

To-do list

1. Exponential family for y not really necessary, it just follows nicely from the latent variable motivation.	2
2. Computational considerations? I think go through the entire chapter without discussing computational issues, and discuss them here. Less cluttered this way.	5
3. How is this calculated? Simulation usually, but also quadrature methods not too bad if m not too large. Stata sheet useful? Talk about if iid errors. . . .	7
4. can use Hamiltonian Monte Carlo?	7
5. Chapter 3	7
6. Lemma X	25
7. Section 4.3.3	29
8. expression XXX	31

Contents

5 I-priors for categorical responses	2
5.1 A naïve model	5
5.2 A latent variable motivation: the I-probit model	5
5.3 Identifiability and IIA	5
5.4 Estimation	5
5.5 A variational algorithm	5
5.6 Post-estimation	5
5.7 Computational consideration	5
5.8 Examples	5
5.9 Discussion	5
5.10 Miscellanea	7
5.10.1 A brief introduction to variational inference	7

5.10.2	Similarity between EM algorithm and variational Bayes	7
5.10.3	A note on computing the multivariate normal integral	7
5.11	Some distributions and their properties	7
5.11.1	Multivariate normal distribution	7
5.11.2	Matrix normal distribution	9
5.11.3	Truncated univariate normal distribution	11
5.11.4	Truncated multivariate normal distribution	13
5.11.5	Wishart distribution	15
5.11.6	Gamma distribution	16
5.12	Proofs related to conically truncated multivariate normal distribution . .	17
5.12.1	Proof of Lemma 5.4: Pdf	17
5.12.2	Proof of Lemma 5.4: Moments	17
5.12.3	Proof of Lemma 5.4: Entropy	22
5.13	Derivation of the CAVI algorithm	22
5.13.1	Derivation of $\tilde{q}(\mathbf{y}^*)$	25
5.13.2	Derivation of $\tilde{q}(\mathbf{w})$	26
5.13.3	Derivation of $\tilde{q}(\eta)$	29
5.13.4	Derivation of $\tilde{q}(\Psi)$	31
5.13.5	Derivation of $\tilde{q}(\alpha)$	33
5.14	Deriving the ELBO expression	34
Bibliography		38

Haziq Jamil

Department of Statistics

London School of Economics and Political Science

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

Chapter 5

I-priors for categorical responses

In a regression setting, consider polytomous response variables y_1, \dots, y_n , where each y_i takes on exactly one of the values $\{1, \dots, m\}$ from a set of m possible choices. Modelling categorical response variables is of profound interest in statistics, econometrics and machine learning, with applications aplenty. In the social sciences, categorical variables often arise from survey responses, and one may be interested in studying correlations between explanatory variables and the categorical response of interest. Economists are often interested in discrete choice models to explain and predict choices between several alternatives, such as consumer choice of goods or modes of transport. In this age of big data, machine learning algorithms are used for classification of observations based on what is usually a large set of variables or features.

As an extension to the I-prior methodology, we propose a flexible modelling framework suitable for regression of categorical response variables.

In the spirit of generalised linear models (McCullagh and Nelder, 1989), we relate the class probabilities of the observations to the I-prior regression model via a link function. Perhaps though, it is more intuitive to view it as machine learners do: Since the regression function is ranged on the entire real line, it is necessary to “squash” it through some sigmoid function to conform it to the interval $[0, 1]$ suitable for probability measures. As in GLMs, the y_i ’s are assumed to follow an exponential family distribution, and in this case, the categorical distribution. We denote this by

$$y_i \sim \text{Cat}(p_{i1}, \dots, p_{im}),$$

1. Exponential family for y not really necessary, it just follows nicely from the latent variable motivation.

with the class probabilities satisfying $p_{ij} \geq 0, \forall j = 1, \dots, m$ and $\sum_{j=1}^m p_{ij} = 1$. The probability mass function (PMF) of y_i is given by

$$p(y_i) = p_{i1}^{[y_i=1]} \dots p_{im}^{[y_i=m]} \quad (5.1)$$

where the notation $[\cdot]$ refers to the Iverson bracket¹. The dependence of the class probabilities on the covariates is specified through the relationship

$$g(p_{ij}) = (\alpha_j + f_j(x_i))_{j=1}^m$$

where $g : [0, 1] \rightarrow \mathbb{R}^m$ is some specified link function. As we will see later, the normality assumption of the errors naturally implies a *probit* link function, i.e., g is the inverse cumulative distribution function (CDF) of a standard normal distribution (or more precisely, a function that *involves* the standard normal CDF). Normality is also a required assumption for I-priors to be specified on the regression functions. We call this method of probit regression using I-priors the *I-probit* regression model.

Note that the probabilities are modelled per class $j \in \{1, \dots, m\}$ by individual regression curves f_j , and in the most general setting, m sets of intercepts α_j and kernel hyperparameters η_j must be estimated. The dependence of these m curves are specified through covariances $\sigma_{jk} := \text{Cov}[\epsilon_{ij}, \epsilon_{ik}]$, for each $j, k \in \{1, \dots, m\}$ and $j \neq k$. While it may be of interest to estimate these covariances, this paper considers cases where the regression functions are class independent, i.e. $\sigma_{jk} = 0, \forall j \neq k$. This violates the independence of irrelevant alternatives (IIA) assumption (see Section 5.3 for details) crucial in choice models, but not so much necessary for classification when the alternatives are distinctively different.

The many advantages of the I-prior methodology of [Jamil and Bergsma, 2017](#) transfer over quite well to the I-probit model for classification and inference. In particular, by choosing appropriate RKHSs for the regression functions, we are able to fit a multitude of binary and multinomial models, including multilevel or random-effects models, linear and non-linear classification models, and even spatio-temporal models. Examples of these models applied to real-world data is shown in Section ???. Working in a Bayesian setting together with variational inference allows us to estimate the model much faster than traditional MCMC sampling methods, yet provides us with the conveniences that come with posterior estimates. For example, inferences around log-odds is usually cumbersome

¹ $[A]$ returns 1 if the proposition A is true, and 0 otherwise. The Iverson bracket is a generalisation of the Kronecker delta.

for probit models, but a credibility interval can easily be obtained by resampling methods from the relevant posteriors, which are normally exponential family distributions in the I-probit model.

5.1 A naïve model

5.2 A latent variable motivation: the I-probit model

5.3 Identifiability and IIA

sec:iaa

5.4 Estimation

5.5 A variational algorithm

sec:iprobit
var

5.6 Post-estimation

5.7 Computational consideration

Computational considerations? I think go through the entire chapter without discussing computational issues, and discuss them here. Less cluttered this way.

This is where talk about computational complexity. Of course, $O(n^3)$ (at least) for binary, otherwise $O(mn^3)$ in general, although can be $O((m-1)n^3)$. Worst case is $O(m^3n^3)$, but manage to reduce this. Storage is $O(n^2)$. Prediction is $O(mn^2)$.

Next, issue with probit link function (so to speak) and that is to compute the truncated normal probabilities. Accuracy? But in the variational algorithm, also require moments involving this truncated normal distribution. For independent probit, this is easier. Otherwise, concerned about accuracy as well.

5.8 Examples

5.9 Discussion

I-prior extended to non-normal data. Naive works good, but can be better. Simply transform the normal model through a squashing function. All the nice things about I-

prior can be applied here too. Probit model variety of binary and multinomial regression models.

Laplace slow, unreliable modes. MCMC also slow. Variational has similarity to EM, but advantageous: easier to calculate posterior s.d., ability to do inference on transformed parameters.

As with the normal model, storage and time requirements slow. again, look to machine learning. improvements in variational algorithm.

Extend to include class-specific covariates.

improvement in calculating the normal integral? Need to see timing where takes longest

In terms of similarity to other works, the generalised additive models (GAMs) of [Hastie and Tibshirani, 1986](#) comes close. The setup of GAMs is near identical to the I-probit model, although estimation is done differently. GAMs do not assume smooth functions from any RKHS, but instead estimates the f 's using a local scoring method or a local likelihood method. Kernel methods for classification are extremely popular in computer science and machine learning; examples include support vector machines ([Schölkopf and Smola, 2002](#)) and Gaussian process classification ([Rasmussen and Williams, 2006](#)), with the latter being more closely related to the I-probit method. I-priors differ from Gaussian process priors in the specification of the covariance kernel. Gaussian process classification typically uses the logistic link function (or squashing function, to use machine learning nomenclature), and estimation is done most commonly using the Laplace approximation, but other methods such as expectation propagation ([Minka, 2001](#)) and MCMC ([Neal, 1999](#)) have been explored as well. Variational inference for Gaussian process probit models have been studied by [Girolami and Rogers, 2006](#), with their work providing a close reference to the variational algorithm employed by us.

5.10 Miscellanea

5.10.1 A brief introduction to variational inference

5.10.2 Similarity between EM algorithm and variational Bayes

5.10.3 A note on computing the multivariate normal integral

How is this calculated? Simulation usually, but also quadrature methods not too bad if m not too large. Stata sheet useful? Talk about iid errors.

Much research has been devoted into developing efficient computational methods for computing these integral, and MCMC methods seem to be the tool of choice in Bayesian analysis (R. McCulloch and Rossi, 1994; Nobile, 1998; R. E. McCulloch et al., 2000). Things get more tractable if Σ is assumed to be diagonal (which corresponds to abandoning the independence of irrelevant alternatives assumption) and much more so if we assume that $\Sigma = \mathbf{I}_m$. The latter yields the *normalised I-probit model*, and a discussion of the merits of this model is given later.

4. can use Hamiltonian Monte Carlo?

Appendix

5.11 Some distributions and their properties

This is a reference relating to the multivariate normal, matrix normal, truncated univariate and multivariate normal, Wishart, and gamma distributions which are collated from various sources for convenience. Of interest are probability density functions, first and second moments, and entropy (as defined in Chapter 3).

5.11.1 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.** $p(X|\mu, \Sigma) = (2\pi)^{-d/2} |\Sigma|^{-1/2} \exp\left(-\frac{1}{2}(X - \mu)^\top \Sigma^{-1}(X - \mu)\right)$.

misc:mnint

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

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

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 5.2. *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 \(2008, §8.1.6\)](#). □

5.11.2 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 5.3 (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.**

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

- **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 $X_i \stackrel{\text{iid}}{\sim} N_m(\mu, \Psi)$ 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 $X \sim \text{MN}(1_n \mu^\top, I_n, \Psi)$.

5.11.3 Truncated univariate normal distribution

Let $X \sim N(\mu, \sigma^2)$ with X lying in the interval (a, b) . Then we say that X follows a truncated normal distribution, and we denote this by $X \sim {}^tN(\mu, \sigma^2, a, b)$. 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.**

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

- **Entropy.**

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

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

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 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 $\text{N}(\mu, \sigma^2)$ 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.

5.11.4 Truncated multivariate normal distribution

Consider the restriction of $X \sim N_d(\mu, \Sigma)$ to a convex subset² $\mathcal{A} \subset \mathbb{R}^d$. 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 $E X$ (mean), $E X^2$ (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 \(1995\)](#) and [Damien and Walker \(2001\)](#). In the latter, the authors explore a simple Gibbs-based approach that is easy to implement in practice. Assume that the one-dimensional slices of \mathcal{A}

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

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

$$\begin{aligned} X_j &\sim {}^tN(\tilde{\mu}_j, \tilde{\sigma}_j^2, x_j^-, x_j^+) \\ \tilde{\mu}_j &= \mu_j + \Sigma_{j,-j}^\top \Sigma_{-j,-j}^{-1} (x_{-j} - \mu_{-j}) \\ \tilde{\sigma}_j^2 &= \Sigma_{jj} - \Sigma_{j,-j}^\top \Sigma_{-j,-j}^{-1} \Sigma_{j,-j}. \end{aligned}$$

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} . Introduce a latent variable $Y \in \mathbb{R}$ such that the joint pdf of X and Y is

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

²A 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.

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.

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 5.4. *Let $X \sim \text{N}_d(\mu, \Sigma, \mathcal{C}_j)$, 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

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

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

thm:contrun
cn

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

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

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

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

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 [Section 5.12](#) for the proof. □

5.11.5 Wishart distribution

Let $X \in \mathbb{R}^{m \times m}$ be a symmetric, positive-definite matrix. The Wishart distribution with scale matrix Ψ and $s > m - 1$ degrees of freedom is denoted $X \sim \text{Wis}_m(\Psi, s)$, and its pdf, moments and entropy are

- **Pdf.**

$$p(X) = \frac{|X|^{(m-s-1)/2} e^{-\text{tr}(\Psi^{-1}X)/2}}{2^{sm/2} |\Psi|^{s/2} \Gamma_m(s/2)}.$$

- **Moments.** $\mathbb{E} X = s\Psi$, $\text{Var } X_{ij} = s(\Psi_{ij}^2 + \Psi_{ii}\Psi_{jj})$.
- **Entropy.**

$$H(p) = \frac{m+1}{2} \log |\Psi| + \frac{1}{2} m(m+1) \log 2 + \log \Gamma_p \left(\frac{s}{2} \right) - \frac{s-m-1}{2} \psi_m \left(\frac{s}{2} \right) + \frac{sm}{2}.$$

In the above, $\Gamma_m(\cdot)$ and $\psi_m(\cdot)$ are the multivariate gamma and digamma functions, respectively, given by

$$\Gamma_m(a) = \int_{U>0} \exp(-\text{tr } U) |U|^{a-(m+1)/2} dU$$

for positive-definite, real, $m \times m$ matrices U , and

$$\psi_m(a) = \frac{\partial}{\partial a} \log \Gamma_p(a).$$

5.11.6 Gamma distribution

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.** $E X = s/r$, $\text{Var } X_{ij} = s/r^2$.
- **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.

apx:contrun
proof

5.12 Proofs related to conically truncated multivariate normal distribution

5.12.1 Proof of Lemma 5.4: Pdf

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

$$\begin{aligned}
& \int \cdots \int \mathbb{1}[x_i < x_j, \forall i \neq j] \prod_{i=1}^d \phi(x_i | \mu_i, \sigma_i^2) dx_1 \cdots dx_d \\
&= \int \cdots \int \mathbb{1}[x_i < x_j, \forall i \neq j] \prod_{i=1}^d \left[\frac{1}{\sigma_i} \phi\left(\frac{x_i - \mu_i}{\sigma_i}\right) \right] dx_1 \cdots dx_d \\
&= \int \cdots \int \mathbb{1}[x_i < x_j, \forall i \neq j] \frac{1}{\sigma_j} \phi\left(\frac{x_j - \mu_j}{\sigma_j}\right) \prod_{\substack{i=1 \\ i \neq j}}^d \left[\frac{1}{\sigma_i} \phi\left(\frac{x_i - \mu_i}{\sigma_i}\right) \right] dx_1 \cdots dx_d \\
&= \int \prod_{\substack{i=1 \\ i \neq j}}^d \Phi\left(\frac{x_j - \mu_i}{\sigma_i}\right) \frac{1}{\sigma_j} \phi\left(\frac{x_j - \mu_j}{\sigma_j}\right) dx_j \\
&= \int \prod_{\substack{i=1 \\ i \neq j}}^d \Phi\left(\frac{\sigma_j z + \mu_j - \mu_i}{\sigma_i}\right) \phi(z) dz \\
&\quad \text{(by using the standardisation } z = (x_j - \mu_j)/\sigma_j) \\
&= \mathbb{E}_Z \left[\prod_{\substack{i=1 \\ i \neq j}}^d \Phi\left(\frac{\sigma_j}{\sigma_i} Z + \frac{\mu_j - \mu_i}{\sigma_i}\right) \right]
\end{aligned}$$

the proof follows directly.

5.12.2 Proof of Lemma 5.4: Moments

Recall that for $Y \sim {}^t\text{N}(\mu, \sigma^2, -\infty, b)$, 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

$$\mathbb{E}[Y - \mu] = -\sigma \frac{\phi(\beta)}{\Phi(\beta)} \quad (5.2)$$

$$\mathbb{E}[Y - \mu]^2 - \sigma^2 = -\sigma^2 \frac{\beta \phi(\beta)}{\Phi(\beta)} \quad (5.3)$$

where $\beta = (b - \mu)/\sigma$. For the conically truncated multivariate normal distribution $X \sim {}^t\text{N}_d(\mu, \Sigma, \mathcal{A}_j)$, 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

$$\begin{aligned} \mathbb{E} g(X_i) &= C^{-1} \int \cdots \int g(x_i) \mathbb{1}[x_k < x_j, \forall k \neq j] \prod_{k=1}^d p(x_k) dx_1 \cdots dx_d \\ &= C^{-1} \frac{\Phi((x_j - \mu_j)/\sigma_j)}{\Phi((x_j - \mu_j)/\sigma_j)} \iint g(x_i) \mathbb{1}[x_i < x_j] p(x_i) p(x_j) \prod_{\substack{k=1 \\ k \neq i, j}}^d \Phi\left(\frac{x_j - \mu_k}{\sigma_k}\right) dx_i dx_j \\ &= C^{-1} \int \mathbb{E}_{X_i \sim {}^t\text{N}(\mu_i, \sigma_i^2, -\infty, x_j)} g(X_i) \prod_{\substack{k=1 \\ k \neq j}}^d \Phi\left(\frac{x_j - \mu_k}{\sigma_k}\right) p(x_j) dx_j \end{aligned} \quad (5.4)$$

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

$$\begin{aligned} \mathbb{E} g(X_j) &= C^{-1} \int \cdots \int g(x_j) \mathbb{1}[x_k < x_j, \forall k \neq j] \prod_{k=1}^d p(x_k) dx_1 \cdots dx_d \\ &= C^{-1} \int g(x_j) \prod_{\substack{k=1 \\ k \neq j}}^d \Phi\left(\frac{x_j - \mu_k}{\sigma_k}\right) p(x_j) dx_j. \end{aligned} \quad (5.5)$$

Plugging in (5.2) for $g(X_i) = X_i - \mu_i$ in (5.4) we get

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

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 (5.5) 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 5.5 in the second last step.

For the second moments, plug in (5.3) for $g(X_i) = (X_i - \mu_i)^2 - \sigma_i^2$ in (5.4) to get

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

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 5.5. *Let $Z \sim N(0, 1)$. 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

5.12.3 Proof of [Lemma 5.4](#): Entropy

As a direct consequence of the definition of entropy,

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

5.13 Derivation of the CAVI algorithm

Let $\mathcal{Z} = \{\mathbf{y}^*, \mathbf{w}, \alpha, \eta, \Psi\}$. Approximate the posterior for \mathcal{Z} by a mean-field variational distribution

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

The first line is by assumption, while the second line follows from an induced factorisation on the latent propensities, as we will see later. If needed, we also assume that $q(\eta)$ factorises into its constituents components. Recall that, for each $\xi \in \mathcal{Z}$, the optimal mean-field variational density \tilde{q} for ξ satisfies

$$\log \tilde{q}(\xi) = \mathbb{E}_{-\xi}[\log p(\mathbf{y}, \mathcal{Z})] + \text{const.} \quad (??)$$

Write $\mathbf{f} = \mathbf{H}_\eta \mathbf{w} \in \mathbb{R}^{n \times m}$. The joint likelihood $p(\mathbf{y}, \mathcal{Z})$ is given by

$$\begin{aligned} p(\mathbf{y}, \mathcal{Z}) &= p(\mathbf{y}|\mathcal{Z})p(\mathcal{Z}) \\ &= p(\mathbf{y}|\mathbf{y}^*)p(\mathbf{y}^*|\boldsymbol{\alpha}, \mathbf{w}, \eta, \boldsymbol{\Psi})p(\mathbf{w}|\boldsymbol{\Psi})p(\eta)p(\boldsymbol{\Psi})p(\boldsymbol{\alpha}). \end{aligned}$$

For reference, the 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.

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

- $p(\mathbf{y}^*|\boldsymbol{\alpha}, \mathbf{w}, \eta, \boldsymbol{\Psi})$. 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

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

where $\mathbf{y}_i^* \in \mathbb{R}^m$ and $\boldsymbol{\mu}_i \in \mathbb{R}^m$ 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^* are independent multivariate normal with mean $\boldsymbol{\mu}_i$ and variance $\boldsymbol{\Psi}^{-1}$.

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

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

- $p(\eta)$. The most common scenario would be $\eta = \{\lambda_1, \dots, \lambda_p\}$ only. In this case, choose independent normal priors for each $\lambda_k \sim N(m_k, v_k)$, $k = 1, \dots, p$, whose pdf is

$$p(\eta) = \prod_{k=1}^p \exp \left[-\frac{1}{2} \log 2\pi - \frac{1}{2} \log v_k - \frac{1}{2v_k} (\lambda_k - m_k)^2 \right].$$

An improper prior $p(\eta) \propto \text{const.}$ can be used as well, and this is the same as letting $m_k \rightarrow 0$ and $v_k \rightarrow 0$. The resulting posterior will be proper. If η contains other parameters as well, such as the Hurst coefficient $\gamma \in (0, 1)$, SE lengthscale $l > 0$ or polynomial offset $c > 0$, then appropriate priors should be used to match the support of the parameter. Choices include $p(\gamma) = \mathbb{1}(\gamma \in (0, 1))$ and $l, c \sim \Gamma(a, b)$.

- $p(\Psi)$. For the precision matrix, a Wishart prior with scale matrix \mathbf{G}^{-1} and g degrees of freedom, denoted $\Psi \sim \text{Wis}_m(\mathbf{G}^{-1}, g)$, is convenient. It has pdf

$$p(\Psi) = \exp \left[\text{const.} + \frac{g - m - 1}{2} \log |\Psi| - \frac{1}{2} \text{tr}(\mathbf{G}\Psi) \right].$$

For the independent I-probit model, $\Psi = \text{diag}(\psi_1, \dots, \psi_m)$, and we choose independent Gamma distributions for each precision $\sigma_j^{-2} \sim \Gamma(s_j, r_j)$, where s_j and r_j are the shape and rate parameters. Then,

$$p(\Psi) = \prod_{j=1}^m \exp [\text{const.} + (s_j - 1) \log \psi_j - r_j \psi_j].$$

- $p(\alpha)$. Choose independent normal priors for the intercept, $\alpha_j \sim N(a_j, A_j)$ for $j = 1, \dots, m$. The pdf is

$$p(\alpha) = \prod_{j=1}^m \exp \left[\log 2\pi - \log A_j - \frac{1}{2A_j} (\alpha_j - a_j)^2 \right].$$

Remark 5.1. The priors on the parameters $\{\boldsymbol{\alpha}, \eta\}$ can be set to very vague or even improper priors, and the resulting posterior will still yield a proper distribution. Using improper priors eases the algebra slightly. For the precision matrix $\boldsymbol{\Psi}$, it is best to stick with the Wishart prior to avoid positive-definite issues, unless the independent I-probit model is used, in which case Jeffreys' prior for the precisions $p(\sigma_j^{-2}) \propto \sigma_j^2$ is a convenient choice.

5.13.1 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 $j \in \{1, \dots, m\}$. The mean-field density $q(\mathbf{y}_i^*)$ for each $i = 1, \dots, n$ is found to be

$$\begin{aligned} \log \tilde{q}(\mathbf{y}_i^*) &= \mathbb{1}[y_{ij}^* = \max_k y_{ik}^*] \mathbb{E}_{\mathcal{Z} \setminus \{\mathbf{y}^*\} \sim q} \left[-\frac{1}{2} (\mathbf{y}_i^* - \boldsymbol{\mu}_i)^\top \boldsymbol{\Psi} (\mathbf{y}_i^* - \boldsymbol{\mu}_i) \right] + \text{const.} \\ &= \mathbb{1}[y_{ij}^* = \max_k y_{ik}^*] \left[-\frac{1}{2} (\mathbf{y}_i^* - \tilde{\boldsymbol{\mu}}_i)^\top \tilde{\boldsymbol{\Psi}} (\mathbf{y}_i^* - \tilde{\boldsymbol{\mu}}_i) \right] + \text{const.} \quad (\star) \\ &\equiv \begin{cases} \phi(\mathbf{y}_i^* | \tilde{\boldsymbol{\mu}}_i, \tilde{\boldsymbol{\Psi}}) & \text{if } y_{ij}^* > y_{ik}^*, \forall k \neq j \\ 0 & \text{otherwise} \end{cases} \end{aligned}$$

where $\tilde{\boldsymbol{\mu}}_i = \mathbb{E} \boldsymbol{\alpha} + (\mathbb{E} \mathbf{H}_\eta \mathbb{E} \mathbf{w})_i$, and expectations are taken under the optimal mean-field distribution \tilde{q} . The distribution $q(\mathbf{y}_i^*)$ is a truncated m -variate normal distribution such that the j 'th component is always largest. Unfortunately, the expectation of this distribution cannot be found in closed-form, and must be approximated by techniques such as Monte Carlo integration. If, however, the independent I-probit model is used and $\tilde{\boldsymbol{\Psi}}$ is diagonal, then [Lemma X](#) provides a simplification.

Remark 5.2. In (\star) above, we needn't consider the second order terms in the expectations because they do not involve \mathbf{y}^* and can be absorbed into the constant. To see this,

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

We will see this occurring a lot later on and we shall take note of this fact.

5.13.2 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,

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

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

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

and making a first-order approximation $(E \mathbf{A})^{-1} \approx E[\mathbf{A}^{-1}]^3$,

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

Ideally, we do not want to work with the $nm \times nm$ matrix \mathbf{V}_w , since its inverse is expensive to compute. We can exploit the Kronecker product structure to compute the inverse efficiently. Perform an orthogonal eigendecomposition of \mathbf{H}_η to obtain $\mathbf{H}_\eta = \mathbf{V} \mathbf{U} \mathbf{V}^\top$ and of Ψ to obtain $\Psi = \mathbf{Q} \mathbf{P} \mathbf{Q}^\top$. This process takes $O(n^3 + m^3) \approx O(n^3)$ time if $m \ll n$. Then, manipulate \mathbf{V}_w^{-1} as follows (for clarity, we drop the tildes from the notations):

$$\begin{aligned} \mathbf{V}_w^{-1} &= (\Psi \otimes \mathbf{H}_\eta^2) + (\Psi^{-1} \otimes \mathbf{I}_n) \\ &= (\mathbf{Q} \mathbf{P} \mathbf{Q}^\top \otimes \mathbf{V} \mathbf{U}^2 \mathbf{V}^\top) + (\mathbf{Q} \mathbf{P}^{-1} \mathbf{Q}^\top \otimes \mathbf{V} \mathbf{V}^\top) \\ &= (\mathbf{Q} \otimes \mathbf{V})(\mathbf{P} \otimes \mathbf{U}^2)(\mathbf{Q}^\top \otimes \mathbf{V}^\top) + (\mathbf{Q} \otimes \mathbf{V})(\mathbf{P}^{-1} \otimes \mathbf{I}_n)(\mathbf{Q}^\top \otimes \mathbf{V}^\top) \\ &= (\mathbf{Q} \otimes \mathbf{V})(\mathbf{P} \otimes \mathbf{U}^2 + \mathbf{P}^{-1} \otimes \mathbf{I}_n)(\mathbf{Q}^\top \otimes \mathbf{V}^\top) \end{aligned}$$

Its inverse is

$$\begin{aligned} \mathbf{V}_w &= (\mathbf{Q}^\top \otimes \mathbf{V}^\top)^{-1} (\mathbf{P} \otimes \mathbf{U}^2 + \mathbf{P}^{-1} \otimes \mathbf{I}_n)^{-1} (\mathbf{Q} \otimes \mathbf{V})^{-1} \\ &= (\mathbf{Q} \otimes \mathbf{V})(\mathbf{P} \otimes \mathbf{U}^2 + \mathbf{P}^{-1} \otimes \mathbf{I}_n)^{-1} (\mathbf{Q}^\top \otimes \mathbf{V}^\top) \end{aligned}$$

which is easy to compute since the middle term is an inverse of diagonal matrices.

In the case of the I-probit model, where $\Psi = \text{diag}(\sigma_1^{-2}, \dots, \sigma_m^{-2})$, then the covariance \mathbf{V}_w takes a simpler form. Specifically, it has the block diagonal structure:

$$\begin{aligned} \mathbf{V}_w &= (\text{diag}(\tilde{\sigma}_1^{-2}, \dots, \tilde{\sigma}_m^{-2}) \otimes \tilde{\mathbf{H}}_\eta^2 + (\text{diag}(\tilde{\sigma}_1^2, \dots, \tilde{\sigma}_m^2) \otimes \mathbf{I}_n)^{-1})^{-1} \\ &= \text{diag} \left((\tilde{\sigma}_1^{-2} \tilde{\mathbf{H}}_\eta^2 + \tilde{\sigma}_1^2 \mathbf{I}_n)^{-1}, \dots, (\tilde{\sigma}_m^{-2} \tilde{\mathbf{H}}_\eta^2 + \tilde{\sigma}_m^2 \mathbf{I}_n)^{-1} \right) \\ &=: \text{diag}(\tilde{\mathbf{V}}_{w_1}, \dots, \tilde{\mathbf{V}}_{w_m}). \end{aligned}$$

³Groves and Rothenberg (1969) show that $E[\mathbf{A}^{-1}] = (E \mathbf{A})^{-1} + \mathbf{B}$, where \mathbf{B} is a positive-definite matrix.

The mean $\tilde{\mathbf{w}}$ in matrix form is

$$\begin{aligned}
 \tilde{\mathbf{w}} &= \tilde{\mathbf{V}}_w (\text{diag}(\tilde{\sigma}_1^{-2}, \dots, \tilde{\sigma}_m^{-2}) \otimes \tilde{\mathbf{H}}_\eta) (\tilde{\mathbf{y}}^* - \mathbf{1}_n \tilde{\boldsymbol{\alpha}}^\top) \\
 &= \text{diag}(\tilde{\mathbf{V}}_{w_1}, \dots, \tilde{\mathbf{V}}_{w_m}) \text{diag}(\tilde{\sigma}_1^{-2} \tilde{\mathbf{H}}_\eta, \dots, \tilde{\sigma}_m^{-2} \tilde{\mathbf{H}}_\eta) (\tilde{\mathbf{y}}^* - \mathbf{1}_n \tilde{\boldsymbol{\alpha}}^\top) \\
 &= \text{diag}(\tilde{\sigma}_1^{-2} \tilde{\mathbf{V}}_{w_1} \tilde{\mathbf{H}}_\eta, \dots, \tilde{\sigma}_m^{-2} \tilde{\mathbf{V}}_{w_m} \tilde{\mathbf{H}}_\eta) (\tilde{\mathbf{y}}^* - \mathbf{1}_n \tilde{\boldsymbol{\alpha}}^\top) \\
 &= \begin{pmatrix} \tilde{\mathbf{w}}_{\cdot 1} & \dots & \tilde{\mathbf{w}}_{\cdot m} \end{pmatrix} \\
 &= \begin{pmatrix} \tilde{\sigma}_1^{-2} \tilde{\mathbf{V}}_{w_1} \tilde{\mathbf{H}}_\eta (\tilde{\mathbf{y}}_{\cdot 1}^* - \tilde{\alpha}_1 \mathbf{1}_n) & \dots & \tilde{\sigma}_m^{-2} \tilde{\mathbf{V}}_{w_m} \tilde{\mathbf{H}}_\eta (\tilde{\mathbf{y}}_{\cdot m}^* - \tilde{\alpha}_m \mathbf{1}_n) \end{pmatrix}.
 \end{aligned}$$

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

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

A quantity that we will be requiring time and again will be $\text{tr}(\mathbf{C} \mathbf{E}[\mathbf{w}^\top \mathbf{D} \mathbf{w}])$, 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

$$\begin{aligned}
 \text{tr}(\mathbf{C} \mathbf{E}[\mathbf{w}^\top \mathbf{D} \mathbf{w}]) &= \sum_{i,j=1}^m \mathbf{C}_{ij} \mathbf{E}[\mathbf{w}^\top \mathbf{D} \mathbf{w}]_{ij} \\
 &= \sum_{i,j=1}^m \mathbf{C}_{ij} \mathbf{E}[\mathbf{w}_{\cdot i}^\top \mathbf{D} \mathbf{w}_{\cdot j}].
 \end{aligned} \tag{5.6}$$

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 (5.6) 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

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

5.13.3 Derivation of $\tilde{q}(\eta)$

By looking at only the terms involving η in ??, we deduce that \tilde{q} for η satisfies

$$\begin{aligned} \log \tilde{q}(\eta) &= -\frac{1}{2} \text{tr} \mathbf{E}_{\mathcal{Z} \setminus \{\eta\} \sim q} \left[(\mathbf{y}^* - \mathbf{1}_n \boldsymbol{\alpha}^\top - \mathbf{H}_\eta \mathbf{w}) \boldsymbol{\Psi} (\mathbf{y}^* - \mathbf{1}_n \boldsymbol{\alpha}^\top - \mathbf{H}_\eta \mathbf{w})^\top \right] + \log p(\eta) \\ &\quad + \text{const.} \\ &= -\frac{1}{2} \text{tr} \mathbf{E}_{\mathcal{Z} \setminus \{\eta\} \sim q} \left(\boldsymbol{\Psi} \mathbf{w}^\top \mathbf{H}_\eta^2 \mathbf{w} - 2 \boldsymbol{\Psi} \mathbf{w}^\top \mathbf{H}_\eta (\mathbf{y}^* - \boldsymbol{\alpha}) \right) + \log p(\eta) + \text{const.} \\ &= -\frac{1}{2} \text{tr} \left(\tilde{\boldsymbol{\Psi}} \mathbf{E}[\mathbf{w}^\top \mathbf{H}_\eta^2 \mathbf{w}] - 2 \tilde{\boldsymbol{\Psi}} \tilde{\mathbf{w}}^\top \mathbf{H}_\eta (\tilde{\mathbf{y}}^* - \tilde{\boldsymbol{\alpha}}) \right) + \log p(\eta) + \text{const.} \end{aligned}$$

with some appropriate prior $p(\eta)$. In general, this does not have a recognisable form in η , especially when it is not linearly dependent on the kernel matrix. This happens when considering parameters other than the scales of the RKHSs. Our interest would be to obtain $\tilde{\mathbf{H}}_\eta := \mathbf{E}_{\eta \sim q} \mathbf{H}_\eta$ and $\tilde{\mathbf{H}}_\eta^2 := \mathbf{E}_{\eta \sim q} \mathbf{H}_\eta^2$. We use a Metropolis random-walk algorithm to obtain these quantities, as detailed in the algorithm below.

Now consider the case where $\eta = \{\lambda_1, \dots, \lambda_p\}$ (RKHS scale parameters only), and the scenario described in the exponential family EM algorithm of [Section 4.3.3](#) applies. In particular, for $k = 1, \dots, p$, we can decompose the kernel matrix as $\mathbf{H}_\eta = \lambda_k \mathbf{R}_k + \mathbf{S}_k$ and its square as $\mathbf{H}_\eta^2 = \lambda_k^2 \mathbf{R}_k^2 + \lambda_k \mathbf{U}_k + \mathbf{S}_k^2$. Then, for $j = 1, \dots, m$, assuming each of

Algorithm 1 Metropolis random-walk to sample η

- 1: **inputs** $\tilde{\alpha}$, $\tilde{\mathbf{w}}$, $\tilde{\Psi}$, and s Metropolis sampling s.d.
- 2: **initialise** $\eta^{(0)} \in \mathbb{R}^q$ and $t \leftarrow 0$
- 3: **for** $t = 1, \dots, T$ **do**
- 4: Draw $\eta^* \sim N_q(\eta^{(t)}, s^2)$
- 5: Accept/reject proposal state, i.e.

$$\eta^{(t+1)} \leftarrow \begin{cases} \eta^* & \text{if } u \sim \text{Unif}(0, 1) < \pi_{\text{acc}} \\ \eta^{(t)} & \text{otherwise} \end{cases}$$

where

$$\pi_{\text{acc}} = \min \left(1, \exp \left(\log \tilde{q}(\eta^*) - \log \tilde{q}(\eta^{(t)}) \right) \right).$$

6: **end for**

$$7: \tilde{\mathbf{H}}_\eta \leftarrow \frac{1}{T} \sum_{i=1}^T \mathbf{H}_{\eta^{(i)}} \text{ and } \tilde{\mathbf{H}}_\eta^2 \leftarrow \frac{1}{T} \sum_{i=1}^T \mathbf{H}_{\eta^{(i)}}^2$$

the $q(\lambda_k)$ densities are independent of each other, we find that

$$\begin{aligned} \log \tilde{q}(\lambda_k) &= \mathbb{E}_{\mathcal{Z} \setminus \{\eta\} \sim q} \left[-\frac{1}{2} \text{tr} \left((\mathbf{y}^* - \boldsymbol{\mu}) \Psi (\mathbf{y}^* - \boldsymbol{\mu})^\top \right) \right] - \frac{1}{2v_k^2} (\lambda_k - m_k)^2 + \text{const.} \\ &= -\frac{1}{2} \text{tr} \mathbb{E}_{\mathcal{Z} \setminus \{\eta\} \sim q} \left[\Psi \mathbf{w}^\top \mathbf{H}_\eta^2 \mathbf{w} - 2\Psi (\mathbf{y}^* - \mathbf{1}\boldsymbol{\alpha}^\top)^\top \mathbf{H}_\eta \mathbf{w} \right] \\ &\quad - \frac{1}{2v_k^2} (\lambda_k - m_k)^2 + \text{const.} \\ &= -\frac{1}{2} \text{tr} \mathbb{E}_{\mathcal{Z} \setminus \{\eta\} \sim q} \left[\Psi \mathbf{w}^\top (\lambda_k^2 \mathbf{R}_k^2 + \lambda_k \mathbf{U}_k) \mathbf{w} - 2\Psi (\mathbf{y}^* - \mathbf{1}\boldsymbol{\alpha}^\top)^\top (\lambda_k \mathbf{R}_k) \mathbf{w} \right] \\ &\quad - \frac{1}{2v_k^2} (\lambda_k^2 - 2m_k \lambda_k) + \text{const.} \\ &= -\frac{1}{2} \text{tr} \mathbb{E}_{\mathcal{Z} \setminus \{\eta\} \sim q} \left[\lambda_k^2 \Psi \mathbf{w}^\top \mathbf{R}_k^2 \mathbf{w} - 2\lambda_k \left(\Psi (\mathbf{y}^* - \mathbf{1}\boldsymbol{\alpha}^\top)^\top \mathbf{R}_k \mathbf{w} - \frac{1}{2} \Psi \mathbf{w}^\top \mathbf{U}_k \mathbf{w} \right) \right] \\ &\quad - \frac{1}{2} \left(\frac{1}{v_k^2} \lambda_k^2 - 2\frac{m_k}{v_k^2} \lambda_k \right) + \text{const.} \\ &= -\frac{1}{2} \left[\lambda_k^2 \overbrace{(\text{tr}(\tilde{\Psi} \mathbb{E}[\mathbf{w}^\top \mathbf{R}_k^2 \mathbf{w}]) + v_k^{-2})}^{c_k} \right. \\ &\quad \left. - 2\lambda_k \overbrace{\left(\text{tr} \left(\tilde{\Psi} (\tilde{\mathbf{y}}^* - \mathbf{1}\tilde{\boldsymbol{\alpha}}^\top)^\top \mathbf{R}_k \tilde{\mathbf{w}} - \frac{1}{2} \tilde{\Psi} \mathbb{E}[\mathbf{w}^\top \mathbf{U}_k \mathbf{w}] \right) + m_k v_k^{-2} \right)}^{d_k} \right] \end{aligned}$$

By completing the squares, we recognise this is as the kernel of a univariate normal density. Specifically, $\lambda_k \sim N(d_k/c_k, 1/c_k)$. The quantity $\tilde{\mathbf{H}}_\eta$ can be obtained by substituting

tuting $\lambda_k \mapsto \mathbb{E}_{\lambda_k \sim q}[\lambda_k]$ in the **expression XXX**. However, in the calculation of $\tilde{\mathbf{H}}_\eta^2$, we must replace $\lambda_k^2 \mapsto \mathbb{E}_{\lambda_k \sim q}[\lambda_k]^2 + \text{Var}_{\lambda_k \sim q}[\lambda_k]$ in all occurrences of square terms. This can be cumbersome, so if felt necessary, use the approximation $\lambda_k^2 \mapsto \mathbb{E}_{\lambda_k \sim q}[\lambda_k]^2$ instead.

Example 5.1. Suppose $k = 1$, and we only have λ to estimate. Then, $\mathbf{H}_\eta = \lambda \mathbf{H}$, $\mathbf{R}_k = \mathbf{H}$, $\mathbf{R}_k^2 = \mathbf{H}^2$, and $\mathbf{U}_k = \mathbf{0}$. Suppose also we use an improper prior $\lambda_k \propto \text{const.}$, which is the same as having $v_k^2 \rightarrow 0$ and $m_k v_k^{-2} \rightarrow 0$. The mean field distribution for λ is then

$$\lambda \sim \text{N} \left(\frac{\text{tr}(\tilde{\Psi}(\tilde{\mathbf{y}}^* - \mathbf{1}\tilde{\alpha}^\top)^\top \mathbf{H}\tilde{\mathbf{w}})}{\text{tr}(\tilde{\Psi} \mathbb{E}[\mathbf{w}^\top \mathbf{H}^2 \mathbf{w}])}, \frac{1}{\text{tr}(\tilde{\Psi} \mathbb{E}[\mathbf{w}^\top \mathbf{H}^2 \mathbf{w}])} \right)$$

Further, if $\tilde{\Psi} = \tilde{\psi} \mathbf{I}_m$, then

$$\lambda \sim \text{N} \left(\frac{\sum_{j=1}^m (\tilde{\mathbf{y}}_{\cdot,j}^* - \tilde{\alpha}_j \mathbf{1})^\top \mathbf{H} \tilde{\mathbf{w}}_{\cdot,j}}{\sum_{j=1}^m \text{tr}(\mathbf{H}^2 \mathbb{E}[\mathbf{w}_{\cdot,j} \mathbf{w}_{\cdot,j}^\top])}, \frac{1}{\sum_{j=1}^m \text{tr}(\mathbf{H}^2 \mathbb{E}[\mathbf{w}_{\cdot,j} \mathbf{w}_{\cdot,j}^\top])} \right)$$

which bears a resemblance to the exponential family EM algorithm solutions described in Chapter 4. Now, $\tilde{\mathbf{H}}_\eta = \mathbb{E}[\lambda \mathbf{H}] = \tilde{\lambda} \mathbf{H}$, and $\tilde{\mathbf{H}}_\eta^2 = \mathbb{E}[\lambda^2 \mathbf{H}^2] = (\text{Var } \lambda + \tilde{\lambda}^2) \mathbf{H}^2$.

5.13.4 Derivation of $\tilde{q}(\Psi)$

Introduce the transformed random matrix $\mathbf{u} = \mathbf{w} \Psi^{-1} \in \mathbb{R}^{n \times m}$. Since we have that $\text{vec } \mathbf{u} = (\text{vec } \mathbf{w})^\top (\Psi^{-1} \otimes \mathbf{I}_n)$, the optimal mean-field distribution for \mathbf{u} is normal with mean $\text{vec } \tilde{\mathbf{u}} = \text{vec}(\tilde{\mathbf{w}} \tilde{\Psi}^{-1})$ and variance

$$\tilde{\mathbf{V}}_u = (\tilde{\Psi}^{-1} \otimes \mathbf{I}_n) \tilde{\mathbf{V}}_w (\tilde{\Psi}^{-1} \otimes \mathbf{I}_n).$$

In the case of the independent model, its mean is $\tilde{\mathbf{u}}_{\cdot,j} = \tilde{\psi}_j^{-1} \tilde{\mathbf{u}}_{\cdot,j}$ for $j = 1, \dots, m$ and its variance is

$$\tilde{\mathbf{V}}_u = \text{diag}(\tilde{\psi}_1^{-2} \tilde{\mathbf{V}}_{w_1}, \dots, \tilde{\psi}_m^{-2} \tilde{\mathbf{V}}_{w_m}).$$

Now, to derive $\tilde{q}(\Psi)$ for the full I-probit model, we inspect the equation

$$\begin{aligned} \log \tilde{q}(\Psi) &= \mathbb{E}_{\mathcal{Z} \setminus \{\Psi\} \sim q} \left[\frac{n}{2} \log |\Psi| - \frac{1}{2} \text{tr}((\mathbf{y}^* - \boldsymbol{\mu})^\top (\mathbf{y}^* - \boldsymbol{\mu}) \Psi) + \frac{n}{2} \log |\Psi| - \frac{1}{2} \text{tr}(\mathbf{u}^\top \mathbf{u} \Psi) \right] \\ &\quad + \frac{g - m - 1}{2} \log |\Psi| - \frac{1}{2} \text{tr}(\mathbf{G} \Psi) + \text{const.} \\ &= -\frac{1}{2} \text{tr} \left((\mathbf{G} + \overbrace{\mathbb{E}[(\mathbf{y}^* - \boldsymbol{\mu})^\top (\mathbf{y}^* - \boldsymbol{\mu})]}^{\mathbf{G}_1} + \overbrace{\mathbb{E}[\mathbf{u}^\top \mathbf{u}]}^{\mathbf{G}_2}) \Psi \right) \\ &\quad + \frac{2n + g - m - 1}{2} \log |\Psi| + \text{const.} \end{aligned}$$

which we recognise to be a Wishart distribution with scale matrix $(\mathbf{G} + \mathbf{G}_1 + \mathbf{G}_2)^{-1}$ and $2n + g - m$ degrees of freedom. Note that using an improper prior, i.e. $\mathbf{G} = \mathbf{0}$ and $g = m$, will still yield a proper posterior distribution. The mean of this distribution is $\tilde{\Psi} = (2n + g - m)(\mathbf{G} + \mathbf{G}_1 + \mathbf{G}_2)^{-1}$. The matrix \mathbf{G}_1 is given as

$$\begin{aligned} \mathbf{G}_1 &= \mathbb{E}[(\mathbf{y}^* - \boldsymbol{\mu})^\top (\mathbf{y}^* - \boldsymbol{\mu})] \\ &= \mathbb{E}[\mathbf{y}^{*\top} \mathbf{y}^* + \boldsymbol{\alpha} \mathbf{1}_n^\top \mathbf{1}_n \boldsymbol{\alpha}^\top + \mathbf{w}^\top \mathbf{H}_\eta \mathbf{w} - 2\mathbf{y}^{*\top} \mathbf{1}_n \boldsymbol{\alpha}^\top - 2\mathbf{y}^{*\top} \mathbf{H}_\eta \mathbf{w} - 2\boldsymbol{\alpha} \mathbf{1}_n^\top \mathbf{H}_\eta \mathbf{w}] \\ &= \mathbb{E}[\mathbf{y}^{*\top} \mathbf{y}^*] + n \mathbb{E}[\boldsymbol{\alpha} \boldsymbol{\alpha}^\top] + \mathbb{E}[\mathbf{w}^\top \mathbf{H}_\eta \mathbf{w}] - 2(\tilde{\mathbf{y}}^{*\top} \mathbf{1}_n \tilde{\boldsymbol{\alpha}}^\top + \tilde{\mathbf{y}}^{*\top} \tilde{\mathbf{H}}_\eta \tilde{\mathbf{w}} + \tilde{\boldsymbol{\alpha}} \mathbf{1}_n^\top \tilde{\mathbf{H}}_\eta \tilde{\mathbf{w}}) \end{aligned}$$

This involves second order moments of a conically truncated multivariate normal distribution, which needs to be obtained via simulation. Meanwhile,

$$\begin{aligned} \mathbf{G}_{2,ij} &= \mathbb{E}[\mathbf{u}^\top \mathbf{u}]_{ij} \\ &= \mathbb{E}[\mathbf{u}_{\cdot i}^\top \mathbf{u}_{\cdot j}] \\ &= \tilde{\mathbf{V}}_u[i, j] + \tilde{\mathbf{u}}_{\cdot i}^\top \tilde{\mathbf{u}}_{\cdot j}. \end{aligned}$$

In the case of the I-probit model, we use a gamma prior on each of the precisions in the diagonal entries of $\Psi = \text{diag}(\psi_1, \dots, \psi_m)$. Then, the variational density for each ψ_j

is found to be

$$\begin{aligned}
\log \tilde{q}(\psi_j) &= \mathbb{E}_{\mathcal{Z} \setminus \{\Psi\} \sim q} \left[\frac{n}{2} \log(\psi_1 \cdots \psi_m) - \frac{1}{2} \sum_{j=1}^m \sum_{i=1}^n \psi_j (\mathbf{y}_{ij}^* - \boldsymbol{\mu}_{ij})^2 \right] \\
&\quad + \mathbb{E}_{\mathcal{Z} \setminus \{\Psi\} \sim q} \left[-\frac{n}{2} \log(\psi_1 \cdots \psi_m) - \frac{1}{2} \sum_{j=1}^m \sum_{i=1}^n \psi_j \mathbf{u}_{ij}^2 \right] \\
&\quad + \sum_{j=1}^m ((s_j - 1) \log \psi_j - r_j \psi_j) + \text{const.} \\
&= (s_j - 1) \log \psi_j - \psi_j \left(\frac{1}{2} \mathbb{E} \|\mathbf{y}_{\cdot j} - \boldsymbol{\mu}_{\cdot j}\|^2 + \frac{1}{2} \mathbb{E} \|\mathbf{u}_{\cdot j}\|^2 + r_j \right) + \text{const.}
\end{aligned}$$

which is again a gamma distribution, and the shape and rate parameters can be read directly. The mean is given by $\tilde{\psi}_j = s_j (\frac{1}{2} \mathbb{E} \|\mathbf{y}_{\cdot j} - \boldsymbol{\mu}_{\cdot j}\|^2 + \frac{1}{2} \mathbb{E} \|\mathbf{u}_{\cdot j}\|^2 + r_j)^{-1}$. Recall that each of the n components of $\mathbf{y}_{\cdot j} - \boldsymbol{\mu}_{\cdot j}$ are independent, and can be calculated using the methods described above. Also, we have $\mathbf{u}_{\cdot j} \sim N_n(\tilde{\mathbf{u}}_{\cdot j}, \tilde{\mathbf{V}}_{u_j})$, and so $\mathbb{E} \|\mathbf{u}_{\cdot j}\|^2 = \text{tr}(\tilde{\mathbf{V}}_{u_j} + \tilde{\mathbf{u}}_{\cdot j} \tilde{\mathbf{u}}_{\cdot j}^\top)$.

5.13.5 Derivation of $\tilde{q}(\alpha)$

The terms involving α_j in ?? are

$$\begin{aligned}
\log \tilde{q}(\alpha_j) &= \mathbb{E}_{\mathcal{Z} \setminus \{\alpha\} \sim q} \left[-\frac{1}{2} \sum_{k=1}^m \sum_{i=1}^n \psi_{ik} (y_{ik}^* - \alpha_j - f_{ik})^2 \right] - \frac{A_j^{-1}}{2} (\alpha_j - a_j)^2 + \text{const.} \\
&= -\frac{1}{2} \mathbb{E} \left[\alpha_j^2 \sum_{i=1}^n \psi_{ij} - 2\alpha_j \sum_{i=1}^n \psi_{ij} (y_{ij}^* - f_{ij}) \right] - \frac{1}{2} (A_j^{-1} \alpha_j^2 - 2A_j^{-1} a_j \alpha_j) + \text{const.} \\
&= -\frac{\sum_{i=1}^n \tilde{\psi}_{ij} + A_j^{-1}}{2} \left(\alpha_j - \frac{\sum_{i=1}^n \tilde{\psi}_{ij} (\tilde{y}_{ij}^* - \tilde{f}_{ij}) + A_j^{-1} a_j}{\sum_{i=1}^n \tilde{\psi}_{ij} + A_j^{-1}} \right)^2 + \text{const.}
\end{aligned}$$

which implies a normal distribution for α_j whose mean and variance can be read directly. Here, we used the notation \tilde{f}_{ij} to mean the (i, j) 'th element of $\mathbb{E}[\mathbf{H}_\eta \mathbf{w}] = \tilde{\mathbf{H}}_\eta \tilde{\mathbf{w}} \in \mathbb{R}^{n \times m}$.

As a remark, due to identifiability, only $m - 1$ of these intercept are estimable. We can either put a constraint that one of the intercepts is fixed at zero, or the sum of the intercepts equals zero. The latter constraint is implemented in this thesis, and this is realised by estimating all the intercepts and then centring them.

5.14 Deriving the ELBO expression

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

$$\begin{aligned}
 \mathcal{L} &= \int q(\mathbf{y}^*, \mathbf{w}, \lambda, \alpha) \log \left[\frac{p(\mathbf{y}, \mathbf{y}^*, \mathbf{w}, \lambda, \alpha)}{q(\mathbf{y}^*, \mathbf{w}, \lambda, \alpha)} \right] d\mathbf{y}^* d\mathbf{w} d\lambda d\alpha \\
 &= \mathbb{E}[\log p(\mathbf{y}, \mathbf{y}^*, \mathbf{w}, \lambda, \alpha)] - \mathbb{E}[\log q(\mathbf{y}^*, \mathbf{w}, \lambda, \alpha)] \\
 &= \mathbb{E} \left[\log \prod_{i=1}^n \prod_{j=1}^m p(y_i | y_{ij}^*) \right] + \mathbb{E}[\log p(\mathbf{y}^* | \mathbf{f})] + \mathbb{E}[\log p(\mathbf{w})] + \mathbb{E}[\log p(\lambda)] + \mathbb{E}[\log p(\alpha)] \\
 &\quad - \mathbb{E}[\log q(\mathbf{y}^*)] - \mathbb{E}[\log q(\mathbf{w})] - \mathbb{E}[\log q(\lambda)] - \mathbb{E}[\log q(\alpha)]
 \end{aligned}$$

Note that the categorical pmf $p(y_i | y_{ij}^*)$ becomes degenerate once the latent variables are known, so this term is cancelled out. With the exception of $q(\mathbf{y}^*)$, all of the distributions are Gaussian. The following results will be helpful.

Terms involving distributions of \mathbf{y}^*

$$\begin{aligned}
 \mathbb{E}[\log p(\mathbf{y}^* | \mathbf{f})] - \mathbb{E}[\log q(\mathbf{y}^*)] &= \sum_{i=1}^n \sum_{j=1}^m \mathbb{E}[\log p(y_{ij}^* | f_{ij})] + \sum_{i=1}^n \mathcal{H}(q(y_i^*)) \\
 &= \sum_{i=1}^n \sum_{j=1}^m \left(-\frac{1}{2} \log 2\pi - \frac{1}{2} \mathbb{E}[y_{ij}^* - f_{ij}]^2 \right) \\
 &\quad + \sum_{i=1}^n \sum_{j=1}^m \left(\frac{1}{2} \log 2\pi + \frac{1}{2} \mathbb{E}[y_{ij}^* - f_{ij}]^2 \right) + \sum_{i=1}^n \log C_i
 \end{aligned}$$

Terms involving distributions of \mathbf{w}

$$\begin{aligned}
 \mathbb{E} [\log p(\mathbf{w})] - \mathbb{E} [\log q(\mathbf{w})] &= \sum_{j=1}^m \left(\mathbb{E} [\log p(\mathbf{w}_j)] - \mathbb{E} [\log q(\mathbf{w}_j)] \right) \\
 &= \sum_{j=1}^m \left(-\frac{n}{2} \log 2\pi - \frac{1}{2} \mathbb{E} [\mathbf{w}_j^\top \mathbf{w}_j] + \mathcal{H}(q(\mathbf{w}_j)) \right) \\
 &= \sum_{j=1}^m \left(-\cancel{\frac{n}{2} \log 2\pi} - \frac{1}{2} \text{tr} \left(\mathbb{E} [\mathbf{w}_j \mathbf{w}_j^\top] \right) + \frac{n}{2} (1 + \log 2\pi) - \frac{1}{2} \log |\mathbf{A}_j| \right) \\
 &= \frac{nm}{2} - \frac{1}{2} \sum_{j=1}^m \left(\text{tr} \widetilde{\mathbf{W}}_j + \log |\mathbf{A}_j| \right)
 \end{aligned}$$

Terms involving distribution of $q(\lambda)$

$$\begin{aligned}
 -\mathbb{E} [\log q(\lambda)] &= \sum_{j=1}^m \mathcal{H}(q(\lambda_j)) \\
 &= \sum_{j=1}^m \left(\frac{1}{2} (1 + \log 2\pi) - \frac{1}{2} \log c_j \right) \\
 &= \frac{m}{2} (1 + \log 2\pi) - \frac{1}{2} \sum_{j=1}^m \log c_j
 \end{aligned}$$

or if using single λ

$$-\mathbb{E} [\log q(\lambda)] = \frac{1}{2} (1 + \log 2\pi) - \frac{1}{2} \log \sum_{j=1}^m c_j.$$

Terms involving distribution of $q(\alpha)$

$$\begin{aligned}
 -\mathbb{E} [\log q(\alpha)] &= \sum_{j=1}^m \mathcal{H}(q(\alpha_j)) \\
 &= \frac{m}{2} (1 + \log 2\pi - \log n)
 \end{aligned}$$

or if using single α

$$- \mathbb{E} [\log q(\alpha)] = \frac{1}{2}(1 + \log 2\pi - \log nm).$$

The lower bound

$$\begin{aligned} \mathcal{L} &= \sum_{i=1}^n \log C_i + \frac{nm}{2} - \frac{1}{2} \sum_{j=1}^m \left(\text{tr } \widetilde{\mathbf{W}}_j + \log |\mathbf{A}_j| \right) \\ &\quad + \frac{m}{2}(1 + \log 2\pi) - \frac{1}{2} \sum_{j=1}^m \log c_j + \frac{m}{2}(1 + \log 2\pi - \log n) \\ &= \frac{m}{2}(n + 2(1 + \log 2\pi) - \log n) - \frac{1}{2} \sum_{j=1}^m \left(\text{tr } \widetilde{\mathbf{W}}_j + \log |\mathbf{A}_j| + \log c_j \right) + \sum_{i=1}^n \log C_i \end{aligned}$$

Of course, if using either single α or single λ , then the formula needs to be adjusted accordingly.

Bibliography

- | | |
|-------------------------|---|
| chopin2011fast | Chopin, Nicolas (2011). “Fast simulation of truncated Gaussian distributions”. In: <i>Statistics and Computing</i> 21.2, pp. 275–288. |
| damien2001sampling | Damien, Paul and Stephen G Walker (2001). “Sampling truncated normal, beta, and gamma densities”. In: <i>Journal of Computational and Graphical Statistics</i> 10.2, pp. 206–215. |
| girolami2006variational | Girolami, Mark and Simon Rogers (2006). “Variational Bayesian Multinomial Probit Regression with Gaussian Process Priors”. In: <i>Neural Computation</i> 18.8, pp. 1790–1817. |
| groves1969note | Groves, Theodore and Thomas Rothenberg (1969). “A note on the expected value of an inverse matrix”. In: <i>Biometrika</i> 56.3, pp. 690–691. |
| hastie1986 | Hastie, Trevor and Robert Tibshirani (Aug. 1986). “Generalized Additive Models”. In: <i>Statist. Sci.</i> 1.3, pp. 297–310. DOI: 10.1214/ss/1177013604 . URL: https://doi.org/10.1214/ss/1177013604 . |
| jamil2017 | Jamil, Haziq and Wicher Bergsma (2017). “iprior: An R Package for Regression Modelling using I-priors”. In: <i>Manuscript in submission</i> . |
| marsaglia2000ziggurat | Marsaglia, George and Wai Wan Tsang (2000). “The ziggurat method for generating random variables”. In: <i>Journal of statistical software</i> 5.8, pp. 1–7. |
| mccullagh1989 | McCullagh, P. and John A. Nelder (1989). <i>Generalized Linear Models</i> . 2nd. Chapman & Hall/CRC Press. |
| mcculloch2000bayesian | McCulloch, Robert E, Nicholas G Polson, and Peter E Rossi (2000). “A Bayesian analysis of the multinomial probit model with fully identified parameters”. In: <i>Journal of econometrics</i> 99.1, pp. 173–193. |

mcculloch1994exact	McCulloch, Robert and Peter E Rossi (1994). “An exact likelihood analysis of the multinomial probit model”. In: <i>Journal of Econometrics</i> 64.1, pp. 207–240.
minka2001expectation	Minka, Thomas P (2001). “Expectation propagation for approximate Bayesian inference”. In: <i>Proceedings of the Seventeenth conference on Uncertainty in artificial intelligence</i> . Morgan Kaufmann Publishers Inc., pp. 362–369.
neal1999	Neal, Radford M. (1999). “Regression and Classification using Gaussian Process Priors”. In: <i>Bayesian Statistics</i> . Ed. by J M Bernardo, J O Berger, A P Dawid, and A F M Smith. Vol. 6. Oxford University Press. (with discussion), pp. 475–501.
nobile1998hybrid	Nobile, Agostino (1998). “A hybrid Markov chain for the Bayesian analysis of the multinomial probit model”. In: <i>Statistics and Computing</i> 8.3, pp. 229–242.
petersen2008matrix	Petersen, Kaare Brandt and Michael Syskind Pedersen (2008). “The matrix cookbook”. In: <i>Technical University of Denmark</i> 7.15, p. 510.
rasmussen2006gaussian	Rasmussen, Carl Edward and Christopher K I Williams (2006). <i>Gaussian Processes for Machine Learning</i> . The MIT Press.
robert1995simulation	Robert, Christian P (1995). “Simulation of truncated normal variables”. In: <i>Statistics and computing</i> 5.2, pp. 121–125.
scholkopf2002learning	Schölkopf, Bernhard and Alexander J Smola (2002). <i>Learning with Kernels: Support Vector Machines, Regularization, Optimization, and Beyond</i> . MIT Press.
zhang2013kronecker	Zhang, Huamin and Feng Ding (2013). “On the Kronecker products and their applications”. In: <i>Journal of Applied Mathematics</i> 2013.