

Binary probit regression with I-priors

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Social Statistics (Year 3)

London School of Economics and Political Science

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PhD Presentation Event

<http://phd3.haziqj.ml>

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① Introduction

- I-priors

- PhD Roadmap

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- The latent variable motivation

- Using I-priors

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③ Variational inference

- Introduction

- Mean-field factorisation

④ Implementation

- R/iprobit

- Examples

⑤ Summary

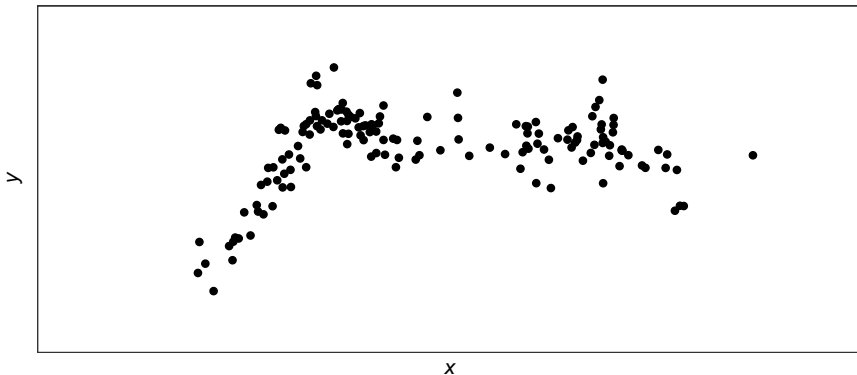
The regression model

- For $i = 1, \dots, n$, consider the regression model

$$y_i = f(x_i) + \epsilon_i \quad (1)$$

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

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



l-priors

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

$$(f(x_1), \dots, f(x_n))^T \sim N(f_0, \mathcal{I}(f))$$

with f_0 a prior mean, and \mathcal{I} the Fisher information for f , given by

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

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- The l-prior regression model for $i = 1, \dots, n$ becomes

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

$$(w_1, \dots, w_n) \sim N(\mathbf{0}, \Psi)$$

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

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

I-priors (cont.)

- Of interest is the posterior regression function characterised by the distribution

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

HJ (2017a). *iprior: Linear Regression using I-Priors*. R Package version 0.6.4:
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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 $f_{\text{new}} = f(x_{\text{new}})$.

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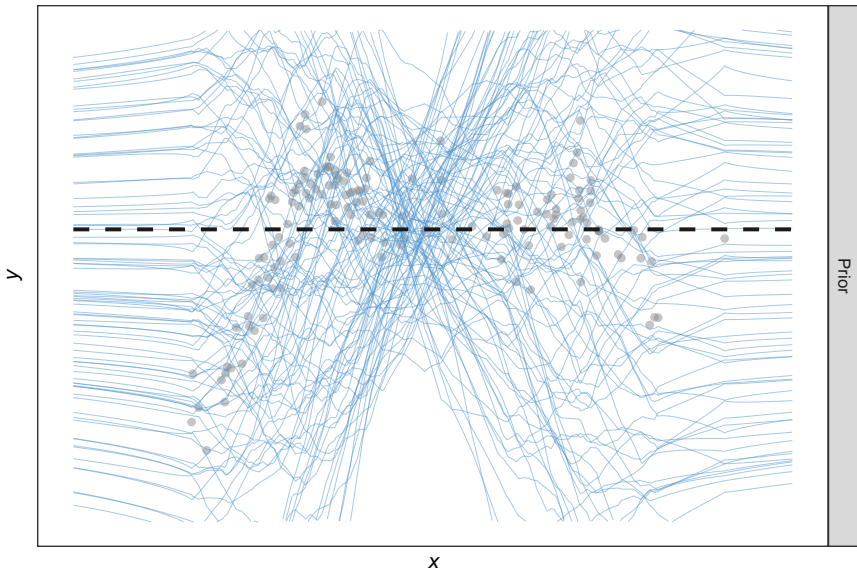
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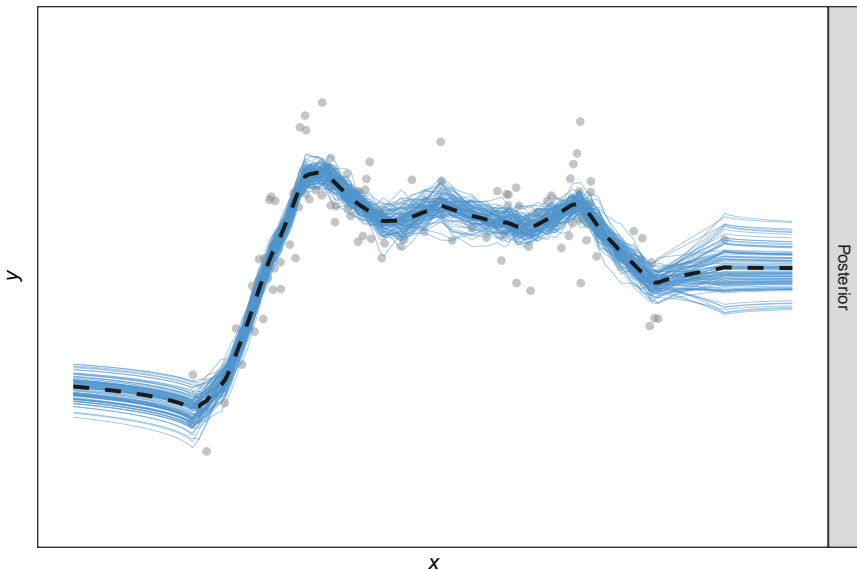
- Estimation using EM algorithm or direct maximisation of the marginal likelihood $\log p(y)$.
- Complete Bayesian estimation also possible.

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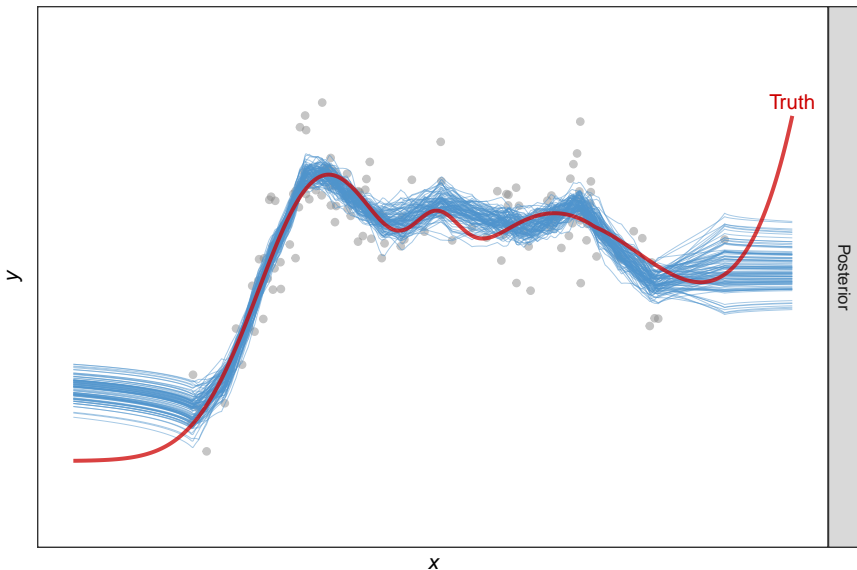
Fractional Brownian motion (FBM) RKHS



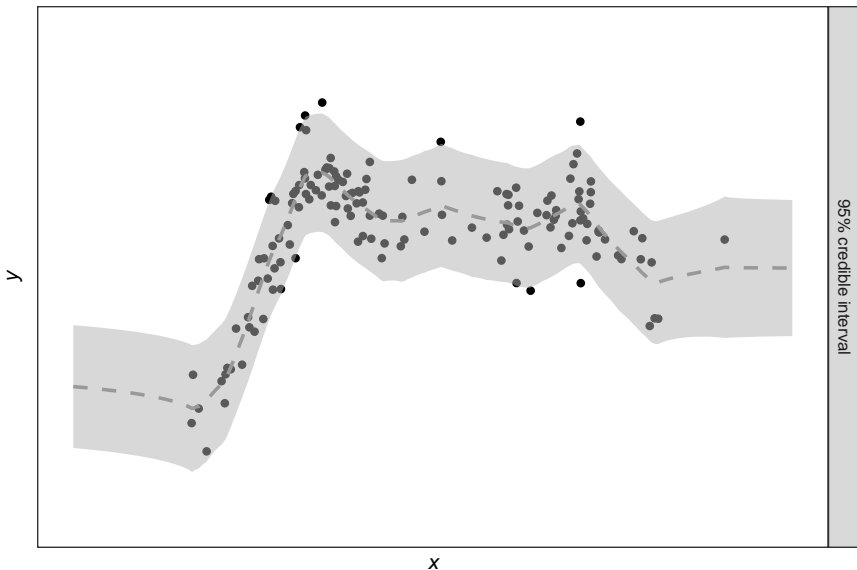
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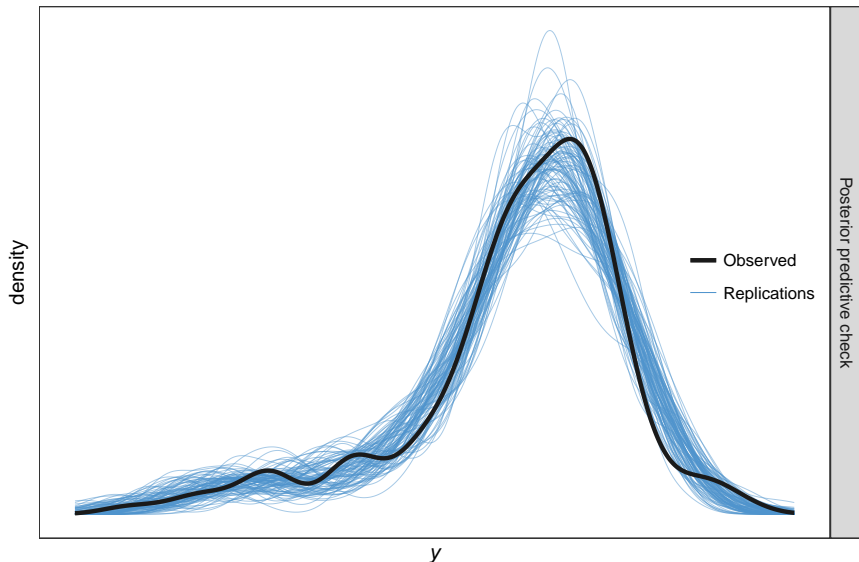
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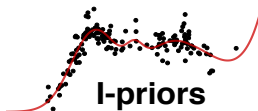
Posterior predictive distribution



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PhD Roadmap



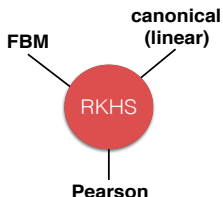
I-priors

Unified methodology for

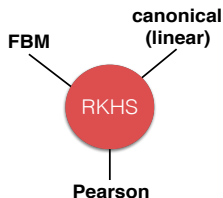
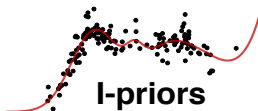
- additive models
- multilevel models
- models with functional covariates

Advantages

- Minimal assumptions
- Straightforward inference
- Performance competitive



PhD Roadmap



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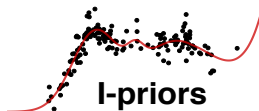
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Estimation:

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- **EM algorithm**
- MCMC (Gibbs/HMC)

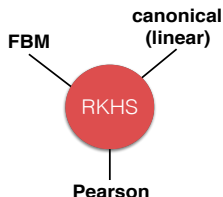
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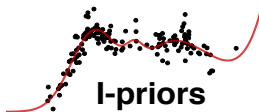
Bayesian Variable Selection

(using I-priors in the canonical RKHS)

✓ ✓ ✗ ✗ ✓
 X_1 X_2 X_3 X_4 X_5

Good performance in cases with multicollinearity

PhD Roadmap



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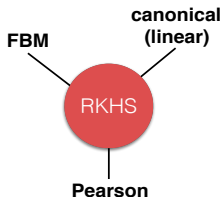
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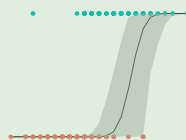
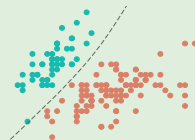
✓ X₁ ✓ X₂ ✗ X₃ ✗ X₄ ✓ X₅

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Binary probit models with I-priors

Extension to binary responses

Estimation using variational inference



- ① Introduction
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The latent variable motivation

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

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

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

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- Model these continuous latent variables according to

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

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

Using I-priors

- Assume an I-prior on f . Then,

$$f(x_i) = f_0(x_i) + \sum_{k=1}^n h_{\lambda}(x_i, x_k) w_k$$
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$$\begin{aligned} p_i &= \mathbf{P}[y_i = 1] = \mathbf{P}[y_i^* \geq 0] \\ &= \mathbf{P}[\epsilon_i \leq f(x_i)] \\ &= \Phi\left(\psi^{1/2}(\alpha + \sum_{k=1}^n h_{\lambda}(x_i, x_k) w_k)\right) \end{aligned}$$

where Φ is the CDF of a standard normal.

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

Estimation

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

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

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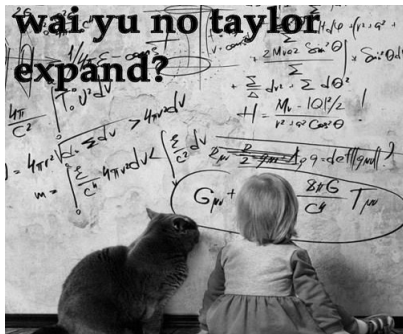
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 - ✓ Laplace approximation

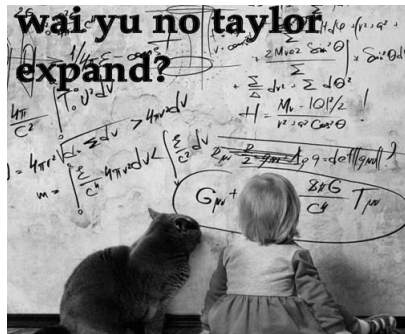


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Variational inference

- Consider a statistical model where we have observations (y_1, \dots, y_n) and also some latent variables (z_1, \dots, z_n) .

C. M. Bishop (2006). *Pattern Recognition and Machine Learning*. Springer, Ch. 10
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- **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.

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Decomposition of the log marginal

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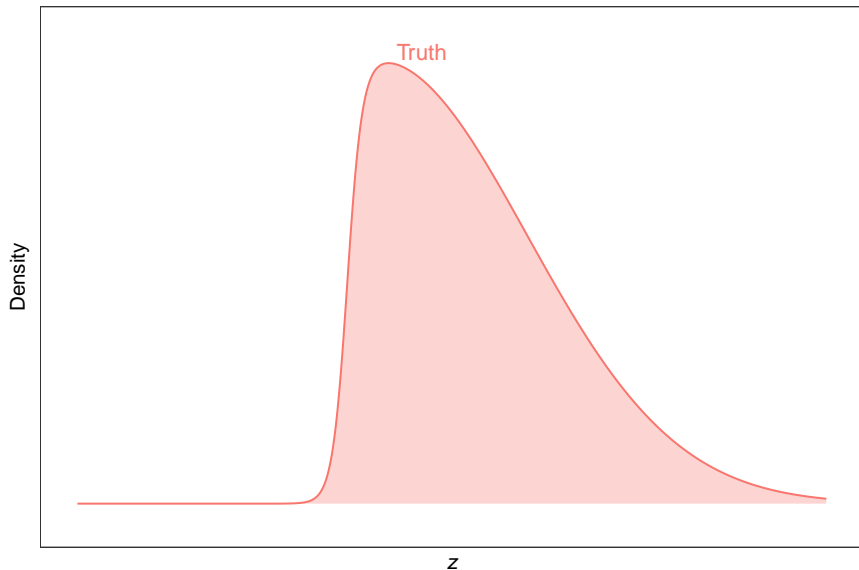
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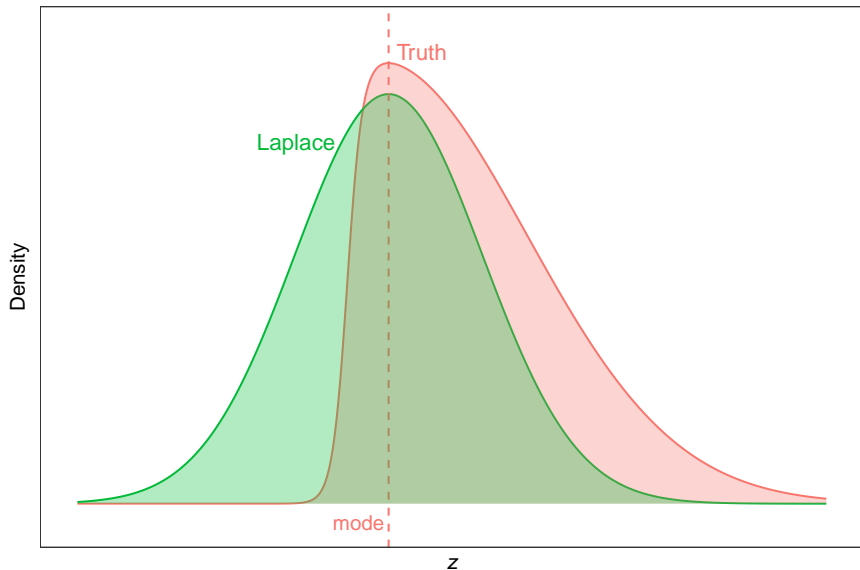
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- \mathcal{L} is referred to as the “lower-bound”, and it serves as a surrogate function to the marginal.
- Maximising $\mathcal{L}(q)$ is equivalent to minimising $\text{KL}(q\|p)$.
- Although $\text{KL}(q\|p)$ is minimised at $q(\mathbf{z}) \equiv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

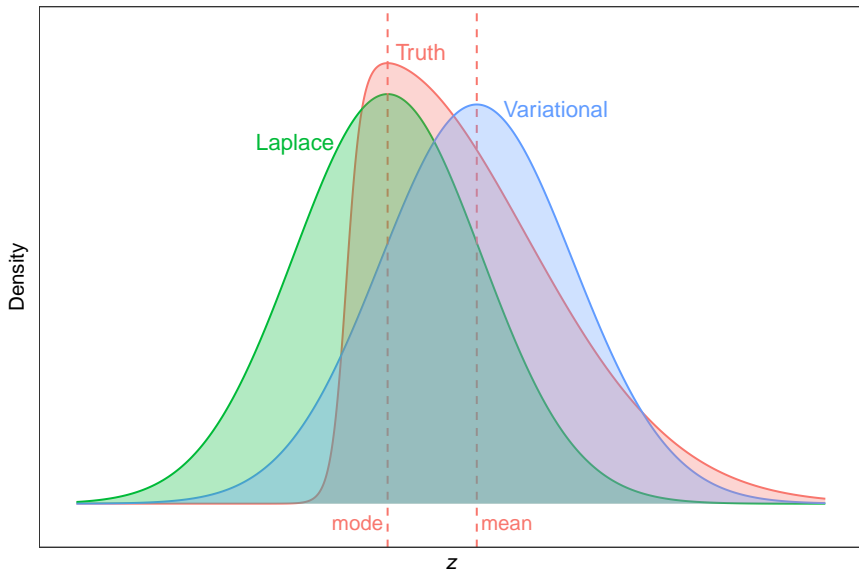
Comparison of approximations (density)



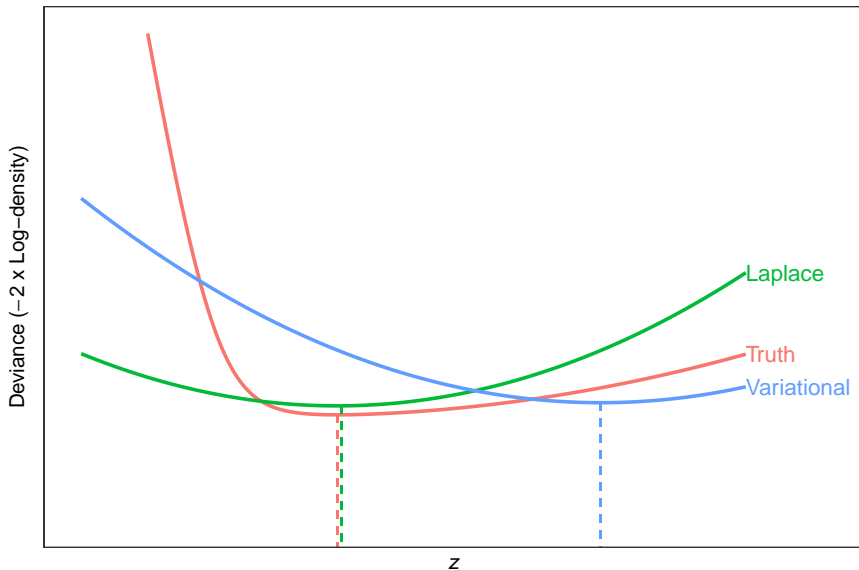
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Comparison of approximations (density)



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 \mathbf{z} into m disjoint groups $\mathbf{z} = (\mathbf{z}^{(1)}, \dots, \mathbf{z}^{(m)})$, and assume

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

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

$$\tilde{q}_j(\mathbf{z}^{(j)}) \propto \exp (E_{-j}[\log p(\mathbf{y}, \mathbf{z})]) \quad (2)$$

for $j \in \{1, \dots, m\}$.

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

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Coordinate ascent mean-field variational inference (CAVI)

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

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

Algorithm 1 CAVI

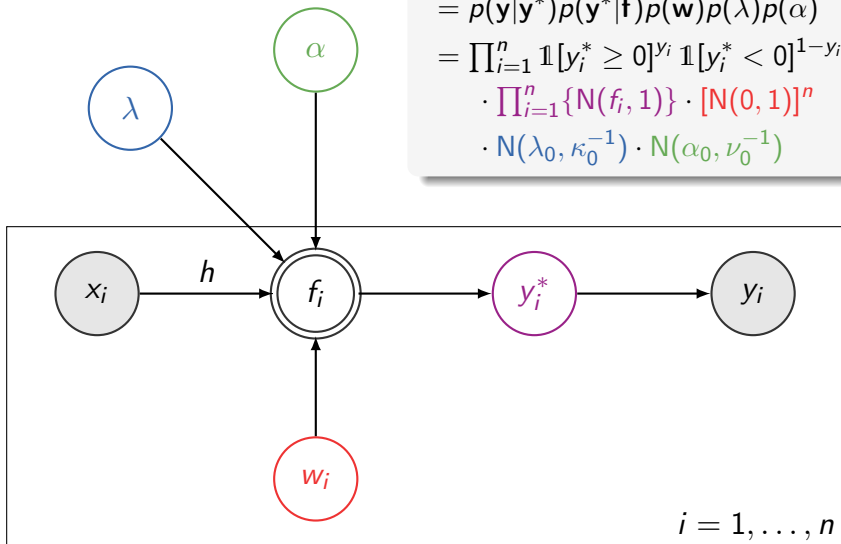
- 1: **initialise** Variational factors $q_j(\mathbf{z}^{(j)})$
- 2: **while** $\mathcal{L}(q)$ not converged **do**
- 3: **for** $j = 1, \dots, m$ **do**
- 4: $\log q_j(\mathbf{z}^{(j)}) \leftarrow \mathbb{E}_{-j}[\log p(\mathbf{y}, \mathbf{z})] + \text{const.}$
- 5: **end for**
- 6: $\mathcal{L}(q)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

[example](#)

- ① Introduction
- ② Probit models with l-priors
- ③ Variational inference
- ④ Implementation**
- ⑤ Summary

Variational I-prior probit

$$\begin{aligned} p(\mathbf{y}, \mathbf{y}^*, \mathbf{w}, \alpha, \lambda) &= p(\mathbf{y}|\mathbf{y}^*)p(\mathbf{y}^*|\mathbf{f})p(\mathbf{w})p(\lambda)p(\alpha) \\ &= \prod_{i=1}^n \mathbb{1}[y_i^* \geq 0]^{y_i} \mathbb{1}[y_i^* < 0]^{1-y_i} \\ &\quad \cdot \prod_{i=1}^n \{N(f_i, 1)\} \cdot [N(0, 1)]^n \\ &\quad \cdot N(\lambda_0, \kappa_0^{-1}) \cdot N(\alpha_0, \nu_0^{-1}) \end{aligned}$$



Posterior distribution

- Approximate the posterior by a mean-field variational density

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

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where

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

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

Posterior distribution

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

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

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

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

Posterior predictive distribution

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

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

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

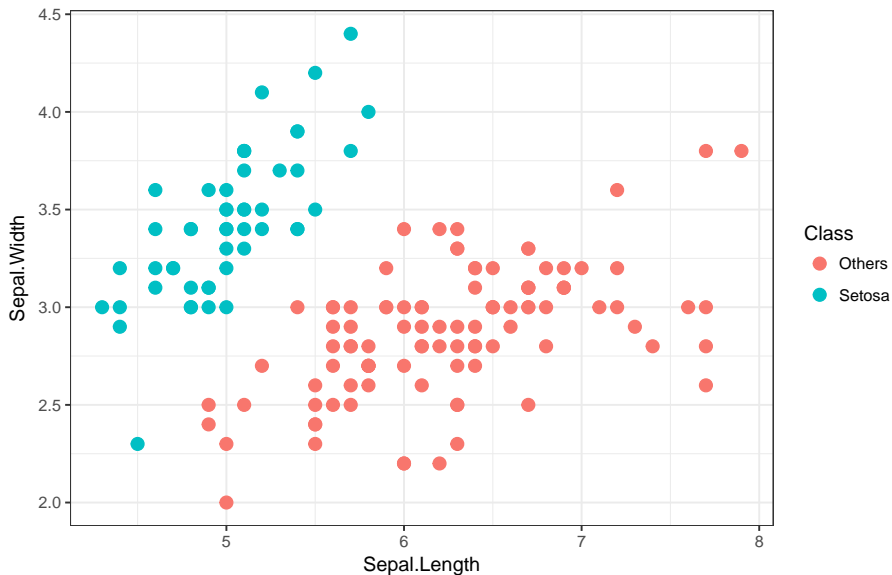
- \tilde{f}_{new} represents the estimate of the latent propensity for y_{new} , and its uncertainty is described by $q(y_{\text{new}}^*)$.

Variational lower bound

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

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

Fisher's Iris data set



Fisher's Iris data set - Model fitting

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

```
R> system.time(  
+   (mod <- iprobit(y, X))  
+ )  
  
##  
## |=====| 61%  
## Converged after 6141 iterations.  
## Training error rate: 0 %  
##      user  system elapsed  
## 67.857   6.396   74.277
```

HJ (2017b). *iprobit: Binary Probit Regression with I-priors*. R Package version 0.1.0: [GitHub](https://github.com/haziqj/iprobit)

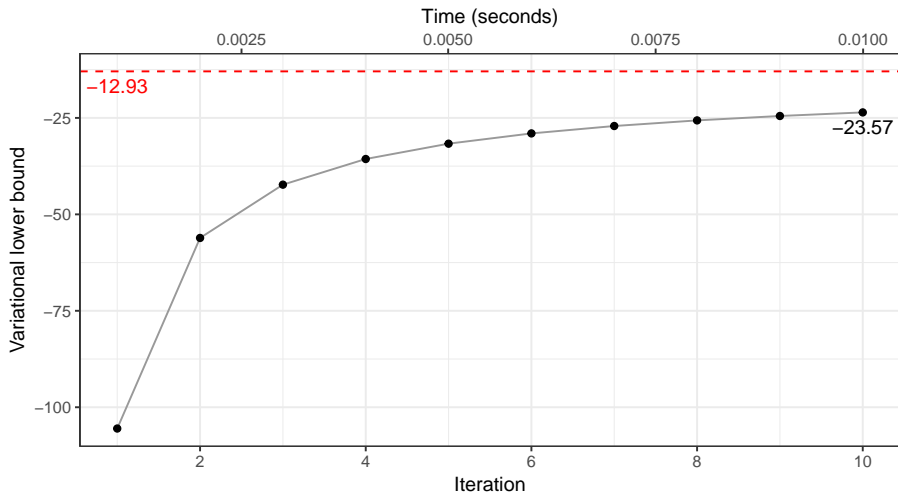
Fisher's Iris data set - Model summary

```
R> summary(mod)

##
## Call:
## iprobit(y = y, X, maxit = 10000)
##
## RKHS used: Canonical
##
##               Mean      S.E.      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
```

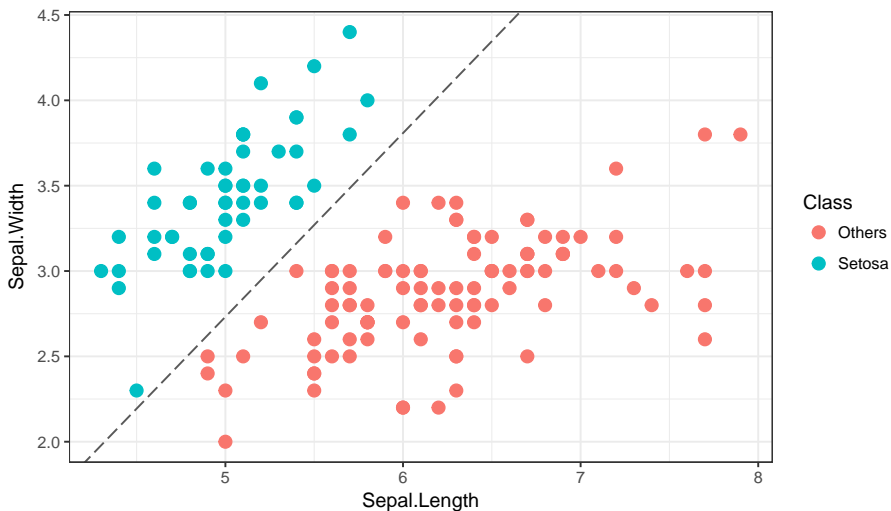

Fisher's Iris data set - Lower bound

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



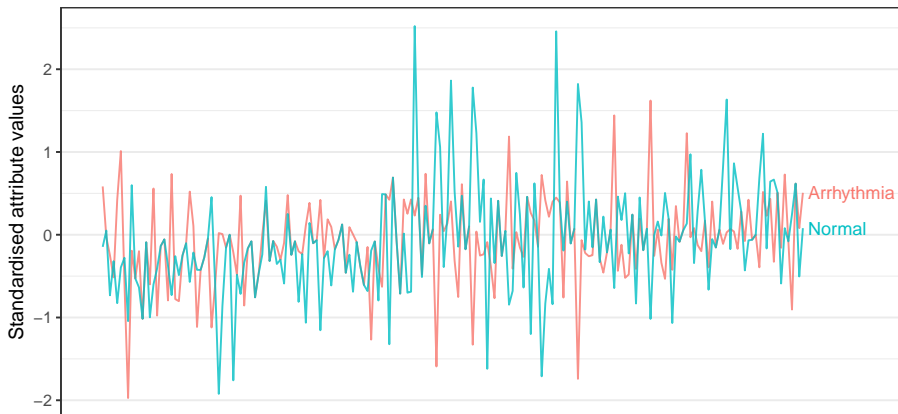
Fisher's Iris data set - Decision boundary

```
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 Set*. URL: <https://archive.ics.uci.edu/ml/datasets/Arrhythmia>

Cardiac arrhythmia data set - Model fit

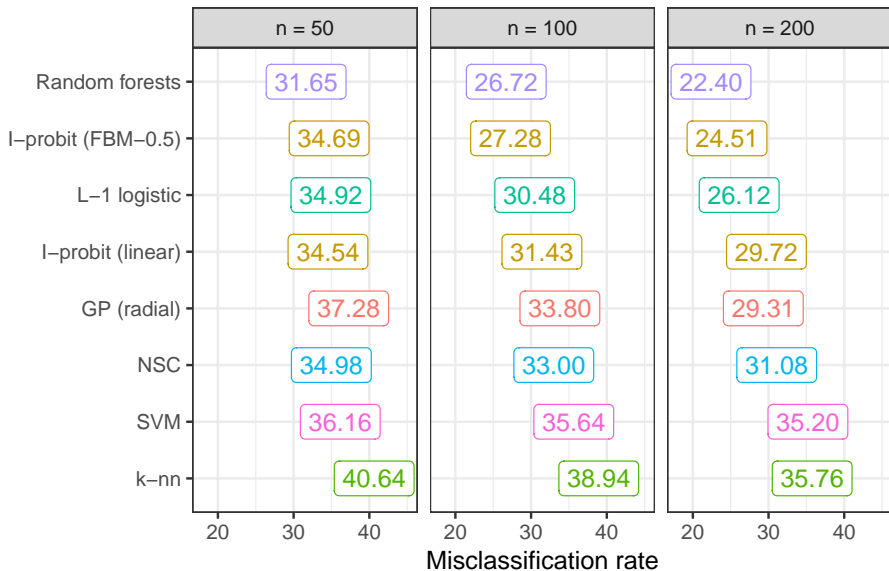
- Fit an I-prior probit model using Canonical and FBM kernels. The full data set takes about 35 seconds.

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

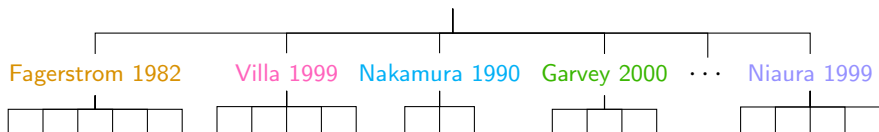
- Compare against popular classifiers: 1) k -nearest neighbours; 2) support vector machine; 3) Gaussian process classification; 4) random forests; 5) nearest shrunken centroids (Tibshirani et al. 2003); and 6) L-1 penalised logistic regression.
- Experiment set-up:
 - ▶ Form training set by sub-sampling $n_{\text{sub}} \in \{50, 100, 200\}$ 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

Meta-analysis of smoking cessation - model

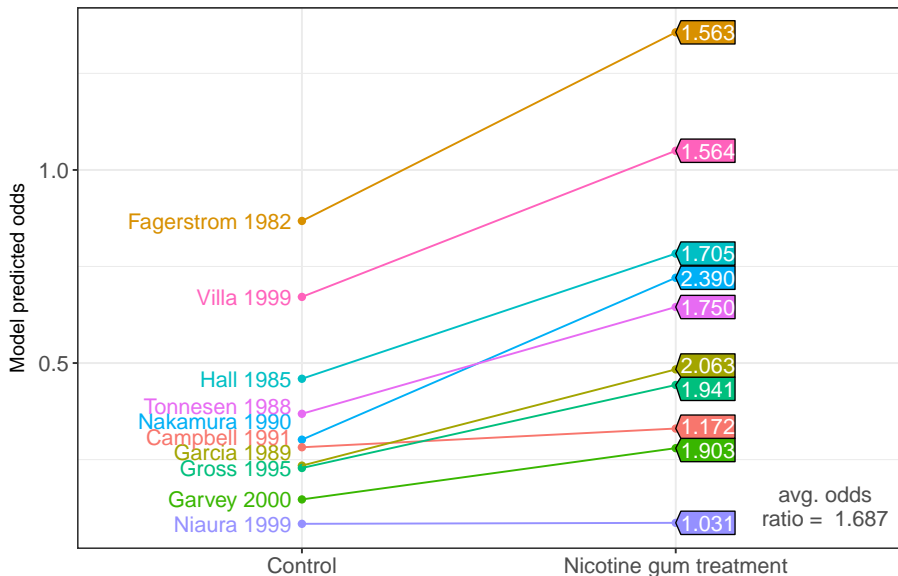
- Let $i = 1, \dots, n_j$ index the patients in study group $j \in 1, \dots, 27$.
- Denote y_{ij} as the binary response variable indicating Quit (1) or Remain (0), and x_{ij} as patient ij 's treatment group indicator.
- Model binary data using I-probit model

$$\begin{aligned}\Phi^{-1}(p_{ij}) &= f(x_{ij}, j) \\ &= f_1(x_{ij}) + f_2(j) + f_{12}(x_{ij}, j)\end{aligned}$$

with $f_1, f_2 \in$ Pearson RKHS, and $f_{12} \in$ 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!

References I

- Bergsma, W. (2017). "Regression with I-priors". *Manuscript in preparation*.
- Bishop, C. M. (2006). *Pattern Recognition and Machine Learning*. Springer.
- Blei, D. M., A. Kucukelbir, and J. D. McAuliffe (2016). "Variational Inference: A Review for Statisticians". [arXiv: 1601.00670](https://arxiv.org/abs/1601.00670).
- Cannings, T. I. and R. J. Samworth (2017). "Random-projection ensemble classification". *Journal of the Royal Statistical Society. Series B: Statistical Methodology (with discussion)*, to appear.
- Guvenir, H. A., M. Burak Acar, and H. Muderrisoglu (1998). *UCI Machine Learning Repository: Arrhythmia Data Set*. URL: <https://archive.ics.uci.edu/ml/datasets/Arrhythmia>.
- Jamil, H. (2017a). *iprior: Linear Regression using I-Priors*. R Package version 0.6.4: CRAN/GitHub.

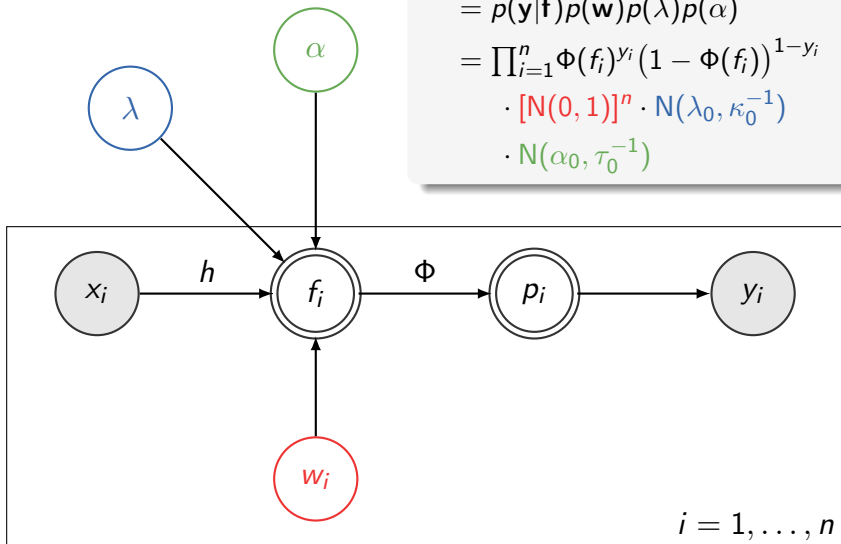
References II

- Jamil, H. (2017b). *iprobbit: Binary Probit Regression with I-priors*. R Package version 0.1.0: GitHub.
- Kass, R. and A. Raftery (1995). “Bayes Factors”. *Journal of the American Statistical Association* 90.430, pp. 773–795.
- Murphy, K. P. (2012). *Machine Learning: A Probabilistic Perspective*. The MIT Press.
- Skrondal, A. and S. Rabe-Hesketh (2004). *Generalized Latent Variable Modeling: Multilevel, Longitudinal, and Structural Equation Models*. Chapman & Hall/CRC.
- 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

The I-prior probit model

$$\begin{aligned}
 p(\mathbf{y}, \mathbf{w}, \alpha, \lambda) &= p(\mathbf{y}|\mathbf{f})p(\mathbf{w})p(\lambda)p(\alpha) \\
 &= \prod_{i=1}^n \Phi(f_i)^{y_i} (1 - \Phi(f_i))^{1-y_i} \\
 &\quad \cdot [\mathbf{N}(0, 1)]^n \cdot \mathbf{N}(\lambda_0, \kappa_0^{-1}) \\
 &\quad \cdot \mathbf{N}(\alpha_0, \tau_0^{-1})
 \end{aligned}$$



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 $\mathbf{A} = -D^2Q(\mathbf{f})$ being the negative Hessian of Q evaluated at $\tilde{\mathbf{f}}$.

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

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

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

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

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

Laplace's method

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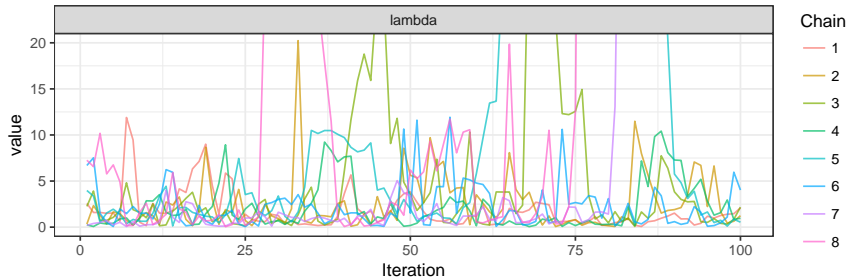
$$p(\mathbf{y}) \approx (2\pi)^{n/2} |\mathbf{A}|^{-1/2} p(\mathbf{y}|\tilde{\mathbf{f}}) p(\tilde{\mathbf{f}})$$

- 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 l-prior, e.g.
 - ▶ $\lambda^2 \sim \Gamma^{-1}(a, b)$
 - ▶ $\alpha \sim N(c, d^2)$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)

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

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

- Using variational calculus, we can solve

$$\arg \max_p \mathcal{H}(p) =: \tilde{p}$$

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

Estimation of a 1-dim Gaussian mean and variance

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

$$y_i \stackrel{\text{iid}}{\sim} \text{N}(\mu, \psi^{-1}) \quad \text{Data}$$

$$\mu | \psi \sim \text{N}(\mu_0, (\kappa_0 \psi)^{-1}) \quad \text{Priors}$$

$$\psi \sim \Gamma(a_0, b_0)$$

$$i = 1, \dots, n$$

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

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

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

Estimation of a 1-dim Gaussian mean and variance

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

- Under the mean-field restriction, the solution to $\arg \max_q \mathcal{L}(q)$ is

$$\tilde{q}_j(\mathbf{z}^{(j)}) \propto \exp \left(\mathbb{E}_{-j}[\log p(\mathbf{y}, \mathbf{z})] \right) \quad (1)$$

for $j \in \{1, \dots, m\}$.

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

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

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

$$\log \tilde{q}_\mu(\mu) = \mathbb{E}_\psi[\log p(\mathbf{y}|\mu, \psi)] + \mathbb{E}_\psi[\log p(\mu|\psi)] + \text{const.}$$

$$\begin{aligned} \log \tilde{q}_\psi(\psi) &= \mathbb{E}_\mu[\log p(\mathbf{y}|\mu, \psi)] + \mathbb{E}_\mu[\log p(\mu|\psi)] + \log p(\psi) \\ &\quad + \text{const.} \end{aligned}$$

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for $j \in \{1, \dots, m\}$.

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

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

$$\tilde{q}_\mu(\mu) \equiv \mathcal{N} \left(\frac{\kappa_0 \mu_0 + n \bar{y}}{\kappa_0 + n}, \frac{1}{(\kappa_0 + n) \mathbb{E}_q[\psi]} \right)$$

Estimation of a 1-dim Gaussian mean and variance

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for $j \in \{1, \dots, m\}$.

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

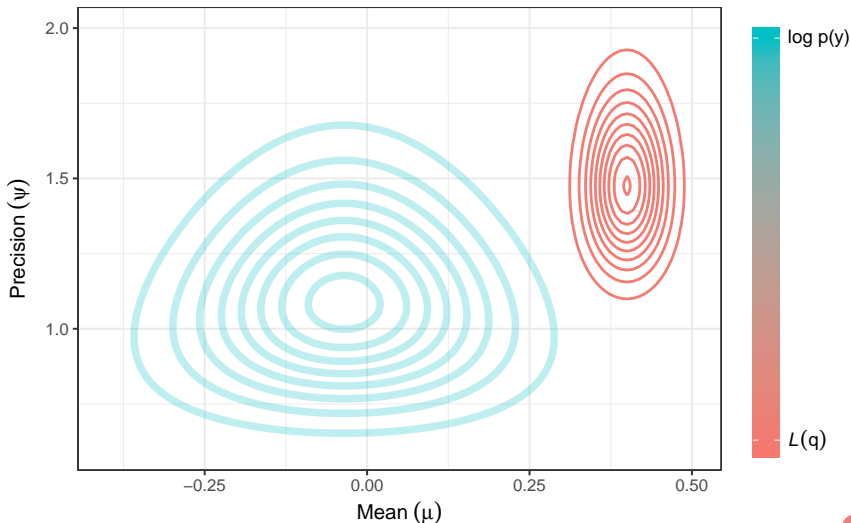
- From (2), we can work out the solutions

$$\tilde{q}_\mu(\mu) \equiv \mathcal{N} \left(\frac{\kappa_0 \mu_0 + n \bar{y}}{\kappa_0 + n}, \frac{1}{(\kappa_0 + n) \mathbb{E}_q[\psi]} \right) \quad \text{and} \quad \tilde{q}_\psi(\psi) \equiv \Gamma(\tilde{a}, \tilde{b})$$

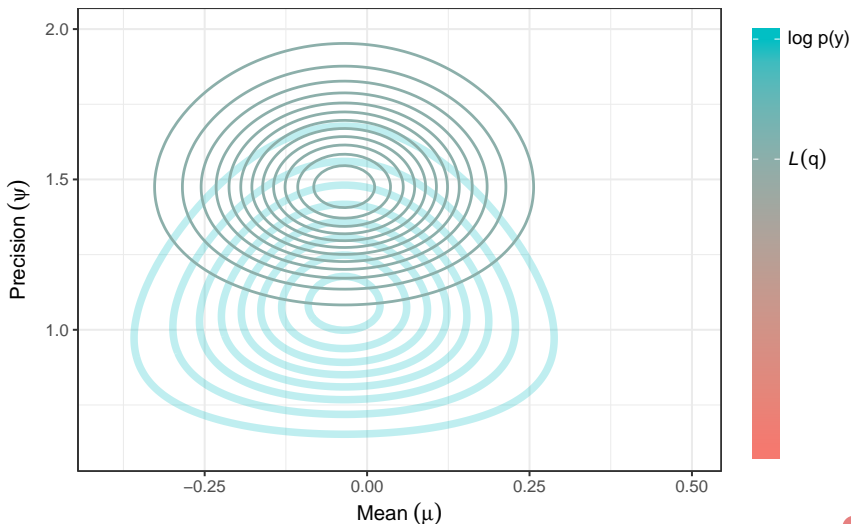
$$\tilde{a} = a_0 + \frac{n}{2} \quad \tilde{b} = b_0 + \frac{1}{2} \mathbb{E}_q \left[\sum_{i=1}^n (y_i - \mu)^2 + \kappa_0 (\mu - \mu_0)^2 \right]$$

Estimation of a 1-dim Gaussian mean and variance (cont.)

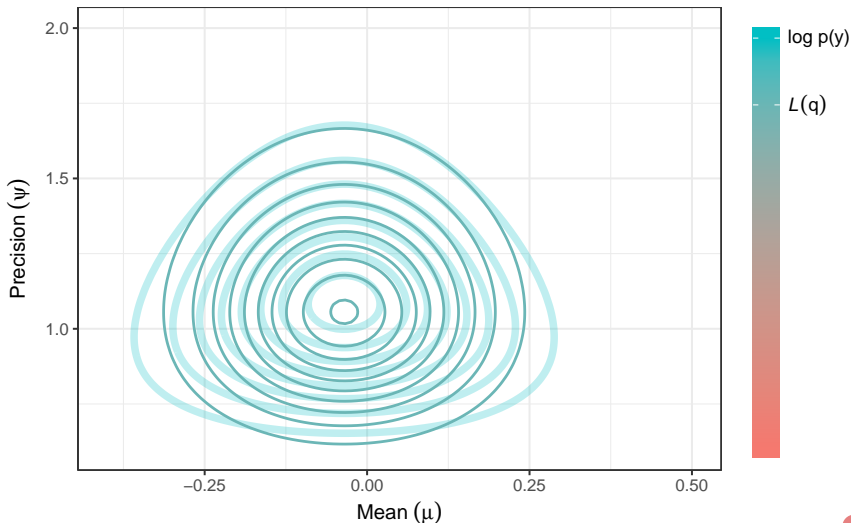
Iteration 0 (initialisation)



Estimation of a 1-dim Gaussian mean and variance (cont.)

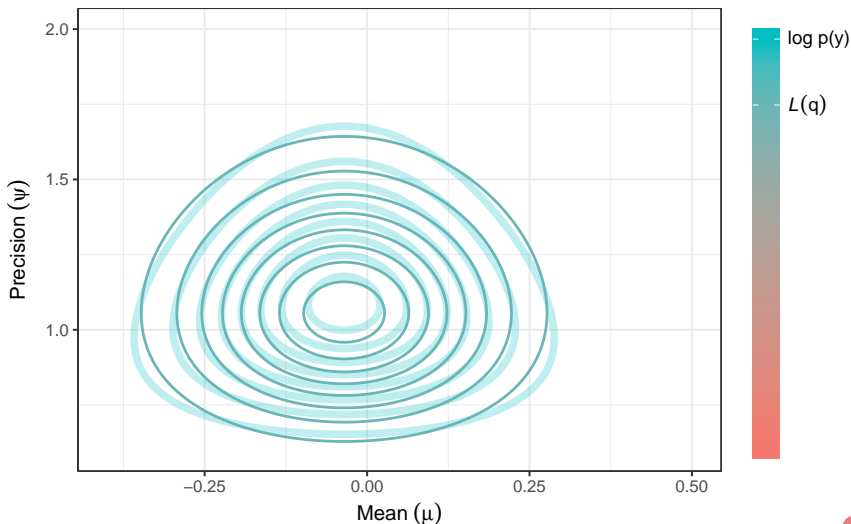
Iteration 1 (μ update)

Estimation of a 1-dim Gaussian mean and variance (cont.)

Iteration 1 (ψ update)

Estimation of a 1-dim Gaussian mean and variance (cont.)

Iteration 2 (μ update)



Estimation of a 1-dim Gaussian mean and variance (cont.)

Iteration 2 (ψ update)