Bayesian Kernel Models: theory and applications

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Learning gradients: simultaneous regression and inverse regression

This talk concerns models on high-dimensional data that are simultaneously predictive – regression – and also infer the underlying geometric structure of the data relevant to prediction – inverse regression.

Theory as well as applications to gene expression analysis and digit recognition will be presented.

The word Bayes will not appear in tomorrow’s talk. However, there will be differential geometry, graphical models, and animal husbandry.
High dimensional inference and random matrices
Spring semester continuation – Geometry and random matrices

Misha Belkin – CSE
Yoon Lee – Statistics

Working group in computational statistics.
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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Regression

data = \{L_i = (x_i, y_i)\}_{i=1}^n\text{ with } L_i \overset{\text{iid}}{\sim} \rho(X, Y).

X \in \mathcal{X} \subset \mathbb{R}^p \text{ and } Y \subset \mathbb{R} \text{ and } p \gg n.

A natural idea

f(x) = \mathbb{E}_Y[Y|x].
An excellent estimator

\[ \hat{f}(x) = \arg \min_{f \in \mathcal{B}s} \left[ \text{error on data} + \text{smoothness of function} \right] \]
An excellent estimator

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

Error on data: \[ L(f, \text{data}) = (f(x) - y)^2 \]

Smoothness of function: \[ \|f\|_K^2 = \int |f'(x)|^2 dx \]

Big function space: \[ \text{reproducing kernel Hilbert space} = \mathcal{H}_K \]
An excellent estimator

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

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

The RKHS

\[ \mathcal{H}_K = \left\{ f \mid f(x) = \sum_{i=1}^{\ell} \alpha_i K(x, x_i), \ x_i \in \mathcal{X}, \ \alpha_i \in \mathbb{R}, \ \ell \in \mathbb{N} \right\} . \]
Representer theorem

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

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

Great when \( p \gg n \).
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

\[ \hat{f}(x) = \arg \min_{f \in \mathcal{H}_K} \left[ \sum_{i=1}^{n} \ln \left( 1 + e^{-y_i \cdot f(x_i)} \right) + \lambda \|f\|_K^2 \right]. \]
Why go Bayes – uncertainty
Priors via spectral expansion

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

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

\[ \lambda_i \phi_i(x) = \int_{\mathcal{X}} K(x, u) \phi_i(u) d\gamma(u). \]
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Specify a prior on \( \mathcal{H}_K \) via a prior on \( \mathcal{A} \)

\[ \mathcal{A} = \left\{ (a_k)_{k=1}^{\infty} \mid \sum_{k} \frac{a_k^2}{\lambda_k} < \infty \right\}. \]
Priors via spectral expansion

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

\[ f(\cdot) \notin \mathcal{H}_K \text{ almost surely.} \]
Integral operators

Integral operator $L_K : \Gamma \rightarrow G$

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

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

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

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

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

A prior on $\Gamma$ implies a prior on $\mathcal{G}$. 

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Equivalence with RKHS

For what \( \Gamma \) is \( \mathcal{H}_K = \text{span}(\mathcal{G}) \)?

What is \( \mathcal{L}_K^{-1}(\mathcal{H}_K) = \)?? This is hard to characterize.
Equivalence with RKHS

For what $\Gamma$ is $\mathcal{H}_K = \text{span}(\mathcal{G})$?

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

The candidates for $\Gamma$ will be

1. square integrable functions
2. integrable functions
3. discrete measures
4. the union or integrable functions and discrete measures.
Square integrable functions are too small

**Proposition**

For every \( \gamma \in L^2(\mathcal{X}) \), \( \mathcal{L}_K[\gamma] \in \mathcal{H}_K \). Consequently, \( L^2(\mathcal{X}) \subset \mathcal{L}^{-1}_K(\mathcal{H}_K) \).
Square integrable functions are too small

**Proposition**

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

**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.
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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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, \( \mathcal{M}_D \subset \mathcal{L}^{-1}_K(\mathcal{H}_K) \).
Signed measures are (almost) just right

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

**Proposition**

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

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

**Proposition**

$\mathcal{B}(\mathcal{X}) \not\subseteq \mathcal{L}_K^{-1}(\mathcal{H}_K(\mathcal{X}))$. 
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.
Bayesian kernel model

\[ y_i = f(x_i) + \varepsilon, \quad \varepsilon \sim \text{iid No}(0, \sigma^2). \]

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

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

\[ y_i = f(x_i) + \varepsilon, \quad \varepsilon \sim \text{No}(0, \sigma^2). \]

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

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

\[ \pi(Z|\text{data}) \propto L(\text{data}|Z) \pi(Z), \]

this implies a posterior on \( f \).
A stochastic process $Z := \{Z_u \in \mathbb{R} : u \in \mathcal{X}\}$ is called a Lévy process if it satisfies the following conditions:

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

Theorem (Lévy-Khintchine)

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

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

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

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

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

Two modelling approaches

1. 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.
A Gaussian process prior on $Z(du)$ is a signed measure so $\text{span}(\mathcal{G}) \subset \mathcal{H}_K$. 
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

\[
P(Z \cdot \in \mathcal{H}_K) = 0.
\]

The sample paths are almost surely outside \( \mathcal{H}_K \).
There exists a unique linear operator $L : \mathcal{H}_R \rightarrow \mathcal{H}_R$ 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

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

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

$$K(s, t) = \langle LR_s, R_t \rangle_R, \quad s, t \in X$$ 

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

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

Characterize $\mathcal{H}_R$ by $\mathcal{L}_K^{-1}(\mathcal{H}_K)$. 
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.
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: \( \text{DP}(\alpha, F_0) \)
Bayesian representer form

Given $X_n = (x_1, ..., x_n) \overset{iid}{\sim} F$

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

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

$$a_n = \frac{\alpha}{\alpha + n}.$$
Bayesian representer form

Taking \( \lim \alpha \rightarrow 0 \) to represent a non-informative prior:

**Proposition (Bayesian representor theorem)**

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

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

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

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

where $\iota = (1, \ldots, 1)'$. 
Prior specification

Factor: $K = F \Delta F'$ with $\Delta := \text{diag}(\lambda_1^2, \ldots, \lambda_n^2)$ and $w = F \Delta^{-1} \beta$. 
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\[
\pi(w_0, \sigma^2) \propto \frac{1}{\sigma^2} \\
\tau_i^{-1} \sim \text{Ga}(a_\tau/2, b_\tau/2) \\
T := \text{diag}(\tau_1, \ldots, \tau_n) \\
\beta \sim \text{No}(0, T) \\
w|K, T \sim \text{No}(0, F \Delta^{-1} T \Delta^{-1} F').
\]
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Factor: \( K = F \Delta F' \) with \( \Delta := \text{diag}(\lambda_1^2, \ldots, \lambda_n^2) \) and \( w = F \Delta^{-1} \beta \).

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\pi(w_0, \sigma^2) \propto 1/\sigma^2 \\
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\]

Standard Gibbs sampler simulates \( p(w, w_0, \sigma^2|\text{data}) \).
Kernel model extension

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

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

\[ k_\nu(x, u) = \sum_{k=1}^{p} \nu_k x_k u_k, \]

\[ k_\nu(x, u) = \left( 1 + \sum_{k=1}^{p} \nu_k x_k u_k \right)^d, \]

\[ k_\nu(x, u) = \exp \left( -\sum_{k=1}^{p} \nu_k (x_k - u_k)^2 \right). \]
Prior specification

\[ \begin{align*}
\nu_k & \sim (1 - \gamma)\delta_0 + \gamma \, \text{Ga}(a_\nu, a_\nu s), \quad (k = 1, \ldots, p), \\
s & \sim \text{Exp}(a_s), \quad \gamma \sim \text{Be}(a_\gamma, b_\gamma)
\end{align*} \]
Prior specification

\[ \nu_k \sim (1 - \gamma)\delta_0 + \gamma \text{Ga}(a_\nu, a_\nu s), \quad (k = 1, \ldots, p), \]
\[ s \sim \text{Exp}(a_s), \quad \gamma \sim \text{Be}(a_\gamma, b_\gamma) \]

Standard Gibbs sampler does not work: Metropolis-Hastings.
Could use help – Chris?
Problem setup

Labelled data: \((Y^p, X^p) = \{(y^p_i, x^p_i); \ i = 1 : n_p\} \overset{iid}{\sim} \rho(Y, X|\phi, \theta).\)

Unlabelled data: \(X^m = \{x^m_i, \ i = (1):(n_m)\} \overset{iid}{\sim} \rho(X|\theta).\)
Problem setup

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

Unlabelled data: \(X^m = \{x_i^m, \ i = (1) : (n_m)\} \overset{iid}{\sim} \rho(X|\theta)\).

How can the unlabelled data help our a predictive model ?

data = \{Y, X, X^m\}

\[p(\phi, \theta|\text{data}) \propto \pi(\phi, \theta)p(Y|X, \phi)p(X|\theta)p(X^m|\theta).\]

Need very strong dependence between \(\theta\) and \(\phi\).
Bayesian kernel model

Result of DP prior

\[ \hat{f}_n(x) = \sum_{i=1}^{np+nm} w_i K(x, x_i). \]
Result of DP prior

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

Same as in Belkin and Niyogi but without

\[
\min_{f \in \mathcal{H}_K} \left[ L(f, \text{data}) + \lambda_1 \| f \|_K^2 + \lambda_2 \| f \|_I^2 \right].
\]
Result of DP prior

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

1. \( \theta = F(\cdot) \) so that \( p(x|\theta)dx = dF(x) \) - the parameter is the full distribution function itself;

2. \( p(y|x, \phi) \) depends intimately on \( \theta = F \); in fact, \( \theta \subseteq \phi \) in this case and dependence of \( \theta \) and \( \phi \) is central to the model.
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Simulated data – semi-supervised

Kernel models and penalized loss
Bayesian kernel model
Priors on measures
Estimation and inference
Results on data
Open problems
Simulated data – semi-supervised
Simulated data – semi-supervised
Cancer classification – semi-supervised

![Graph showing error rate vs. percentage of labelled examples with and without unlabelled data.]
MNIST digits – feature selection
MNIST digits – feature selection

![Graph showing feature selection with and without variable selection.](image-url)
Discussion

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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- Bayesian variable selection: Efficient sampling and search in high-dimensional space.
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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.
Summary

It's extra work but it pays to be Bayes :)

Sayan Mukherjee
Bayesian Kernel Models: theory and applications