Binary probit regression with I-priors

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PhD Presentation Event

http://phd3.haziqj.ml

Outline

- 2 Probit models with I-priors
 The latent variable motivation
 Using I-priors
 Estimation (and challenges)
- Variational inference Introduction Mean-field factorisation
- 4 Implementation R/iprobit Examples
- Summary

The regression model

Introduction

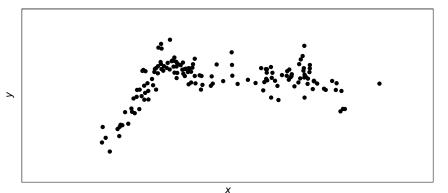
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• For i = 1, ..., n, consider the regression model

$$y_i = f(x_i) + \epsilon_i$$

$$(\epsilon_1, \dots, \epsilon_n) \sim N(\mathbf{0}, \Psi^{-1})$$
(1)

where $f \in \mathcal{F}$, $y_i \in \mathbb{R}$, and $x_i = (x_{i1}, \dots, x_{ip}) \in \mathcal{X}$.



I-priors

Introduction

• Let \mathcal{F} be a reproducing kernel Hilbert space (RKHS) with reproducing kernel $h_{\lambda}: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$. An I-prior on f is

$$(f(x_1),\ldots,f(x_n))^{\top}\sim \mathsf{N}\left(\mathsf{f}_0,\mathcal{I}(f)\right)$$

with \mathbf{f}_0 a prior mean, and \mathcal{I} the Fisher information for f, given by

$$\mathcal{I}(f(x), f(x')) = \sum_{k=1}^{n} \sum_{l=1}^{n} \psi_{kl} h_{\lambda}(x, x_k) h_{\lambda}(x', x_l).$$

• The I-prior regression model for i = 1, ..., n becomes

$$y_i = f_0(x_i) + \sum_{k=1}^n h_\lambda(x_i, x_k) w_k + \epsilon_i$$

 $(w_1, \dots, w_n) \sim \mathsf{N}(\mathbf{0}, \mathbf{\Psi})$
 $(\epsilon_1, \dots, \epsilon_n) \sim \mathsf{N}(\mathbf{0}, \mathbf{\Psi}^{-1})$

W. Bergsma (2017). "Regression with I-priors". Manuscript in preparation

I-priors (cont.)

Introduction

 Of interest is the posterior regression function characterised by the distribution

$$p(\mathbf{f}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{f})p(\mathbf{f})}{\int p(\mathbf{y}|\mathbf{f})p(\mathbf{f})\,\mathrm{d}\mathbf{f}},$$

and also the posterior predictive distribution for new data points x_{new}

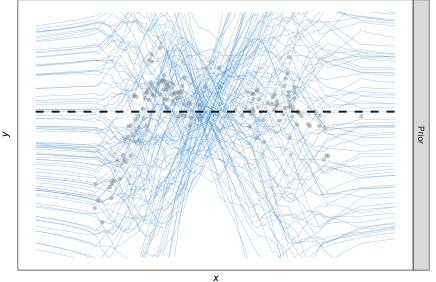
$$p(y_{\text{new}}|\mathbf{y}) = \int p(y_{\text{new}}|\mathbf{y}, f_{\text{new}}) p(f_{\text{new}}|\mathbf{y}) \, df_{\text{new}}$$

with $f_{\text{new}} = f(x_{\text{new}})$.

- Estimation using EM algorithm or direct maximisation of the marginal likelihood $\log p(y)$.
- Complete Bayesian estimation also possible.

HJ (2017a). iprior: Linear Regression using I-Priors. R Package version 0.6.4: CRAN/GitHub

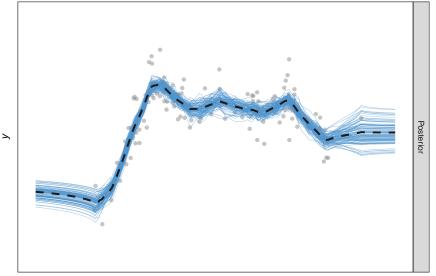
Fractional Brownian motion (FBM) RKHS



Introduction

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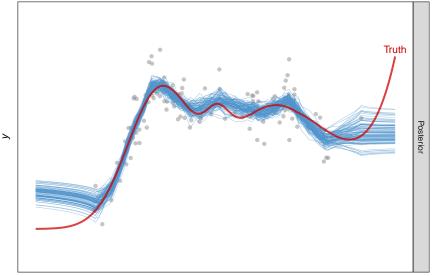
Fractional Brownian motion (FBM) RKHS



Introduction

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Fractional Brownian motion (FBM) RKHS



Probit with I-priors

Introduction

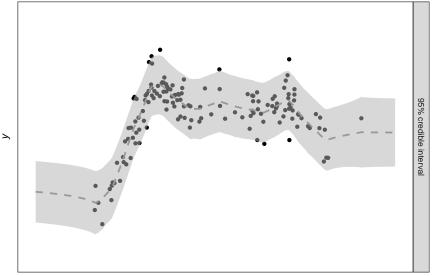
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Variational

Implementation

Summary

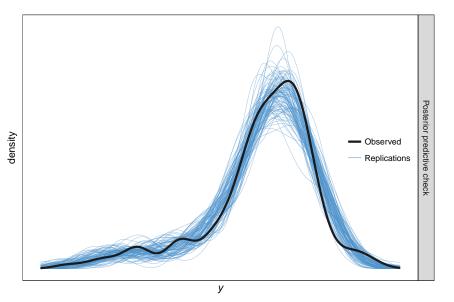
Posterior predictive distribution



Introduction

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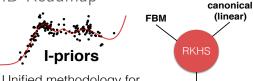
Posterior predictive distribution



Introduction Probit with I-priors Summary 000000

Pearson

PhD Roadmap



Unified methodology for

- additive models
- multilevel models
- models with functional covariates

<u>Advantages</u>

- Minimal assumptions
- Straightforward inference
- Performance competetive

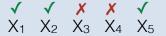
R/iprior

Estimation:

- Direct maximisation
- EM algorithm
- MCMC (Gibbs/HMC)

Bayesian Variable Selection (using I-priors in the

canonical RKHS)



Good performance in cases with multicollinearity

Binary probit models with I-priors

Extension to binary responses Estimation using variational inference



classification



inference / fitted probabilities

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The latent variable motivation

- Consider binary responses y_1, \ldots, y_n together with their corresponding covariates x_1, \ldots, x_n .
- For i = 1, ..., n, model the responses as

$$y_i \sim \mathsf{Bern}(p_i)$$
.

 Assume that there exists continuous, underlying latent variables y_1^*, \ldots, y_n^* , such that

$$y_i = \begin{cases} 1 & \text{if } y_i^* \ge 0 \\ 0 & \text{if } y_i^* < 0. \end{cases}$$

Model these continuous latent variables according to

$$y_i^* = f(x_i) + \epsilon_i$$

where $(\epsilon_1, \dots, \epsilon_n) \sim \mathsf{N}(\mathbf{0}, \Psi^{-1})$ and $f \in \mathcal{F}$ (some RKHS).

Using I-priors

Assume an I-prior on f. Then,

$$f(x_i) = \overbrace{f_0(x_i)}^{\alpha} + \sum_{k=1}^{n} h_{\lambda}(x_i, x_k) w_k$$
$$(w_1, \dots, w_n) \sim \mathsf{N}(\mathbf{0}, \mathbf{\Psi})$$

• For now, consider iid errors $\Psi = \psi \mathbf{I}_n$. In this case,

$$p_i = P[y_i = 1] = P[y_i^* \ge 0]$$

$$= P[\epsilon_i \le f(x_i)]$$

$$= \Phi\left(\psi^{1/2}(\alpha + \sum_{k=1}^n h_\lambda(x_i, x_k)w_k)\right)$$

where Φ is the CDF of a standard normal.

ullet No loss of generality compared with using an arbitrary threshold au or error precision ψ . Thus, set $\psi = 1$.

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Estimation

- Denote $f_i = f(x_i)$ for short.
- The marginal density

$$p(\mathbf{y}) = \int p(\mathbf{y}|\mathbf{f})p(\mathbf{f}) d\mathbf{f}$$

$$= \int \prod_{i=1}^{n} \left[\Phi(f_i)^{y_i} (1 - \Phi(f_i))^{1-y_i} \right] \cdot N(\alpha \mathbf{1}_n, \mathbf{H}_{\lambda}^2) d\mathbf{f}$$

for which $p(\mathbf{f}|\mathbf{y})$ depends, cannot be evaluated analytically.

- Some strategies:
 - Naive Monte-Carlo integral
 - X EM algorithm with a MCMC E-step
 - ✓ Laplace approximation
 - ✓ MCMC sampling

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Variational inference

- Consider a statistical model where we have observations (y_1, \ldots, y_n) and also some latent variables (z_1, \ldots, z_n) .
- The z_i could be random effects or some auxiliary latent variables.
- In a Bayesian setting, this could also include the parameters to be estimated.
- GOAL: Find approximations for
 - ▶ The posterior distribution $p(\mathbf{z}|\mathbf{y})$; and
 - ▶ The marginal likelihood (or model evidence) $p(\mathbf{y})$.
- Variational inference is a deterministic approach, unlike MCMC.

C. M. Bishop (2006). Pattern Recognition and Machine Learning. Springer, Ch. 10 K. P. Murphy (2012). Machine Learning: A Probabilistic Perspective. The MIT Press. Ch. 21

Decomposition of the log marginal

• Let q(z) be some density function to approximate p(z|y). Then the log-marginal density can be decomposed into

$$\log p(\mathbf{y}) = \log p(\mathbf{y}, \mathbf{z}) - \log p(\mathbf{z}|\mathbf{y})$$

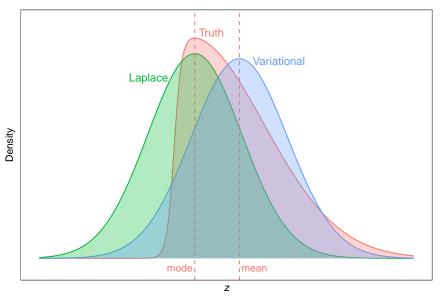
$$= \int \left\{ \log \frac{p(\mathbf{y}, \mathbf{z})}{q(\mathbf{z})} - \log \frac{p(\mathbf{z}|\mathbf{y})}{q(\mathbf{z})} \right\} q(\mathbf{z}) d\mathbf{z}$$

$$= \mathcal{L}(q) + \mathsf{KL}(q||p)$$

$$\geq \mathcal{L}(q)$$

- \bullet L is referred to as the "lower-bound", and it serves as a surrogate function to the marginal.
- Maximising $\mathcal{L}(q)$ is equivalent to minimising $\mathsf{KL}(q||p)$.
- Although KL(q||p) is minimised at $q(z) \equiv p(z|y)$ (c.f. EM algorithm), we are unable to work with $p(\mathbf{z}|\mathbf{y})$.

Comparison of approximations (density)



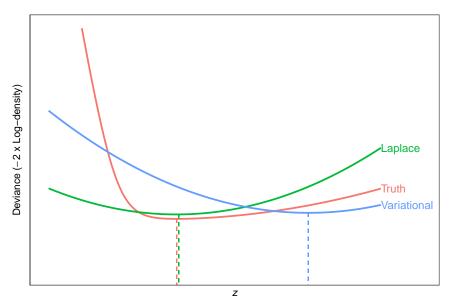
End

Probit with I-priors Varia

Variational Implementation

ntation Summary

Comparison of approximations (deviance)



Factorised distributions (Mean-field theory)

- Maximising \mathcal{L} over all possible q not feasible. Need some restrictions, but only to achieve tractability.
- Suppose we partition elements of z into m disjoint groups $z = (z^{(1)}, ..., z^{(m)})$, and assume

$$q(\mathsf{z}) = \prod_{j=1}^m q_j(\mathsf{z}^{(j)})$$

• Under this restriction, the solution to arg max_q $\mathcal{L}(q)$ is

$$\tilde{q}_j(\mathbf{z}^{(j)}) \propto \exp\left(\mathsf{E}_{-j}[\log p(\mathbf{y}, \mathbf{z})]\right)$$
 (2)

for $i \in \{1, ..., m\}$.

 In practice, these unnormalised densities are of recognisable form (especially if conjugate priors are used).

D. M. Blei et al. (2016). "Variational Inference: A Review for Statisticians". arXiv: 1601.00670

Coordinate ascent mean-field variational inference (CAVI)

- The optimal distributions are coupled with another, i.e. each $\tilde{q}_i(\mathbf{z}^{(j)})$ depends on the optimal moments of $\mathbf{z}^{(k)}$, $k \in \{1, \dots, m : k \neq i\}$.
- One way around this to employ an iterative procedure.
- Assess convergence by monitoring the lower bound

$$\mathcal{L}(q) = \mathsf{E}_q[\log p(\mathbf{y}, \mathbf{z})] - \mathsf{E}_q[\log q(\mathbf{z})].$$

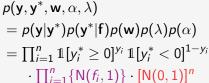
Algorithm 1 CAVI

- 1: **initialise** Variational factors $q_i(\mathbf{z}^{(j)})$
- 2: while $\mathcal{L}(q)$ not converged do
- 3. for $j = 1, \ldots, m$ do
- $\log q_i(\mathbf{z}^{(j)}) \leftarrow \mathsf{E}_{-i}[\log p(\mathbf{y}, \mathbf{z})] + \mathsf{const.}$ 4.
- end for 5:
- $\mathcal{L}(q) \leftarrow \mathsf{E}_q[\log p(\mathsf{y},\mathsf{z})] \mathsf{E}_q[\log q(\mathsf{z})]$
- 7. end while
- 8: **return** $\tilde{q}(z) = \prod_{i=1}^{m} \tilde{q}_i(z^{(i)})$

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 y_i^* y_i

 $i=1,\ldots,n$

Posterior distribution

• Approximate the posterior by a mean-field variational density

$$p(\mathbf{y}^*, \mathbf{w}, \alpha, \lambda | \mathbf{y}) \approx \prod_{i=1}^n q(y_i^*) q(\mathbf{w}) q(\alpha) q(\lambda)$$

where

$$q(y_i^*) \equiv \begin{cases} \mathbb{1}[y_i^* \geq 0] \, \mathsf{N}(\tilde{f}_i, 1) & \text{if } y_i = 1 \\ \mathbb{1}[y_i^* < 0] \, \mathsf{N}(\tilde{f}_i, 1) & \text{if } y_i = 0 \end{cases} \qquad q(\mathbf{w}) \equiv \mathsf{N}(\tilde{\mathbf{w}}, \tilde{\mathbf{V}}_w)$$

$$q(\lambda) \equiv \mathsf{N}(\tilde{\lambda}, \tilde{v}_w) \qquad q(\alpha) \equiv \mathsf{N}(\tilde{\alpha}, 1/n)$$

$$\tilde{f}_i = \tilde{\alpha} + \sum_{k=1}^n h_{\tilde{\lambda}}(x_i, x_k) \tilde{w}_k \qquad \tilde{\alpha} = \frac{1}{n} \sum_{k=1}^n \left(\mathsf{E}[y_i^*] - h_{\tilde{\lambda}}(x_i, x_k) \tilde{w}_k \right)$$

$$\tilde{\mathbf{w}} = \tilde{\mathbf{V}}_w \mathbf{H}_{\tilde{\lambda}}(\mathsf{E}[\mathbf{y}^*] - \tilde{\alpha} \mathbf{1}_n) \qquad \tilde{\mathbf{V}}_w^{-1} = \mathbf{H}_{\tilde{\lambda}}^2 + \mathbf{I}_n$$

$$\tilde{\lambda} = (\mathsf{E}[\mathbf{y}^*] - \tilde{\alpha} \mathbf{1}_n) \mathsf{H} \tilde{\mathbf{w}} / \tilde{v}_{\lambda} \qquad \tilde{v}_{\lambda} = \mathsf{tr}(\mathbf{H}^2(\tilde{\mathbf{V}}_w + \tilde{\mathbf{w}} \tilde{\mathbf{w}}^\top))$$

Posterior predictive distribution

• Given new data points x_{new} , interested in

$$\begin{split} p(y_{\mathsf{new}}|\mathbf{y}) &= \int p(y_{\mathsf{new}}|y_{\mathsf{new}}^*, \mathbf{y}) p(y_{\mathsf{new}}^*|\mathbf{y}) \, \mathrm{d}y_{\mathsf{new}}^* \\ &\approx \int p(y_{\mathsf{new}}|y_{\mathsf{new}}^*) q(y_{\mathsf{new}}^*) \, \mathrm{d}y_{\mathsf{new}}^* \\ &= \begin{cases} \Phi(\tilde{f}_{\mathsf{new}}) & \text{if } y_{\mathsf{new}} = 1 \\ 1 - \Phi(\tilde{f}_{\mathsf{new}}) & \text{if } y_{\mathsf{new}} = 0 \end{cases} \end{split}$$

where
$$\tilde{f}_{\text{new}} = \tilde{\alpha} + \sum_{k=1}^{n} h_{\tilde{\lambda}}(x_{\text{new}}, x_k) \tilde{w}_k$$
.

• f_{new} represents the estimate of the latent propensity for y_{new} , and its uncertainty is described by $q(y_{\text{new}}^*)$.

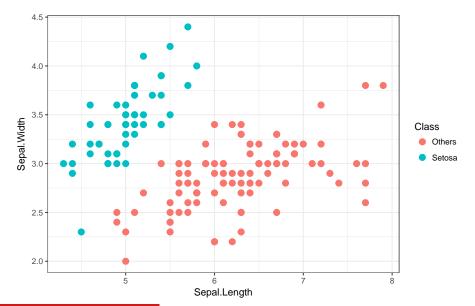
Variational lower bound

- Since the solutions are coupled, we implement an iterative scheme (as per Algorithm 1)
- Assess convergence by monitoring the lower bound

$$\begin{split} \mathcal{L} &= \mathsf{E}_q[\log p(\mathbf{y}, \mathbf{y}^*, \mathbf{w}, \alpha, \lambda)] - \mathsf{E}_q[\log q(\mathbf{y}^*, \mathbf{w}, \alpha, \lambda)] \\ &= \mathsf{const.} + \sum_{i=1}^n \left(y_i \log \Phi(\tilde{f}_i) + (1 - y_i) \log \left(1 - \Phi(\tilde{f}_i) \right) \right) \\ &- \frac{1}{2} \left(\mathsf{tr} \, \tilde{\mathbf{V}}_w + \mathsf{tr}(\tilde{\mathbf{w}} \tilde{\mathbf{w}}^\top) - \log |\tilde{\mathbf{V}}_w| + \log \tilde{v}_{\lambda} \right) \end{split}$$

Probit with I-priors Variational Implementation Summary End

Fisher's Iris data set



Fisher's Iris data set - Model fitting

 Varitional inference for I-prior probit models implemented in R package iprobit (still lots of work to do!).

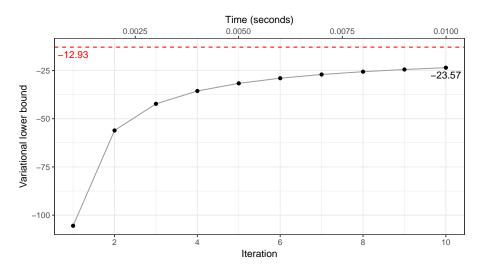
HJ (2017b). iprobit: Binary Probit Regression with I-priors. R Package version 0.1.0: GitHub

Fisher's Iris data set - Model summary

```
R> summary(mod)
##
## Call:
## iprobit(y = y, X, maxit = 10000)
##
## RKHS used: Canonical
##
            Mean S.D. 2.5% 97.5%
##
## alpha -4.1730 0.0816 -4.3330 -4.0129
## lambda 1.2896 0.0142 1.2618 1.3175
##
## Converged to within 1e-05 tolerance. No. of iterations: 6141
## Model classification error rate (%): 0
## Variational lower bound: -12.93486
```

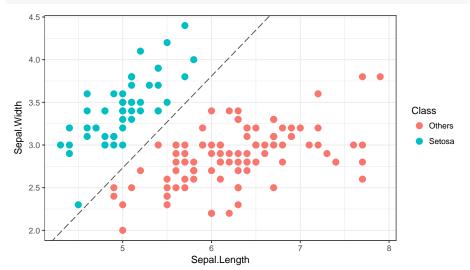
Fisher's Iris data set - Lower bound

R> iplot_lb(mod, niter.plot = 10)



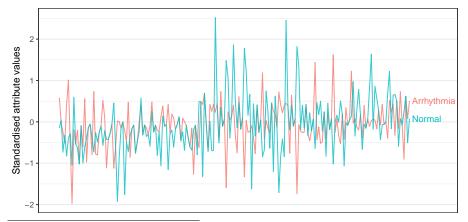
Fisher's Iris data set - Decision boundary

R> iplot_decbound(mod)



Cardiac arrhythmia data set

Detect the presence of cardiac arrhythmia based on various ECG data and other attributes such as age and weight (n = 451, p = 194).



H. A. Guvenir et al. (1998). UCI Machine Learning Repository: Arrhythmia Data URL: https://archive.ics.uci.edu/ml/datasets/Arrhythmia Set.

Cardiac arrhythmia data set - Model fit

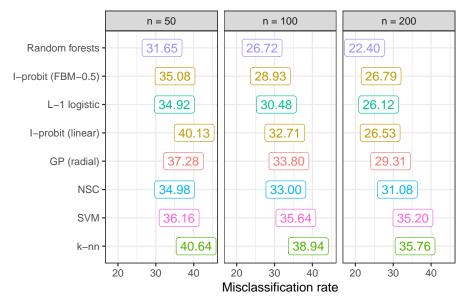
• Fit an I-prior probit model using Canonical and FBM kernels. The full data set takes about 35 seconds.

```
R> mod <- iprior(y, X, kernel = "FBM")</pre>
```

- Compare against popular classifiers: 1) k-nearest neighbours; 2) support vector machine; 3) Gaussian process classification; 4) random forests; 5) nearest shrunken centroids (Tibshirani et al. 2003); and 6) L-1 penalised logistic regression.
- Experiment set-up:
 - ▶ Form training set by sub-sampling $n_{\text{sub}} \in \{50, 100, 200\}$ data points.
 - Use remaining data as test set.
 - ► Fit model on training set and obtain test error rates.
 - Repeat 100 times.

T. I. Cannings and R. J. Samworth (2017). "Random-projection ensemble classification". J. R. Stat. Soc. Ser. B: Stat. Methodol (w. discussion), to appear

Cardiac arrhythmia data set - Results



Meta-analysis of smoking cessation



- Data from 27 separate smoking cessation studies, where participants subjected to nicotine gum treatment or placed in control group.
- Some summary statistics:

	Min.	Avg.	Max.	Prop. quit	Odds quit
Control	20	101	617	0.207	0.261
Treated	21	117	600	0.320	0.470

- Raw odds ratio: 1.801.
- Random-effects analysis using a multilevel logistic model estimates this odds ratio as 1.768.

A. Skrondal and S. Rabe-Hesketh (2004). Generalized Latent Variable Modeling: Multilevel, Longitudinal, and Structural Equation Models. Chapman & Hall/CRC, §9.5

Summary

- Let $i = 1, ..., n_i$ index the patients in study group $j \in 1, ..., 27$.
- Denote y_{ii} as the binary response variable indicating Quit (1) or Remain (0), and x_{ii} as patient; 's treatment group indicator.
- Model binary data using I-probit model

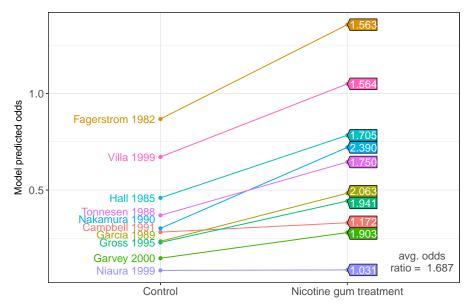
$$\Phi^{-1}(p_{ij}) = f(x_{ij}, j)$$

= $f_1(x_{ij}) + f_2(j) + f_{12}(x_{ij}, j)$

with $f_1, f_2 \in \text{Pearson RKHS}$, and $f_{12} \in \text{ANOVA RKHS}$.

	Model	Lower bound	Brier score	No. of RKHS
				param.
1	f_1	-3210.79	0.0311	1
2	$f_1 + f_2$	-3097.24	0.0294	2
3	$f_1 + f_2 + f_{12}$	-3091.21	0.0294	2

Meta-analysis of smoking cessation - results



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Summary

- An extension of the I-prior methodology to binary responses.
- Variational inference used to approximate the intractable likelihood.
 - ▶ A deterministic approximation of the posterior density by a "close" (in the KL divergence sense), tractable density.
 - ▶ It's somewhere between Laplace's method and MCMC sampling.
- Several real-world examples demonstrated the use of I-probit models for classification and inference.
- Further work:
 - R package iprobit.
 - Extend to non-iid errors case.
 - Extend to multinomial probit models.
 - Other algorithms (e.g. expectation propagation).

Slides, source code and results are made available at: http://phd3.haziqj.ml

End

Thank you!

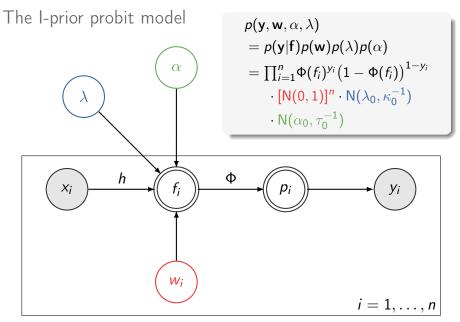
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 - https://archive.ics.uci.edu/ml/datasets/Arrhythmia.
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- Tibshirani, R., T. Hastie, B. Narasimhan, and G. Chu (2003). "Class prediction by nearest shrunken centroids, with applications to DNA microarrays". *Statistical Science* 18.1, pp. 104–117.

6 Additional material



Laplace's method

• Interested in $p(\mathbf{f}|\mathbf{y}) \propto p(\mathbf{y}|\mathbf{f})p(\mathbf{f}) =: e^{Q(\mathbf{f})}$, with normalising constant $p(\mathbf{y}) = \int e^{Q(\mathbf{f})} d\mathbf{f}$. The Taylor expansion of Q about its mode $\tilde{\mathbf{f}}$

$$Q(\mathbf{f}) \approx Q(\tilde{\mathbf{f}}) - \frac{1}{2}(\mathbf{f} - \tilde{\mathbf{f}})^{\top} \mathbf{A}(\mathbf{f} - \tilde{\mathbf{f}})$$

is recognised as the logarithm of an unnormalised Gaussian density, with ${\bf A}=-{\sf D}^2 Q({\bf f})$ being the negative Hessian of Q evaluated at $\tilde{{\bf f}}$.

• The posterior $p(\mathbf{f}|\mathbf{y})$ is approximated by $N(\tilde{\mathbf{f}}, \mathbf{A}^{-1})$, and the marginal by

$$p(\mathbf{y}) \approx (2\pi)^{n/2} |\mathbf{A}|^{-1/2} p(\mathbf{y}|\tilde{\mathbf{f}}) p(\tilde{\mathbf{f}})$$

• Won't scale with large *n*; difficult to find modes in high dimensions.

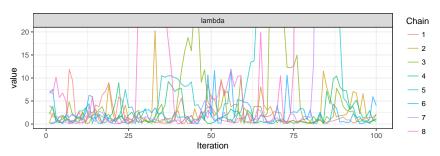
R. Kass and A. Raftery (1995). "Bayes Factors". *Journal of the American Statistical Association* 90.430, pp. 773–795, §4.1, pp. 777-778.

Full Bayesian analysis using MCMC

- · Assign hyperpriors on parameters of the I-prior, e.g.
 - $\lambda^2 \sim \Gamma^{-1}(a,b)$
 - $\sim \alpha \sim N(c, d^2)$

for a hierarchical model to be estimated fully Bayes.

- No closed-form posteriors need to resort to MCMC sampling.
- Computationally slow, and sampling difficulty results in unreliable posterior samples.



Variational inference

 Name derived from calculus of variations which deals with maximising or minimising functionals.

Functions
$$p: \theta \mapsto \mathbb{R}$$
 (standard calculus)
Functionals $\mathcal{H}: p \mapsto \mathbb{R}$ (variational calculus)

• Using standard calculus, we can solve

$$\underset{\theta}{\operatorname{arg\,max}} p(\theta) =: \hat{\theta}$$

e.g. p is a likelihood function, and $\hat{\theta}$ is the ML estimate.

• Using variational calculus, we can solve

$$\operatorname{arg\,max}_{p} \mathcal{H}(p) =: \tilde{p}$$

e.g. \mathcal{H} is the entropy $\mathcal{H} = -\int p(x) \log p(x) dx$, and \tilde{p} is the entropy maximising distribution.

• GOAL: Bayesian inference of mean μ and variance ψ^{-1}

$$y_i \stackrel{\mathsf{iid}}{\sim} \mathsf{N}(\mu, \psi^{-1})$$
 Data $\mu | \psi \sim \mathsf{N}\left(\mu_0, (\kappa_0 \psi)^{-1}\right)$ $\psi \sim \mathsf{\Gamma}(a_0, b_0)$ Priors $i = 1, \dots, n$

• Substitute $p(\mu, \psi|\mathbf{y})$ with the mean-field approximation

$$q(\mu,\psi)=q_{\mu}(\mu)q_{\psi}(\psi)$$

• From (2), we can work out the solutions

$$ilde{q}_{\mu}(\mu) \equiv \mathsf{N}\left(rac{\kappa_0\mu_0 + nar{y}}{\kappa_0 + n}, rac{1}{(\kappa_0 + n)\,\mathsf{E}_q[\psi]}
ight) \quad \mathsf{and} \quad ilde{q}_{\psi}(\psi) \equiv \Gamma(ilde{a}, ilde{b})$$

$$\tilde{a} = a_0 + \frac{n}{2}$$
 $\tilde{b} = b_0 + \frac{1}{2} E_q \left[\sum_{i=1}^n (y_i - \mu)^2 + \kappa_0 (\mu - \mu_0)^2 \right]$

