \, \mathcal{K}(x, x_i).$$

Same as in Belkin and Niyogi but without

$$\min_{f \in \mathcal{H}_{K}} \left[L(f, \mathsf{data}) + \lambda_{1} \| f \|_{K}^{2} + \lambda_{2} \| f \|_{I}^{2} \right].$$

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Results on data Open problems Likelihood and prior specification Variable selection Semi-supervised learning

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- θ = F(·) so that p(x|θ)dx = dF(x) the parameter is the full distribution function itself;
- *p*(y|x, φ) depends intimately on θ = F; in fact, θ ⊆ φ in this case and dependence of θ and φ is central to the model.

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Results on data Open problems Likelihood and prior specification Variable selection Semi-supervised learning

Bayesian kernel model

Result of DP prior

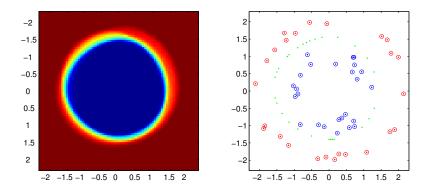
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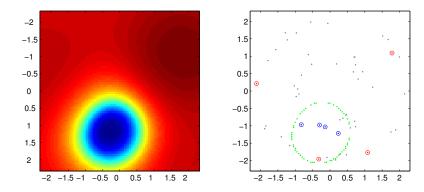
Open problems

Simulated data - semi-supervised



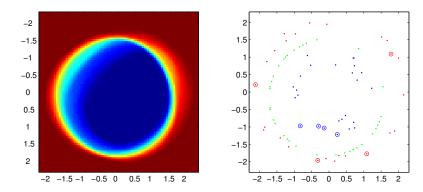
Open problems

Simulated data - semi-supervised

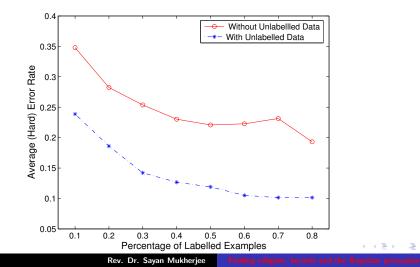


Open problems

Simulated data - semi-supervised

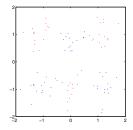


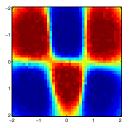
Cancer classification – semi-supervised



Open problems

Simulated data – feature selection

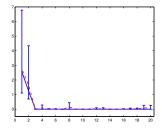




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Open problems

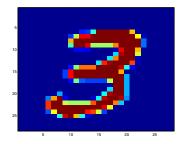
Simulated data – feature selection

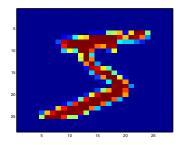


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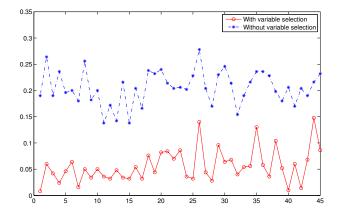
Open problems

MNIST digits – feature selection





MNIST digits - feature selection





Lots of work left:

• Further refinement of integral operators and priors in terms of Sobolev spaces.



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- Semi-supervised setting: relation of kernel model and priors with Laplace-Beltrami and graph Laplacian operators.

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Lots of work left:

- Further refinement of integral operators and priors in terms of Sobolev spaces.
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- Semi-supervised setting: Duality between diffusion processes on manifolds and Markov chains.

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- Semi-supervised setting: relation of kernel model and priors with Laplace-Beltrami and graph Laplacian operators.
- Semi-supervised setting: Duality between diffusion processes on manifolds and Markov chains.
- Bayesian variable selection: Efficient sampling and search in high-dimensional space.
- Numeric stability and statistical robustness.

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Its extra work but it pays to be Bayes :)

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