

## 1 Variational inference for I-prior models

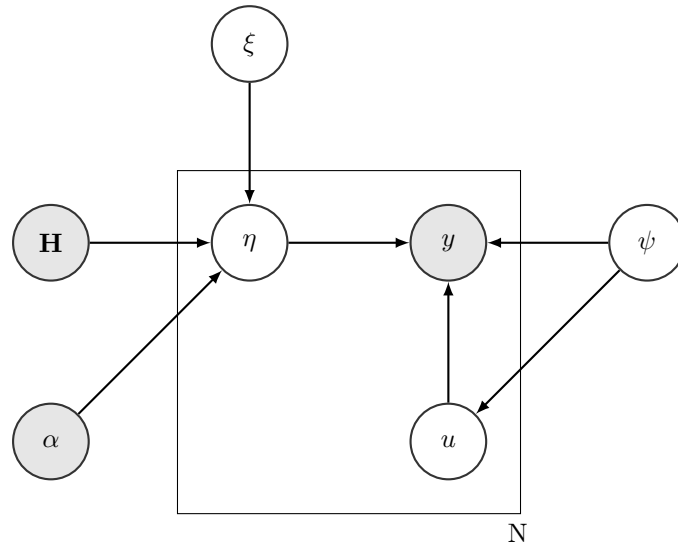
The model:

$$\begin{aligned}\mathbf{y} &= \boldsymbol{\alpha} + \lambda \mathbf{H} \mathbf{w} + \boldsymbol{\epsilon} \\ \boldsymbol{\epsilon} &\sim \mathcal{N}(\mathbf{0}, \psi^{-1} \mathbf{I}_n) \\ \mathbf{w} &\sim \mathcal{N}(\mathbf{0}, \psi \mathbf{I}_n)\end{aligned}$$

Let  $\mathbf{u} \sim \mathcal{N}(\mathbf{0}, \psi^{-1} \mathbf{I}_n)$ . Reparameterise  $\xi = \lambda \psi$ . Then  $\psi^{-1} \mathbf{w}$  will have the same distribution as  $\mathbf{u}$ . Substituting this into the I-prior model, we have

$$\begin{aligned}\mathbf{y} &= \boldsymbol{\alpha} + \xi \mathbf{H} \mathbf{u} + \boldsymbol{\epsilon} \\ \mathbf{u} &\sim \mathcal{N}(\mathbf{0}, \psi^{-1} \mathbf{I}_n) \\ \boldsymbol{\epsilon} &\sim \mathcal{N}(\mathbf{0}, \psi^{-1} \mathbf{I}_n)\end{aligned}$$

### 1.1 DAG for the I-prior model



## 1.2 Distributions

### 1.2.1 Priors

$$p(u_1, \dots, u_n) \equiv [\mathcal{N}(0, \psi^{-1})]^n$$
$$p(\xi, \psi) \propto \text{const.}$$

### 1.2.2 Joint data and latent

$$p(\mathbf{y}, \mathbf{u}, \xi, \psi) = p(\mathbf{y}|\mathbf{u}, \xi, \psi)p(\mathbf{u}, \xi, \psi)$$
$$= p(\mathbf{y}|\boldsymbol{\eta})p(\mathbf{u})p(\xi, \psi)$$

where

$$\boldsymbol{\eta} = \boldsymbol{\alpha} + \xi \mathbf{H} \mathbf{u}$$

### 1.2.3 pdf/pmf

$$\begin{aligned} \log p(\mathbf{y}|\boldsymbol{\eta}) &= \log \mathcal{N}(\boldsymbol{\eta}, \psi^{-1} \mathbf{I}_n) \\ &= -\frac{n}{2} \log 2\pi + \frac{n}{2} \log \psi - \frac{\psi}{2} \|\mathbf{y} - \boldsymbol{\eta}\|^2 \\ &= -\frac{n}{2} \log 2\pi + \frac{n}{2} \log \psi - \frac{\psi}{2} \|\mathbf{y} - \boldsymbol{\alpha} - \xi \mathbf{H} \mathbf{u}\|^2 \\ &= -\frac{n}{2} \log 2\pi + \frac{n}{2} \log \psi - \frac{\psi}{2} \sum_{i=1}^n (y_i - \alpha - \xi \mathbf{H}_i \mathbf{u})^2 \end{aligned}$$

$$\begin{aligned} \log p(\mathbf{u}) &= \log \mathcal{N}(\mathbf{0}, \psi^{-1} \mathbf{I}_n) \\ &= -\frac{n}{2} \log 2\pi + \frac{n}{2} \log \psi - \frac{\psi}{2} \|\mathbf{u}\|^2 \\ &= -\frac{n}{2} \log 2\pi + \frac{n}{2} \log \psi - \frac{\psi}{2} \sum_{i=1}^n u_i^2 \end{aligned}$$

## 1.3 Mean field approximation

$$q(\mathbf{u}, \xi, \psi) \equiv q(\mathbf{u})q(\xi)q(\psi)$$

### 1.3.1 Distribution of $\tilde{q}(\mathbf{u})$

$$\begin{aligned}
\log \tilde{q}(\mathbf{u}) &= \mathbb{E}_{\xi, \psi} \left[ -\frac{\psi}{2} \|\mathbf{y} - \boldsymbol{\alpha} - \xi \mathbf{H} \mathbf{u}\|^2 + \|\mathbf{u}\|^2 \right] + \text{const.} \\
&= -\frac{\mathbb{E} \psi}{2} \mathbb{E}_{\xi, \psi} [\xi^2 \mathbf{u}^\top \mathbf{H}^2 \mathbf{u} + \mathbf{u}^\top \mathbf{u} - 2\xi (\mathbf{y} - \boldsymbol{\alpha})^\top \mathbf{H} \mathbf{u}] + \text{const.} \\
&= -\frac{\mathbb{E} \psi}{2} \left( \mathbf{u}^\top (\mathbb{E}[\xi^2] \mathbf{H}^2 + \mathbf{I}_n) \mathbf{u} - 2 \mathbb{E} \xi (\mathbf{y} - \boldsymbol{\alpha})^\top \mathbf{H} \mathbf{u} \right) + \text{const.}
\end{aligned}$$

Let  $\mathbf{A} = \mathbb{E}[\xi^2] \mathbf{H}^2 + \mathbf{I}_n$  and  $\mathbf{a} = \mathbb{E}[\xi] \mathbf{H}(\mathbf{y} - \boldsymbol{\alpha})$ . Then, using the fact that

$$\mathbf{u}^\top \mathbf{A} \mathbf{u} - 2 \mathbf{a}^\top \mathbf{u} = (\mathbf{u} - \mathbf{A}^{-1} \mathbf{a})^\top \mathbf{A} (\mathbf{u} - \mathbf{A}^{-1} \mathbf{a}),$$

we see the  $\tilde{q}(\mathbf{u})$  is quadratic in  $\mathbf{u}$ , and we recognise this as the kernel of a multivariate normal density. Therefore,

$$\tilde{q}(\mathbf{u}) \equiv \mathcal{N}(\mathbf{A}^{-1} \mathbf{a}, \mathbf{A}^{-1} / \mathbb{E} \psi)$$

For convenience later in deriving the lower bound, we note that the second moment of  $\tilde{q}(\mathbf{w})$  is equal to  $\mathbb{E}[\mathbf{u} \mathbf{u}^\top] = \mathbf{A}^{-1} (\mathbb{E}^{-1}[\psi] \mathbf{I}_n + \mathbf{a} \mathbf{a}^\top \mathbf{A}^{-1}) =: \tilde{\mathbf{U}}$ .

### 1.3.2 Distribution of $\tilde{q}(\xi)$

$$\begin{aligned}
\log \tilde{q}(\xi) &= \mathbb{E}_{\mathbf{u}, \psi} \left[ -\frac{\psi}{2} \|\mathbf{y} - \boldsymbol{\alpha} - \xi \mathbf{H} \mathbf{u}\|^2 \right] + \text{const.} \\
&= -\frac{\mathbb{E} \psi}{2} \mathbb{E}_{\mathbf{u}, \psi} [\xi^2 \text{tr}(\mathbf{H}^2 \mathbf{u} \mathbf{u}^\top) - 2\xi (\mathbf{y} - \boldsymbol{\alpha})^\top \mathbf{H} \mathbf{u}] + \text{const.} \\
&= -\frac{\mathbb{E} \psi}{2} \left[ \xi^2 \text{tr}(\mathbf{H}^2 \mathbb{E}[\mathbf{u} \mathbf{u}^\top]) - 2\xi (\mathbf{y} - \boldsymbol{\alpha})^\top \mathbf{H} \mathbb{E} \mathbf{u} \right] + \text{const.}
\end{aligned}$$

By completing the square, we get that  $\tilde{q}(\xi) \equiv \mathcal{N}(d/c, (c \mathbb{E}[\psi])^{-1})$ , where

$$c = \text{tr}(\mathbf{H}^2 \mathbb{E}[\mathbf{u} \mathbf{u}^\top]) \quad \text{and} \quad d = (\mathbf{y} - \boldsymbol{\alpha})^\top \mathbf{H} \mathbb{E} \mathbf{u}$$

### 1.3.3 Distribution of $\tilde{q}(\psi)$

$$\begin{aligned}
\log \tilde{q}(\psi) &= \mathbb{E}_{\mathbf{u}, \xi} \left[ \frac{n}{2} \log \psi - \frac{\psi}{2} \|\mathbf{y} - \boldsymbol{\eta}\|^2 + \frac{n}{2} \log \psi - \frac{\psi}{2} \|\mathbf{u}\|^2 \right] + \text{const.} \\
&= n \log \psi - \mathbb{E}_{\mathbf{u}, \xi} \left[ \frac{\psi}{2} (\|\mathbf{y} - \boldsymbol{\eta}\|^2 + \|\mathbf{u}\|^2) \right] + \text{const.} \\
&= (n + 1 - 1) \log \psi \\
&\quad - \psi \cdot \left( \frac{1}{2} \sum_{i=1}^n (y_i - \alpha)^2 + \frac{1}{2} \text{tr} \left( (\mathbb{E}[\xi^2] \mathbf{H}^2 + \mathbf{I}_n) \tilde{\mathbf{U}} \right) - \mathbb{E}[\xi] (\mathbf{y} - \boldsymbol{\alpha})^\top \mathbf{H} \mathbb{E}[\mathbf{u}] \right) + \text{const.}
\end{aligned}$$

This is a gamma distribution with shape  $s = n + 1$  and rate  $r = \frac{1}{2} \sum_{i=1}^n (y_i - \alpha)^2 + \frac{1}{2} \text{tr} \left( (\mathbb{E}[\xi^2] \mathbf{H}^2 + \mathbf{I}_n) \tilde{\mathbf{U}} \right) - \mathbb{E}[\xi] (\mathbf{y} - \boldsymbol{\alpha})^\top \mathbf{H} \mathbb{E}[\mathbf{u}]$ . The mean is  $s/r$ , and the mean of  $\log \psi$  is  $\Psi(s) - \log r$ , where  $\Psi$  is the digamma function.

## 1.4 Monitoring the lower bound

A convergence criterion would be when there is no more significant increase in the lower bound  $\mathcal{L}$ , as defined by

$$\begin{aligned}
\mathcal{L} &= \int q(\mathbf{u}, \xi, \psi) \log \left[ \frac{p(\mathbf{y}, \mathbf{u}, \xi, \psi)}{q(\mathbf{u}, \xi, \psi)} \right] d\mathbf{u} d\xi d\psi \\
&= \mathbb{E}[\log p(\mathbf{y}, \mathbf{u}, \xi, \psi)] - \mathbb{E}[\log q(\mathbf{u}, \xi, \psi)] \\
&= \mathbb{E}[\log p(\mathbf{y}|\boldsymbol{\eta})] + \mathbb{E}[\log p(\mathbf{u})] + \mathbb{E}[\log p(\xi)] + \mathbb{E}[\log p(\psi)] \\
&\quad - \mathbb{E}[\log q(\mathbf{u})] - \mathbb{E}[\log q(\xi)] - \mathbb{E}[\log q(\psi)]
\end{aligned}$$

**Definition 1** (Differential entropy). *The differential entropy  $\mathcal{H}$  of a pdf  $p(x)$  is given by*

$$\mathcal{H}(p) = - \int p(x) \log p(x) dx = - \mathbb{E}_p[\log p(x)].$$

**Lemma 1.** *Let  $p(x)$  be the pdf of a random variable  $x$ . Then if*

(i)  *$p$  is a univariate normal distribution with mean  $\mu$  and variance  $\psi^{-1}$ ,*

$$\mathcal{H}(p) = \frac{1}{2}(1 + \log 2\pi) - \frac{1}{2} \log \psi$$

(ii)  *$p$  is a  $d$ -dimensional normal distribution with mean  $\mu$  and variance  $\Sigma$ ,*

$$\mathcal{H}(p) = \frac{d}{2}(1 + \log 2\pi) + \frac{1}{2} \log |\Sigma|$$

(iii)  $p$  is the pdf of a gamma distribution with shape  $s$  and rate  $r$ ,

$$\mathcal{H}(p) = s - \log r + \log \Gamma(s) + (1 - s)\Psi(s)$$

where  $\Psi(s) = d \log \Gamma(s) / ds = \Gamma'(s) / \Gamma(s)$  is the digamma function.

#### 1.4.1 Terms involving distributions of $\mathbf{u}$

$$\begin{aligned} \mathbb{E} [\log p(\mathbf{y}|\boldsymbol{\eta})] + \mathbb{E} [\log p(\mathbf{u})] - \mathbb{E} [\log q(\mathbf{u})] &= \mathbb{E} \left[ -\frac{n}{2} \log 2\pi + \frac{n}{2} \log \psi - \frac{\psi}{2} \|\mathbf{y} - \boldsymbol{\alpha} - \xi \mathbf{H} \mathbf{u}\|^2 \right] \\ &\quad + \mathbb{E} \left[ -\frac{n}{2} \log 2\pi + \frac{n}{2} \log \psi - \frac{\psi}{2} \|\mathbf{u}\|^2 \right] + \mathcal{H}(q(\mathbf{u})) \\ &= -\cancel{\frac{n}{2} \log 2\pi} + \frac{n}{2} \mathbb{E} [\log \psi] - \frac{\mathbb{E} \psi}{2} \mathbb{E} [\|\mathbf{y} - \boldsymbol{\alpha} - \xi \mathbf{H} \mathbf{u}\|^2] \\ &\quad - \frac{n}{2} \log 2\pi + \frac{n}{2} \mathbb{E} [\log \psi] - \frac{\mathbb{E} \psi}{2} \mathbb{E} [\|\mathbf{u}\|^2] \\ &\quad + \frac{n}{2} (1 + \log 2\pi) - \frac{1}{2} \log |\mathbf{A}| - \frac{n}{2} \log \mathbb{E} \psi \\ &= \frac{n}{2} (1 + 2 \mathbb{E} [\log \psi] - \log \mathbb{E} \psi - \log 2\pi) - r \mathbb{E} \psi - \frac{1}{2} \log |\mathbf{A}| \\ &= \frac{n}{2} (1 + 2(\Psi(s) - \log r) - \log(s/r) - \log 2\pi) - r(s/r) - \frac{1}{2} \log |\mathbf{A}| \\ &= \frac{n}{2} (1 + 2\Psi(n+1) - \log r - \log(n+1) - \log 2\pi) - \frac{1}{2} \log |\mathbf{A}| - (n+1) \end{aligned}$$

#### 1.4.2 Terms involving distribution of $q(\xi)$

$$\begin{aligned} -\mathbb{E} [\log q(\xi)] &= \mathcal{H}(q(\xi)) \\ &= \frac{1}{2} (1 + \log 2\pi) - \frac{1}{2} \log \text{tr} \left( \mathbf{H}^2 \tilde{\mathbf{U}} \right) - \frac{1}{2} \log \mathbb{E} [\psi] \end{aligned}$$

#### 1.4.3 Terms involving distribution of $q(\psi)$

$$\begin{aligned} -\mathbb{E} [\log q(\alpha)] &= \mathcal{H}(q(\psi)) \\ &= (n+1) - \log r + \log \Gamma(n+1) - n\Psi(n+1) \end{aligned}$$



## 1.5 The variational Bayes EM algorithm

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**Algorithm 1** VB-EM algorithm for the probit I-prior model

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1: procedure INITIALISE
2:    $\hat{\alpha} \leftarrow \sum_{i=1}^n y_i / n$ 
3:    $\tilde{\xi}^{(0)} \leftarrow 1$ 
4:    $\tilde{\xi}^{sq(0)} \leftarrow 1$   $\triangleright$  this is  $E[\xi^2]$ 
5:    $\tilde{\psi}^{(0)} \leftarrow 1$ 
6:    $\tilde{\mathbf{u}}^{(0)} \leftarrow \mathbf{0}_n$   $\triangleright$  or draw  $u_i^{(0)} \sim N(0, 1)$  for  $i = 1, \dots, n$ .
7: end procedure

8: procedure UPDATE FOR  $\mathbf{u}$  (time  $t$ )
9:    $\mathbf{A} \leftarrow \tilde{\xi}^{sq(t)} \mathbf{H}^2 + \mathbf{I}_n$ 
10:   $\mathbf{a} \leftarrow \tilde{\xi}^{(t)} \mathbf{H}(\mathbf{y} - \hat{\alpha})$ 
11:   $\tilde{\mathbf{u}}^{(t+1)} \leftarrow \mathbf{A}^{-1} \mathbf{a}$ 
12:   $\tilde{\mathbf{U}}^{(t+1)} \leftarrow \mathbf{A}^{-1} ((1/\tilde{\psi}^{(t)}) \mathbf{I}_n + \mathbf{a} \mathbf{a}^\top \mathbf{A}^{-1})$ 
13:   $\log \det \mathbf{A}^{(t+1)} \leftarrow \log |\mathbf{A}|$ 
14: end procedure

15: procedure UPDATE FOR  $\xi$  (time  $t$ )
16:   $c \leftarrow c^{(t+1)} \leftarrow \text{tr} \left( \mathbf{H}^2 \tilde{\mathbf{U}}^{(t+1)} \right)$ 
17:   $d \leftarrow (\mathbf{y} - \hat{\alpha})^\top \mathbf{H} \tilde{\mathbf{u}}^{(t+1)}$ 
18:   $\tilde{\xi}^{(t+1)} \leftarrow d/c$ 
19:   $\tilde{\xi}^{sq(t+1)} \leftarrow 1/(\tilde{\psi}^{(t)} c) + (d/c)^2$ 
20: end procedure

21: procedure UPDATE FOR  $\psi$  (time  $t$ )
22:   $r \leftarrow r^{(t+1)} \leftarrow \frac{1}{2} \sum_{i=1}^n (y_i - \hat{\alpha})^2 + \frac{1}{2} \text{tr} \left( (\tilde{\xi}^{sq(t+1)} \mathbf{H}^2 + \mathbf{I}_n) \tilde{\mathbf{U}}^{(t+1)} \right) - \tilde{\xi}^{(t+1)} (\mathbf{y} - \hat{\alpha})^\top \mathbf{H} \tilde{\mathbf{u}}^{(t+1)}$ 
23:   $\tilde{\psi}^{(t+1)} \leftarrow (n+1)/r$ 
24: end procedure

25: procedure CALCULATE LOWER BOUND (time  $t$ )
26:   $\mathcal{L}^{(t)} \leftarrow \frac{n+1}{2} (1 - \log r^{(t+1)} - \log(n+1)) - \frac{n-1}{2} \log 2\pi + \log \Gamma(n+1) - \frac{1}{2} (\log \det \mathbf{A}^{(t+1)} + \log c^{(t+1)})$ 
27: end procedure

28: procedure THE VB-EM ALGORITHM
29:   $t \leftarrow 0$ 
30:  while  $\mathcal{L}^{(t+1)} - \mathcal{L}^{(t)} > \delta$  or  $t < t_{max}$  do
31:    call UPDATE FOR  $\mathbf{u}$ 
32:    call UPDATE FOR  $\xi$ 
33:    call UPDATE FOR  $\psi$ 
34:    call CALCULATE LOWER BOUND
35:     $t \leftarrow t + 1$ 
36:  end while
37: end procedure

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38: return ( $\hat{\mathbf{w}}, \hat{\alpha}, \hat{\lambda}, \hat{\psi}$ )  $\leftarrow (\tilde{\mathbf{u}}^{(t)} / \tilde{\psi}^{2(t)}, \hat{\alpha}, \tilde{\xi}^{(t)} / \tilde{\psi}^{2(t)}, \tilde{\psi}^{-2(t)})$      $\triangleright$  converged parameter estimates
39: return ( $\hat{y}_1, \dots, \hat{y}_n$ )  $\leftarrow \hat{\alpha} \mathbf{1} + \hat{\lambda} \mathbf{H} \hat{\mathbf{w}}$      $\triangleright$  fitted values

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