

To-do list

1. insert scatterplot and density plot of conically truncated samples	17
2. eq:standmultilevel	28
3. Cite this with correct version.	46

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PhD thesis: ‘Regression modelling using Fisher information covariance kernels (I-priors)’

Chapter 1

Preceding chapters

Appendix A

Functional derivatives

Typically, the problem of finding the maxima of $H(p)$ in (3.6) is tackled using calculus of variations. The following is an alternative route to obtain the functional derivative of the entropy.

Definition A.1 (Directional derivative and gradient). Let $(\mathcal{H}, \langle \cdot, \cdot \rangle_{\mathcal{H}})$ be an inner product space, and consider a function $g : \mathcal{H} \rightarrow \mathbb{R}$. Denote the directional derivate of g in the direction z by $\nabla_z g$, that is,

$$\nabla_z g(x) = \lim_{\delta \rightarrow 0} \frac{g(x + \delta z) - g(x)}{\delta}.$$

The gradient of g , denoted by ∇g , is the unique vector field satisfying

$$\langle \nabla g(x), z \rangle_{\mathcal{H}} = \nabla_z g(x), \quad \forall x, z \in \mathcal{H}.$$

Definition A.2 (Functional derivative). Given a manifold M representing continuous/smooth functions ρ with certain boundary conditions, and a functional $F : M \rightarrow \mathbb{R}$, the functional derivative of $F[\rho]$ with respect to ρ , denoted $\partial F / \partial \rho$, is defined by

$$\begin{aligned} \int \frac{\partial F}{\partial \rho}(x) \phi(x) dx &= \lim_{\epsilon \rightarrow 0} \frac{F[\rho + \epsilon \phi] - F[\rho]}{\epsilon} \\ &= \left[\frac{d}{d\epsilon} F[\rho + \epsilon \phi] \right]_{\epsilon=0}, \end{aligned}$$

where ϕ is an arbitrary function. The function $\partial F/\partial \rho$ as the gradient of F at the point ρ , and

$$\partial F(\rho, \phi) = \int \frac{\partial F}{\partial \rho}(x) \phi(x) dx$$

as the directional derivative at point ρ in the direction of ϕ . Analogous to vector calculus, the inner product with the gradient gives the directional derivative.

Example A.1 (Functional derivative of entropy). Let X be a discrete random variable with probability mass function $p(x) \geq 0$, for $\forall x \in \Omega$, a finite set. The entropy is a functional of p , namely

$$\mathcal{E}[p] = - \sum_{x \in \Omega} p(x) \log p(x).$$

Equivalently, using the counting measure ν on Ω , we can write

$$\mathcal{E}[p] = - \int_{\Omega} p(x) \log p(x) d\nu(x).$$

$$\begin{aligned} \int_{\Omega} \frac{\partial \mathcal{E}}{\partial p}(x) \phi(x) dx &= \left[\frac{d}{d\epsilon} \mathcal{E}[p + \epsilon \phi] \right]_{\epsilon=0} \\ &= \left[- \frac{d}{d\epsilon} (p(x) + \epsilon \phi(x)) \log (p(x) + \epsilon \phi(x)) \right]_{\epsilon=0} \\ &= - \int_{\Omega} \left(\frac{p(x) \phi(x)}{p(x) + \epsilon \phi(x)} + \frac{\epsilon \phi(x)}{p(x) + \epsilon \phi(x)} + \phi(x) \log (p(x) + \epsilon \phi(x)) \right) dx \\ &= - \int_{\Omega} (1 + \log p(x)) \phi(x) dx. \end{aligned}$$

Thus, $(\partial \mathcal{E}/\partial p)(x) = -1 - \log p(x)$.

Appendix B

Kronecker product and vectorisation

The Kronecker product crops up in the definition of matrix normal distributions, which is used in [Chapter 5](#) for the I-probit model.

def:kroneck
erprod

Definition B.1 (Kronecker product). The Kronecker matrix product, denoted by \otimes , for two matrices $A \in \mathbb{R}^{n \times m}$ and $B \in \mathbb{R}^{p \times q}$ is defined by

$$A \otimes B = \begin{pmatrix} A_{11}B & A_{12}B & \cdots & A_{1m}B \\ A_{21}B & A_{22}B & \cdots & A_{2m}B \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1}B & A_{n2}B & \cdots & A_{nm}B \end{pmatrix} \in \mathbb{R}^{np \times mq}.$$

The Kronecker product is a generalisation of the outer product for vectors to matrices. Of use will be these properties of the Kronecker product ([Zhang and Ding, 2013](#)):

- **Bilinearity and associativity.** For appropriately sized matrices A , B and C , and a scalar λ ,

$$A \otimes (B + C) = A \otimes B + A \otimes C$$

$$(A + B) \otimes C = A \otimes C + B \otimes C$$

$$\lambda A \otimes B = A \otimes \lambda B = \lambda(A \otimes B)$$

$$(A \otimes B) \otimes C = A \otimes (B \otimes C)$$

- **Non-commutative.** In general, $A \otimes B \neq B \otimes A$, but they are *permutation equivalent*, i.e. $A \otimes B \neq P(B \otimes A)Q$ for some permutation matrices P and Q .
- **The mixed product property.** $(A \otimes B)(C \otimes D) = AC \otimes BD$.
- **Inverse.** $A \otimes B$ is invertible if and only if A and B are both invertible, and $(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$.
- **Transpose.** $(A \otimes B)^\top = A^\top \otimes B^\top$.
- **Determinant.** If A is $n \times n$ and B is $m \times m$, then $|A \otimes B| = |A|^m |B|^n$. Note that the exponent of $|A|$ is the order of B and vice versa.
- **Trace.** Suppose A and B are square matrices. Then $\text{tr}(A \otimes B) = \text{tr } A \text{tr } B$.
- **Rank.** $\text{rank}(A \otimes B) = \text{rank } A \text{rank } B$.
- **Matrix equations.** $AXB = C \Leftrightarrow (B^\top \otimes A) \text{vec } X = \text{vec}(AXB) = \text{vec } C$.

The equivalence between matrix normal and multivariate normal distributions are established making use of vectorisation for matrices. This is defined below.

Definition B.2. The vectorisation operation ‘vec’ stacks the columns of the matrices into one long vector, for instance, for the matrix $A \in \mathbb{R}^{n \times m}$

$$\text{vec } A = (A_{11}, \dots, A_{n1}, A_{12}, \dots, A_{n2}, \dots, A_{1m}, \dots, A_{nm})^\top \in \mathbb{R}^{nm}.$$

def:vectori
sation

Appendix C

Statistical distributions and their properties

This is a reference relating to the multivariate normal, matrix normal, truncated univariate and multivariate normal, which are collated from various sources for convenience. Of interest are probability density functions, first and second moments, and entropy ([Definition 3.5](#), page 19).

C.1 Multivariate normal distribution

Let $X \in \mathbb{R}^d$ be distributed according to a multivariate normal (Gaussian) distribution with mean $\mu \in \mathbb{R}^d$ and covariance matrix $\Sigma \in \mathbb{R}^d$ (a square, symmetric, positive-definite matrix). We say that $X \sim N_d(\mu, \Sigma)$. Then,

- **Pdf.** $p(X|\mu, \Sigma) = (2\pi)^{-d/2} |\Sigma|^{-1/2} \exp\left(-\frac{1}{2}(X - \mu)^\top \Sigma^{-1}(X - \mu)\right)$.
- **Moments.** $E X = \mu$, $E[XX^\top] = \Sigma + \mu\mu^\top$.
- **Entropy.** $H(p) = \frac{1}{2} \log|2\pi e \Sigma| = \frac{d}{2}(1 + \log 2\pi) + \frac{1}{2} \log|\Sigma|$.

Lemma C.1 (Properties of multivariate normal). *Assume that $X \sim N_d(\mu, \Sigma)$ and $Y \sim N_d(\nu, \Psi)$, where*

$$X = \begin{pmatrix} X_a \\ X_b \end{pmatrix}, \quad \mu = \begin{pmatrix} \mu_a \\ \mu_b \end{pmatrix}, \quad \text{and} \quad \Sigma = \begin{pmatrix} \Sigma_a & \Sigma_{ab} \\ \Sigma_{ab}^\top & \Sigma_b \end{pmatrix}.$$

apx:fisherm
ultinormal

Then,

- **Marginal distributions.**

$$X_a \sim N_{\dim X_a}(\mu_a, \Sigma_a) \quad \text{and} \quad X_b \sim N_{\dim X_b}(\mu_b, \Sigma_b).$$

- **Conditional distributions.**

$$X_a|X_b \sim N_{\dim X_a}(\tilde{\mu}_a, \tilde{\Sigma}_a) \quad \text{and} \quad X_b \sim N_{\dim X_b}(\tilde{\mu}_b, \tilde{\Sigma}_b),$$

where

$$\begin{aligned} \tilde{\mu}_a &= \mu_a + \Sigma_{ab}\Sigma_b^{-1}(X_b - \mu_b) & \tilde{\mu}_b &= \mu_b + \Sigma_{ab}^\top\Sigma_a^{-1}(X_a - \mu_a) \\ \tilde{\Sigma}_a &= \Sigma_a - \Sigma_{ab}\Sigma_b^{-1}\Sigma_{ab}^\top & \tilde{\Sigma}_b &= \Sigma_b - \Sigma_{ab}^\top\Sigma_a^{-1}\Sigma_{ab} \end{aligned}$$

- **Linear combinations.**

$$AX + BY + C \sim N_d(A\mu + B\nu + C, A\Sigma A^\top + B\Psi B^\top)$$

where A and B are appropriately sized matrices, and $C \in \mathbb{R}^d$.

- **Product of Gaussian densities.**

$$p(X|\mu, \Sigma)p(Y|\nu, \Psi) \propto p(Z|m, S)$$

where $p(Z)$ is a Gaussian density, $m = S(\Sigma^{-1}\mu + \Psi^{-1}\nu)$ and $S = (\Sigma^{-1} + \Psi^{-1})^{-1}$.
The normalising constant is equal to the density of $\mu \sim N(\nu, \Sigma + \Psi)$.

Proof. Omitted—see [Petersen and Pedersen \(2008, §8\)](#). □

Frequently, in Bayesian statistics especially, the following identities will be useful in deriving posterior distributions involving multivariate normals.

Lemma C.2. Let $x, b \in \mathbb{R}^d$ be a vector, $X, B \in \mathbb{R}^{n \times d}$ a matrix, and $A \in \mathbb{R}^{d \times d}$ a symmetric, invertible matrix. Then,

$$\begin{aligned} -\frac{1}{2}x^\top Ax + b^\top x &= -\frac{1}{2}(x - A^{-1}b)^\top A(x - A^{-1}b) + \frac{1}{2}b^\top A^{-1}b \\ -\frac{1}{2}\text{tr}(X^\top AX) + \text{tr}(B^\top X) &= -\frac{1}{2}\text{tr}((X - A^{-1}B)^\top A(X - A^{-1}B)) + \frac{1}{2}\text{tr}(B^\top A^{-1}B). \end{aligned}$$

Proof. Omitted—see [Petersen and Pedersen \(2008, §8.1.6\)](#). \square

Lemma C.3. Let $X \sim N_p(\mu_\theta, \Sigma_\theta)$, that is, the mean vector μ_θ and covariance matrix Σ_θ depends on a real, q -dimensional vector θ . The Fisher information matrix $U \in \mathbb{R}^{q \times q}$ for θ has (i, j) entries given by

$$U_{ij} = \frac{\partial \mu_\theta^\top}{\partial \theta_i} \Sigma_\theta^{-1} \frac{\partial \mu_\theta}{\partial \theta_j} + \frac{1}{2} \text{tr} \left(\Sigma_\theta^{-1} \frac{\partial \Sigma_\theta}{\partial \theta_i} \Sigma_\theta^{-1} \frac{\partial \Sigma_\theta}{\partial \theta_j} \right) \quad (\text{C.1})$$

for $i, j = 1, \dots, q$.

Proof. Define the derivative of a matrix $\Sigma \in \mathbb{R}^{p \times p}$ with respect to a scalar z , denoted $\partial \Sigma / \partial z \in \mathbb{R}^{p \times p}$, by $(\partial \Sigma / \partial z)_{ij} = \partial \Sigma_{ij} / \partial z$, i.e. derivatives are taken element-wise. The two identities below are useful:

$$\frac{\partial}{\partial z} \text{tr} \Sigma = \text{tr} \frac{\partial \Sigma}{\partial z} \quad (\text{C.2})$$

$$\frac{\partial}{\partial z} \log |\Sigma| = \text{tr} \left(\Sigma^{-1} \frac{\partial \Sigma}{\partial z} \right) \quad (\text{C.3})$$

$$\frac{\partial \Sigma^{-1}}{\partial z} = -\Sigma^{-1} \frac{\partial \Sigma}{\partial z} \Sigma^{-1} \quad (\text{C.4})$$

A useful reference for these identities is [Petersen and Pedersen \(2008\)](#).

Differentiating the log-likelihood for θ with respect to the i 'th component of θ yields

$$\begin{aligned} \frac{\partial}{\partial \theta_i} L(\theta|X) &= -\frac{1}{2} \frac{\partial}{\partial \theta_i} \log |\Sigma_\theta| - \frac{1}{2} \frac{\partial}{\partial \theta_i} \text{tr}(\Sigma_\theta^{-1} (X - \mu_\theta)(X - \mu_\theta)^\top) \\ &= -\frac{1}{2} \text{tr} \left(\Sigma_\theta^{-1} \frac{\partial \Sigma_\theta}{\partial \theta_i} \right) - \frac{1}{2} \text{tr} \left(\frac{\partial \Sigma_\theta^{-1}}{\partial \theta_i} (X - \mu_\theta)(X - \mu_\theta)^\top \right) \\ &\quad - \frac{1}{2} \text{tr} \left(\Sigma_\theta^{-1} \frac{\partial}{\partial \theta_i} ((X - \mu_\theta)(X - \mu_\theta)^\top) \right) \\ &= \underbrace{-\frac{1}{2} \text{tr} \left(\Sigma_\theta^{-1} \frac{\partial \Sigma_\theta}{\partial \theta_i} \right)}_{(A)} - \underbrace{\frac{1}{2} \text{tr} \left(\Sigma_\theta^{-1} \frac{\partial \Sigma_\theta}{\partial \theta_i} \Sigma_\theta^{-1} (X - \mu_\theta)(X - \mu_\theta)^\top \right)}_{(B)} \\ &\quad + \underbrace{\text{tr} \left(\Sigma_\theta^{-1} (X - \mu_\theta) \frac{\partial \mu_\theta^\top}{\partial \theta_i} \right)}_{(C)}. \end{aligned}$$

Taking derivatives again, this time with respect to θ_j , of the three parts (A), (B) and (C) above, we get:

• (A)

$$\frac{1}{2} \frac{\partial}{\partial \theta_j} \text{tr} \left(\Sigma_\theta^{-1} \frac{\partial \Sigma_\theta}{\partial \theta_i} \right) = \frac{1}{2} \text{tr} \left(\frac{\partial \Sigma_\theta^{-1}}{\partial \theta_j} \frac{\partial \Sigma_\theta}{\partial \theta_i} + \Sigma_\theta^{-1} \frac{\partial^2 \Sigma_\theta}{\partial \theta_i \partial \theta_j} \right)$$

• (B)

$$\begin{aligned} & \frac{1}{2} \frac{\partial}{\partial \theta_j} \text{tr} \left(\Sigma_\theta^{-1} \frac{\partial \Sigma_\theta}{\partial \theta_i} \Sigma_\theta^{-1} (X - \mu_\theta)(X - \mu_\theta)^\top \right) \\ &= \frac{1}{2} \text{tr} \left(\frac{\partial \Sigma_\theta^{-1}}{\partial \theta_j} \frac{\partial \Sigma_\theta}{\partial \theta_i} \Sigma_\theta^{-1} (X - \mu_\theta)(X - \mu_\theta)^\top \right) \\ & \quad + \frac{1}{2} \text{tr} \left(\Sigma_\theta^{-1} \frac{\partial^2 \Sigma_\theta}{\partial \theta_i \partial \theta_j} \Sigma_\theta^{-1} (X - \mu_\theta)(X - \mu_\theta)^\top \right) \\ & \quad + \frac{1}{2} \text{tr} \left(\Sigma_\theta^{-1} \frac{\partial \Sigma_\theta}{\partial \theta_i} \frac{\partial \Sigma_\theta^{-1}}{\partial \theta_j} (X - \mu_\theta)(X - \mu_\theta)^\top \right) \\ & \quad - \text{tr} \left(\Sigma_\theta^{-1} \frac{\partial \Sigma_\theta}{\partial \theta_i} \Sigma_\theta^{-1} \frac{\partial \mu_\theta}{\partial \theta_j} (X - \mu_\theta)^\top \right) \end{aligned}$$

• (C)

$$\begin{aligned} \frac{\partial}{\partial \theta_j} \text{tr} \left(\Sigma_\theta^{-1} (X - \mu_\theta) \frac{\partial \mu_\theta^\top}{\partial \theta_i} \right) &= \text{tr} \left(\frac{\partial \Sigma_\theta^{-1}}{\partial \theta_j} (X - \mu_\theta) \frac{\partial \mu_\theta^\top}{\partial \theta_i} - \Sigma_\theta^{-1} \frac{\partial \mu_\theta}{\partial \theta_j} \frac{\partial \mu_\theta^\top}{\partial \theta_i} \right. \\ & \quad \left. - \Sigma_\theta^{-1} (X - \mu_\theta) \frac{\partial^2 \mu_\theta}{\partial \theta_i \partial \theta_j} \right) \end{aligned}$$

The Fisher information matrix U contains (i, j) entries equal to the expectation of $-\frac{\partial^2}{\partial \theta_i \partial \theta_j} L(\theta|X)$. Using the fact that 1) $E[X - \mu_\theta] = 0$; 2) $E[\text{tr} \Sigma] = \text{tr}(E \Sigma)$; 3) $E[XX^\top] = \Sigma_\theta$; and 4) the trace is invariant under cyclic permutations, we get

$$\begin{aligned} U_{ij} &= \text{tr} \left(\Sigma_\theta^{-1} \frac{\partial \mu_\theta}{\partial \theta_j} \frac{\partial \mu_\theta^\top}{\partial \theta_i} \right) \\ & \quad + \frac{1}{2} \text{tr} \left(\cancel{\frac{\partial \Sigma_\theta^{-1}}{\partial \theta_j} \frac{\partial \Sigma_\theta}{\partial \theta_i}} + \cancel{\Sigma_\theta^{-1} \frac{\partial^2 \Sigma_\theta}{\partial \theta_i \partial \theta_j}} - \cancel{\frac{\partial \Sigma_\theta^{-1}}{\partial \theta_j} \frac{\partial \Sigma_\theta}{\partial \theta_i}} - \cancel{\Sigma_\theta^{-1} \frac{\partial^2 \Sigma_\theta}{\partial \theta_i \partial \theta_j}} - \frac{\partial \Sigma_\theta}{\partial \theta_i} \frac{\partial \Sigma_\theta^{-1}}{\partial \theta_j} \right) \\ &= \frac{\partial \mu_\theta^\top}{\partial \theta_i} \Sigma_\theta^{-1} \frac{\partial \mu_\theta}{\partial \theta_j} + \frac{1}{2} \text{tr} \left(\Sigma_\theta^{-1} \frac{\partial \Sigma_\theta}{\partial \theta_i} \Sigma_\theta^{-1} \frac{\partial \Sigma_\theta}{\partial \theta_j} \right) \end{aligned}$$

as required. □

C.2 Matrix normal distribution

The matrix normal distribution is an extension of the Gaussian distribution to matrices. Let $X \in \mathbb{R}^{n \times m}$ matrix, and let X follow a matrix normal distribution with mean $\mu \in \mathbb{R}^{n \times m}$ and row and column variances $\Sigma \in \mathbb{R}^{n \times n}$ and $\Psi \in \mathbb{R}^{m \times m}$ respectively, which we denote by $X \sim \text{MN}_{n,m}(\mu, \Sigma, \Psi)$. Then,

- **Pdf.** $p(X|\mu, \Sigma, \Psi) = (2\pi)^{-nm/2} |\Sigma|^{-m/2} |\Psi|^{-n/2} e^{-\frac{1}{2} \text{tr}(\Psi^{-1}(X-\mu)^\top \Sigma^{-1}(X-\mu))}$.
- **Moments.** $\mathbb{E} X = \mu$, $\text{Var}(X_{i.}) = \Psi$ for $i = 1, \dots, n$, and $\text{Var}(X_{.j}) = \Sigma$ for $j = 1, \dots, m$.
- **Entropy.** $H(p) = \frac{1}{2} \log |2\pi e(\Psi \otimes \Sigma)| = \frac{nm}{2} (1 + \log 2\pi) + \frac{1}{2} \log |\Sigma|^m |\Psi|^n$.

In the above, ' \otimes ' denotes the Kronecker matrix product defined by

$$\Psi \otimes \Sigma = \begin{pmatrix} \Psi_{11}\Sigma & \Psi_{12}\Sigma & \cdots & \Psi_{1m}\Sigma \\ \Psi_{21}\Sigma & \Psi_{22}\Sigma & \cdots & \Psi_{2m}\Sigma \\ \vdots & \vdots & \ddots & \vdots \\ \Psi_{m1}\Sigma & \Psi_{m2}\Sigma & \cdots & \Psi_{mm}\Sigma \end{pmatrix} \in \mathbb{R}^{nm \times nm}.$$

Of use will be these properties of the Kronecker product ([Zhang and Ding, 2013](#)).

- **Bilinearity and associativity.** For appropriately sized matrices A , B and C , and a scalar λ ,

$$\begin{aligned} A \otimes (B + C) &= A \otimes B + A \otimes C \\ (A + B) \otimes C &= A \otimes C + B \otimes C \\ \lambda A \otimes B &= A \otimes \lambda B = \lambda(A \otimes B) \\ (A \otimes B) \otimes C &= A \otimes (B \otimes C) \end{aligned}$$

- **Non-commutative.** In general, $A \otimes B \neq B \otimes A$, but they are *permutation equivalent*, i.e. $A \otimes B \neq P(B \otimes A)Q$ for some permutation matrices P and Q .
- **The mixed product property.** $(A \otimes B)(C \otimes D) = AC \otimes BD$.
- **Inverse.** $A \otimes B$ is invertible if and only if A and B are both invertible, and $(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$.
- **Transpose.** $(A \otimes B)^\top = A^\top \otimes B^\top$.

- **Determinant.** If A is $n \times n$ and B is $m \times m$, then $|A \otimes B| = |A|^m |B|^n$. Note that the exponent of $|A|$ is the order of B and vice versa.
- **Trace.** Suppose A and B are square matrices. Then $\text{tr}(A \otimes B) = \text{tr } A \text{tr } B$.
- **Rank.** $\text{rank}(A \otimes B) = \text{rank } A \text{rank } B$.
- **Matrix equations.** $AXB = C \Leftrightarrow (B^\top \otimes A) \text{vec } X = \text{vec}(AXB) = \text{vec } C$.

The vectorisation operation ‘vec’ stacks the columns of the matrices into one long vector, for instance,

$$\text{vec } \Psi = (\Psi_{11}, \dots, \Psi_{m1}, \Psi_{12}, \dots, \Psi_{m2}, \dots, \Psi_{1m}, \dots, \Psi_{mm})^\top \in \mathbb{R}^{m \times m}.$$

Lemma C.4 (Equivalence between matrix and multivariate normal). $X \sim \text{MN}_{n,m}(\mu, \Sigma, \Psi)$ if and only if $\text{vec } X \sim \text{N}_{nm}(\text{vec } \mu, \Psi \otimes \Sigma)$.

Proof. In the exponent of the matrix normal pdf, we have

$$\begin{aligned} -\frac{1}{2} \text{tr}(\Psi^{-1}(X - \mu)^\top \Sigma^{-1}(X - \mu)) \\ &= -\frac{1}{2} \text{vec}(X - \mu)^\top \text{vec}(\Sigma^{-1}(X - \mu) \Psi^{-1}) \\ &= -\frac{1}{2} \text{vec}(X - \mu)^\top (\Psi^{-1} \otimes \Sigma^{-1}) \text{vec}(X - \mu) \\ &= -\frac{1}{2} (\text{vec } X - \text{vec } \mu)^\top (\Psi \otimes \Sigma)^{-1} (\text{vec } X - \text{vec } \mu). \end{aligned}$$

Also, $|\Sigma|^{-m/2} |\Psi|^{-n/2} = |\Psi \otimes \Sigma|^{-1/2}$. This converts the matrix normal pdf to that of a multivariate normal pdf. \square

Some useful properties of the matrix normal distribution are listed:

- **Expected values.**

$$\begin{aligned} \text{E}(X - \mu)(X - \mu)^\top &= \text{tr}(\Psi) \Sigma \in \mathbb{R}^{n \times n} \\ \text{E}(X - \mu)^\top (X - \mu) &= \text{tr}(\Sigma) \Psi \in \mathbb{R}^{m \times m} \\ \text{E } X A X^\top &= \text{tr}(A^\top \Psi) \Sigma + \mu A \mu^\top \\ \text{E } X^\top B X &= \text{tr}(\Sigma B^\top) \Psi + \mu^\top B \mu \\ \text{E } X C X &= \Sigma C^\top \Psi + \mu C \mu \end{aligned}$$

- **Transpose.** $X^\top \sim \text{MN}_{m,n}(\mu^\top, \Psi, \Sigma)$.
- **Linear transformation.** Let $A \in \mathbb{R}^{a \times n}$ be of full-rank $a \leq n$ and $B \in \mathbb{R}^{m \times b}$ be of full-rank $b \leq m$. Then $AXB \sim \text{MN}_{a,b}(\mu^\top, A\Sigma A^\top, B^\top \Psi B)$.
- **Iid.** If $X_i \stackrel{\text{iid}}{\sim} \text{N}_m(\mu, \Psi)$ for $i = 1, \dots, n$, and we arranged these vectors row-wise into the matrix $X = (X_1^\top, \dots, X_n^\top)^\top \in \mathbb{R}^{n \times m}$, then $X \sim \text{MN}(1_n \mu^\top, I_n, \Psi)$.

C.3 Truncated univariate normal distribution

Let $X \sim \text{N}(\mu, \sigma^2)$ with the random variable X restricted to the interval $(a, b) \subset \mathbb{R}$. Then we say that X follows a truncated normal distribution, and we denote this by $X \sim {}^t\text{N}(\mu, \sigma^2, a, b)$. Let $\alpha = (a - \mu)/\sigma$, $\beta = (b - \mu)/\sigma$, and $C = \Phi(\beta) - \Phi(\alpha)$. Then,

- **Pdf.** $p(X|\mu, \sigma, a, b) = C^{-1}(2\pi\sigma^2)^{-1/2}e^{-\frac{1}{2\sigma^2}(X-\mu)^2} = \sigma C^{-1}\phi(\frac{X-\mu}{\sigma})$.
- **Moments.**

$$\begin{aligned} \text{E } X &= \mu + \sigma \frac{\phi(\alpha) - \phi(\beta)}{C} \\ \text{E } X^2 &= \sigma^2 + \mu^2 + \sigma^2 \frac{\alpha\phi(\alpha) - \beta\phi(\beta)}{C} + 2\mu\sigma \frac{\phi(\alpha) - \phi(\beta)}{C} \\ \text{Var } X &= \sigma^2 \left[1 + \frac{\alpha\phi(\alpha) - \beta\phi(\beta)}{C} - \left(\frac{\phi(\alpha) - \phi(\beta)}{C} \right)^2 \right] \end{aligned}$$

- **Entropy.**

$$\begin{aligned} H(p) &= \frac{1}{2} \log 2\pi e \sigma^2 + \log C + \frac{\alpha\phi(\alpha) - \beta\phi(\beta)}{2C} \\ &= \frac{1}{2} \log 2\pi e \sigma^2 + \log C + \frac{1}{2\sigma^2} \cdot \overbrace{\sigma^2 \frac{\alpha\phi(\alpha) - \beta\phi(\beta)}{C}}^{\text{Var } X - \sigma^2 + (\text{E } X - \mu)^2} \\ &= \frac{1}{2} \log 2\pi \sigma^2 + \log C + \frac{1}{2\sigma^2} \text{E}[X - \mu]^2 \end{aligned}$$

$$\text{because } \text{Var } X + (\text{E } X - \mu)^2 = \text{E } X^2 - (\text{E } X)^2 + (\text{E } X)^2 + \mu^2 - 2\mu \text{E } X.$$

For binary probit models, the distributions that come up are one-sided truncations at zero, i.e. ${}^t\text{N}(\mu, \sigma^2, 0, +\infty)$ (upper tail/positive part) and ${}^t\text{N}(\mu, \sigma^2, -\infty, 0)$ (lower tail/negative part), for which their moments are of interest. As an aside, if $\mu = 0$ then the truncation ${}^t\text{N}(0, \sigma^2, 0, +\infty)$ is called the *half-normal* distribution. For the positive

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one-sided truncation at zero, $C = \Phi(+\infty) - \Phi(-\mu/\sigma) = 1 - \Phi(-\mu/\sigma) = \Phi(\mu/\sigma)$, and for the negative one-sided truncation at zero, $C = \Phi(-\mu/\sigma) - \Phi(-\infty) = 1 - \Phi(\mu/\sigma)$.

One may simulate random draws from a truncated normal distribution by drawing from $N(\mu, \sigma^2)$ and discarding samples that fall outside (a, b) . Alternatively, the inverse-transform method using

$$X = \mu + \sigma \Phi^{-1}(\Phi(\alpha) + UC)$$

with $U \sim \text{Unif}(0, 1)$ will work too. Either of these methods will work reasonably well as long as the truncation region is not too far away from μ , but neither is particularly fast. Efficient algorithms have been explored which are along the lines of either accept/reject algorithms (Robert, 1995), Gibbs sampling (Damien and Walker, 2001), or pseudo-random number generation algorithms (Chopin, 2011). The latter algorithm is inspired by the Ziggurat algorithm (Marsaglia and Tsang, 2000) which is considered to be the fastest Gaussian random number generator.

C.4 Truncated multivariate normal distribution

Consider the restriction of $X \sim N_d(\mu, \Sigma)$ to a convex subset¹ $\mathcal{A} \subset \mathbb{R}^d$. Call this distribution the truncated multivariate normal distribution, and denote it $X \sim {}^tN_d(\mu, \Sigma, \mathcal{A})$. The pdf is $p(X|\mu, \Sigma, \mathcal{A}) = C^{-1}\phi(X|\mu, \Sigma) \mathbb{1}[X \in \mathcal{A}]$, where

$$C = \int_{\mathcal{A}} \phi(x|\mu, \Sigma) dx = P(X \in \mathcal{A}).$$

Generally speaking, there are no closed-form expressions for $Eg(X)$ for any well-defined functions g on X . One strategy to obtain values such as EX (mean), EX^2 (second moment) and $E \log p(X)$ (entropy) would be Monte Carlo integration. If $X^{(1)}, \dots, X^{(T)}$ are samples from $X \sim {}^tN_d(\mu, \Sigma, \mathcal{A})$, then $\widehat{Eg(X)} = \frac{1}{T} \sum_{i=1}^T g(X^{(i)})$.

Sampling from a truncated multivariate normal distribution is described by Robert (1995), who used a Gibbs-based approach, which we now describe. Assume that the one-dimensional slices of \mathcal{A}

$$\mathcal{A}_k(X_{-j}) = \{X_j | (X_1, \dots, X_{j-1}, X_j, X_{j+1}, \dots, X_d) \in \mathcal{A}\}$$

¹A convex subset is a subset of a space that is closed under convex combinations. In Euclidean space, for every pair of points in a convex set, all the points that lie on the straight line segment which joins the pair of points are also in the set.

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are readily available so that the bounds or anti-truncation region of X_j given the rest of the components X_{-j} are known to be (x_j^-, x_j^+) . Using properties of the normal distribution, the full conditionals of X_j given X_{-j} is

$$\begin{aligned} X_j | X_{-j} &\sim {}^t\text{N}(\tilde{\mu}_j, \tilde{\sigma}_j^2, x_j^-, x_j^+) \\ \tilde{\mu}_j &= \mu_j + \Sigma_{j,-j}^\top \Sigma_{-j,-j} (x_{-j} - \mu_{-j}) \\ \tilde{\sigma}_j^2 &= \Sigma_{11} - \Sigma_{j,-j}^\top \Sigma_{-j,-j} \Sigma_{j,-j}. \end{aligned}$$

According to [Robert \(1995\)](#), if $\Psi = \Sigma^{-1}$, then

$$\Sigma_{-j,-j}^{-1} = \Psi_{-j,-j} - \Psi_{j,-j} \Psi_{-j,-j}^\top / \Psi_{jj}$$

which means that we need only compute one global inverse Σ^{-1} . Therefore, the Gibbs sampler makes draws from truncated normal distributions in the following sequence, given initial values $X^{(0)}$:

- Draw $X_1^{(t)} | X_2^{(t)}, \dots, X_d^{(t)} \sim {}^t\text{N}(\tilde{\mu}_1, \tilde{\sigma}_1^2, x_1^-, x_1^+)$.
- Draw $X_2^{(t)} | X_1^{(t+1)}, X_3^{(t)}, \dots, X_d^{(t)} \sim {}^t\text{N}(\tilde{\mu}_2, \tilde{\sigma}_2^2, x_2^-, x_2^+)$.
- ...
- Draw $X_d^{(t)} | X_1^{(t+1)}, \dots, X_{d-1}^{(t+1)} \sim {}^t\text{N}(\tilde{\mu}_d, \tilde{\sigma}_d^2, x_d^-, x_d^+)$.

In a later work, [Damien and Walker \(2001\)](#) introduce a latent variable $Y \in \mathbb{R}$ such that the joint pdf of X and Y is

$$p(X_1, \dots, X_d, Y) \propto \exp(-Y/2) \mathbb{1}[y > (x - \mu)^\top \Sigma^{-1}(x - \mu)] \mathbb{1}[X \in \mathcal{A}].$$

Now, the Gibbs conditional densities for the X_k 's are given by

$$p(X_j | X_{-j}, Y) \propto \mathbb{1}[X_j \in \mathcal{B}_j]$$

where

$$\mathcal{B}_j \in (x_j^-, x_j^+) \cap \{X_j | (X - \mu)^\top \Sigma^{-1}(X - \mu) < Y\}.$$

Thus, given values for X_{-j} and Y , the bounds for X_j involves solving a quadratic equation in X_j . The Gibbs conditional density for $Y | X$ is a shifted exponential distribution, which can be sampled using the inverse-transform method. Thus, both X and Y can be sampled directly from uniform variates.

For probit models, we are interested in the conical truncations $\mathcal{C}_j = \{X_j > X_k | k \neq j, \text{ and } k = 1, \dots, m\}$ for which the j 'th component of X is largest. These truncations form cones in d -dimensional space such that $\mathcal{C}_1 \cup \dots \cup \mathcal{C}_d = \mathbb{R}^d$, and hence the name.

insert scatterplot and density plot of conically truncated samples

In the case where Σ is a diagonal matrix, the conically truncated multivariate normal distributions are easier to deal with due to the independence structure in the covariance matrix. In particular, most calculations of interest involve only a one dimensional integral of products of normal cdfs. We present some results that we have not previously seen before elsewhere.

Lemma C.5. Let $X \sim {}^t\text{N}_d(\mu, \Sigma, \mathcal{C}_j)$, with $\mu = (\mu_1, \dots, \mu_d)^\top$ and $\Sigma = \text{diag}(\sigma_1^2, \dots, \sigma_d^2)$, and $\mathcal{C}_j = \{X_j > X_k | k \neq j, \text{ and } k = 1, \dots, m\}$ a conical truncation of \mathbb{R}^d such that the j 'th component is largest. Then,

(i) **Pdf.** The pdf of X has the following functional form:

$$p(X) = \frac{C^{-1}}{\sigma_1 \dots \sigma_d (2\pi)^{d/2}} \exp \left[-\frac{1}{2} \sum_{i=1}^d \left(\frac{x_i - \mu_i}{\sigma_i} \right)^2 \right]$$

where ϕ is the pdf of a standard normal distribution and

$$C = \text{E}_Z \left[\prod_{\substack{i=1 \\ i \neq j}}^d \Phi \left(\frac{\sigma_j}{\sigma_i} Z + \frac{\mu_j - \mu_i}{\sigma_i} \right) \right]$$

where $Z \sim \text{N}(0, 1)$.

(ii) **Moments.** The expectation $\text{E} X = (\text{E} X_1, \dots, \text{E} X_d)^\top$ is given by

$$\text{E} X_i = \begin{cases} \mu_i - \sigma_i C^{-1} \text{E}_Z \left[\phi_i \prod_{k \neq i, j} \Phi_k \right] & \text{if } i \neq j \\ \mu_j - \sigma_j \sum_{i \neq j} (\text{E} X_i - \mu_i) & \text{if } i = j \end{cases}$$

and the second moments $\text{E}[X - \mu]^2$ are given by

$$\text{E}[X_i - \mu_i]^2 = \begin{cases} \sigma_i^2 + (\mu_j - \mu_i)(\text{E} X_i - \mu_i) + \sigma_i \sigma_j C^{-1} \text{E}_Z \left[Z \phi_i \prod_{k \neq i, j} \Phi_k \right] & \text{if } i \neq j \\ C^{-1} \sigma_j^2 \text{E}_Z \left[Z^2 \prod_{k \neq j} \Phi_k \right] & \text{if } i = j \end{cases}$$

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where we had defined

$$\phi_i = \phi_i(Z) = \phi\left(\frac{\sigma_j Z + \mu_j - \mu_i}{\sigma_i}\right), \text{ and}$$

$$\Phi_i = \Phi_i(Z) = \Phi\left(\frac{\sigma_j Z + \mu_j - \mu_i}{\sigma_i}\right).$$

(iii) **Entropy.** The entropy is given by

$$H(p) = \log C + \frac{d}{2} \log 2\pi + \frac{1}{2} \sum_{i=1}^d \log \sigma_i^2 + \frac{1}{2} \sum_{i=1}^d \frac{1}{\sigma_i^2} \mathbb{E}[x_i - \mu_i]^2.$$

Proof. See [Appendix D](#) for the proof. □

C.5 Gamma distribution

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For $X \in \mathbb{R}^+$, let X be distributed according to the gamma distribution with shape s and rate r , denoted $X \sim \Gamma(s, r)$. Then,

- **Pdf.** $p(X) = \Gamma(s)^{-1} r^s X^{s-1} e^{-rX}$.
- **Moments.** $\mathbb{E} X = s/r$, $\text{Var } X = s/r^2$.
- **Entropy.** $H(p) = s - \log r + \log \Gamma(s) + (1-s)\psi(s)$.

In the above, $\Gamma(\cdot) = \Gamma_1(\cdot)$ and $\psi(\cdot) = \psi_1(\cdot)$ are the gamma and digamma functions, defined by

$$\Gamma(a) = \begin{cases} (a-1)! & \text{if } a \in \mathbb{Z}^+ \\ \int_0^\infty u^{a-1} e^{-u} du & \text{otherwise} \end{cases}$$

and

$$\psi(a) = \frac{\partial}{\partial a} \log \Gamma(a) = \frac{\partial \Gamma(a) / \partial a}{\Gamma(a)}.$$

Often, the gamma distribution is parameterised according to shape s and scale $\sigma = 1/r$ parameters, $X \sim \Gamma(s, \sigma)$.

C.6 Inverse gamma distribution

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For $X \in \mathbb{R}^+$, a random variable X distributed according to an inverse gamma distribution with parameters s (shape) and σ (scale) is denoted by $X \sim \Gamma^{-1}(s, \sigma)$. Then,

- **Pdf.** $p(X) = \Gamma(s)^{-1} \sigma^s X^{-(s+1)} e^{-\sigma/X}$.
- **Moments.** $E X = \sigma/(s-1)$, $\text{Var } X = \sigma^2((s-1)^2(s-2))^{-1}$.
- **Entropy.** $H(p) = s + \log(\sigma \Gamma(s)) - (1+s)\psi(s)$.

with $\Gamma(\cdot)$ and $\psi(\cdot)$ representing the gamma and digamma functions respectively, as defined in [Appendix C.5](#).

Lemma C.6. *If X has a Gamma distribution with shape and rate s and r , then $1/X \sim \Gamma^{-1}(s, r)$.*

Proof. Let $Y = 1/X$. Then the pdf of Y is

$$\begin{aligned} p_Y(Y) &= p_X(1/Y) \left| \frac{\partial}{\partial Y}(1/Y) \right| \\ &= \Gamma(s)^{-1} r^s (1/Y)^{s-1} e^{-r/Y} (1/Y^2) \\ &= \Gamma(s)^{-1} r^s Y^{-(s+1)} e^{-r/Y} \end{aligned}$$

which is the pdf of an inverse gamma with shape s and scale r . □

Appendix D

Proofs related to the conically truncated independent multivariate normal distribution

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proof

We present the proof for [Lemma C.5](#) related to the conically truncated independent multivariate normal distribution, which we had not encountered in the literature.

D.1 Proof of [Lemma C.5](#): Pdf

Using the fact that $\int p(x) dx = 1$, and that

$$\begin{aligned}
 & \int \cdots \int \mathbb{1}[x_i < x_j, \forall i \neq j] \prod_{i=1}^d \phi(x_i | \mu_i, \sigma_i^2) dx_1 \cdots dx_d \\
 &= \int \cdots \int \mathbb{1}[x_i < x_j, \forall i \neq j] \prod_{i=1}^d \left[\frac{1}{\sigma_i} \phi\left(\frac{x_i - \mu_i}{\sigma_i}\right) \right] dx_1 \cdots dx_d \\
 &= \int \cdots \int \mathbb{1}[x_i < x_j, \forall i \neq j] \frac{1}{\sigma_j} \phi\left(\frac{x_j - \mu_j}{\sigma_j}\right) \prod_{\substack{i=1 \\ i \neq j}}^d \left[\frac{1}{\sigma_i} \phi\left(\frac{x_i - \mu_i}{\sigma_i}\right) \right] dx_1 \cdots dx_d \\
 &= \int \prod_{\substack{i=1 \\ i \neq j}}^d \Phi\left(\frac{x_j - \mu_i}{\sigma_i}\right) \frac{1}{\sigma_j} \phi\left(\frac{x_j - \mu_j}{\sigma_j}\right) dx_j
 \end{aligned}$$

$$\begin{aligned}
 &= \int \prod_{\substack{i=1 \\ i \neq j}}^d \Phi\left(\frac{\sigma_j z + \mu_j - \mu_i}{\sigma_i}\right) \phi(z) \, dz \\
 &\quad \text{(by using the standardisation } z = (x_j - \mu_j)/\sigma_j) \\
 &= \mathbb{E}_Z \left[\prod_{\substack{i=1 \\ i \neq j}}^d \Phi\left(\frac{\sigma_j}{\sigma_i} Z + \frac{\mu_j - \mu_i}{\sigma_i}\right) \right]
 \end{aligned}$$

the proof follows directly.

D.2 Proof of Lemma C.5: Moments

Recall that for $Y \sim {}^t\mathcal{N}(\mu, \sigma^2, -\infty, b)$, for some function g of Y , we have that

$$\mathbb{E} g(Y) = \Phi(\beta)^{-1} \int g(y) \mathbb{1}[y < b] \phi(y|\mu, \sigma^2) \, dy,$$

and in particular, we have

$$\mathbb{E}[Y - \mu] = -\sigma \frac{\phi(\beta)}{\Phi(\beta)} \tag{D.1}$$

$$\mathbb{E}[Y - \mu]^2 - \sigma^2 = -\sigma^2 \frac{\beta \phi(\beta)}{\Phi(\beta)} \tag{D.2}$$

where $\beta = (b - \mu)/\sigma$. For the conically truncated multivariate normal distribution $X \sim {}^t\mathcal{N}_d(\mu, \Sigma, \mathcal{A}_j)$, where $\Sigma = \text{diag}(\sigma_1^2, \dots, \sigma_d^2)$, the independence structure of Σ makes it possible to consider the expectations of each of the components separately by marginalising out the rest of the components. For simplicity, denote $p(x_k) = \phi(x_k|\mu_k, \sigma_k) = \sigma_k^{-1} \phi(\frac{x_k - \mu_k}{\sigma_k})$. For $i \neq j$, we have

$$\begin{aligned}
 \mathbb{E} g(X_i) &= C^{-1} \int \dots \int g(x_i) \mathbb{1}[x_k < x_j, \forall k \neq j] \prod_{k=1}^d p(x_k) \, dx_1 \dots dx_d \\
 &= C^{-1} \frac{\Phi((x_j - \mu_j)/\sigma_j)}{\Phi((x_j - \mu_j)/\sigma_j)} \iint g(x_i) \mathbb{1}[x_i < x_j] p(x_i) p(x_j) \prod_{\substack{k=1 \\ k \neq i, j}}^d \Phi\left(\frac{x_j - \mu_k}{\sigma_k}\right) \, dx_i \, dx_j \\
 &= C^{-1} \int \mathbb{E}_{X_i \sim {}^t\mathcal{N}(\mu_i, \sigma_i^2, -\infty, x_j)} g(X_i) \prod_{\substack{k=1 \\ k \neq j}}^d \Phi\left(\frac{x_j - \mu_k}{\sigma_k}\right) p(x_j) \, dx_j \tag{D.3}
 \end{aligned}$$

where C is the normalising constant for X , while for the j 'th component we have

$$\begin{aligned} \mathbb{E} g(X_j) &= C^{-1} \int \cdots \int g(x_j) \mathbb{1}[x_k < x_j, \forall k \neq j] \prod_{k=1}^d p(x_k) dx_1 \cdots dx_d \\ &= C^{-1} \int g(x_j) \prod_{\substack{k=1 \\ k \neq j}}^d \Phi\left(\frac{x_j - \mu_k}{\sigma_k}\right) p(x_j) dx_j. \end{aligned} \quad (\text{D.4})$$

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Plugging in (D.1) for $g(X_i) = X_i - \mu_i$ in (D.3) we get

$$\begin{aligned} \mathbb{E} X_i - \mu_i &= -C^{-1} \int \left(\sigma_i \phi\left(\frac{x_j - \mu_i}{\sigma_i}\right) / \Phi\left(\frac{x_j - \mu_i}{\sigma_i}\right) \right) \prod_{\substack{k=1 \\ k \neq j}}^d \Phi\left(\frac{x_j - \mu_k}{\sigma_k}\right) p(x_j) dx_j \\ &= -\sigma_i C^{-1} \int \phi\left(\frac{x_j - \mu_i}{\sigma_i}\right) \prod_{\substack{k=1 \\ k \neq j}}^d \Phi\left(\frac{x_j - \mu_k}{\sigma_k}\right) p(x_j) dx_j \\ &= -\sigma_i C^{-1} \int \phi\left(\frac{\sigma_j z + \mu_j - \mu_i}{\sigma_i}\right) \prod_{\substack{k=1 \\ k \neq j}}^d \Phi\left(\frac{\sigma_j z + \mu_j - \mu_k}{\sigma_k}\right) \phi(z) dz \\ &= -\sigma_i C^{-1} \mathbb{E}_Z \left[\phi\left(\frac{\sigma_j Z + \mu_j - \mu_i}{\sigma_i}\right) \prod_{\substack{k=1 \\ k \neq j}}^d \Phi\left(\frac{\sigma_j Z + \mu_j - \mu_k}{\sigma_k}\right) \right] \end{aligned}$$

where Z is the distribution of $N(0, 1)$, and we had used a change of variable $x_j = \sigma_j z + \mu_j$, so that $p(x_j) = \sigma_j^{-1} \phi(z)$ and $dx_j = \sigma_j dz$. For the j 'th component, substitute $g(x_j) =$

$x_j - \mu_j$ in (D.4) to get

$$\begin{aligned}
 \mathbb{E} X_j - \mu_j &= C^{-1} \int (x_j - \mu_j) \prod_{\substack{k=1 \\ k \neq j}}^d \Phi\left(\frac{x_j - \mu_k}{\sigma_k}\right) p(x_j) dx_j \\
 &= C^{-1} \sigma_j \int z \prod_{\substack{k=1 \\ k \neq j}}^d \Phi\left(\frac{\sigma_j z + \mu_j - \mu_k}{\sigma_k}\right) \phi(z) dz \\
 &= \sigma_j \sum_{\substack{i=1 \\ i \neq j}}^d \sigma_i C^{-1} \mathbb{E} \left[\phi\left(\frac{\sigma_j Z + \mu_j - \mu_i}{\sigma_i}\right) \prod_{\substack{k=1 \\ k \neq i, j}}^d \Phi\left(\frac{\sigma_j Z + \mu_j - \mu_k}{\sigma_k}\right) \right] \\
 &= -\sigma_j \sum_{\substack{i=1 \\ i \neq j}}^d (\mathbb{E} X_i - \mu_i),
 \end{aligned}$$

where we have made use of Lemma D.1 in the second last step.

For the second moments, plug in (D.2) for $g(X_i) = (X_i - \mu_i)^2 - \sigma_i^2$ in (D.3) to get

$$\begin{aligned}
 \mathbb{E}[X_i - \mu_i]^2 - \sigma_i^2 &= -\sigma_i^2 C^{-1} \int \overbrace{\frac{x_j - \mu_i}{\sigma_i}}^{x_j - \mu_i - \mu_j + \mu_j} \cdot \frac{\phi((x_j - \mu_i)/\sigma_i)}{\Phi((x_j - \mu_i)/\sigma_i)} \prod_{\substack{k=1 \\ k \neq j}}^d \Phi\left(\frac{x_j - \mu_k}{\sigma_k}\right) p(x_j) dx_j \\
 &= -\sigma_i C^{-1} \int (x_j - \mu_j) \phi\left(\frac{x_j - \mu_i}{\sigma_i}\right) \prod_{\substack{k=1 \\ k \neq i, j}}^d \Phi\left(\frac{x_j - \mu_k}{\sigma_k}\right) p(x_j) dx_j \\
 &\quad + \overbrace{(\mu_j - \mu_i) \cdot -\sigma_i C^{-1} \int \phi\left(\frac{x_j - \mu_i}{\sigma_i}\right) \prod_{\substack{k=1 \\ k \neq i, j}}^d \Phi\left(\frac{x_j - \mu_k}{\sigma_k}\right) p(x_j) dx_j}^{\mathbb{E} X_i - \mu_i} \\
 &= (\mu_j - \mu_i)(\mathbb{E} X_i - \mu_i) \\
 &\quad + \sigma_i C^{-1} \int \sigma_j z \phi\left(\frac{x_j - \mu_i}{\sigma_i}\right) \prod_{\substack{k=1 \\ k \neq i, j}}^d \Phi\left(\frac{\sigma_j z + \mu_j - \mu_k}{\sigma_k}\right) \phi(z) dz \\
 &= (\mu_j - \mu_i)(\mathbb{E} X_i - \mu_i) \\
 &\quad + \sigma_i \sigma_j C^{-1} \mathbb{E} \left[Z \phi\left(\frac{\sigma_j Z + \mu_j - \mu_i}{\sigma_i}\right) \prod_{\substack{k=1 \\ k \neq i, j}}^d \Phi\left(\frac{\sigma_j Z + \mu_j - \mu_k}{\sigma_k}\right) \right]
 \end{aligned}$$

And similarly, for the j 'th component

$$\begin{aligned}
 \mathbb{E}[X_j - \mu_j]^2 &= C^{-1} \int (x_j - \mu_j)^2 \prod_{\substack{k=1 \\ k \neq j}}^d \Phi\left(\frac{x_j - \mu_k}{\sigma_k}\right) p(x_j) dx_j \\
 &= C^{-1} \sigma_j^2 \int z^2 \prod_{\substack{k=1 \\ k \neq j}}^d \Phi\left(\frac{z\sigma_j + \mu_j - \mu_k}{\sigma_k}\right) p(x_j) dz \\
 &= C^{-1} \sigma_j^2 \mathbb{E}_Z \left[Z^2 \prod_{\substack{k=1 \\ k \neq j}}^d \Phi\left(\frac{Z\sigma_j + \mu_j - \mu_k}{\sigma_k}\right) \right].
 \end{aligned}$$

Lastly, we use the following result in the derivation above.

lem:EZgZ

Lemma D.1. *Let $Z \sim \mathcal{N}(0, 1)$. Then for all $m \in \{\mathbb{N} \mid m > 1\}$ and $(\mu, \sigma) \in \mathbb{R} \times \mathbb{R}^+$,*

$$\mathbb{E} \left[Z \prod_{\substack{k=1 \\ k \neq j}}^m \Phi(\sigma_k Z + \mu_k) \right] = \sum_{\substack{i=1 \\ i \neq j}}^m \mathbb{E} \left[\sigma_i \phi(\sigma_i Z + \mu_i) \prod_{\substack{k=1 \\ k \neq i, j}}^m \Phi(\sigma_k Z + \mu_k) \right]$$

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

Proof. Use the fact that for any differentiable function g , $\mathbb{E}[Zg(Z)] = \mathbb{E}[g'(Z)]$, and apply the result with the function $g_m : z \mapsto \prod_{k \neq j} \Phi(\sigma_k z + \mu_k)$. All that is left is to derive the derivative of g , and we use an inductive proof to do this. Introduce the following notation for convenience:

$$\begin{aligned}
 \phi_i &= \phi(\sigma_i z + \mu_i) \\
 \Phi_i &= \Phi(\sigma_i z + \mu_i)
 \end{aligned}$$

The simplest case is when $m = 2$, which can be trivially shown to be true. Without loss of generality, let $j = 1$. Then

$$\begin{aligned}
 g_2(z) &= \Phi_2 \\
 \Rightarrow \dot{g}_2(z) &= \sigma_2 \phi_2 = \sum_{\substack{i=1 \\ i \neq 1}}^2 \left[\sigma_i \phi_i \sum_{\substack{k=1 \\ k \neq 1, 2}}^2 \Phi_k \right].
 \end{aligned}$$

Now assume that the inductive hypothesis holds for some $m \in \{\mathbb{N} \mid m > 1\}$. That is, the derivative of $g_m(z) = \prod_{k \neq j} \Phi_k$,

$$\dot{g}_m(z) = \sum_{\substack{i=1 \\ i \neq j}}^m \left[\sigma_i \phi_i \prod_{\substack{k=1 \\ k \neq i, j}}^m \Phi_k \right],$$

is assumed to be true. Also assume that, without loss of generality, $j \neq m+1$. Then, the derivative of

$$g_{m+1}(z) = \prod_{\substack{k=1 \\ k \neq j}}^{m+1} \Phi_k = g_m(z) \Phi_{m+1}$$

is found to be

$$\begin{aligned} \dot{g}_{m+1}(z) &= \sigma_{m+1} \phi_{m+1} g_m(z) + \dot{g}_m(z) \Phi_{m+1} \\ &= \sigma_{m+1} \phi_{m+1} \prod_{\substack{k=1 \\ k \neq j}}^m \Phi_k + \sum_{\substack{i=1 \\ i \neq j}}^m \left[\sigma_i \phi_i \prod_{\substack{k=1 \\ k \neq i, j}}^m \Phi_k \right] \Phi_{m+1} \\ &= \sigma_{m+1} \phi_{m+1} \prod_{\substack{k=1 \\ k \neq j, m+1}}^{m+1} \Phi_k + \sum_{\substack{i=1 \\ i \neq j}}^m \left[\sigma_i \phi_i \prod_{\substack{k=1 \\ k \neq i, j}}^{m+1} \Phi_k \right] \\ &= \sum_{\substack{i=1 \\ i \neq j}}^{m+1} \left[\sigma_i \phi_i \prod_{\substack{k=1 \\ k \neq i, j}}^{m+1} \Phi_k \right], \end{aligned}$$

as required for the inductive proof. Using linearity of expectations, the proof is complete. \square

D.3 Proof of **Lemma C.5**: Entropy

As a direct consequence of the definition of entropy,

$$\begin{aligned} H(p) &= -\mathbb{E}[\log p(X)] \\ &= -\mathbb{E} \left[-\log C - \frac{d}{2} \log 2\pi - \frac{1}{2} \sum_{i=1}^d \log \sigma_i^2 - \frac{1}{2} \sum_{i=1}^d \left(\frac{x_i - \mu_i}{\sigma_i} \right)^2 \right] \\ &= \log C + \frac{d}{2} \log 2\pi + \frac{1}{2} \sum_{i=1}^d \log \sigma_i^2 + \frac{1}{2} \sum_{i=1}^d \frac{1}{\sigma_i^2} \mathbb{E}[x_i - \mu_i]^2. \end{aligned}$$

Appendix E

I-prior interpretation of the g -prior

misc:gprior

The I-prior for β in a standard linear model resembles the objective g -prior (Zellner, 1986) for regression coefficients,

$$\beta \sim N_p(\mathbf{0}, g(\mathbf{X}^\top \Psi \mathbf{X})^{-1}),$$

although they are quite different objects. The g -prior for β has the *inverse* (scaled) Fisher information matrix as its covariance matrix. This, in itself, has a much different and arguably counterintuitive meaning: large amounts of Fisher information about β corresponds to a small prior variance, and hence less deviation away from the prior mean of zero in estimating β . The choice of the hyperparameter g has been the subject of much debate, with choices ranging from fixing $g = n$ (corresponding to the concept of *unit Fisher information*), to fully Bayesian and empirical Bayesian methods of estimating g from the data.

On the other hand, we note that the g -prior has an I-prior interpretation when argued as follows. Assume that the regression function f lies in the continual dual space of \mathbb{R}^p equipped with the inner product $\langle \mathbf{x}, \mathbf{x}' \rangle_{\mathcal{X}} = \mathbf{x}^\top (\mathbf{X}^\top \Psi \mathbf{X})^{-1} \mathbf{x}$. With this inner product

and from (3.3) (p. 12), the Fisher information for β is

$$\begin{aligned}\mathcal{I}_g(\beta) &= \sum_{i=1}^n \sum_{j=1}^n \psi_{ij} (\mathbf{X}^\top \Psi \mathbf{X})^{-1} \mathbf{x}_i \otimes (\mathbf{X}^\top \Psi \mathbf{X})^{-1} \mathbf{x}_j \\ &= (\mathbf{X}^\top \Psi \mathbf{X})^{-1} (\mathbf{X}^\top \Psi \mathbf{X}) (\mathbf{X}^\top \Psi \mathbf{X})^{-1} \\ &= (\mathbf{X}^\top \Psi \mathbf{X})^{-1},\end{aligned}$$

and this, rather than the usual $\mathbf{X}^\top \Psi \mathbf{X}$ as the prior covariance matrix for β , means that the I-prior is in fact the standard g -prior.

The metric induced by the inner product is actually the *Mahalanobis distance*, a scale-invariant natural distance if the covariates are measured on different scales. To expand on this idea, circle back to the regression function and write it as $f(\mathbf{x}) = \langle \mathbf{x}, \beta \rangle_{\mathcal{X}}$. In usual least squares regression, the choice of inner product is irrelevant, so the usual dot product is commonly used (however, as we have seen above, the choice of inner product determines the form of the Fisher information for β). In particular, suppose that all the x_{ik} 's, $k = 1, \dots, p$ for each unit $i = 1, \dots, n$ are measured on the same scale; for instance, these could be measurements in centimetres. In this case, the dot product is reasonable, because $\langle \mathbf{x}_i, \mathbf{x}_j \rangle = \sum_{k=1}^p x_{ik} x_{jk}$ and the inner product has a coherent unit, namely the squared unit of the x_{ik} 's. However, if they were a mix of various scaled measurements, then obviously the inner product's unit is incoherent—one would be resorted to adding measurements in different units, for example, cm^2 and kg^2 and so on. In such a case, a unitless inner product is appropriate, like the Mahalanobis inner product, which technically rescales the x_{ik} 's to unity. In summary, if the covariates are all measured on the same scale, then the I-prior is appropriate, and if not, the g -prior is appropriate.

Appendix F

I-prior for standard multilevel models

misc:multilevelmodels

We show the corresponding I-prior for the regression coefficients of the standard linear multilevel model [eq:standmultilevel](#). Write $\alpha = \beta_0$, and for simplicity, assume iid errors, i.e., $\Psi = \psi \mathbf{I}_n$. The form of $f \in \mathcal{F}$ is now $f(\mathbf{x}_i^{(j)}, j) = \sum_{i'=1}^{n_{j'}} \sum_{j'=1}^m h_\lambda((\mathbf{x}_i^{(j)}, j), (\mathbf{x}_{i'}^{(j')}, j')) w_{i'j'}$, where each $w_{i'j'} \sim N(0, \psi^{-1})$.

Now, functions in the scaled RKHS \mathcal{F}_2 have the form

$$\begin{aligned} f_2(j) &= \sum_{i=1}^{n_{j'}} \sum_{j'=1}^m \lambda_2 \left(\frac{\delta_{jj'}}{p_j} - 1 \right) w_{ij'} \\ &= \lambda_2 \left(\frac{w_{++}}{p_j} - w_{++} \right), \end{aligned}$$

where a ‘+’ in the index of w_{ik} indicates a summation over that index, and p_j is the empirical distribution over \mathcal{M} , i.e. $p_j = n_j/n$. Clearly $f_2(j)$ is a variable depending on j , so write $f_2(j) = \beta_{0j}$. The distribution of β_{0j} is normal with zero mean and variance

$$\begin{aligned} \text{Var } \beta_{0j} &= \lambda_2^2 \left(\frac{n_j \psi}{n_j^2/n^2} + n\psi \right) \\ &= n\psi \lambda_2^2 \left(\frac{1}{p_j} + 1 \right). \end{aligned}$$

The covariance between any two random intercepts β_{0j} and $\beta_{0j'}$ is

$$\begin{aligned}
\text{Cov}(\beta_{0j}, \beta_{0j'}) &= \text{Cov}\left(\lambda_2 \left(\frac{w_{+j}}{p_j} - w_{++}\right), \lambda_2 \left(\frac{w_{+j'}}{p_{j'}} - w_{++}\right)\right) \\
&= \frac{\lambda_2^2}{p_j p_{j'}} \text{Cov}(w_{+j}, w_{+j'}) - \frac{\lambda_2^2}{p_j} \text{Cov}(w_{+j}, w_{++}) - \frac{\lambda_2^2}{p_{j'}} \text{Cov}(w_{++}, w_{+j'}) \\
&\quad + \lambda_2^2 \text{Cov}(w_{++}, w_{++}) \\
&= -\frac{\lambda_2^2}{n_j/n} n_j \psi - \frac{\lambda_2^2}{n_{j'}/n} n_{j'} \psi + \lambda_2^2 n \psi \\
&= -n \psi \lambda_2^2.
\end{aligned}$$

Functions in \mathcal{F}_{12} , on the other hand, have the form

$$\begin{aligned}
f_{12}(\mathbf{x}_i, j) &= \sum_{i'=1}^{n_{j'}} \sum_{j'=1}^m \lambda_1 \lambda_2 \cdot \tilde{\mathbf{x}}_i^{(j)\top} \tilde{\mathbf{x}}_{i'}^{(j')} \cdot \left(\frac{\delta_{jj'}}{p_j} - 1\right) w_{i'j'} \\
&= \tilde{\mathbf{x}}_i^{(j)\top} \underbrace{\left(\frac{\lambda_1 \lambda_2}{p_j} \sum_{i'=1}^{n_j} \tilde{\mathbf{x}}_{i'}^{(j)} w_{i'j} - \lambda_1 \lambda_2 \sum_{i'=1}^{n_{j'}} \sum_{j'=1}^m \tilde{\mathbf{x}}_{i'}^{(j')} w_{i'j'} \right)}_{\beta_{1j}},
\end{aligned}$$

and this is, as expected, a linear form dependent on cluster j . We can calculate the variance for β_{1j} to be

$$\begin{aligned}
\text{Var } \beta_{1j} &= \lambda_1^2 \lambda_2^2 \text{Var} \left(\frac{1}{p_j} \tilde{\mathbf{X}}_j^\top \mathbf{w}_j - \tilde{\mathbf{X}}^\top \mathbf{w} \right) \\
&= \lambda_1^2 \lambda_2^2 \left(\frac{\psi}{n_j^2/n^2} \tilde{\mathbf{X}}_j^\top \tilde{\mathbf{X}}_j + \psi \tilde{\mathbf{X}}^\top \tilde{\mathbf{X}} - \frac{1}{p_j} \tilde{\mathbf{X}}_j^\top \text{Cov}(\mathbf{w}_j, \mathbf{w}) \tilde{\mathbf{X}}^\top \right) \\
&= n \psi \lambda_1^2 \lambda_2^2 \left(\frac{1}{p_j} \mathbf{S}_j + \mathbf{S} - \mathbf{S}_j \right) \\
&= n \psi \lambda_1^2 \lambda_2^2 \left(\left(\frac{1}{p_j} - 1 \right) \mathbf{S}_j + \mathbf{S} \right)
\end{aligned}$$

where $\mathbf{S}_j = \frac{1}{n_j} \sum_{i=1}^{n_j} (\mathbf{x}_i^{(j)} - \bar{\mathbf{x}})^\top (\mathbf{x}_i^{(j)} - \bar{\mathbf{x}})$, $\mathbf{S} = \frac{1}{n} \sum_{i=1}^{n_j} \sum_{j=1}^m (\mathbf{x}_i^{(j)} - \bar{\mathbf{x}})^\top (\mathbf{x}_i^{(j)} - \bar{\mathbf{x}})$, and $\bar{\mathbf{x}} = \frac{1}{n} \sum_{i=1}^{n_j} \sum_{j=1}^m \mathbf{x}_i^{(j)}$. The covariance between two vectors of the random slopes is

$$\begin{aligned} \text{Cov}(\boldsymbol{\beta}_{1j}, \boldsymbol{\beta}_{1j'}) &= \lambda_1^2 \lambda_2^2 \text{Cov} \left(\frac{1}{p_j} \tilde{\mathbf{X}}_j^\top \mathbf{w}_j - \tilde{\mathbf{X}}^\top \mathbf{w}, \frac{1}{p_{j'}} \tilde{\mathbf{X}}_{j'}^\top \mathbf{w}_{j'} - \tilde{\mathbf{X}}^\top \mathbf{w} \right) \\ &= \psi \lambda_1^2 \lambda_2^2 \left(\tilde{\mathbf{X}}^\top \tilde{\mathbf{X}} - \frac{1}{p_j} \tilde{\mathbf{X}}_j^\top \tilde{\mathbf{X}}_j - \frac{1}{p_{j'}} \tilde{\mathbf{X}}_{j'}^\top \tilde{\mathbf{X}}_{j'} \right) \\ &= n \psi \lambda_1^2 \lambda_2^2 (\mathbf{S} - \mathbf{S}_j - \mathbf{S}_{j'}). \end{aligned}$$

Another quantity of interest is the covariance between the random intercepts and random slopes:

$$\begin{aligned} \text{Cov}(\beta_{0j}, \boldsymbol{\beta}_{1j}) &= \lambda_1 \lambda_2^2 \text{Cov} \left(\frac{1}{p_j} \mathbf{1}_{n_j}^\top \mathbf{w}_j - \mathbf{1}_n^\top \mathbf{w}, \frac{1}{p_j} \tilde{\mathbf{X}}_j^\top \mathbf{w}_j - \tilde{\mathbf{X}}^\top \mathbf{w} \right) \\ &= \psi \lambda_1 \lambda_2^2 \left(\mathbf{1}_n^\top \tilde{\mathbf{X}}^0 + \frac{1}{p_j^2} \mathbf{1}_{n_j}^\top \tilde{\mathbf{X}}_j - \frac{2}{p_j} \mathbf{1}_{n_j}^\top \tilde{\mathbf{X}}_j \right) \\ &= n \psi \lambda_1 \lambda_2^2 \left(\left(\frac{1}{p_j} - 2 \right) \frac{1}{n_j} \sum_{i=1}^{n_j} (\mathbf{x}_i^{(j)} - \bar{\mathbf{x}}) \right) \\ &= n \psi \lambda_1 \lambda_2^2 \left(\frac{1}{p_j} - 2 \right) (\bar{\mathbf{x}}^{(j)} - \bar{\mathbf{x}}) \end{aligned}$$

and

$$\begin{aligned} \text{Cov}(\beta_{0j}, \boldsymbol{\beta}_{1j'}) &= \lambda_1 \lambda_2^2 \text{Cov} \left(\frac{1}{p_j} \mathbf{1}_{n_j}^\top \mathbf{w}_j - \mathbf{1}_n^\top \mathbf{w}, \frac{1}{p_{j'}} \tilde{\mathbf{X}}_{j'}^\top \mathbf{w}_{j'} - \tilde{\mathbf{X}}^\top \mathbf{w} \right) \\ &= \psi \lambda_1 \lambda_2^2 \left(\mathbf{1}_n^\top \tilde{\mathbf{X}}^0 + \frac{1}{p_j p_{j'}} \mathbf{1}_{n_j}^\top \text{Cov}(\mathbf{w}_j, \mathbf{w}_{j'}) \tilde{\mathbf{X}}_{j'}^0 - \frac{1}{p_j} \mathbf{1}_{n_j}^\top \tilde{\mathbf{X}}_j - \frac{1}{p_{j'}} \mathbf{1}_{n_{j'}}^\top \tilde{\mathbf{X}}_{j'} \right) \\ &= n \psi \lambda_1 \lambda_2^2 \left(-\frac{1}{n_j} \sum_{i=1}^{n_j} (\mathbf{x}_i^{(j)} - \bar{\mathbf{x}}) - \frac{1}{n_{j'}} \sum_{i=1}^{n_{j'}} (\mathbf{x}_i^{(j')} - \bar{\mathbf{x}}) \right) \\ &= n \psi \lambda_1 \lambda_2^2 (2\bar{\mathbf{x}} - \bar{\mathbf{x}}^{(j)} - \bar{\mathbf{x}}^{(j')}). \end{aligned}$$

Appendix G

Posterior distribution of the I-prior regression function

We derive the posterior distribution for the I-prior random effects $\mathbf{w} = (w_1, \dots, w_n)^\top$, which is related to the I-prior regression function via $f(x_i) = \sum_{k=1}^n h_\eta(x_i, x_k) w_k$, or in matrix terms, $\mathbf{f} := (f(x_1), \dots, f(x_n))^\top = \mathbf{H}_\eta \mathbf{w}$, and $f \in \mathcal{F}$ an RKHS with kernel h_η . A closely related distribution of interest is the posterior predictive distribution of y_{new} , the prediction at a new data point x_{new} .

G.1 Deriving the posterior distribution for \mathbf{w}

apx:posterior
orw

In the following derivation, we implicitly assume the dependence on \mathbf{f}_0 and θ . The distribution of $\mathbf{y}|\mathbf{w}$ is $N_n(\alpha + \mathbf{f}_0 + \mathbf{H}_\eta \mathbf{w}, \Psi^{-1})$, where $\alpha = \alpha \mathbf{1}_n$, while the prior distribution for \mathbf{w} is $N_n(\mathbf{0}, \Psi)$. Since $p(\mathbf{w}|\mathbf{y}) \propto p(\mathbf{y}|\mathbf{w})p(\mathbf{w})$, we have that

$$\begin{aligned} \log p(\mathbf{w}|\mathbf{y}) &= \log p(\mathbf{y}|\mathbf{w}) + \log p(\mathbf{w}) \\ &= \text{const.} + \frac{1}{2} \log |\Psi| - \frac{1}{2} (\mathbf{y} - \alpha - \mathbf{f}_0 - \mathbf{H}_\eta \mathbf{w})^\top \Psi (\mathbf{y} - \alpha - \mathbf{f}_0 - \mathbf{H}_\eta \mathbf{w}) \\ &\quad - \frac{1}{2} \log |\Psi| - \frac{1}{2} \mathbf{w}^\top \Psi^{-1} \mathbf{w} \\ &= \text{const.} - \frac{1}{2} \mathbf{w}^\top (\mathbf{H}_\eta \Psi \mathbf{H}_\eta + \Psi^{-1}) \mathbf{w} + (\mathbf{y} - \alpha - \mathbf{f}_0)^\top \Psi \mathbf{H}_\eta \mathbf{w}. \end{aligned}$$

Setting $\mathbf{A} = \mathbf{H}_\eta \boldsymbol{\Psi} \mathbf{H}_\eta + \boldsymbol{\Psi}^{-1}$, $\mathbf{a}^\top = (\mathbf{y} - \boldsymbol{\alpha} - \mathbf{f}_0)^\top \boldsymbol{\Psi} \mathbf{H}_\eta$, and using the fact that

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

we have that $\mathbf{w}|\mathbf{y}$ is normally distributed with the required mean and variance.

Alternatively, one could have shown this using standard results of multivariate normal distributions. Noting that the covariance between \mathbf{y} and \mathbf{w} is

$$\begin{aligned} \text{Cov}(\mathbf{y}, \mathbf{w}) &= \text{Cov}(\boldsymbol{\alpha} + \mathbf{f}_0 + \mathbf{H}_\eta \mathbf{w} + \boldsymbol{\epsilon}, \mathbf{w}) \\ &= \mathbf{H}_\eta \text{Cov}(\mathbf{w}, \mathbf{w}) \\ &= \mathbf{H}_\eta \boldsymbol{\Psi} \end{aligned}$$

and that $\text{Cov}(\mathbf{w}, \mathbf{y}) = \boldsymbol{\Psi} \mathbf{H}_\eta = \mathbf{H}_\eta \boldsymbol{\Psi} = \text{Cov}(\mathbf{y}, \mathbf{w})$ by symmetry, the joint distribution (\mathbf{y}, \mathbf{w}) is

$$\begin{pmatrix} \mathbf{y} \\ \mathbf{w} \end{pmatrix} \sim N_{n+n} \left(\begin{pmatrix} \boldsymbol{\alpha} + \mathbf{f}_0 \\ \mathbf{0} \end{pmatrix}, \begin{pmatrix} \mathbf{V}_y & \mathbf{H}_\eta \boldsymbol{\Psi} \\ \mathbf{H}_\eta \boldsymbol{\Psi} & \boldsymbol{\Psi} \end{pmatrix} \right).$$

Thus,

$$\begin{aligned} \mathbb{E}[\mathbf{w}|\mathbf{y}] &= \mathbb{E} \mathbf{w} + \text{Cov}(\mathbf{w}, \mathbf{y})(\text{Var} \mathbf{y})^{-1}(\mathbf{y} - \mathbb{E} \mathbf{y}) \\ &= \mathbf{H}_\eta \boldsymbol{\Psi} \mathbf{V}_y^{-1}(\mathbf{y} - \boldsymbol{\alpha} - \mathbf{f}_0), \end{aligned}$$

and

$$\begin{aligned} \text{Var}[\mathbf{w}|\mathbf{y}] &= \text{Var} \mathbf{w} - \text{Cov}(\mathbf{w}, \mathbf{y})(\text{Var} \mathbf{y})^{-1} \text{Cov}(\mathbf{y}, \mathbf{w}) \\ &= \boldsymbol{\Psi} - \mathbf{H}_\eta \boldsymbol{\Psi} \mathbf{V}_y^{-1} \mathbf{H}_\eta \boldsymbol{\Psi} \\ &= \boldsymbol{\Psi} - \boldsymbol{\Psi} \mathbf{H}_\eta (\boldsymbol{\Psi}^{-1} + \mathbf{H}_\eta \boldsymbol{\Psi} \mathbf{H}_\eta)^{-1} \mathbf{H}_\eta \boldsymbol{\Psi} \\ &= (\boldsymbol{\Psi}^{-1} + \mathbf{H}_\eta \boldsymbol{\Psi} \mathbf{H}_\eta)^{-1} \\ &= \mathbf{V}_y^{-1} \end{aligned}$$

as a direct consequence of the Woodbury matrix identity ([Petersen and Pedersen, 2008](#), eq. (156), §3.2.2).

apx:postpre
d

G.2 Deriving the posterior predictive distribution

The posterior predictive distribution is obtained in an empirical Bayesian manner, in which the parameters of the model are replaced with their ML estimates (denoted with hats).

A priori, assume that $y_{\text{new}} \sim \text{N}(\hat{\alpha}, v_{\text{new}})$, where $v_{\text{new}} = \mathbf{h}_{\hat{\eta}}(x_{\text{new}})^\top \hat{\Psi} \mathbf{h}_{\hat{\eta}}(x_{\text{new}}) + \psi_{\text{new}}^{-1}$. Consider the joint distribution of $(y_{\text{new}}, \mathbf{y})^\top$, which is multivariate normal (since both y_{new} and \mathbf{y} are. Write

$$\begin{pmatrix} y_{\text{new}} \\ \mathbf{y} \end{pmatrix} \sim \text{N}_{n+1} \left(\begin{pmatrix} \hat{\alpha} \\ \hat{\alpha} \mathbf{1}_n \end{pmatrix}, \begin{pmatrix} v_{\text{new}} & \text{Cov}(y_{\text{new}}, \mathbf{y}) \\ \text{Cov}(y_{\text{new}}, \mathbf{y})^\top & \hat{\mathbf{V}}_y \end{pmatrix} \right),$$

where

$$\begin{aligned} \text{Cov}(y_{\text{new}}, \mathbf{y}) &= \text{Cov}(f_{\text{new}} + \epsilon_{\text{new}}, \mathbf{f} + \boldsymbol{\epsilon}) \\ &= \text{Cov}(f_{\text{new}}, \mathbf{f}) + \text{Cov}(\epsilon_{\text{new}}, \boldsymbol{\epsilon}) \\ &= \text{Cov} \left(\mathbf{h}_{\hat{\eta}}(x_{\text{new}})^\top \tilde{\mathbf{w}}, \mathbf{H}_{\hat{\eta}} \tilde{\mathbf{w}} \right) + (\sigma_{\text{new},1}, \dots, \sigma_{\text{new},n}) \\ &= \mathbf{h}_{\hat{\eta}}(x_{\text{new}})^\top \hat{\Psi} \mathbf{H}_{\hat{\eta}} + \boldsymbol{\sigma}_{\text{new}}. \end{aligned}$$

The vector of covariances $\boldsymbol{\sigma}_{\text{new}}$ between observations y_1, \dots, y_n and the predicted point y_{new} would need to be prescribed a priori (treated as extra parameters), or estimated again, which seems excessive. Under an iid assumption of the error precisions, then $\boldsymbol{\sigma}_{\text{new}} = \mathbf{0}$ would be acceptable.

In any case, using standard multivariate normal results, we get that $y_{\text{new}}|\mathbf{y}$ is also normally distributed with mean

$$\begin{aligned} E[y_{\text{new}}|\mathbf{y}] &= \hat{\alpha} + (\mathbf{h}_{\hat{\eta}}(x_{\text{new}})^\top \hat{\Psi} \mathbf{H}_{\hat{\eta}} + \boldsymbol{\sigma}_{\text{new}}) \tilde{\mathbf{V}}_y^{-1} \tilde{\mathbf{y}} \\ &= \hat{\alpha} + \mathbf{h}_{\hat{\eta}}(x_{\text{new}})^\top \overbrace{\mathbf{h}_{\hat{\eta}}(x_{\text{new}})^\top \hat{\Psi} \mathbf{H}_{\hat{\eta}} \tilde{\mathbf{V}}_y^{-1}}^{\hat{\mathbf{w}}} \tilde{\mathbf{y}} + \boldsymbol{\sigma}_{\text{new}} \tilde{\mathbf{V}}_y^{-1} \tilde{\mathbf{y}} \\ &= \hat{\alpha} + E[f(x_{\text{new}})|\mathbf{y}] + \text{mean correction term} \end{aligned}$$

and variance

$$\begin{aligned}
\text{Var}[y_{\text{new}}|\mathbf{y}] &= v_{\text{new}} - (\mathbf{h}_{\hat{\eta}}(x_{\text{new}})^\top \hat{\Psi} \mathbf{H}_{\hat{\eta}} + \boldsymbol{\sigma}_{\text{new}}) \tilde{\mathbf{V}}_y^{-1} (\mathbf{h}_{\hat{\eta}}(x_{\text{new}})^\top \hat{\Psi} \mathbf{H}_{\hat{\eta}} + \boldsymbol{\sigma}_{\text{new}})^\top \\
&= \mathbf{h}_{\hat{\eta}}(x_{\text{new}})^\top \hat{\Psi} \hat{\mathbf{h}}_{\hat{\eta}}(x_{\text{new}}) + \psi_{\text{new}}^{-1} - \mathbf{h}_{\hat{\eta}}(x_{\text{new}})^\top \hat{\Psi} \mathbf{H}_{\hat{\eta}} \tilde{\mathbf{V}}_y^{-1} \mathbf{H}_{\hat{\eta}} \hat{\Psi} \mathbf{h}_{\hat{\eta}}(x_{\text{new}}) \\
&\quad + \text{variance correction term} \\
&= \mathbf{h}_{\hat{\eta}}(x_{\text{new}})^\top (\hat{\Psi} - \hat{\Psi} \mathbf{H}_{\hat{\eta}} \tilde{\mathbf{V}}_y^{-1} \mathbf{H}_{\hat{\eta}} \hat{\Psi}) \mathbf{h}_{\hat{\eta}}(x_{\text{new}}) + \psi_{\text{new}}^{-1} \\
&\quad + \text{variance correction term} \\
&= \mathbf{h}_{\hat{\eta}}(x_{\text{new}})^\top \hat{\mathbf{V}}_y^{-1} \mathbf{h}_{\hat{\eta}}(x_{\text{new}}) + \psi_{\text{new}}^{-1} + \text{variance correction term} \\
&= \text{Var}[f(x_{\text{new}})|\mathbf{y}] + \psi_{\text{new}}^{-1} + \text{variance correction term.}
\end{aligned}$$

Appendix H

Variational EM algorithm for I-probit models

The two sections that follow detail the derivation of the variational densities used in the E-step of the variational EM algorithm, and also the lower bound (ELBO) used to monitor convergence.

H.1 Derivation of the variational densities

In what follows, the implicit dependence of the densities on the parameters of the model θ are dropped. We derive a mean-field variational approximation of

$$\begin{aligned} p(\mathbf{y}^*, \mathbf{w} | \mathbf{y}) &\approx q(\mathbf{y}^*)q(\mathbf{w}) \\ &= \prod_{i=1}^n q(\mathbf{y}_i^*)q(\mathbf{w}). \end{aligned}$$

The first line is by assumption, while the second line follows from an induced factorisation on the latent propensities, as we will see later. Recall that the optimal mean-field variational density \tilde{q} satisfy

$$\begin{aligned} \log \tilde{q}(\mathbf{y}^*) &= \mathbb{E}_{\mathbf{w} \sim \tilde{q}} [\log p(\mathbf{y}, \mathbf{y}^*, \mathbf{w})] + \text{const.} && \text{(from ??)} \\ \log \tilde{q}(\mathbf{w}) &= \mathbb{E}_{\mathbf{y}^* \sim \tilde{q}} [\log p(\mathbf{y}, \mathbf{y}^*, \mathbf{w})] + \text{const.} && \text{(from ??)} \end{aligned}$$

The joint likelihood is given by

$$p(\mathbf{y}, \mathbf{y}^*, \mathbf{w}) = p(\mathbf{y}|\mathbf{y}^*)p(\mathbf{y}^*|\mathbf{w})p(\mathbf{w}).$$

For reference, the three relevant distributions are listed below.

- $p(\mathbf{y}|\mathbf{y}^*)$. For each observation $i \in \{1, \dots, n\}$, given the corresponding latent propensities $\mathbf{y}_i^* = (y_{i1}^*, \dots, y_{im}^*)$, the distribution for y_i is a degenerate distribution which depends on the j 'th component of \mathbf{y}_i^* being largest, where the value observed for y_i was j . Since each of the y_i 's are independent, everything is multiplicative.

$$p(\mathbf{y}|\mathbf{y}^*) = \prod_{i=1}^n \prod_{j=1}^m p_{ij}^{[y_i=j]} = \prod_{i=1}^n \prod_{j=1}^m \mathbb{1}[y_{ij}^* = \max_k y_{ik}^*] \mathbb{1}[y_i=j].$$

- $p(\mathbf{y}^*|\mathbf{w})$. Given values for the parameters and I-prior random effects, the distribution of the latent propensities is matrix normal

$$\mathbf{y}^*|\boldsymbol{\alpha}, \mathbf{w}, \eta, \boldsymbol{\Psi} \sim \text{MN}_{n,m}(\mathbf{1}_n \boldsymbol{\alpha}^\top + \mathbf{H}_\eta \mathbf{w}, \mathbf{I}_n, \boldsymbol{\Psi}^{-1}).$$

Write $\boldsymbol{\mu} = \mathbf{1}_n \boldsymbol{\alpha}^\top + \mathbf{H}_\eta \mathbf{w}$. Its pdf is

$$\begin{aligned} p(\mathbf{y}^*|\mathbf{w}) &= \exp \left[-\frac{nm}{2} \log 2\pi + \frac{n}{2} \log |\boldsymbol{\Psi}| - \frac{1}{2} \text{tr}((\mathbf{y}^* - \boldsymbol{\mu}) \boldsymbol{\Psi} (\mathbf{y}^* - \boldsymbol{\mu})^\top) \right] \\ &= \exp \left[-\frac{nm}{2} \log 2\pi + \frac{n}{2} \log |\boldsymbol{\Psi}| - \frac{1}{2} \sum_{i=1}^n (\mathbf{y}_{i\cdot}^* - \boldsymbol{\mu}_{i\cdot})^\top \boldsymbol{\Psi} (\mathbf{y}_{i\cdot}^* - \boldsymbol{\mu}_{i\cdot}) \right], \end{aligned}$$

where $\mathbf{y}_{i\cdot}^* \in \mathbb{R}^m$ and $\boldsymbol{\mu}_{i\cdot} \in \mathbb{R}^m$ are the rows of \mathbf{y}^* and $\boldsymbol{\mu}$ respectively. The second line follows directly from the definition of the trace, but also emanates from the fact that $\mathbf{y}_{i\cdot}^*$ are independent multivariate normal with mean $\boldsymbol{\mu}_{i\cdot}$ and variance $\boldsymbol{\Psi}^{-1}$.

- $p(\mathbf{w})$. The \mathbf{w} 's are normal random matrices $\mathbf{w} \sim \text{MN}_{n,m}(\mathbf{0}, \mathbf{I}_n, \boldsymbol{\Psi})$ with pdf

$$\begin{aligned} p(\mathbf{w}) &= \exp \left[-\frac{nm}{2} \log 2\pi - \frac{n}{2} \log |\boldsymbol{\Psi}| - \frac{1}{2} \text{tr}(\mathbf{w} \boldsymbol{\Psi}^{-1} \mathbf{w}^\top) \right] \\ &= \exp \left[-\frac{nm}{2} \log 2\pi - \frac{n}{2} \log |\boldsymbol{\Psi}| - \frac{1}{2} \sum_{i=1}^n \mathbf{w}_{i\cdot}^\top \boldsymbol{\Psi}^{-1} \mathbf{w}_{i\cdot} \right]. \end{aligned}$$

H.1.1 Derivation of $\tilde{q}(\mathbf{y}^*)$

The rows of \mathbf{y}^* are independent, and thus we can consider the variational density for each \mathbf{y}_i^* separately. Consider the case where y_i takes one particular value $j \in \{1, \dots, m\}$. In such cases, we have that $y_{ij}^* > y_{ik}$ for all $k \neq j$, and that

$$\begin{aligned} \log \tilde{q}(\mathbf{y}_{i.}^*) &= \mathbb{E}_{\mathbf{w} \sim \tilde{q}} \left[-\frac{1}{2} (\mathbf{y}_i^* - \boldsymbol{\mu}_i)^\top \boldsymbol{\Psi} (\mathbf{y}_i^* - \boldsymbol{\mu}_i) \right] + \text{const.} \\ &= \left[-\frac{1}{2} (\mathbf{y}_i^* - \tilde{\boldsymbol{\mu}}_i)^\top \boldsymbol{\Psi} (\mathbf{y}_i^* - \tilde{\boldsymbol{\mu}}_i) \right] + \text{const.} \end{aligned} \quad (\star)$$

where $\tilde{\boldsymbol{\mu}}_{i.} = \boldsymbol{\alpha} + \tilde{\mathbf{w}} \mathbf{h}_\eta(x_i)$, $\tilde{\mathbf{w}} = \mathbb{E}_{\mathbf{w} \sim \tilde{q}}[\mathbf{w}]$. This is recognised as the logarithm of a multivariate normal pdf with mean $\tilde{\boldsymbol{\mu}}_{i.}$ and variance $\boldsymbol{\Psi}^{-1}$. On the other hand, when $y_i \neq j$, the pdf is zero. Thus,

$$\tilde{q}(\mathbf{y}_{i.}^*) = \begin{cases} \phi(\mathbf{y}_{i.}^* | \tilde{\boldsymbol{\mu}}_{i.}, \boldsymbol{\Psi}^{-1}) & \text{if } y_{ij}^* > y_{ik}^*, \forall k \neq j \\ 0 & \text{otherwise,} \end{cases}$$

implying a truncated multivariate normal distribution for $\mathbf{y}_{i.}^*$. The required moments from the truncated multivariate normal distribution can be obtained using the methods described in ??.

Remark H.1. In the above derivation, we needn't consider the second order terms in the expectations because they do not involve $\mathbf{y}_{i.}^*$, and thus, these terms can be absorbed into the constant. To see this,

$$\begin{aligned} \mathbb{E}[(\mathbf{y}_{i.}^* - \boldsymbol{\mu}_{i.})^\top \boldsymbol{\Psi} (\mathbf{y}_{i.}^* - \boldsymbol{\mu}_{i.})] &= \mathbb{E}[\mathbf{y}_{i.}^{*\top} \boldsymbol{\Psi} \mathbf{y}_{i.}^* + \boldsymbol{\mu}_{i.}^\top \boldsymbol{\Psi} \boldsymbol{\mu}_{i.} - 2\boldsymbol{\mu}_{i.}^\top \boldsymbol{\Psi} \mathbf{y}_{i.}^*] \\ &= \mathbf{y}_{i.}^{*\top} \boldsymbol{\Psi} \mathbf{y}_{i.}^* - 2\mathbb{E}[\boldsymbol{\mu}_{i.}^\top] \boldsymbol{\Psi} \mathbf{y}_{i.}^* + \text{const.} \\ &= \mathbf{y}_{i.}^{*\top} \boldsymbol{\Psi} \mathbf{y}_{i.}^* - 2\tilde{\boldsymbol{\mu}}_{i.}^\top \boldsymbol{\Psi} \mathbf{y}_{i.}^* + \text{const.} \\ &= (\mathbf{y}_{i.}^* - \tilde{\boldsymbol{\mu}}_{i.})^\top \boldsymbol{\Psi} (\mathbf{y}_{i.}^* - \tilde{\boldsymbol{\mu}}_{i.}) + \text{const.} \end{aligned}$$

The square is then completed to get the final line, which is the expression for the term (\star) multiplied by a half.

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H.1.2 Derivation of $\tilde{q}(\mathbf{w})$

The terms involving \mathbf{w} in ?? are the $p(\mathbf{y}^*|\boldsymbol{\alpha}, \mathbf{w}, \eta, \boldsymbol{\Psi})$ and $p(\mathbf{w}|\boldsymbol{\Psi})$ terms, and the rest are absorbed into the constant. The easiest way to derive $\tilde{q}(\mathbf{w})$ is to vectorise \mathbf{y}^* and \mathbf{w} . We know that

$$\begin{aligned} \text{vec } \mathbf{y}^*|\boldsymbol{\alpha}, \mathbf{w}, \eta, \boldsymbol{\Psi} &\sim N_{nm}(\text{vec}(\mathbf{1}_n \boldsymbol{\alpha}^\top + \mathbf{H}_\eta \mathbf{w}), \boldsymbol{\Psi}^{-1} \otimes \mathbf{I}_n) \\ &\text{and} \\ \text{vec } \mathbf{w}|\boldsymbol{\Psi} &\sim N_{nm}(\mathbf{0}, \boldsymbol{\Psi} \otimes \mathbf{I}_n) \end{aligned}$$

using properties of matrix normal distributions. We also use the fact that $\text{vec}(\mathbf{H}_\eta \mathbf{w}) = (\mathbf{I}_m \otimes \mathbf{H}_\eta) \text{vec } \mathbf{w}$. For simplicity, write $\bar{\mathbf{y}}^* = \text{vec}(\mathbf{y}^* - \mathbf{1}_n \boldsymbol{\alpha}^\top)$, and $\mathbf{M} = (\mathbf{I}_m \otimes \mathbf{H}_\eta)$. Thus,

$$\begin{aligned} \log \tilde{q}(\mathbf{w}) &= E_{\mathbf{y}^* \sim \tilde{q}} \left[-\frac{1}{2} (\bar{\mathbf{y}}^* - \mathbf{M} \text{vec } \mathbf{w})^\top (\boldsymbol{\Psi}^{-1} \otimes \mathbf{I}_n)^{-1} (\bar{\mathbf{y}}^* - \mathbf{M} \text{vec } \mathbf{w}) \right] \\ &\quad + E_{\mathbf{y}^* \sim \tilde{q}} \left[-\frac{1}{2} (\text{vec } \mathbf{w})^\top (\boldsymbol{\Psi} \otimes \mathbf{I}_n)^{-1} \text{vec } \mathbf{w} \right] + \text{const.} \\ &= -\frac{1}{2} E_{\mathbf{y}^* \sim \tilde{q}} \left[(\text{vec } \mathbf{w})^\top \left(\overbrace{\mathbf{M}^\top (\boldsymbol{\Psi} \otimes \mathbf{I}_n) \mathbf{M} + (\boldsymbol{\Psi}^{-1} \otimes \mathbf{I}_n)}^{\mathbf{A}} \right) \text{vec } \mathbf{w} \right] \\ &\quad + E_{\mathbf{y}^* \sim \tilde{q}} \left[\overbrace{\bar{\mathbf{y}}^{*\top} (\boldsymbol{\Psi} \otimes \mathbf{I}_n) \mathbf{M}}^{\mathbf{a}^\top} \text{vec } \mathbf{w} \right] + \text{const.} \\ &= -\frac{1}{2} E_{\mathbf{y}^* \sim \tilde{q}} \left[(\text{vec } \mathbf{w} - \mathbf{A}^{-1} \mathbf{a})^\top \mathbf{A} (\text{vec } \mathbf{w} - \mathbf{A}^{-1} \mathbf{a}) \right] + \text{const.} \end{aligned}$$

This is recognised as a multivariate normal of dimension nm with mean and precision given by $\text{vec } \tilde{\mathbf{w}} = E[\mathbf{A}^{-1} \mathbf{a}]$ and $\tilde{\mathbf{V}}_w^{-1} = E[\mathbf{A}]$ respectively. With a little algebra, we find that

$$\begin{aligned} \tilde{\mathbf{V}}_w &= \{ E_{\mathbf{y}^* \sim \tilde{q}}[\mathbf{A}] \}^{-1} \\ &= \left\{ E_{\mathbf{y}^* \sim \tilde{q}} \left[(\mathbf{I}_m \otimes \mathbf{H}_\eta)^\top (\boldsymbol{\Psi} \otimes \mathbf{I}_n) (\mathbf{I}_m \otimes \mathbf{H}_\eta) + (\boldsymbol{\Psi}^{-1} \otimes \mathbf{I}_n) \right] \right\}^{-1} \\ &= (\boldsymbol{\Psi} \otimes \mathbf{H}_\eta^2 + \boldsymbol{\Psi}^{-1} \otimes \mathbf{I}_n)^{-1} \end{aligned}$$

and

$$\begin{aligned}
 \text{vec } \tilde{\mathbf{w}} &= \mathbb{E}_{\mathbf{y}^* \sim \tilde{q}}[\mathbf{A}^{-1} \mathbf{a}] \\
 &= \tilde{\mathbf{V}}_w \mathbb{E}_{\mathbf{y}^* \sim \tilde{q}}[(\mathbf{I}_m \otimes \mathbf{H}_\eta)(\Psi \otimes \mathbf{I}_n) \text{vec}(\mathbf{y}^* - \mathbf{1}_n \boldsymbol{\alpha}^\top)] \\
 &= \tilde{\mathbf{V}}_w(\Psi \otimes \mathbf{H}_\eta) \mathbb{E}_{\mathbf{y}^* \sim \tilde{q}}[\text{vec}(\mathbf{y}^* - \mathbf{1}_n \boldsymbol{\alpha}^\top)] \\
 &= \tilde{\mathbf{V}}_w(\Psi \otimes \mathbf{H}_\eta) \text{vec}(\tilde{\mathbf{y}}^* - \mathbf{1}_n \boldsymbol{\alpha}^\top).
 \end{aligned}$$

We will often refer to $\tilde{\mathbf{w}}$ as the $n \times m$ matrix constructed by filling in its entries with $\text{vec } \tilde{\mathbf{w}}$ column-wise (akin to the opposite of vectorisation). This way, the $\tilde{\mathbf{w}}$ contains posterior mean values arranged by class $j = 1, \dots, m$ column-wise, and by observations $i = 1, \dots, n$ row-wise. Ideally, we do not want to work with the $nm \times nm$ matrix \mathbf{V}_w , since its inverse is expensive to compute. Refer to [Section 5.6.2](#) for details.

In the case of the I-probit model, where $\Psi = \text{diag}(\psi_1, \dots, \psi_m)$, then the covariance matrix takes a simpler form. Specifically, it has the block diagonal structure:

$$\begin{aligned}
 \tilde{\mathbf{V}}_w &= (\text{diag}(\psi_1, \dots, \psi_m) \otimes \mathbf{H}_\eta^2 + \text{diag}(\psi_1, \dots, \psi_m) \otimes \mathbf{I}_n)^{-1} \\
 &= \text{diag}\left((\psi_1 \mathbf{H}_\eta^2 + \psi_1^{-1} \mathbf{I}_n)^{-1}, \dots, (\psi_m \mathbf{H}_\eta^2 + \psi_m^{-1} \mathbf{I}_n)^{-1}\right) \\
 &=: \text{diag}(\tilde{\mathbf{V}}_{w_1}, \dots, \tilde{\mathbf{V}}_{w_m}).
 \end{aligned}$$

The mean $\text{vec } \tilde{\mathbf{w}}$ is

$$\begin{aligned}
 \text{vec } \tilde{\mathbf{w}} &= \tilde{\mathbf{V}}_w(\text{diag}(\psi_1, \dots, \psi_m) \otimes \tilde{\mathbf{H}}_\eta) \text{vec}(\tilde{\mathbf{y}}^* - \mathbf{1}_n \boldsymbol{\alpha}^\top) \\
 &= \text{diag}(\tilde{\mathbf{V}}_{w_1}, \dots, \tilde{\mathbf{V}}_{w_m}) \text{diag}(\psi_1 \mathbf{H}_\eta, \dots, \psi_m \mathbf{H}_\eta) \text{vec}(\tilde{\mathbf{y}}^* - \mathbf{1}_n \boldsymbol{\alpha}^\top) \\
 &= \text{diag}(\psi_1 \tilde{\mathbf{V}}_{w_1} \mathbf{H}_\eta, \dots, \psi_m \tilde{\mathbf{V}}_{w_m} \mathbf{H}_\eta)(\tilde{\mathbf{y}}^* - \mathbf{1}_n \boldsymbol{\alpha}^\top) \\
 &= \begin{pmatrix} \tilde{\mathbf{w}}_{\cdot 1}^\top & \dots & \tilde{\mathbf{w}}_{\cdot m}^\top \end{pmatrix}^\top \begin{pmatrix} (\psi_1 \tilde{\mathbf{V}}_{w_1} \mathbf{H}_\eta(\tilde{\mathbf{y}}_{\cdot 1}^* - \alpha_1 \mathbf{1}_n))^\top & \dots & (\psi_m \tilde{\mathbf{V}}_{w_m} \mathbf{H}_\eta(\tilde{\mathbf{y}}_{\cdot m}^* - \alpha_m \mathbf{1}_n))^\top \end{pmatrix}^\top.
 \end{aligned}$$

Therefore, we can consider the distribution of $\mathbf{w} = (\mathbf{w}_{\cdot 1}, \dots, \mathbf{w}_{\cdot m})$ columnwise, and each are normally distributed with mean and variance

$$\tilde{\mathbf{w}}_{\cdot j} = \psi_j \tilde{\mathbf{V}}_{w_j} \mathbf{H}_\eta(\tilde{\mathbf{y}}_{\cdot j}^* - \alpha_j \mathbf{1}_n) \quad \text{and} \quad \tilde{\mathbf{V}}_{w_j} = (\psi_j \mathbf{H}_\eta^2 + \psi_j^{-1} \mathbf{I}_n)^{-1}.$$

A quantity that we will be requiring time and again will be $\text{tr}(\mathbf{C} \mathbb{E}[\mathbf{w}^\top \mathbf{D} \mathbf{w}])$, where $\mathbf{C} \in \mathbb{R}^{m \times m}$ and $\mathbf{D} \in \mathbb{R}^{n \times n}$ are both square and symmetric matrices. Using the definition

of the trace directly, we get

$$\begin{aligned}\text{tr}(\mathbf{C} \mathbf{E}[\mathbf{w}^\top \mathbf{D} \mathbf{w}]) &= \sum_{i,j=1}^m \mathbf{C}_{ij} \mathbf{E}[\mathbf{w}^\top \mathbf{D} \mathbf{w}]_{ij} \\ &= \sum_{i,j=1}^m \mathbf{C}_{ij} \mathbf{E}[\mathbf{w}_{\cdot i}^\top \mathbf{D} \mathbf{w}_{\cdot j}].\end{aligned}\tag{H.1}$$

The expectation of the univariate quantity $\mathbf{w}_{\cdot i}^\top \mathbf{D} \mathbf{w}_{\cdot j}$ is inspected below:

$$\begin{aligned}\mathbf{E}[\mathbf{w}_{\cdot i}^\top \mathbf{D} \mathbf{w}_{\cdot j}] &= \text{tr}(\mathbf{D} \mathbf{E}[\mathbf{w}_{\cdot j} \mathbf{w}_{\cdot i}^\top]) \\ &= \text{tr}(\mathbf{D}(\text{Cov}(\mathbf{w}_{\cdot j}, \mathbf{w}_{\cdot i}) + \mathbf{E}[\mathbf{w}_{\cdot j}] \mathbf{E}[\mathbf{w}_{\cdot i}]^\top)) \\ &= \text{tr}(\mathbf{D}(\mathbf{V}_w[i, j] + \tilde{\mathbf{w}}_{\cdot j} \tilde{\mathbf{w}}_{\cdot i}^\top)).\end{aligned}$$

where $\mathbf{V}_w[i, j] \in \mathbb{R}^{n \times n}$ refers to the (i, j) 'th submatrix block of \mathbf{V}_w . Of course, in the independent the I-probit model, this is equal to

$$\mathbf{V}_w[i, j] = \delta_{ij}(\psi_j \mathbf{H}_\eta^2 + \psi_j^{-1} \mathbf{I}_n)^{-1}$$

where δ is the Kronecker delta. Continuing on (H.1) leads us to

$$\text{tr}(\mathbf{C} \mathbf{E}[\mathbf{w}^\top \mathbf{D} \mathbf{w}]) = \sum_{i,j=1}^m \mathbf{C}_{ij} \left(\text{tr}(\mathbf{D}(\delta_{ij} \mathbf{V}_{w_j} + \tilde{\mathbf{w}}_{\cdot j} \tilde{\mathbf{w}}_{\cdot i}^\top)) \right).$$

If $\mathbf{C} = \text{diag}(c_1, \dots, c_m)$, then

$$\begin{aligned}\text{tr}(\mathbf{C} \mathbf{E}[\mathbf{w}^\top \mathbf{D} \mathbf{w}]) &= \sum_{j=1}^m c_j \left(\text{tr}(\mathbf{D} \tilde{\mathbf{V}}_{w_j}) + \tilde{\mathbf{w}}_{\cdot j}^\top \mathbf{D} \tilde{\mathbf{w}}_{\cdot j} \right) \\ &= \sum_{j=1}^m c_j \text{tr}(\mathbf{D}(\tilde{\mathbf{V}}_{w_j} + \tilde{\mathbf{w}}_{\cdot j} \tilde{\mathbf{w}}_{\cdot j}^\top)).\end{aligned}$$

H.2 Deriving the ELBO expression

The evidence lower bound (ELBO) expression involves the following calculation:

$$\begin{aligned}
\mathcal{L}_q(\theta) &= \int \cdots \int q(\mathbf{y}^*, \mathbf{w}) \log \frac{p(\mathbf{y}, \mathbf{y}^*, \mathbf{w} | \theta)}{q(\mathbf{y}^*, \mathbf{w})} d\mathbf{y}^* d\mathbf{w} d\theta \\
&= \mathbb{E} \left[\overbrace{\log p(\mathbf{y}, \mathbf{y}^*, \mathbf{w} | \theta)}^{\text{joint likelihood}} \right] + \left(-\mathbb{E} \left[\overbrace{\log q(\mathbf{y}^*, \mathbf{w})}^{\text{entropy}} \right] \right) \\
&= \mathbb{E} \left[\sum_{i=1}^n \sum_{j=1}^m \log p(y_i | y_{ij}^*) + \sum_{i=1}^n \log p(\mathbf{y}_{i\cdot}^* | \boldsymbol{\alpha}, \mathbf{w}, \boldsymbol{\Psi}, \eta) + \log p(\mathbf{w} | \boldsymbol{\Psi}) \right] \\
&\quad + \sum_{i=1}^n H[q(\mathbf{y}_{i\cdot}^*)] + H[q(\mathbf{w})].
\end{aligned}$$

As discussed, given the latent propensities \mathbf{y}^* , the pdf of \mathbf{y} is degenerate and hence can be disregarded.

H.2.1 Terms involving distributions of \mathbf{y}^*

$$\begin{aligned}
&\sum_{i=1}^n \left(\mathbb{E} \log p(\mathbf{y}_{i\cdot}^* | \boldsymbol{\alpha}, \mathbf{w}, \boldsymbol{\Psi}, \eta) + H[q(\mathbf{y}_{i\cdot}^*)] \right) \\
&= -\frac{nm}{2} \log 2\pi + \frac{n}{2} \log |\boldsymbol{\Psi}| - \frac{1}{2} \mathbb{E} \sum_{i=1}^n (\mathbf{y}_{i\cdot}^* - \boldsymbol{\mu}_{i\cdot})^\top \boldsymbol{\Psi} (\mathbf{y}_{i\cdot}^* - \boldsymbol{\mu}_{i\cdot}) \\
&\quad + \frac{nm}{2} \log 2\pi - \frac{n}{2} \log |\boldsymbol{\Psi}| + \frac{1}{2} \mathbb{E} \sum_{i=1}^n (\mathbf{y}_{i\cdot}^* - \boldsymbol{\mu}_{i\cdot})^\top \boldsymbol{\Psi} (\mathbf{y}_{i\cdot}^* - \boldsymbol{\mu}_{i\cdot}) + \log C_i \\
&= \sum_{i=1}^n \log C_i
\end{aligned}$$

where C_i is the normalising constant for the distribution of multivariate truncated normal $\mathbf{y}_{i\cdot}^* \sim \text{tN}(\boldsymbol{\mu}(x_i), \boldsymbol{\Psi}^{-1}, \mathcal{C}_{y_i})$.

H.2.2 Terms involving distributions of \mathbf{w}

$$\begin{aligned}
 \mathbb{E} \log p(\mathbf{w}|\Psi) + H[q(\mathbf{w})] &= -\cancel{\frac{nm}{2} \log 2\pi} - \frac{n}{2} \log |\Psi| - \frac{1}{2} \mathbb{E} \operatorname{tr} (\mathbf{w} \Psi^{-1} \mathbf{w}^\top) \\
 &\quad + \frac{nm}{2} (1 + \log 2\pi) + \frac{1}{2} \log |\tilde{\mathbf{V}}_w| \\
 &= \frac{nm}{2} - \frac{n}{2} \log |\Psi| - \frac{1}{2} \sum_{i,j=1}^m \Psi_{ij}^{-1} \operatorname{tr} \mathbb{E} [\tilde{\mathbf{w}}_{\cdot j} \tilde{\mathbf{w}}_{\cdot j}^\top] + \frac{1}{2} \log |\tilde{\mathbf{V}}_w|
 \end{aligned}$$

Appendix I

The Gibbs sampler for the I-prior Bayesian variable selection model

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The I-prior Bayesian variable selection model has the following hierarchical form:

$$\begin{aligned}
\mathbf{y}|\alpha, \boldsymbol{\beta}, \gamma, \sigma^2, \kappa &\sim N_n(\alpha \mathbf{1}_n + \mathbf{X}\boldsymbol{\theta}, \sigma^2 I_n) \\
\boldsymbol{\theta} &= (\gamma_1 \beta_1, \dots, \gamma_p \beta_p)^\top \\
\boldsymbol{\beta}|\sigma^2, \kappa &\sim N_p(\mathbf{0}, \sigma^2 \kappa \mathbf{X}^\top \mathbf{X}) \\
\alpha|\sigma^2 &\sim N(0, \sigma^2 A) \\
\sigma^2, \kappa &\sim \Gamma^{-1}(c, d) \\
\gamma_j &\sim \text{Bern}(\pi_j) \quad j = 1, \dots, p
\end{aligned}$$

In the simulations and real-data examples, we used $\pi_j = 0.5, \forall j$, $A = 100$, and $c = d = 0.001$, and the columns of the matrix \mathbf{X} are standardised.

The first line of the set of equations above is the likelihood, while the joint prior density is given by

$$p(\alpha, \boldsymbol{\beta}, \gamma, \sigma^2, \kappa) = p(\boldsymbol{\beta}|\sigma^2)p(\alpha|\sigma^2)p(\sigma^2)p(\kappa)p(\gamma_1) \cdots p(\gamma_p).$$

For simplicity, in the following subsections we shall denote by Θ the entire set of parameters, while $\Theta_{-\xi}$ implies the set of parameters excluding the parameter ξ .

I.1 Conditional posterior for β

$$\begin{aligned}
\log p(\beta|\mathbf{y}, \Theta_{-\beta}) &= \text{const.} + \log p(\mathbf{y}|\Theta) + \log p(\beta|\sigma^2) \\
&= \text{const.} - \frac{1}{2\sigma^2} \|\mathbf{y} - \alpha\mathbf{1}_n - \mathbf{X}_\gamma\beta\|^2 - \frac{1}{2\sigma^2} \beta^\top (\kappa \mathbf{X}^\top \mathbf{X})^{-1} \beta \\
&= \text{const.} - \frac{1}{2\sigma^2} \left(\beta^\top (\mathbf{X}_\gamma^\top \mathbf{X}_\gamma + (\kappa \mathbf{X}^\top \mathbf{X})^{-1}) \beta - 2(\mathbf{y} - \alpha\mathbf{1}_n)^\top \mathbf{X}_\gamma \beta \right) \\
&= \text{const.} - \frac{1}{2\sigma^2} (\beta - \tilde{\mathbf{B}}(\mathbf{y} - \alpha\mathbf{1}_n))^\top \tilde{\mathbf{B}}^{-1} (\beta - \tilde{\mathbf{B}}(\mathbf{y} - \alpha\mathbf{1}_n))
\end{aligned}$$

where $\tilde{\mathbf{B}} = \mathbf{X}_\gamma^\top \mathbf{X}_\gamma + (\kappa \mathbf{X}^\top \mathbf{X})^{-1}$, and $\mathbf{X}_\gamma = (\gamma_1 X_1 \cdots \gamma_p X_p)$ is the $n \times p$ design matrix \mathbf{X} with each of the p columns multiplied by the indicator variable γ . This is of course recognised as the log density of a p -variate normal distribution with mean and variance

$$\mathbb{E}[\beta|\Theta_{-\beta}] = \tilde{\mathbf{B}}(\mathbf{y} - \alpha\mathbf{1}_n) \text{ and } \text{Var}[\beta|\Theta_{-\beta}] = \sigma^2 \tilde{\mathbf{B}}^{-1}.$$

I.2 Conditional posterior for γ

Consider each γ_j in turn. For $j \in \{1, \dots, p\}$,

$$\begin{aligned}
p(\gamma_j|\mathbf{y}, \Theta_{-\gamma_j}) &\propto p(\mathbf{y}|\Theta) p(\gamma_j) \\
&\propto \exp\left(-\frac{1}{2\sigma^2} \|\mathbf{y} - \alpha\mathbf{1}_n - \mathbf{X}\theta\|^2\right) \pi_j^{\gamma_j} (1 - \pi_j)^{1-\gamma_j}
\end{aligned}$$

Since the support of γ_j is $\{0, 1\}$, the above is a probability mass function which can be normalised easily. When $\gamma_j = 1$, we have

$$p(\gamma_j|\mathbf{y}, \Theta_{-\gamma_j}) \propto \pi_j \exp\left(-\frac{1}{2\sigma^2} \|\mathbf{y} - \alpha\mathbf{1}_n - \mathbf{X}\theta_j^{[1]}\|^2\right) := u_j$$

while for $\gamma_j = 0$, we have

$$p(\gamma_j|\mathbf{y}, \Theta_{-\gamma_j}) \propto (1 - \pi_j) \exp\left(-\frac{1}{2\sigma^2} \|\mathbf{y} - \alpha\mathbf{1}_n - \mathbf{X}\theta_j^{[0]}\|^2\right) := v_j.$$

For $j = 1, \dots, p$, we have used the notation $\theta_j^{[\omega]}$ to mean

$$\theta_j^{[\omega]} = \begin{cases} (\theta_1, \dots, \theta_{j-1}, \beta_j, \theta_{j+1}, \dots, \theta_p) & \omega = 1 \\ (\theta_1, \dots, \theta_{j-1}, 0, \theta_{j+1}, \dots, \theta_p) & \omega = 0. \end{cases}$$

Therefore, the conditions distribution for γ_j is Bernoulli with success probability

$$\tilde{\pi}_j = \frac{u_j}{u_j + v_j}.$$

I.3 Conditional posterior for α

We can obtain the conditional posterior for α in a similar fashion we obtained the conditional posterior for β . That is,

$$\begin{aligned} \log p(\alpha | \mathbf{y}, \Theta_{-\alpha}) &= \text{const.} + \log p(\mathbf{y} | \Theta) + \log p(\alpha | \sigma^2) \\ &= \text{const.} - \frac{1}{2\sigma^2} \|\mathbf{y} - \alpha \mathbf{1}_n - \mathbf{X}\boldsymbol{\theta}\|^2 - \frac{\alpha^2}{2\sigma^2 A} \\ &= \text{const.} - \frac{1}{2\sigma^2} \left((n + A^{-1})\alpha^2 - 2\alpha \sum_{i=1}^n (y_i - \mathbf{x}_i^\top \boldsymbol{\theta}) \right) \\ &= \text{const.} - \frac{1}{2\sigma^2(n + A^{-1})} \left(\alpha - \frac{\sum_{i=1}^n (y_i - \mathbf{x}_i^\top \boldsymbol{\theta})}{n + A^{-1}} \right)^2. \end{aligned}$$

Thus, the conditional posterior for α is normal with mean and variance which can be easily read off the final line above.

I.4 Conditional posterior for σ^2

The conditional density for σ^2 is

$$\begin{aligned} \log p(\sigma^2 | \mathbf{y}, \Theta_{-\sigma^2}) &= \text{const.} + \log p(\mathbf{y} | \Theta) + \log p(\sigma^2) \\ &= \text{const.} - \frac{n}{2} \log \sigma^2 - \frac{1}{2\sigma^2} \|\mathbf{y} - \alpha \mathbf{1}_n - \mathbf{X}\boldsymbol{\theta}\|^2 - (c + 1) \log \sigma^2 - d/\sigma^2 \\ &= \text{const.} - (n/2 + c + 1) \log \sigma^2 - \frac{\|\mathbf{y} - \alpha \mathbf{1}_n - \mathbf{X}\boldsymbol{\theta}\|^2/2 + d}{\sigma^2} \end{aligned}$$

which is an inverse gamma distribution with shape $\tilde{c} = n/2 + c + 1$ and scale $\tilde{d} = \|\mathbf{y} - \alpha \mathbf{1}_n - \mathbf{X}\boldsymbol{\theta}\|^2/2 + d$.

I.5 Conditional posterior for κ

Interestingly, since κ is a hyperparameter to be estimated, it does not actually make use of any data, apart from the appearance of \mathbf{X} in the covariance matrix for $\boldsymbol{\beta}$.

$$\begin{aligned} \log p(\kappa|\mathbf{y}, \Theta_{-\kappa}) &= \text{const.} + \log p(\boldsymbol{\beta}|\sigma^2, \kappa) + \log p(\kappa) \\ &= \text{const.} - \frac{p}{2} \log \kappa - \frac{1}{\kappa} \cdot \frac{1}{2\sigma^2} \boldsymbol{\beta}^\top (\mathbf{X}^\top \mathbf{X})^{-1} \boldsymbol{\beta} - (c+1) \log \kappa - d/\kappa \\ &= \text{const.} - (p/2 + c + 1) \log \kappa - \frac{\boldsymbol{\beta}^\top (\mathbf{X}^\top \mathbf{X})^{-1} \boldsymbol{\beta} / \sigma^2 + d}{\kappa} \end{aligned}$$

This is an inverse gamma distribution with shape $\tilde{c} = p/2 + c + 1$ and scale $\tilde{d} = \boldsymbol{\beta}^\top (\mathbf{X}^\top \mathbf{X})^{-1} \boldsymbol{\beta} / \sigma^2 + d$.

I.6 Computational note

From the above, we see that all of the Gibbs conditionals are of recognisable form, making Gibbs sampling a straightforward MCMC method to implement. We built an R package **ipriorBVS** that uses JAGS (Plummer, 2003), a variation of WinBUGS, internally for the Gibbs sampling, and wrote a wrapper function which takes formula based inputs for convenience. The **ipriorBVS** also performs two-stage BVS, and supported priors are the I-prior, g -prior, and independent prior, as used in this thesis. Although a Gibbs sampler could be coded from scratch, JAGS has the advantage of being tried and tested and has simple controls for tuning (burn-in, adaptation, thinning, etc.). Furthermore, the output from JAGS can be inspected using a myriad of multipurpose MCMC tools to diagnose convergence problems. The **ipriorBVS** package is available at <https://github.com/haziqj/ipriorBVS>.

In all examples, a default setting of 4,000 burn-in samples, 1,000 adaptation size, and 10,000 samples with no thinning seemed adequate. There were no major convergence issues encountered.

3. Cite this with correct version.

Computational complexity is dominated by the inversion of a $p \times p$ matrix, and matrix multiplications of order $O(np^2)$. These occur in the conditional posterior for β . Overall, if $n \gg p$, then time complexity is $O(np^2)$. Storage requirements are $O(np)$.

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