Bayesian Kernel Models: theory and applications

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May 10, 2007

Shameless plug for tomorrow

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.

Fun SAMSI program this spring

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.

Table of contents

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

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

An excellent estimator

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

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$$\begin{aligned}
\text{error on data} &= L(f, \text{data}) = (f(x) - y)^2 \\
\text{smoothness of function} &= \|f\|_K^2 = \int |f'(x)|^2 dx \\
\underline{\text{b}}\text{ig function } \underline{\text{s}}\text{pace} &= \text{reproducing kernel Hilbert space} = \mathcal{H}_K
\end{aligned}$$

An excellent estimator

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

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

The RKHS

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

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 $p \gg n$.

Very popular and useful

1. Support vector machines

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

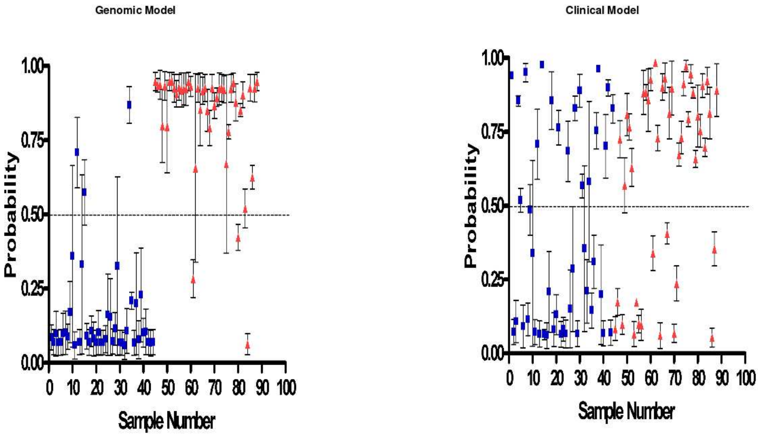
2. Regularized Kernel regression

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

3. 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

$$\mathcal{H}_K = \left\{ f \;\middle|\; f(x) = \sum_{i=1}^{\infty} a_i \phi_i(x) \text{ with } \sum_{i=1}^{\infty} a_i^2/\lambda_i < \infty \right\},$$

$\phi_i(x)$ 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 $\mathcal{A}$

$$\mathcal{A} = \left\{ (a_k)_{k=1}^{\infty} \;\middle|\; \sum_k a_k^2/\lambda_k < \infty \right\}.$$

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

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.

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where K is given by the kernel.

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

Integral operators

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

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

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

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

Equivalence with RKHS

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

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

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The candidates for Γ 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,* $L^2(\mathcal{X}) \subset \mathcal{L}_K^{-1}(\mathcal{H}_K)$.

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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.

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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, $\mathcal{M}_D \subset \mathcal{L}_K^{-1}(\mathcal{H}_K)$.

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

$\mathcal{B}(\mathcal{X}) \subsetneqq \mathcal{L}_K^{-1}(\mathcal{H}_K(\mathcal{X}))$.

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

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

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

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

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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.

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:

1. $Z_0 = 0$ almost surely.
2. For any choice of $m \geq 1$ and $0 \leq u_0 < u_1 < ... < u_m$, the random variables $Z_{u_0}, Z_{u_1} - Z_{u_0}, ..., Z_{u_m} - Z_{u_{m-1}}$ are independent. (Independent increments property)
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 ν 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 σ^2
- $\nu(dw)$ the jump process or Lévy measure.

$$\exp\left\{u\left[i\lambda a - \frac{1}{2}\sigma^2\lambda^2\right]\right\}$$

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

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.

Prior on random measure

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

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

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

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

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

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

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

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

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

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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 $R \succ K$.

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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.

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

Bayesian representer form

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

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

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

$a_n = \alpha/(\alpha + n)$.

Bayesian representer form

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

Proposition (Bayesian representor theorem)

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

$w_i = w(x_i)/n.$

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

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

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

Prior specification

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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\begin{aligned}
\pi(w_0, \sigma^2) &\propto 1/\sigma^2 \\
\tau_i^{-1} &\sim \text{Ga}(a_\tau/2, b_\tau/2) \\
T &:= \text{diag}(\tau_1, ..., \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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\end{aligned}$$

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

$$\begin{aligned} k_\nu(x,u) &= \sum_{k=1}^{p} \nu_k \, x_k \, u_k, \\ k_\nu(x,u) &= \left(1 + \sum_{k=1}^{p} \nu_k \, x_k \, u_k\right)^d, \\ k_\nu(x,u) &= \exp\left(-\sum_{k=1}^{p} \nu_k (x_k - u_k)^2\right). \end{aligned}$$

Prior specification

$$
\begin{aligned}
\nu_k &\sim (1-\gamma)\delta_0 + \gamma\ \mathrm{Ga}(a_\nu, a_\nu s), \quad (k = 1, \ldots, p), \\
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Standard Gibbs sampler does not work: Metropolis-Hastings.
Could use help – Chris ?

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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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 ?

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

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

Need very strong dependence between θ and ϕ.

Bayesian kernel model

Result of DP prior

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

Bayesian kernel model

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

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

Bayesian kernel model

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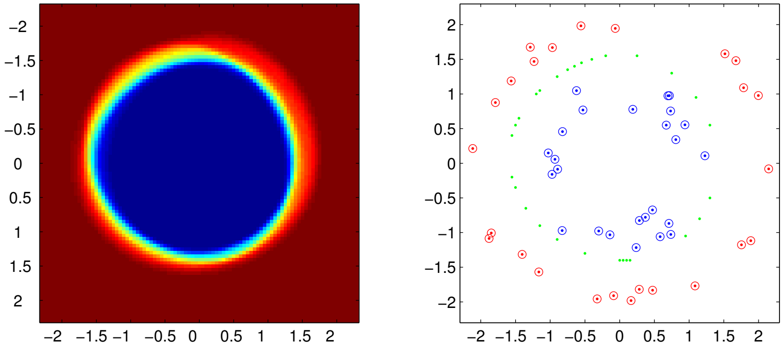

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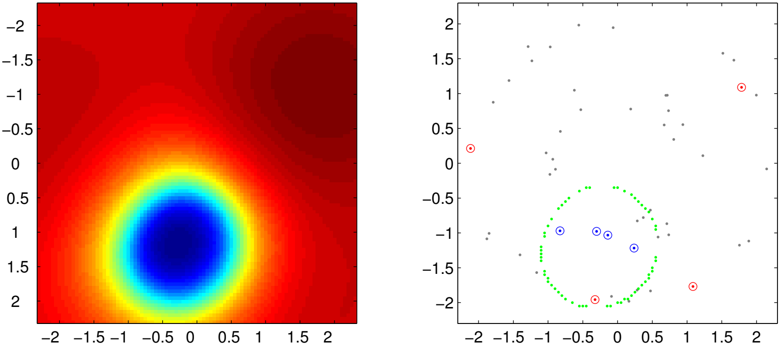

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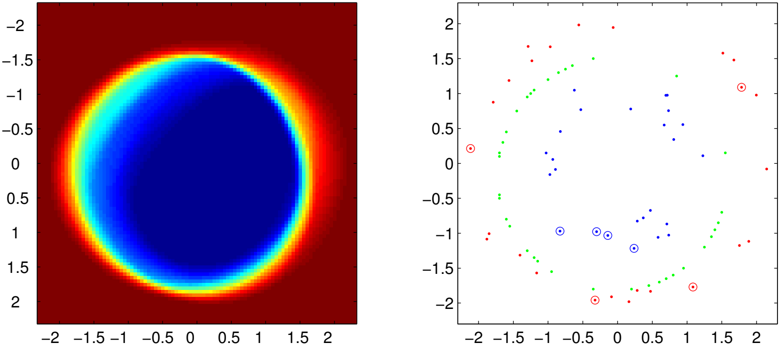
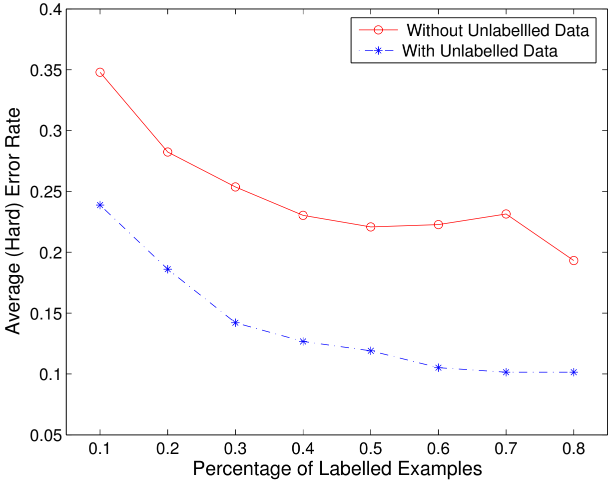
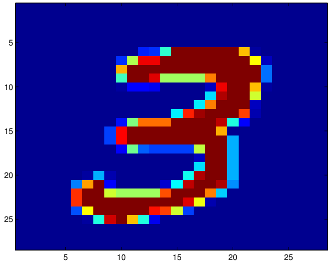
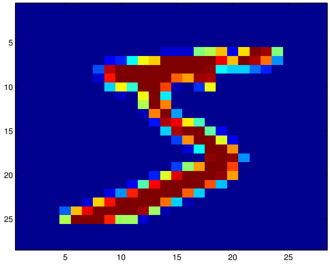


Cancer classification – semi-supervised



MNIST digits – feature selection





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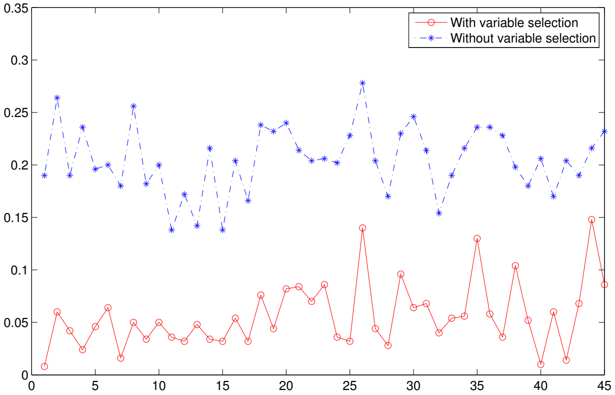

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- Semi-supervised setting: Duality between diffusion processes on manifolds and Markov chains.
- Bayesian variable selection: Efficient sampling and search in high-dimensional space.
- Numeric stability and statistical robustness.

Summary

Its extra work but it pays to be Bayes :)