

Binary probit regression with I-priors

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PhD Presentation Event

<http://phd3.haziqj.ml>

Outline

① Introduction

I-priors

PhD Roadmap

② Probit models with I-priors

The latent variable motivation

Using I-priors

Estimation (and challenges)

③ Variational inference

Introduction

Mean-field factorisation

Variational I-prior probit

④ Examples

Cardiac arrhythmia data set

Meta-analysis of smoking cessation

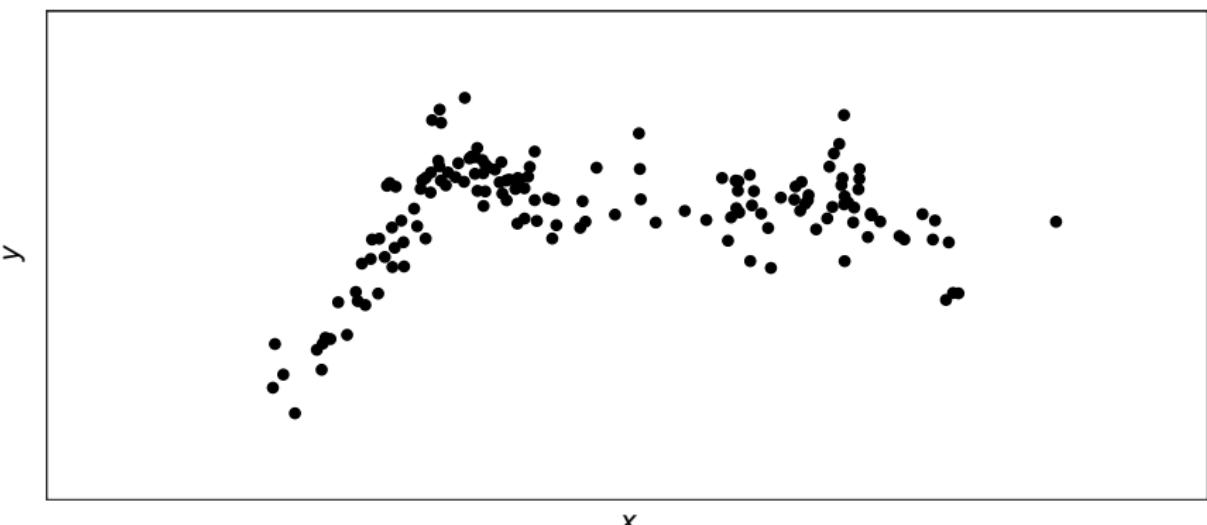
⑤ Summary

The regression model

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

$$\begin{aligned}y_i &= f(x_i) + \epsilon_i \\(\epsilon_1, \dots, \epsilon_n) &\sim N(\mathbf{0}, \Psi^{-1})\end{aligned}\tag{1}$$

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



I-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 I-prior on f is

$$(f(x_1), \dots, f(x_n))^\top \sim N(\mathbf{f}_0, \mathcal{I}(f)),$$

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 $i = 1, \dots, n$ becomes

$$\begin{aligned} y_i &= f_0(x_i) + \sum_{k=1}^n h_\lambda(x_i, x_k) w_k + \epsilon_i \\ (w_1, \dots, w_n) &\sim N(\mathbf{0}, \Psi) \\ (\epsilon_1, \dots, \epsilon_n) &\sim N(\mathbf{0}, \Psi^{-1}). \end{aligned} \tag{2}$$

I-priors (cont.)

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

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

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

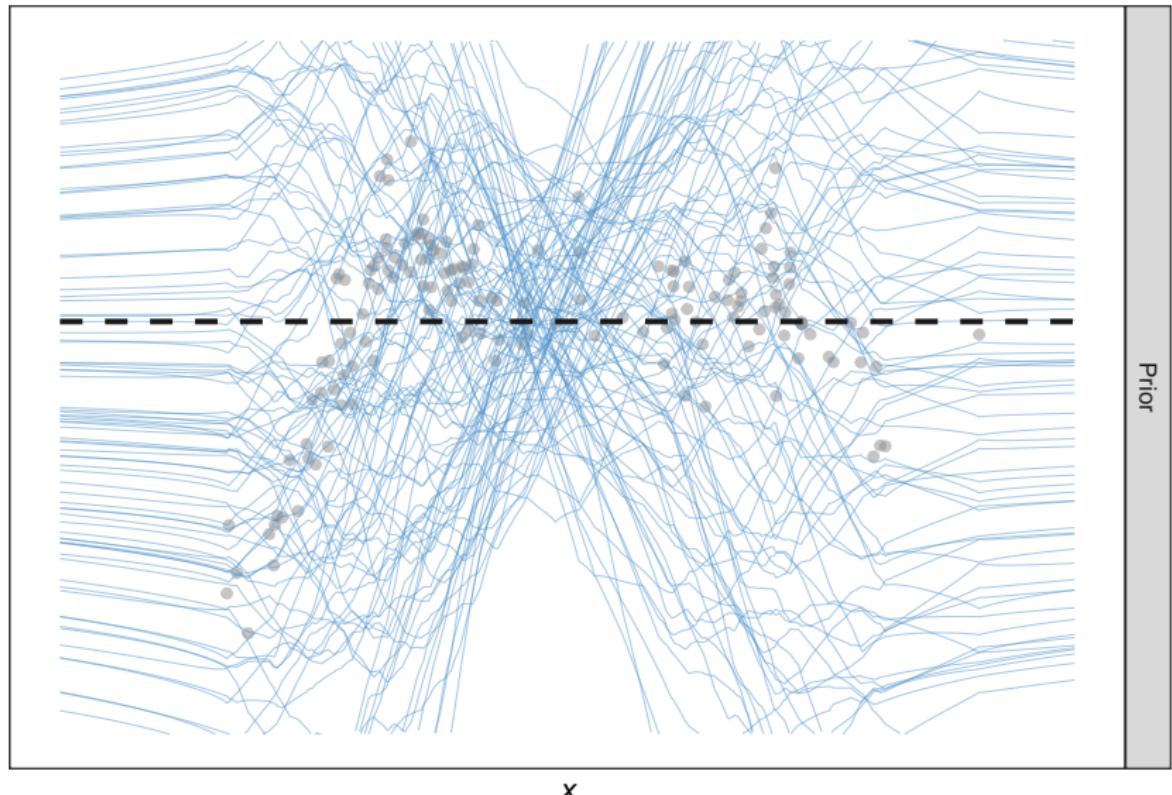
$$p(y_{\text{new}}|\mathbf{y}) = \int p(y_{\text{new}}|\mathbf{y}, f_{\text{new}})p(f_{\text{new}}|\mathbf{y}) df_{\text{new}}$$

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

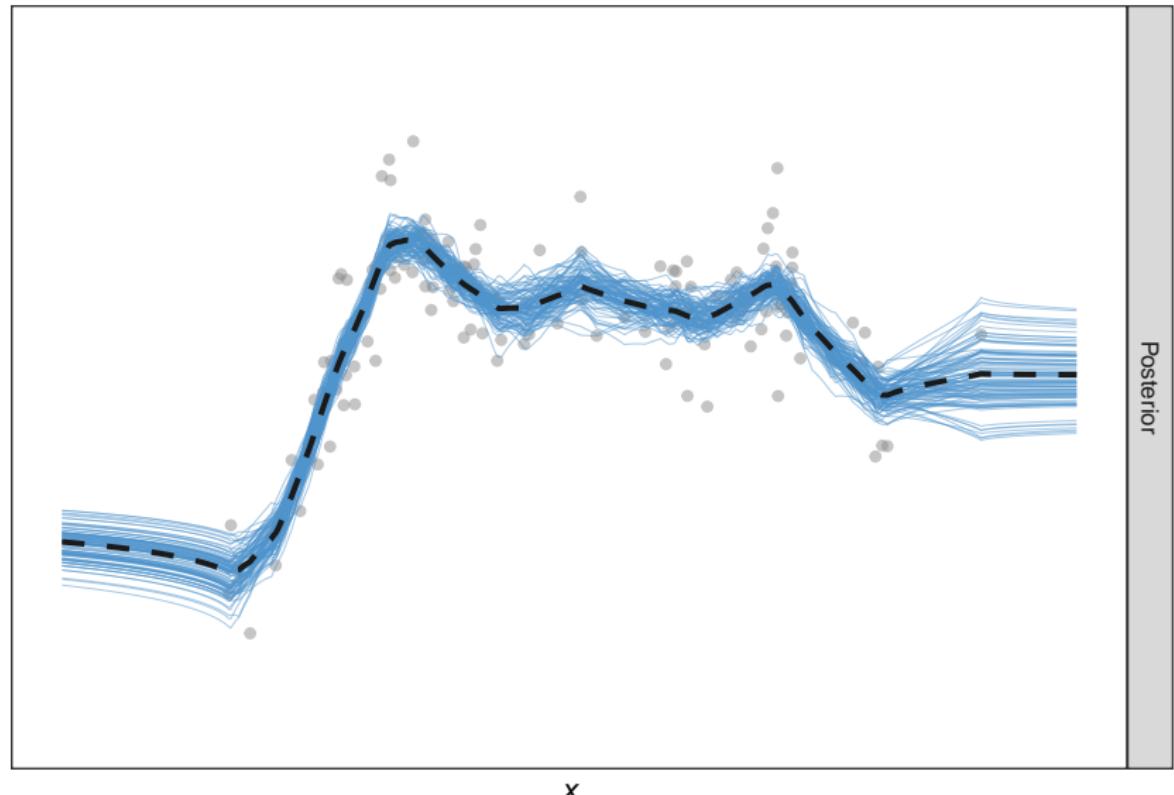
- Estimation using EM algorithm or direct maximisation of the marginal likelihood $\log p(\mathbf{y})$.
- Complete Bayesian estimation also possible.

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

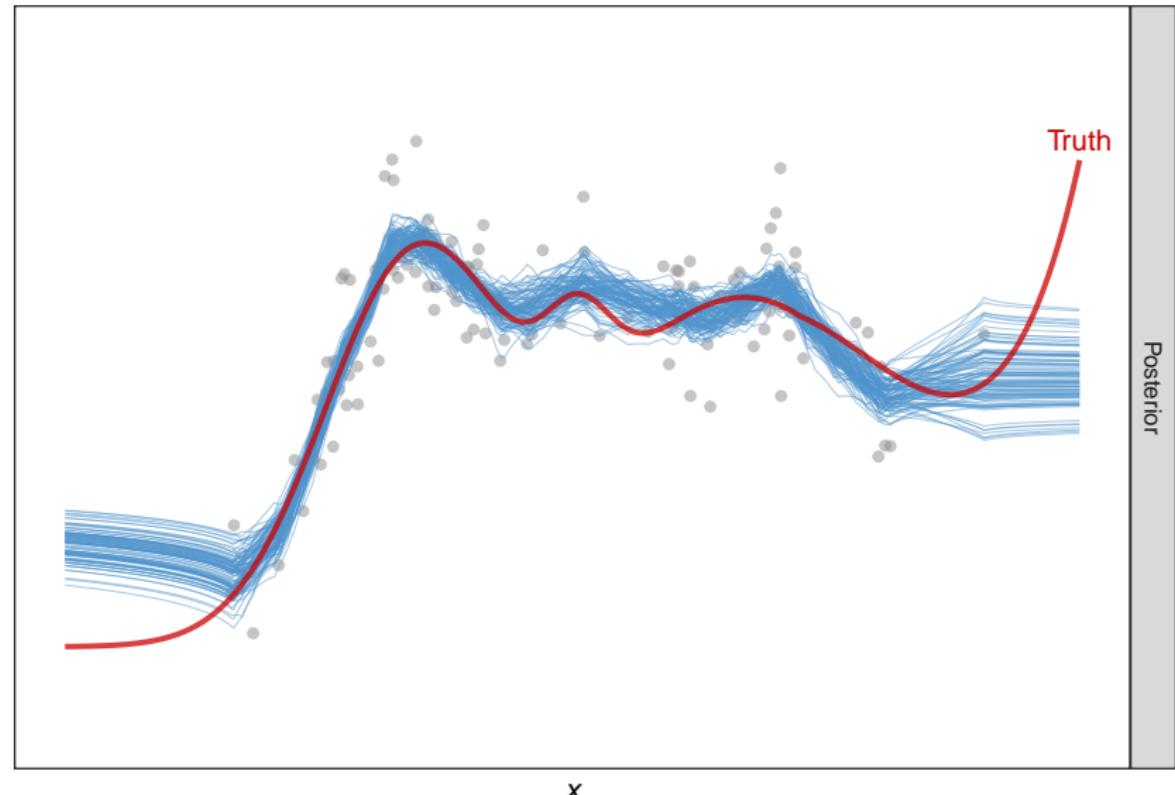
Fractional Brownian motion (FBM) RKHS



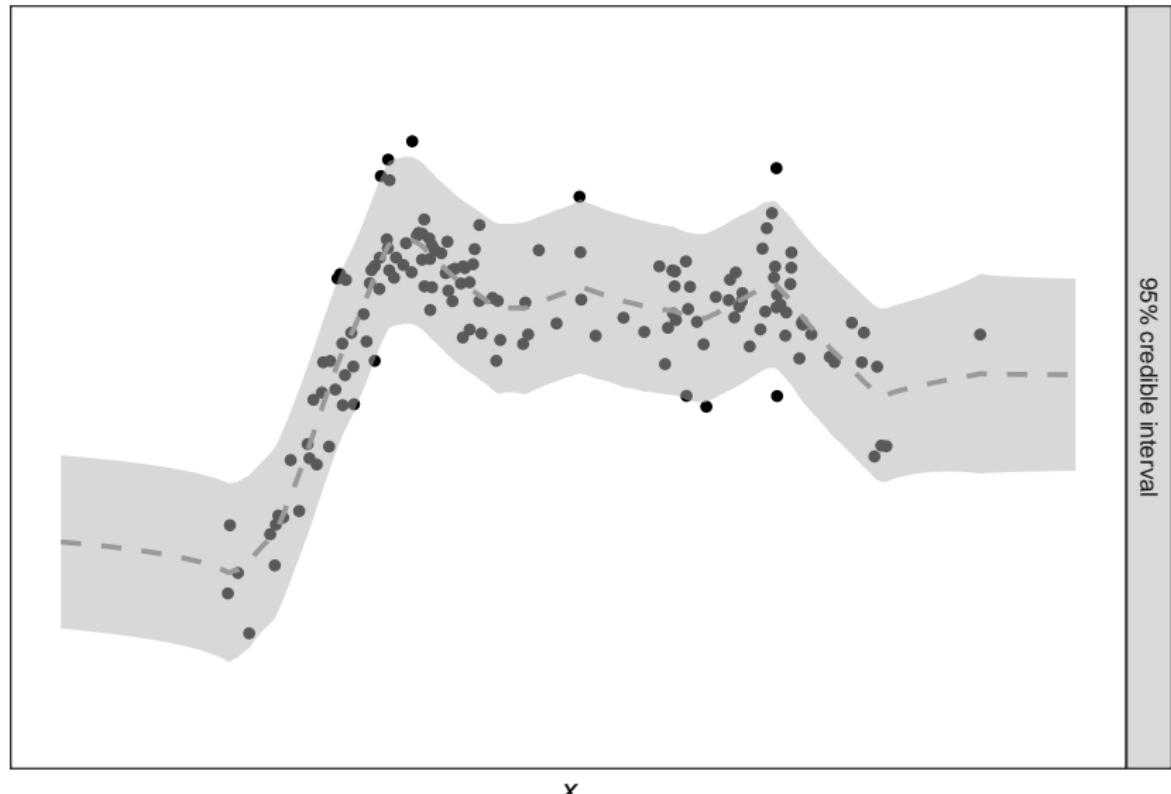
Fractional Brownian motion (FBM) RKHS



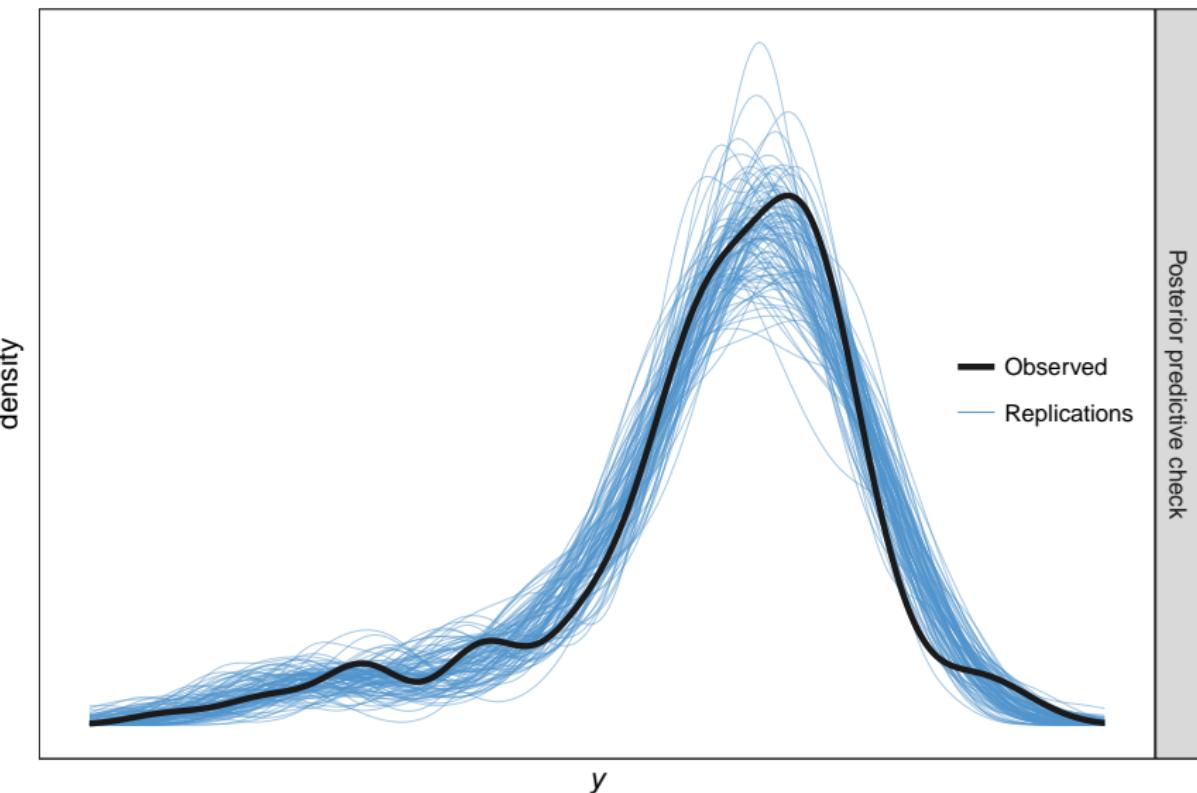
Fractional Brownian motion (FBM) RKHS



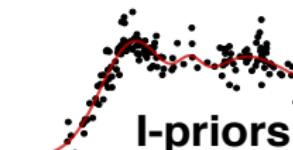
Posterior predictive distribution



Posterior predictive distribution

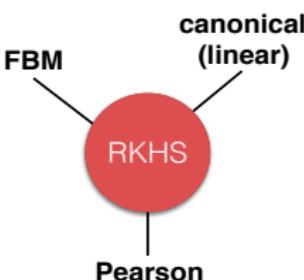


PhD Roadmap



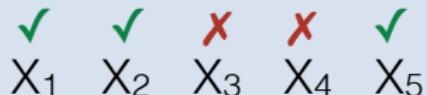
Unified methodology for

- additive models
- multilevel models
- models with functional covariates



Bayesian Variable Selection

(using I-priors in the canonical RKHS)



Good performance in cases with multicollinearity

Advantages

- Minimal assumptions
- Straightforward inference
- Performance competitive

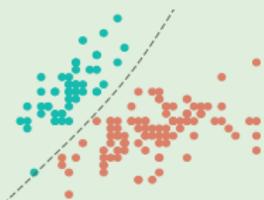
R/iprior

Estimation:

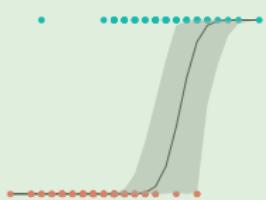
- Direct maximisation
- EM algorithm
- MCMC (Gibbs/HMC)

Binary probit models with I-priors

Extension to binary responses
Estimation using variational inference



classification



inference / fitted probabilities

① Introduction

② Probit models with I-priors

③ Variational inference

④ Examples

⑤ Summary

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

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

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

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

- Model these continuous latent variables according to

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

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

Using I-priors

- Assume an I-prior on f . Then,

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

- For now, consider iid errors $\Psi = \psi I_n$. In this case,

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

where Φ is the CDF of a standard normal.

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

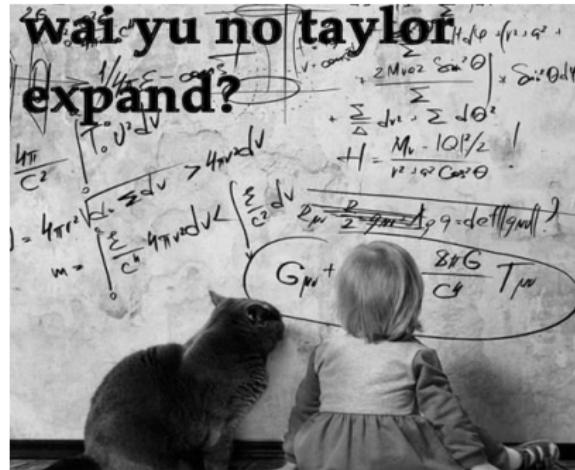
Estimation

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

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

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

- Some strategies:
 - ✗ Naive Monte-Carlo integral
 - ✗ EM algorithm with a MCMC E-step
 - ✓ Laplace approximation [details](#)
 - ✓ MCMC sampling [details](#)



① Introduction

② Probit models with I-priors

③ Variational inference

④ Examples

⑤ Summary

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) .
- 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 $p(z|y)$; and
 - ▶ The marginal likelihood (or model evidence) $p(y)$.
- 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 as follows:

$$\begin{aligned}\log p(y) &= \log p(y, z) - \log p(z|y) \\ &= \int \left\{ \log \frac{p(y, z)}{q(z)} - \log \frac{p(z|y)}{q(z)} \right\} q(z) dz \\ &= \mathcal{L}(q) + \text{KL}(q||p) \\ &\geq \mathcal{L}(q)\end{aligned}$$

- \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 $q(z) \equiv p(z|y)$ (c.f. EM algorithm), we are unable to work with $p(z|y)$.

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 $z = (z^{(1)}, \dots, z^{(m)})$, and assume

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

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

$$\tilde{q}_j(z^{(j)}) \propto \exp(E_{-j}[\log p(y, z)]) \quad (3)$$

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

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

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

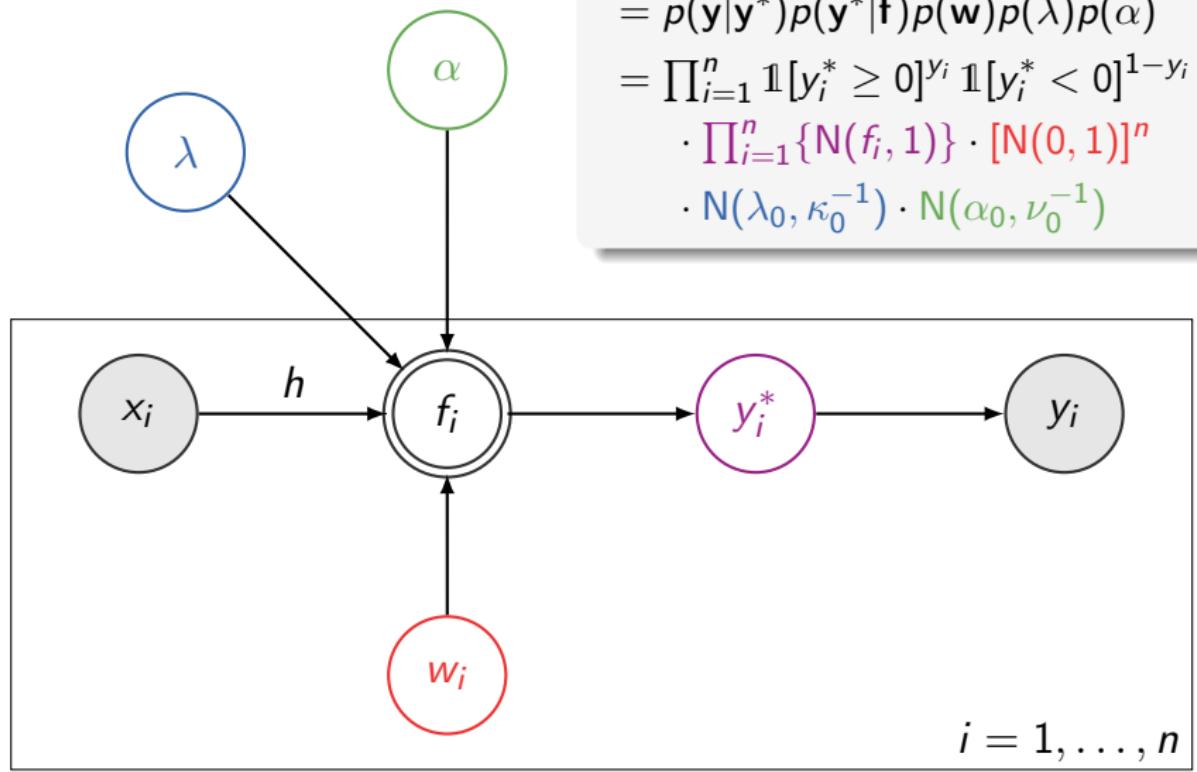
$$\mathcal{L}(q) = E_q[\log p(\mathbf{y}, \mathbf{z})] - E_q[\log q(\mathbf{z})].$$

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: $\log q_j(\mathbf{z}^{(j)}) \leftarrow E_{-\mathbf{j}}[\log p(\mathbf{y}, \mathbf{z})] + \text{const.}$
- 5: **end for**
- 6: $\mathcal{L}(q) \leftarrow E_q[\log p(\mathbf{y}, \mathbf{z})] - E_q[\log q(\mathbf{z})]$
- 7: **end while**
- 8: **return** $\tilde{q}(\mathbf{z}) = \prod_{j=1}^m \tilde{q}_j(\mathbf{z}^{(j)})$

example

Variational I-prior probit



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

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

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

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

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

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

Variational lower bound

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

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

- (possible) ISSUE: Different initialisations lead to different converged lower bound values indicating presence of many local optima.
- From experience, typically local optima gives better predictive abilities.

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

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

① Introduction

② Probit models with I-priors

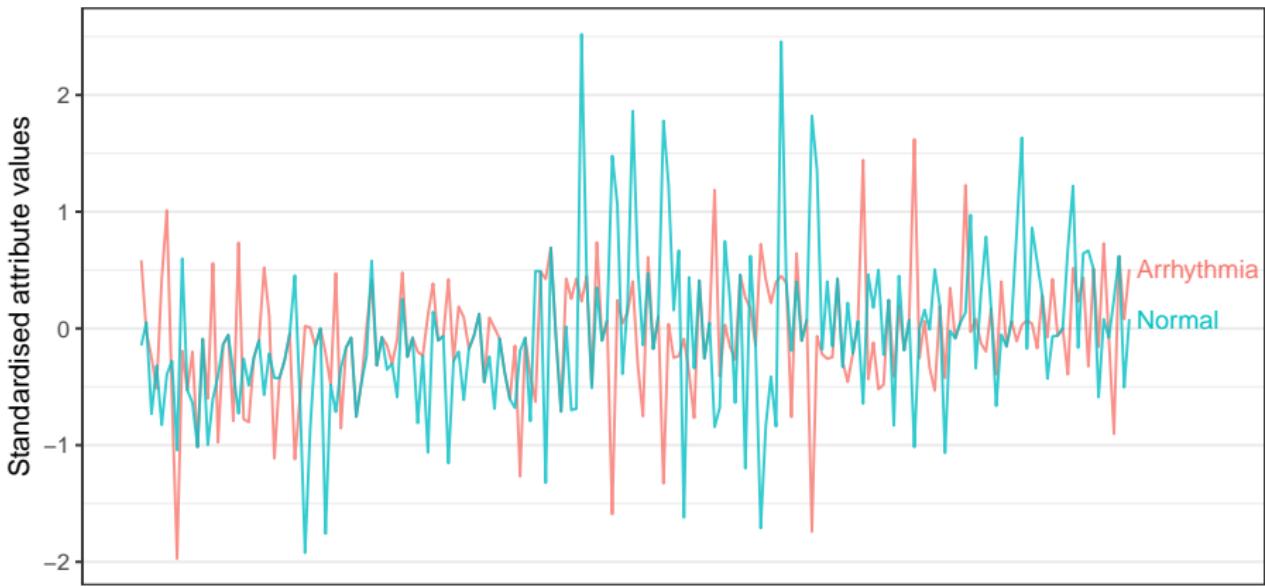
③ Variational inference

④ Examples

⑤ Summary

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

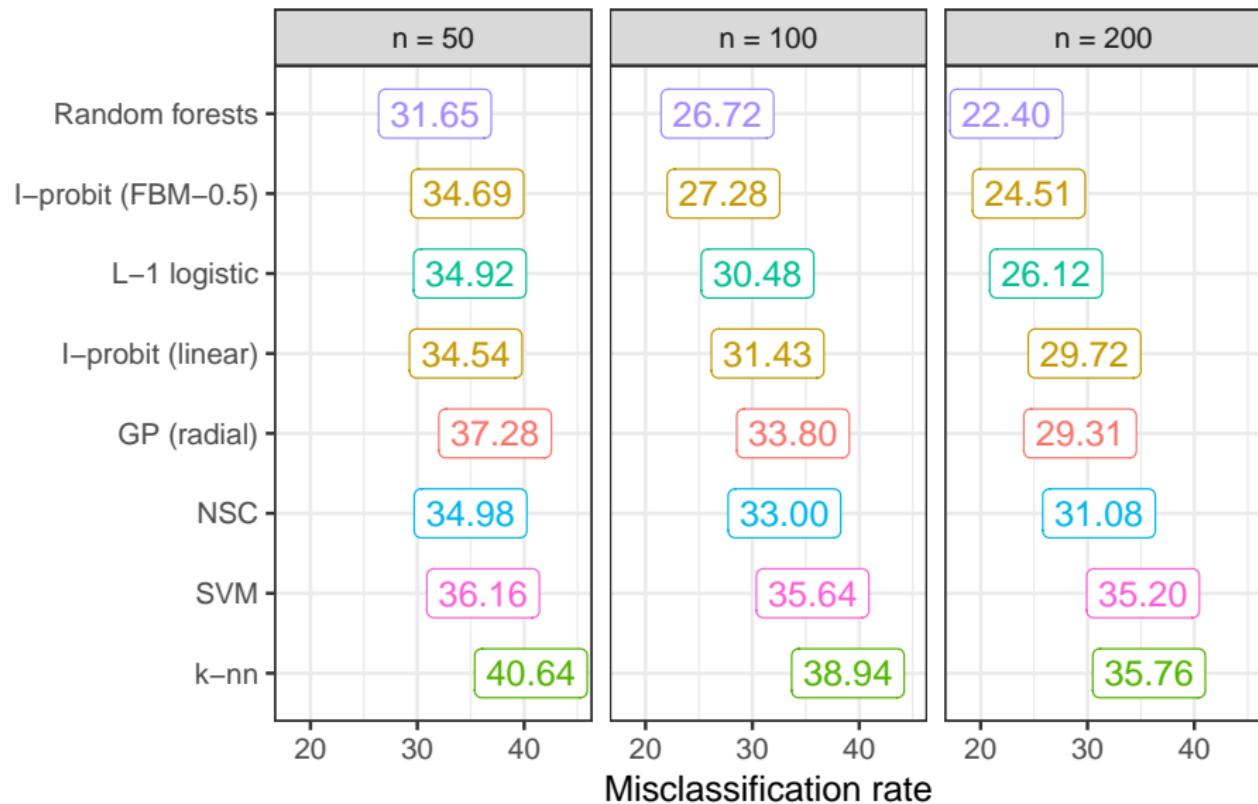
- Fit an I-prior probit model using Canonical and FBM kernels. The full data set takes about 35 seconds.

```
R> mod <- iprobit(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

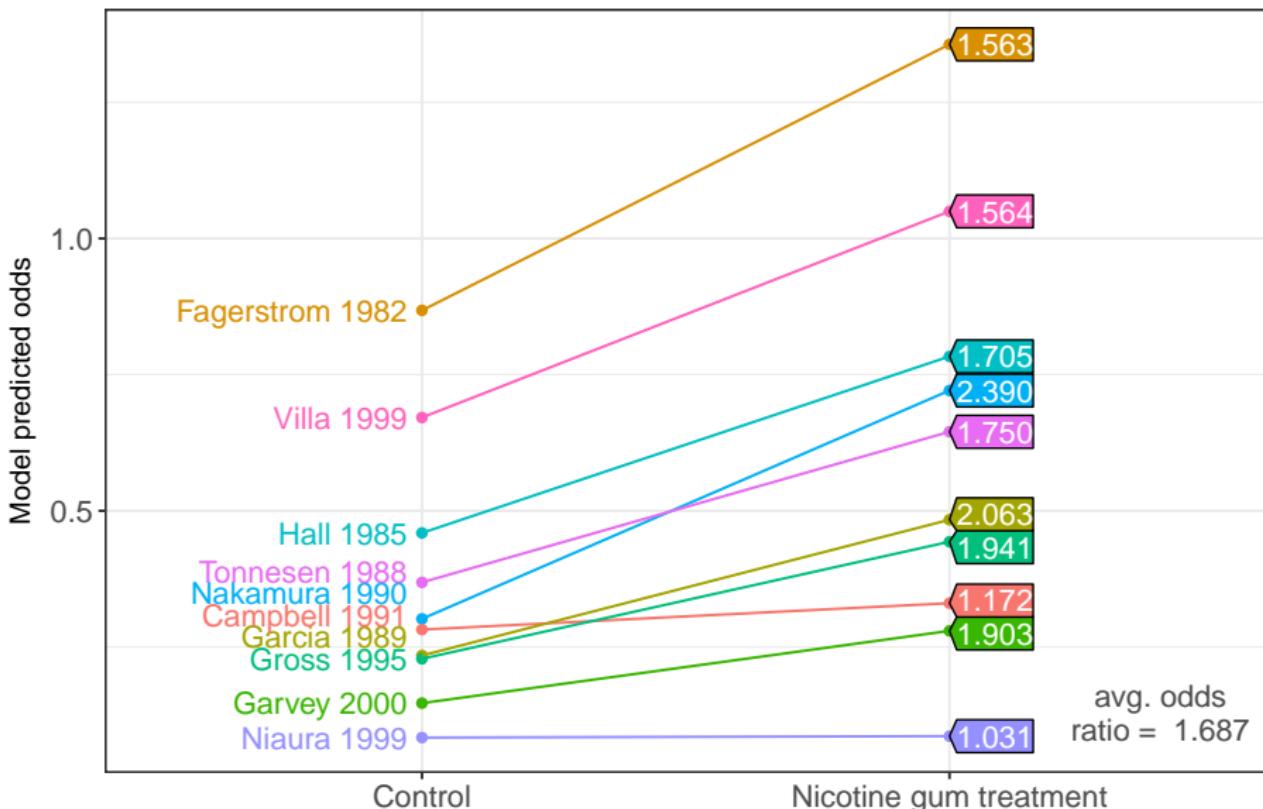
- Let $i = 1, \dots, n_j$ index the patients in study group $j \in 1, \dots, 27$.
- Denote y_{ij} as the binary response variable indicating Quit (1) or Remain (0), and x_{ij} as patient $_{ij}$'s treatment group indicator.
- Model binary data using l-probit model

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

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



① Introduction

② Probit models with I-priors

③ Variational inference

④ Examples

⑤ Summary

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. [details](#)
- 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>

Introduction
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Probit with I-priors
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Variational
oooooooo

Examples
oooooo

Summary

End

End

Thank you!

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⑥ Additional material

The I-prior probit model

Laplace's method

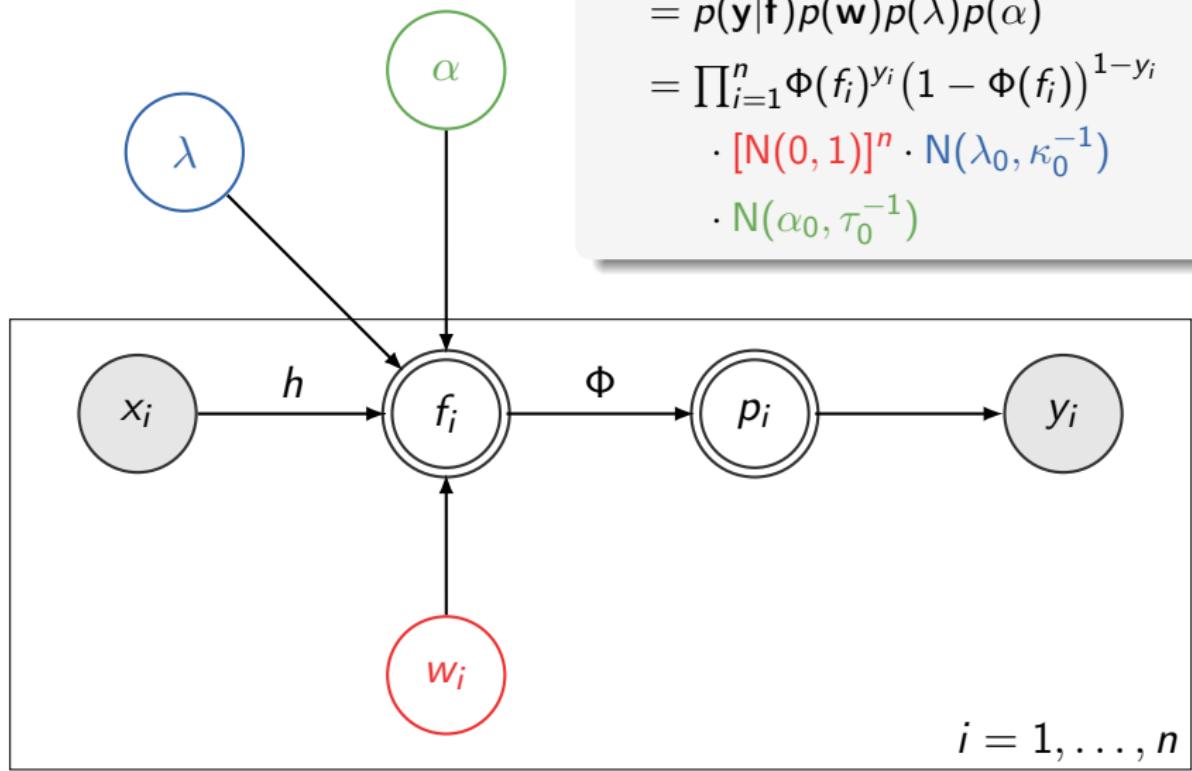
Full Bayesian analysis of I-probit models

Variational inference

A simple variational inference example

Fisher's Iris data set

The I-prior probit model



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 $\mathbf{A} = -D^2 Q(\mathbf{f})$ 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

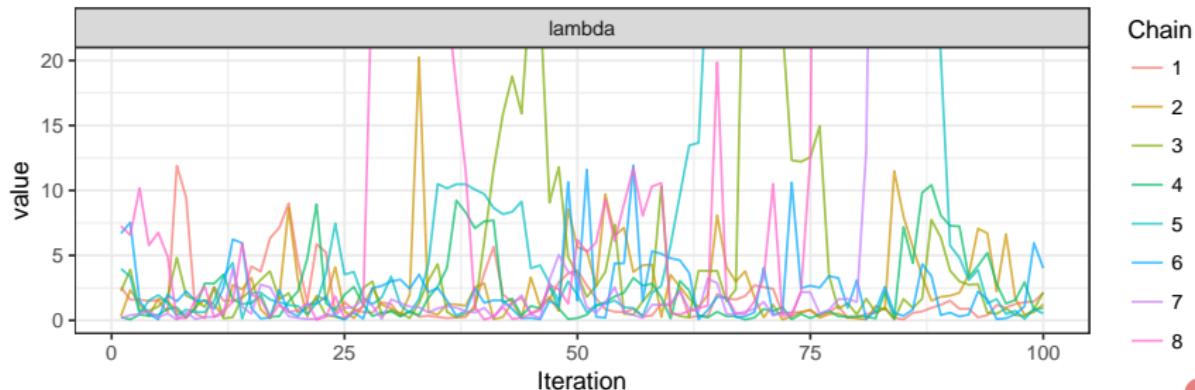
$$p(\mathbf{y}) \approx (2\pi)^{n/2} |\mathbf{A}|^{-1/2} p(\mathbf{y}|\tilde{\mathbf{f}}) p(\tilde{\mathbf{f}})$$

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

$$\begin{array}{ll} \text{Functions} & p : \theta \mapsto \mathbb{R} \quad (\text{standard calculus}) \\ \text{Functionals} & \mathcal{H} : p \mapsto \mathbb{R} \quad (\text{variational calculus}) \end{array}$$

- Using standard calculus, we can solve

$$\arg \max_{\theta} p(\theta) =: \hat{\theta}$$

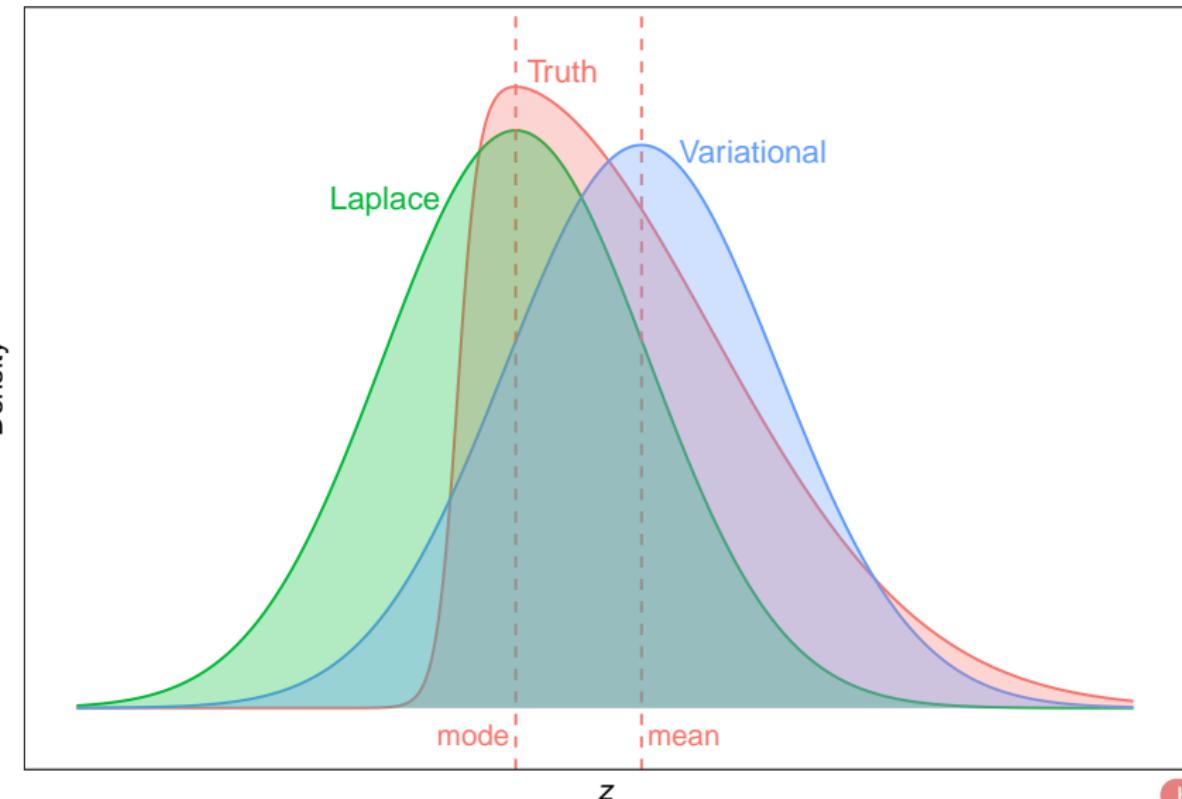
e.g. p is a likelihood function, and $\hat{\theta}$ is the ML estimate.

- Using variational calculus, we can solve

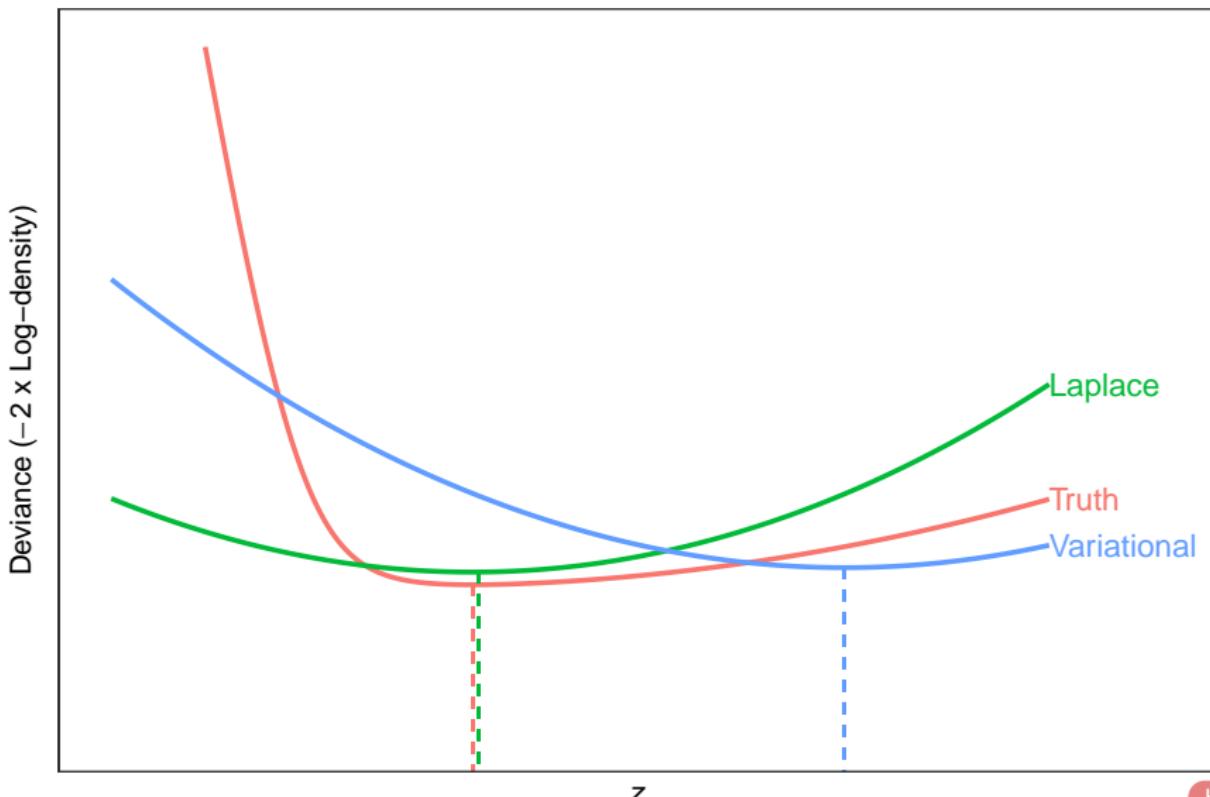
$$\arg \max_p \mathcal{H}(p) =: \tilde{p}$$

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

Comparison of approximations (density)



Comparison of approximations (deviance)



Estimation of a 1-dim Gaussian mean and variance

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

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

$$\begin{aligned} \mu | \psi &\sim N(\mu_0, (\kappa_0 \psi)^{-1}) && \text{Priors} \\ \psi &\sim \Gamma(a_0, b_0) \end{aligned}$$

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

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

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

- From (3), we can work out the solutions

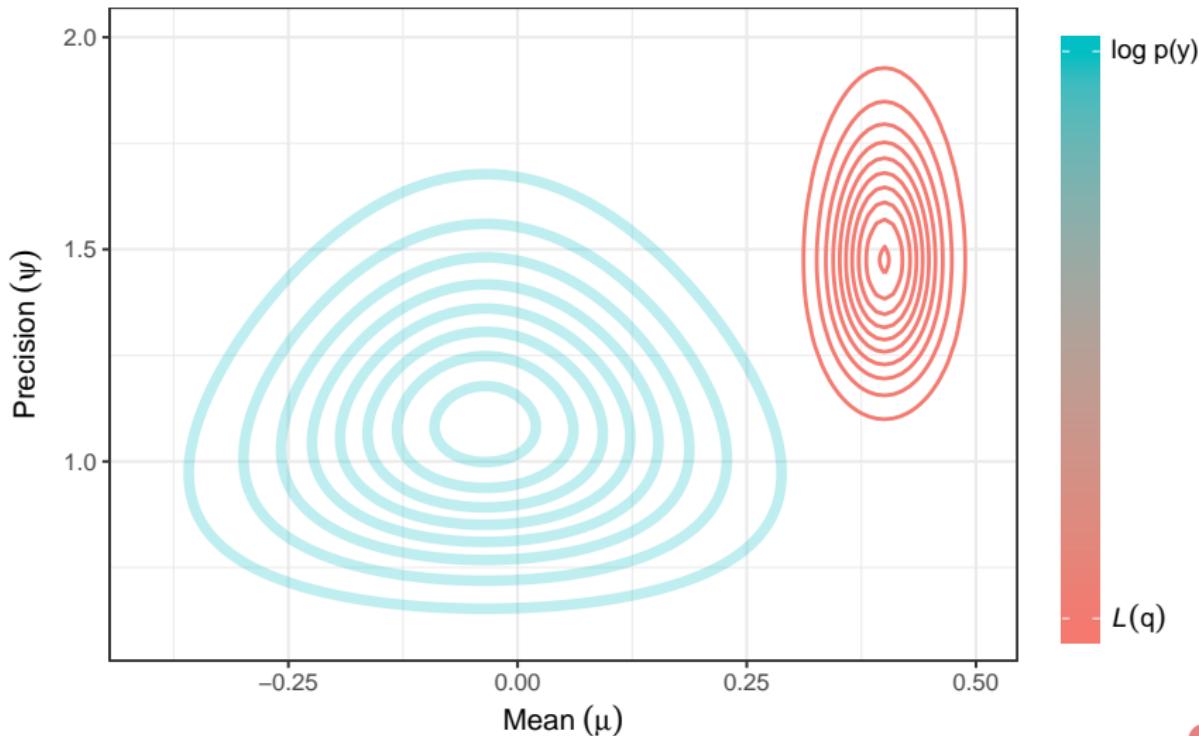
$$\tilde{q}_\mu(\mu) \equiv N\left(\frac{\kappa_0 \mu_0 + n \bar{y}}{\kappa_0 + n}, \frac{1}{(\kappa_0 + n) E_q[\psi]}\right) \quad \text{and} \quad \tilde{q}_\psi(\psi) \equiv \Gamma(\tilde{a}, \tilde{b})$$

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

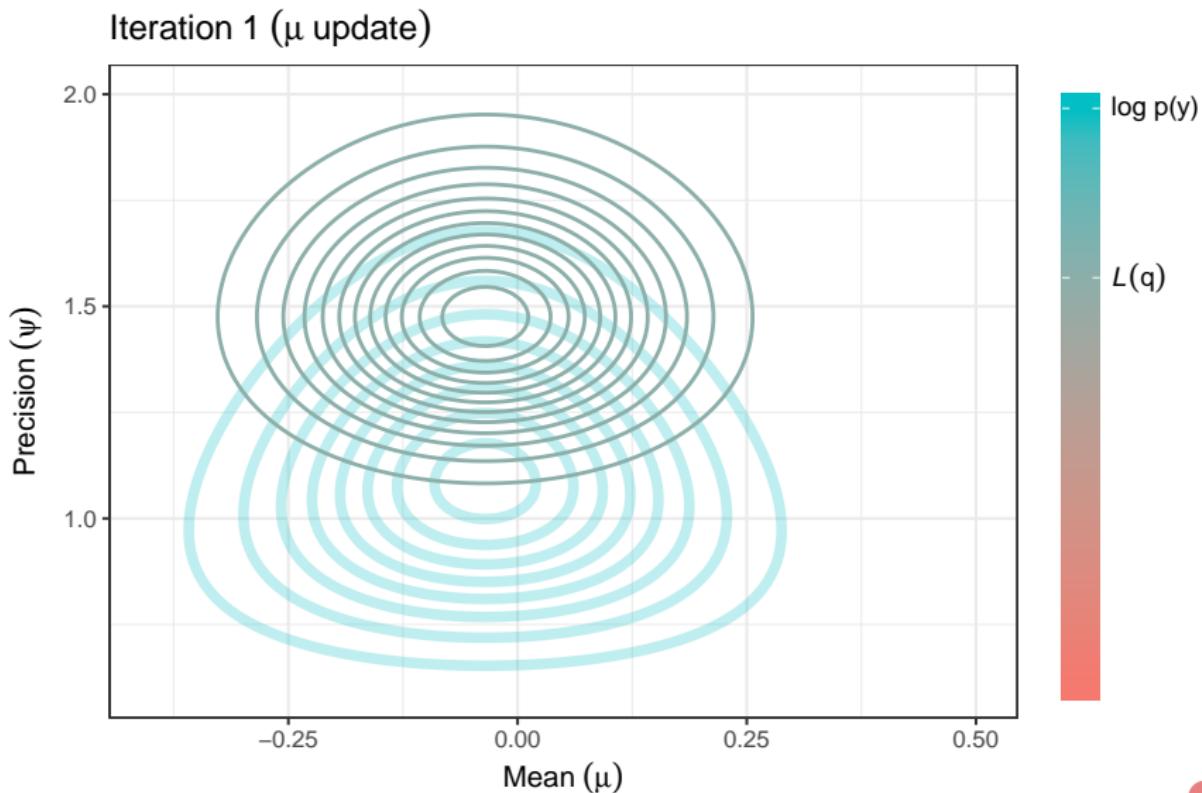
back

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

Iteration 0 (initialisation)

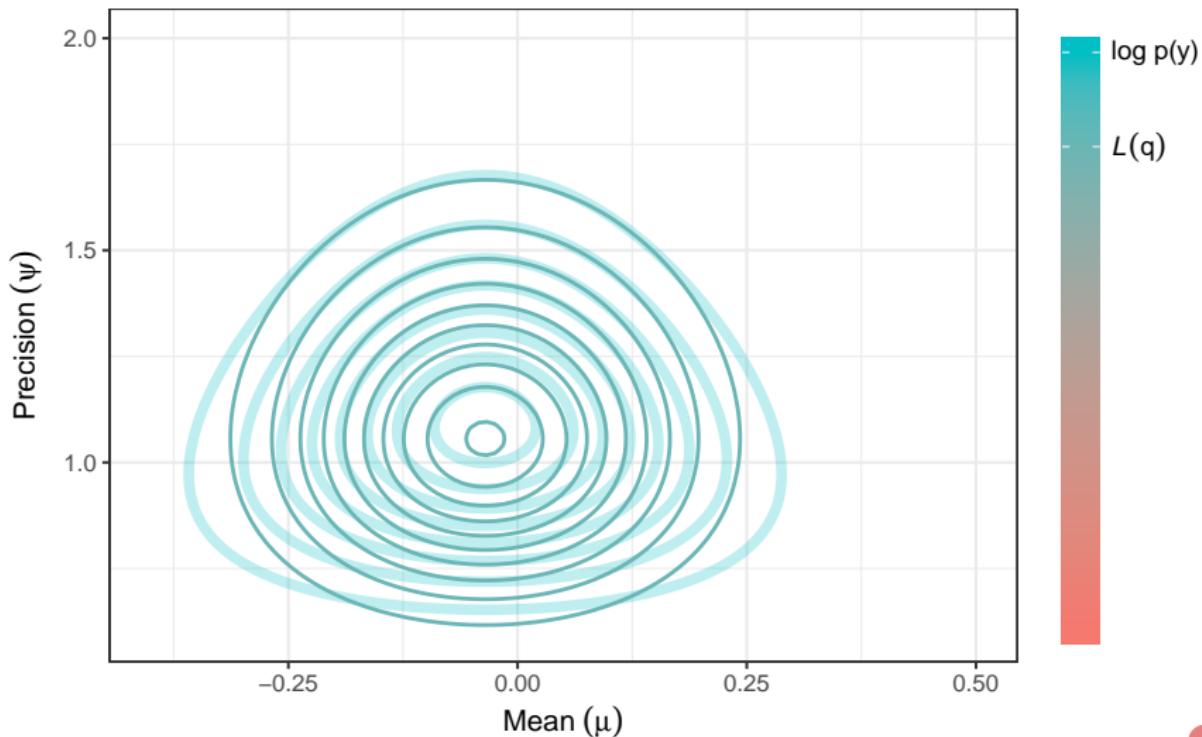


Estimation of a 1-dim Gaussian mean and variance (cont.)



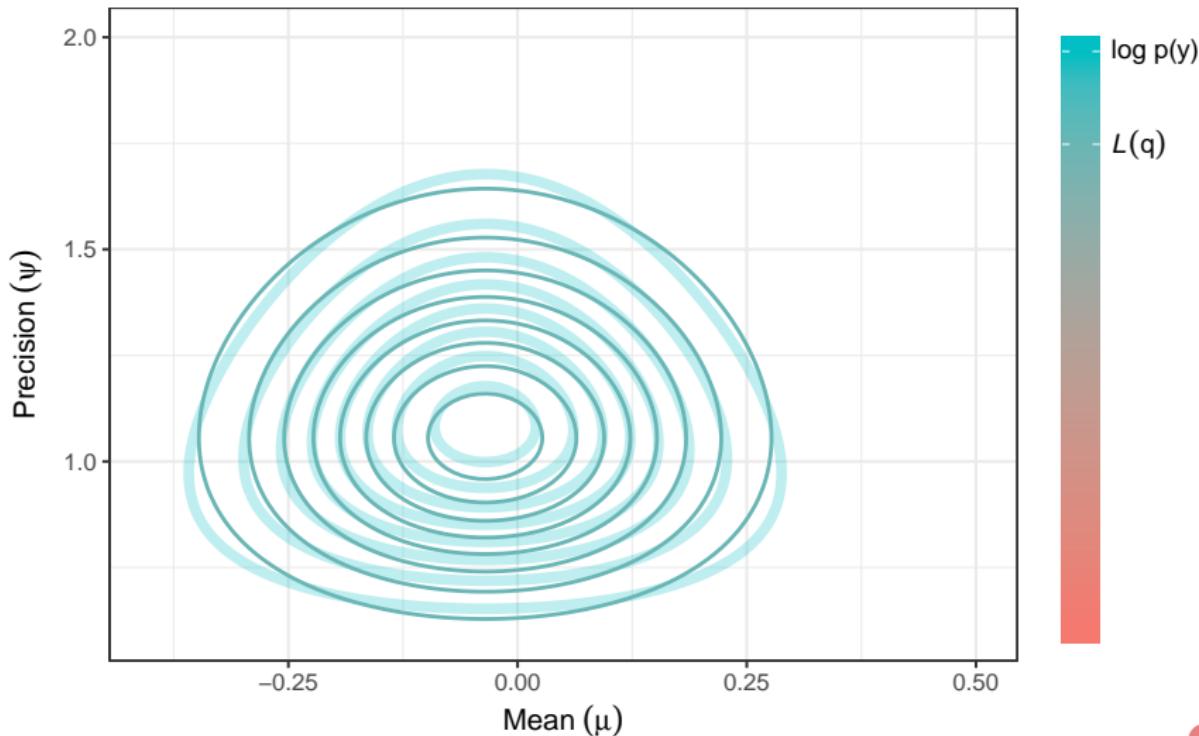
Estimation of a 1-dim Gaussian mean and variance (cont.)

Iteration 1 (ψ update)



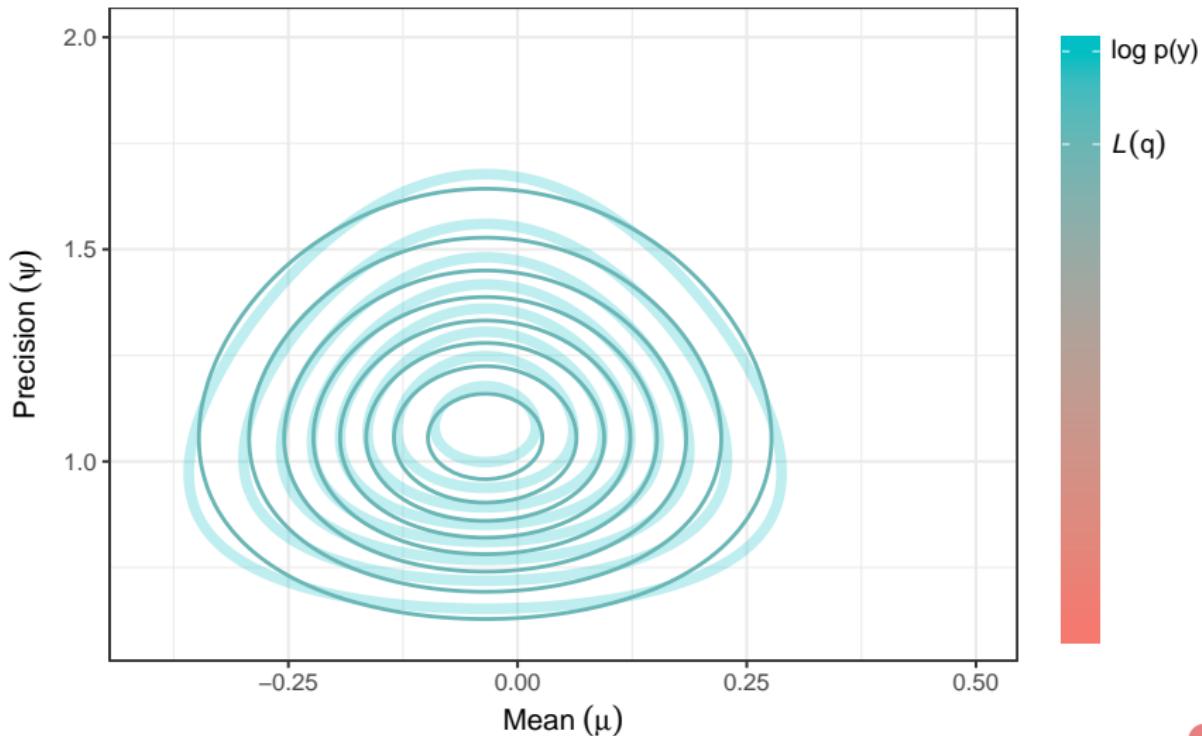
Estimation of a 1-dim Gaussian mean and variance (cont.)

Iteration 2 (μ update)

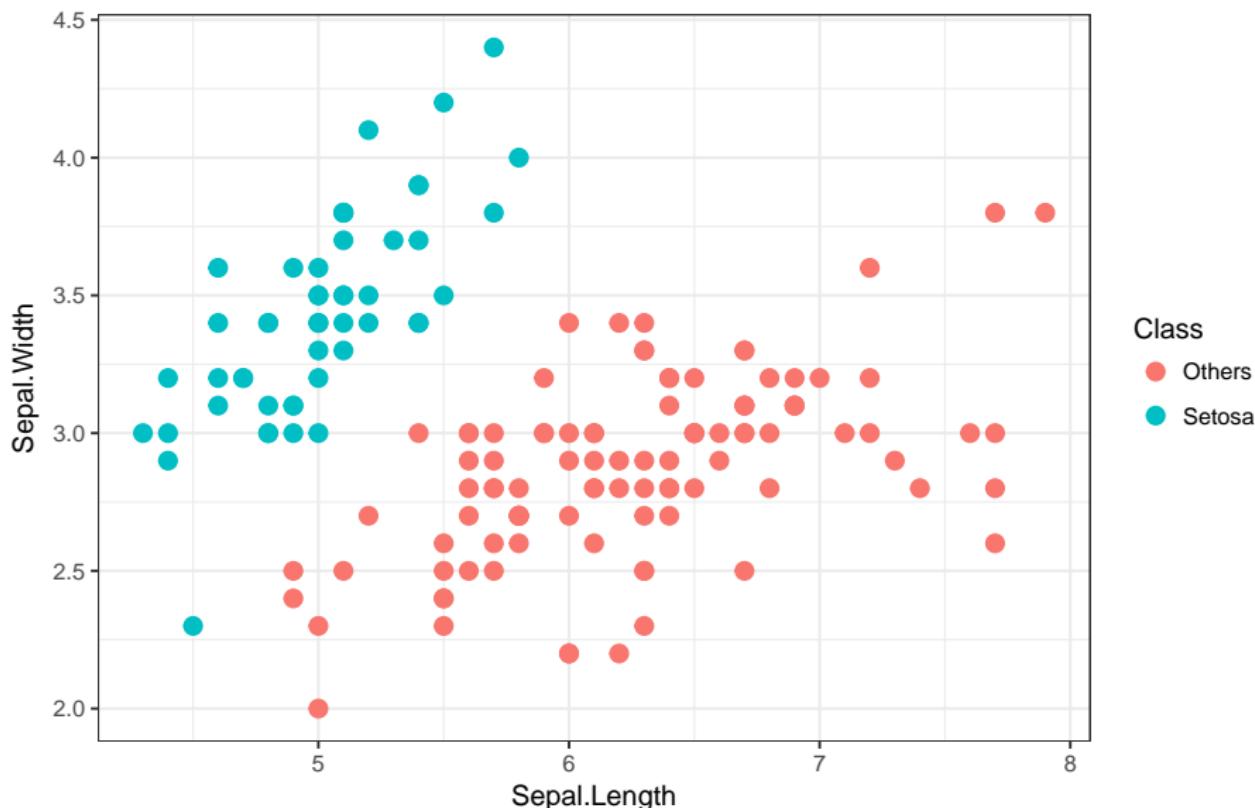


Estimation of a 1-dim Gaussian mean and variance (cont.)

Iteration 2 (ψ update)



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

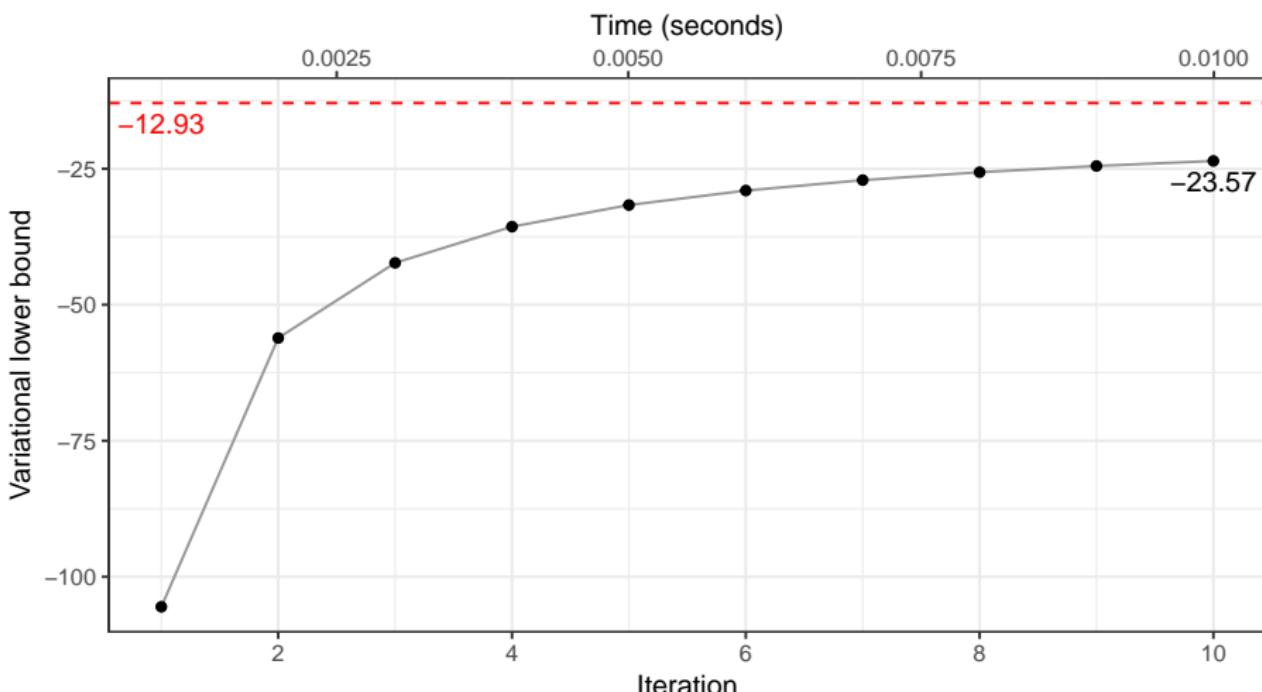
Fisher's Iris data set - Model summary

```
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)
```

