

Cosine basis

Daeyoung Lim*
Department of Statistics
Korea University

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1 Criteo Dataset

1.1 File descriptions

- **train.csv** - The training set consists of a portion of Criteo's traffic over a period of 7 days. Each row corresponds to a display ad served by Criteo. Positive (clicked) and negatives (non-clicked) examples have both been subsampled at different rates in order to reduce the dataset size. The examples are chronologically ordered.
- **test.csv** - The test set is computed in the same way as the training set but for events on the day following the training period.
- **random_submission.csv** - A sample submission file in the correct format.

1.2 Data fields

- **Label** - Target variable that indicates if an ad was clicked (1) or not (0).
- **I1 - I13** - A total of 13 columns of integer features (mostly count features).
- **C1 - C26** - A total of 26 columns of categorical features. The values of these features have been hashed onto 32 bits for anonymization purposes.

The semantics of the features is undisclosed. When a value is missing, the field is empty.

2 Normal

2.1 Model specifications

$$\begin{aligned}y_i &= w_i' \beta + f(x_i) + \epsilon_i, & \epsilon_i &\sim \mathcal{N}(0, \sigma^2) \\ \theta_j | \sigma, \tau, \gamma &\sim \mathcal{N}(0, \sigma^2 \tau^2 \exp[-j\gamma]) \\ \tau^2 &\sim \text{IG}\left(\frac{r_{0,\tau}}{2}, \frac{s_{0,\tau}}{2}\right) \\ \sigma^2 &\sim \text{IG}\left(\frac{r_{0,\sigma}}{2}, \frac{s_{0,\sigma}}{2}\right) \\ \beta &\sim \mathcal{N}(\mu_\beta^0, \Sigma_\beta^0) \\ \gamma &\sim \text{Exp}(\omega_0) \\ |\psi| &= \gamma, \quad \psi \sim \text{DE}(0, \omega_0) \\ \varphi_j(x) &= \sqrt{2} \cos(\pi j x)\end{aligned}$$

*Prof. Taeryon Choi

Joint density:

$$p(y, \Theta) = \mathcal{N}(y|W\beta + f_J, \sigma^2 I_n) \left\{ \prod_{j=1}^J \mathcal{N}(\theta_j|0, \sigma^2 \tau^2 \exp[-j|\psi|]) \right\} \text{IG}\left(\tau^2 \middle| \frac{r_{0,\tau}}{2}, \frac{s_{0,\tau}}{2}\right) \text{IG}\left(\sigma^2 \middle| \frac{r_{0,\sigma}}{2}, \frac{s_{0,\sigma}}{2}\right) \mathcal{N}(\beta|\mu_\beta^0, \Sigma_\beta^0) \\ \text{DE}(\psi|0, \omega_0)$$

We will use the joint density to derive the LB and updating algorithm. The variational distributions are

$$\begin{aligned} q_1(\beta) &= \mathcal{N}(\mu_\beta^q, \Sigma_\beta^q) \\ q_2(\theta_J) &= \mathcal{N}(\mu_\theta^q, \Sigma_\theta^q) \\ q_3(\sigma^2) &= \text{IG}\left(\frac{r_{q,\sigma}}{2}, \frac{s_{q,\sigma}}{2}\right) \\ q_4(\tau^2) &= \text{IG}\left(\frac{r_{q,\tau}}{2}, \frac{s_{q,\tau}}{2}\right) \\ q_5(\psi) &= \mathcal{N}(\mu_\psi^q, \sigma_\psi^{2q}) \quad (\text{NCVMP}). \end{aligned}$$

2.2 Lower bound

2.2.1 LB: $\mathbb{E}[\ln p(y|\Theta)]$

$$\begin{aligned} \mathbb{E}[\ln p(y|\Theta)] &= -\frac{n}{2} \ln(2\pi\sigma^2) - \frac{1}{2} \mathbb{E}[(y - W\beta - \varphi_J \theta)'(y - W\beta - \varphi_J \theta)] \\ &= -\frac{n}{2} \ln(2\pi\sigma^2) - \frac{1}{2} (y - W\mu_\beta^q - \varphi_J \mu_\theta^q)' (y - W\mu_\beta^q - \varphi_J \mu_\theta^q) - \frac{1}{2} (\text{Tr}(W'W\Sigma_\beta^q) + \text{Tr}(\varphi_J' \varphi_J \Sigma_\theta^q)) \end{aligned}$$

2.3 LB: $\mathbb{E}[\ln p(\theta_j|\sigma, \tau, \psi)]$

$$\sum_{j=1}^J \mathbb{E}[\ln p(\theta_j|\sigma, \tau, \psi)] = \sum_{j=1}^J \mathbb{E}\left[-\frac{1}{2} \ln(2\pi) + \ln \frac{1}{\sigma} + \ln \frac{1}{\tau} + \frac{j}{2} |\psi| - \frac{\theta_j^2 e^{j|\psi|}}{2\sigma^2 \tau^2}\right]$$

Let's note the following fact: if $X \sim \mathcal{N}(\mu, \sigma^2)$, then $|X| \sim \text{folded-Normal}(\mu, \sigma^2)$. Then,

$$\begin{aligned} \mathbb{E}|X| &= \sigma \sqrt{\frac{2}{\pi}} \exp\left\{-\frac{\mu^2}{2\sigma^2}\right\} + \mu \left(1 - 2\Phi\left(\frac{-\mu}{\sigma}\right)\right) \\ &= \sigma \sqrt{\frac{2}{\pi}} \exp\left\{-\frac{\mu^2}{2\sigma^2}\right\} - \mu \text{erf}\left(\frac{-\mu}{\sqrt{2}\sigma}\right) \\ \mathbb{E}e^{t|X|} &= \exp\left\{\frac{\sigma^2 t^2}{2} + \mu t\right\} \left[1 - \Phi\left(-\frac{\mu}{\sigma} - \sigma t\right)\right] + \exp\left\{\frac{\sigma^2 t^2}{2} - \mu t\right\} \left[1 - \Phi\left(\frac{\mu}{\sigma} - \sigma t\right)\right]. \end{aligned}$$

3 Probit: No Restriction

3.1 Model specifications

$$\begin{aligned}
\Pr(y_i = 1|f, \beta) &= \Phi(w'_i \beta + f(x_i)) \\
y_i^* &= w'_i \beta + f(x_i) + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, 1) \\
y_i &= \begin{cases} 1, & \text{if } y_i^* \geq 0 \\ 0, & \text{if } y_i^* < 0 \end{cases} \\
\theta_j | \sigma, \tau, \gamma &\sim \mathcal{N}(0, \sigma^2 \tau^2 \exp[-j\gamma]) \\
\tau^2 &\sim \text{IG}\left(\frac{r_{0,\tau}}{2}, \frac{s_{0,\tau}}{2}\right) \\
\sigma^2 &\sim \text{IG}\left(\frac{r_{0,\sigma}}{2}, \frac{s_{0,\sigma}}{2}\right) \\
\beta &\sim \mathcal{N}(\mu_\beta^0, \sigma^2 \Sigma_\beta^0) \quad (p \times 1) \\
\gamma &\sim \text{Exp}(\omega_0) \\
|\psi| &= \gamma, \quad \psi \sim \text{DE}(0, \omega_0) \\
\varphi_j(x) &= \sqrt{2} \cos(\pi j x)
\end{aligned}$$

Joint density:

$$\begin{aligned}
p(y, y^*, \Theta) &= C \left\{ \prod_{j=1}^J \mathcal{N}(\theta_j | 0, \sigma^2 \tau^2 \exp[-j|\psi|]) \right\} \text{IG}\left(\tau^2 \middle| \frac{r_{0,\tau}}{2}, \frac{s_{0,\tau}}{2}\right) \text{IG}\left(\sigma^2 \middle| \frac{r_{0,\sigma}}{2}, \frac{s_{0,\sigma}}{2}\right) \mathcal{N}(\beta | \mu_\beta^0, \sigma^2 \Sigma_\beta^0) \\
&\quad \text{DE}(\psi | 0, \omega_0) \left\{ \prod_{i=1}^n (1[y_i^* \geq 0] 1[y_i = 1] + 1[y_i^* < 0] 1[y_i = 0]) \phi(y_i^* - w'_i \beta - \varphi'_i \theta_J) \right\}
\end{aligned}$$

where C is the normalizing constant. The variational distributions are

$$\begin{aligned}
q_1(\beta) &= \mathcal{N}(\mu_\beta^q, \Sigma_\beta^q) \\
q_2(\theta_J) &= \mathcal{N}(\mu_\theta^q, \Sigma_\theta^q) \\
q_3(\sigma^2) &= \text{IG}\left(\frac{r_{q,\sigma}}{2}, \frac{s_{q,\sigma}}{2}\right) \\
q_4(\tau^2) &= \text{IG}\left(\frac{r_{q,\tau}}{2}, \frac{s_{q,\tau}}{2}\right) \\
q_5(\psi) &= \mathcal{N}(\mu_\psi^q, \sigma_\psi^{2q}) \quad (\text{NCVMP}) \\
q_6(y^*) &= \mathcal{TN}(\mu_{y^*}^q, I_n, 0)
\end{aligned}$$

3.2 Lower bound

3.2.1 LB: $\mathbb{E} [\ln p(y^*|\text{rest})] + \mathbb{H}[y^*]$

$$\begin{aligned} \mathbb{E} [\ln p(y^*|\text{rest})] + \mathbb{H}[y^*] &= \sum_{i=1}^n \mathbb{E} \left[\ln \phi(y_i^* - w_i' \beta - \varphi_i' \theta_J) - \ln \phi(y_i^* - w_i' \mu_\beta^q - \varphi_i' \mu_\theta^q) \right] \\ &\quad + \sum_{i=1}^n \ln \left(\left\{ \Phi(w_i' \mu_\beta^q + \varphi_i' \mu_\theta^q) \right\}^{y_i} \left\{ 1 - \Phi(w_i' \mu_\beta^q + \varphi_i' \mu_\theta^q) \right\}^{1-y_i} \right) \\ &= -\frac{1}{2} \left(\text{Tr}(W' W \Sigma_\beta^q) + \text{Tr}(\varphi_J' \varphi_J \Sigma_\theta^q) \right) \\ &\quad + \sum_{i=1}^n \ln \left(\left\{ \Phi(w_i' \mu_\beta^q + \varphi_i' \mu_\theta^q) \right\}^{y_i} \left\{ 1 - \Phi(w_i' \mu_\beta^q + \varphi_i' \mu_\theta^q) \right\}^{1-y_i} \right) \end{aligned}$$

3.2.2 LB: $\mathbb{E} [\ln p(\theta_j|\sigma, \tau, \psi)]$

Let's note the following fact: if $X \sim \mathcal{N}(\mu, \sigma^2)$, then $|X| \sim \text{folded-Normal}(\mu, \sigma^2)$. Then,

$$\begin{aligned} \mathbb{E}|X| &= \sigma \sqrt{\frac{2}{\pi}} \exp \left\{ -\frac{\mu^2}{2\sigma^2} \right\} + \mu \left(1 - 2\Phi \left(\frac{-\mu}{\sigma} \right) \right) \\ &= \sigma \sqrt{\frac{2}{\pi}} \exp \left\{ -\frac{\mu^2}{2\sigma^2} \right\} - \mu \text{erf} \left(\frac{-\mu}{\sqrt{2}\sigma} \right) \\ \mathbb{E} e^{t|X|} &= \exp \left\{ \frac{\sigma^2 t^2}{2} + \mu t \right\} \left[1 - \Phi \left(-\frac{\mu}{\sigma} - \sigma t \right) \right] + \exp \left\{ \frac{\sigma^2 t^2}{2} - \mu t \right\} \left[1 - \Phi \left(\frac{\mu}{\sigma} - \sigma t \right) \right]. \end{aligned}$$

Therefore,

$$\begin{aligned} \sum_{j=1}^J \mathbb{E} [\ln p(\theta_j|\sigma, \tau, \psi)] + \mathbb{H}[\theta_J] &= \sum_{j=1}^J \mathbb{E} \left[-\frac{1}{2} \ln(2\pi) + \frac{1}{2} \ln \frac{1}{\sigma^2} + \frac{1}{2} \ln \frac{1}{\tau^2} + \frac{j}{2} |\psi| - \frac{\theta_j^2 e^{j|\psi|}}{2\sigma^2 \tau^2} \right] + \mathbb{H}[\theta_J] \\ &= -\frac{J}{2} \left\{ \ln(2\pi) - \left(\text{di} \left(\frac{r_{q,\sigma}}{2} \right) - \ln \left(\frac{s_{q,\sigma}}{2} \right) \right) - \left(\text{di} \left(\frac{r_{q,\tau}}{2} \right) - \ln \left(\frac{s_{q,\tau}}{2} \right) \right) \right\} \\ &\quad + \frac{J(J+1)}{4} \left\{ \sigma_\psi^q \sqrt{\frac{2}{\pi}} \exp \left(-\frac{\mu_\psi^{q^2}}{2\sigma_\psi^{q^2}} \right) + \mu_\psi^q \left(1 - 2\Phi \left(\frac{-\mu_\psi^q}{\sigma_\psi^q} \right) \right) \right\} \\ &\quad - \frac{1}{2} \frac{r_{q,\sigma}}{s_{q,\sigma}} \frac{r_{q,\tau}}{s_{q,\tau}} \left(\text{Tr}(\Sigma_\theta^q) + \mu_\theta^{q'} \mu_\theta^q \right) \sum_{j=1}^J Q_j \left(\mu_\psi^q, \sigma_\psi^{q^2} \right) + \frac{J}{2} (1 + \ln(2\pi)) + \frac{1}{2} \ln |\Sigma_\theta^q| \end{aligned}$$

where

$$\begin{aligned} Q_j \left(\mu_\psi^q, \sigma_\psi^{q^2} \right) &= \mathbb{E} e^{j|\psi|} \\ &= \exp \left\{ \frac{\sigma_\psi^{q^2} j^2}{2} + \mu_\psi^q j \right\} \left[1 - \Phi \left(-\frac{\mu_\psi^q}{\sigma_\psi^q} - \sigma_\psi^q j \right) \right] + \exp \left\{ \frac{\sigma_\psi^{q^2} j^2}{2} - \mu_\psi^q j \right\} \left[1 - \Phi \left(\frac{\mu_\psi^q}{\sigma_\psi^q} - \sigma_\psi^q j \right) \right]. \end{aligned}$$

3.2.3 LB: $\mathbb{E} [\ln p(\tau^2)] + \mathbb{H}[\tau^2]$

$$\begin{aligned} \mathbb{E} [\ln p(\tau^2)] + \mathbb{H}[\tau^2] &= \frac{r_{0,\tau}}{2} \ln \left(\frac{s_{0,\tau}}{2} \right) - \ln \Gamma \left(\frac{r_{0,\tau}}{2} \right) + \left(\frac{r_{0,\tau}}{2} - \frac{r_{q,\tau}}{2} \right) \text{di} \left(\frac{r_{q,\tau}}{2} \right) - \left(\frac{r_{0,\tau}}{2} + 1 \right) \ln \left(\frac{s_{q,\tau}}{2} \right) \\ &\quad - \frac{s_{0,\tau}}{2} \frac{r_{q,\tau}}{s_{q,\tau}} + \frac{r_{q,\tau}}{2} + \ln \left(\frac{s_{q,\tau}}{2} \right) + \ln \Gamma \left(\frac{r_{q,\tau}}{2} \right) \end{aligned}$$

3.2.4 LB: $E[\ln p(\sigma^2)] + H[\sigma^2]$

$$E[\ln p(\sigma^2)] + H[\sigma^2] = \frac{r_{0,\sigma}}{2} \ln\left(\frac{s_{0,\sigma}}{2}\right) - \ln \Gamma\left(\frac{r_{0,\sigma}}{2}\right) + \left(\frac{r_{0,\sigma}}{2} - \frac{r_{q,\sigma}}{2}\right) \text{di}\left(\frac{r_{q,\sigma}}{2}\right) - \left(\frac{r_{0,\sigma}}{2} + 1\right) \ln\left(\frac{s_{q,\sigma}}{2}\right) \\ - \frac{s_{0,\sigma}}{2} \frac{r_{q,\sigma}}{s_{q,\sigma}} + \frac{r_{q,\sigma}}{2} + \ln\left(\frac{s_{q,\sigma}}{2}\right) + \ln \Gamma\left(\frac{r_{q,\sigma}}{2}\right)$$

3.2.5 LB: $E[\ln p(\beta)] + H[\beta]$

$$E[\ln p(\beta)] + H[\beta] = \frac{p+1}{2} + \frac{p+1}{2} \left(\text{di}\left(\frac{r_{q,\sigma}}{2}\right) - \ln\left(\frac{s_{q,\sigma}}{2}\right) \right) + \frac{1}{2} \ln \left| \Sigma_\beta^{0-1} \Sigma_\beta^q \right| \\ - \frac{1}{2} \frac{r_{q,\sigma}}{s_{q,\sigma}} \left\{ \text{Tr}\left(\Sigma_\beta^{0-1} \Sigma_\beta^q\right) + \left(\mu_\beta^q - \mu_\beta^0\right)' \Sigma_\beta^{0-1} \left(\mu_\beta^q - \mu_\beta^0\right) \right\}$$

3.2.6 LB: $E[\ln p(\psi)] + H[\psi]$

$$E[\ln p(\psi)] + H[\psi] = \ln \frac{\omega_0}{2} - \omega_0 \left\{ \sigma_\psi^q \sqrt{\frac{2}{\pi}} \exp\left(-\frac{\mu_\psi^{q2}}{2\sigma_\psi^{q2}}\right) + \mu_\psi^q \left(1 - 2\Phi\left(-\frac{\mu_\psi^q}{\sigma_\psi^q}\right)\right) \right\} \\ + \frac{1}{2} \ln\left(2\pi\sigma_\psi^{q2}\right) - \frac{1}{2}$$

3.2.7 LB

$$\mathcal{L} = -\frac{1}{2} \left(\text{Tr}\left(W'W\Sigma_\beta^q\right) + \text{Tr}\left(\varphi_J'\varphi_J\Sigma_\theta^q\right) \right) + \sum_{i=1}^n \ln \left(\left\{ \Phi\left(w_i'\mu_\beta^q + \varphi_i'\mu_\theta^q\right) \right\}^{y_i} \left\{ 1 - \Phi\left(w_i'\mu_\beta^q + \varphi_i'\mu_\theta^q\right) \right\}^{1-y_i} \right) \\ - \frac{J}{2} \left\{ \ln(2\pi) - \left(\text{di}\left(\frac{r_{q,\sigma}}{2}\right) - \ln\left(\frac{s_{q,\sigma}}{2}\right) \right) - \left(\text{di}\left(\frac{s_{q,\tau}}{2}\right) - \ln\left(\frac{s_{q,\tau}}{2}\right) \right) \right\} \\ S_2\left(\mu_\psi^q, \sigma_\psi^{q2}\right) + \frac{J}{2} (1 + \ln(2\pi)) + \frac{1}{2} \ln |\Sigma_\theta^q| \\ + \frac{r_{0,\tau}}{2} \ln\left(\frac{s_{0,\tau}}{2}\right) - \ln \Gamma\left(\frac{r_{0,\tau}}{2}\right) + \left(\frac{r_{0,\tau}}{2} - \frac{r_{q,\tau}}{2}\right) \text{di}\left(\frac{r_{q,\tau}}{2}\right) - \left(\frac{r_{0,\tau}}{2} + 1\right) \ln\left(\frac{s_{q,\tau}}{2}\right) \\ - \frac{s_{0,\tau}}{2} \frac{r_{q,\tau}}{s_{q,\tau}} + \frac{r_{q,\tau}}{2} + \ln\left(\frac{s_{q,\tau}}{2}\right) + \ln \Gamma\left(\frac{r_{q,\tau}}{2}\right) \\ + \frac{r_{0,\sigma}}{2} \ln\left(\frac{s_{0,\sigma}}{2}\right) - \ln \Gamma\left(\frac{r_{0,\sigma}}{2}\right) + \left(\frac{r_{0,\sigma}}{2} - \frac{r_{q,\sigma}}{2}\right) \text{di}\left(\frac{r_{q,\sigma}}{2}\right) - \left(\frac{r_{0,\sigma}}{2} + 1\right) \ln\left(\frac{s_{q,\sigma}}{2}\right) \\ - \frac{s_{0,\sigma}}{2} \frac{r_{q,\sigma}}{s_{q,\sigma}} + \frac{r_{q,\sigma}}{2} + \ln\left(\frac{s_{q,\sigma}}{2}\right) + \ln \Gamma\left(\frac{r_{q,\sigma}}{2}\right) \\ + \frac{p+1}{2} + \frac{p+1}{2} \left(\text{di}\left(\frac{r_{q,\sigma}}{2}\right) - \ln\left(\frac{s_{q,\sigma}}{2}\right) \right) + \frac{1}{2} \ln \left| \Sigma_\beta^{0-1} \Sigma_\beta^q \right| \\ - \frac{1}{2} \frac{r_{q,\sigma}}{s_{q,\sigma}} \left\{ \text{Tr}\left(\Sigma_\beta^{0-1} \Sigma_\beta^q\right) + \left(\mu_\beta^q - \mu_\beta^0\right)' \Sigma_\beta^{0-1} \left(\mu_\beta^q - \mu_\beta^0\right) \right\} \\ + \ln\left(\frac{\omega_0}{2}\right) + S_1\left(\mu_\psi^q, \sigma_\psi^{q2}\right) + \frac{1}{2} \ln\left(2\pi\sigma_\psi^{q2}\right) - \frac{1}{2}$$

3.3 Update

3.3.1 θ_j

$$\Sigma_\theta^q \leftarrow \left(\varphi_J'\varphi_J + \frac{r_{q,\sigma}}{s_{q,\sigma}} \frac{r_{q,\tau}}{s_{q,\tau}} \text{Dg}(Q_{1:J}) \right)^{-1} \\ \mu_\theta^q \leftarrow \Sigma_\theta^q \varphi_J' \left(\mu_{y^*}^q - W\mu_\beta^q \right)$$

3.3.2 τ^2

$$r_{q,\tau} \leftarrow r_{0,\tau} + J$$

$$s_{q,\tau} \leftarrow s_{0,\tau} + \frac{r_{q,\sigma}}{s_{q,\sigma}} \sum_{j=1}^J \left(\Sigma_{\theta,jj}^q + \mu_{\theta,j}^q \right)^2 Q_j$$

3.3.3 σ^2

$$r_{q,\sigma} \leftarrow r_{0,\sigma} + J + p + 1$$

$$s_{q,\sigma} \leftarrow s_{0,\sigma} + \frac{r_{q,\tau}}{s_{q,\tau}} \sum_{j=1}^J \left(\Sigma_{\theta,jj}^q + \mu_{\theta,j}^q \right)^2 Q_j + \text{Tr} \left(\Sigma_{\beta}^{0^{-1}} \Sigma_{\beta}^q \right) + \left(\mu_{\beta}^q - \mu_{\beta}^0 \right)' \Sigma_{\beta}^{0^{-1}} \left(\mu_{\beta}^q - \mu_{\beta}^0 \right)$$

3.3.4 β

$$\Sigma_{\beta}^q \leftarrow \left(\frac{r_{q,\sigma}}{s_{q,\sigma}} \Sigma_{\beta}^{0^{-1}} + W'W \right)^{-1}$$

$$\mu_{\beta}^q \leftarrow \Sigma_{\beta}^q \left(\frac{r_{q,\sigma}}{s_{q,\sigma}} \Sigma_{\beta}^{0^{-1}} \mu_{\beta}^0 + W' \left(\mu_{y*}^q - \varphi_J \mu_{\theta}^q \right) \right)$$

3.3.5 ψ

$$\begin{aligned}
\frac{\partial S_1}{\partial \mu_\psi^q} &= -\omega_0 \left\{ -\frac{1}{\sigma_\psi^q} \sqrt{\frac{2}{\pi}} \exp \left(-\frac{\mu_\psi^{q^2}}{2\sigma_\psi^{q^2}} \right) + 1 - 2\Phi \left(-\frac{\mu_\psi^q}{\sigma_\psi^q} \right) + 2\frac{\mu_\psi^q}{\sigma_\psi^q} \phi \left(-\frac{\mu_\psi^q}{\sigma_\psi^q} \right) \right\} \\
\frac{\partial S_1}{\partial \sigma_\psi^{q^2}} &= -\omega_0 \left\{ \left(\frac{1}{\sqrt{2\pi}\sigma_\psi^q} + \frac{\mu_\psi^{q^2}}{\sqrt{\pi}(\sigma_\psi^{q^2})^{3/2}} \right) \exp \left(-\frac{\mu_\psi^{q^2}}{\sigma_\psi^{q^2}} \right) - \phi \left(-\frac{\mu_\psi^q}{\sigma_\psi^q} \right) \frac{\mu_\psi^{q^2}}{(\sigma_\psi^{q^2})^{3/2}} \right\} \\
\frac{\partial Q_j}{\partial \mu_\psi^q} &= j \exp \left(\frac{\sigma_\psi^{q^2} j^2}{2} + \mu_\psi^q j \right) \left\{ 1 - \Phi \left(\frac{-\mu_\psi^q}{\sigma_\psi^q} - \sigma_\psi^q j \right) \right\} + \frac{1}{\sigma_\psi^q} \exp \left(\frac{\sigma_\psi^{q^2} j^2}{2} + \mu_\psi^q j \right) \phi \left(-\frac{\mu_\psi^q}{\sigma_\psi^q} - \sigma_\psi^q j \right) \\
&\quad - j \exp \left(\frac{\sigma_\psi^{q^2} j^2}{2} - \mu_\psi^q j \right) \left\{ 1 - \Phi \left(\frac{\mu_\psi^q}{\sigma_\psi^q} - \sigma_\psi^q j \right) \right\} - \frac{1}{\sigma_\psi^q} \exp \left(\frac{\sigma_\psi^{q^2} j^2}{2} - \mu_\psi^q j \right) \phi \left(\frac{\mu_\psi^q}{\sigma_\psi^q} - \sigma_\psi^q j \right) \\
\frac{\partial Q_j}{\partial \sigma_\psi^{q^2}} &= j \exp \left(\frac{\sigma_\psi^{q^2} j^2}{2} + \mu_\psi^q j \right) \left\{ 1 - \Phi \left(-\frac{\mu_\psi^q}{\sigma_\psi^q} - \sigma_\psi^q j \right) \right\} + \left(\frac{1}{2\sigma_\psi^q} j - \frac{\mu_\psi^q}{2(\sigma_\psi^{q^2})^{3/2}} \right) \phi \left(-\frac{\mu_\psi^q}{\sigma_\psi^q} - \sigma_\psi^q j \right) \exp \left(\frac{\sigma_\psi^{q^2} j^2}{2} + \mu_\psi^q j \right) \\
&\quad + j \exp \left(\frac{\sigma_\psi^{q^2} j^2}{2} - \mu_\psi^q j \right) \left\{ 1 - \Phi \left(\frac{\mu_\psi^q}{\sigma_\psi^q} - \sigma_\psi^q j \right) \right\} + \left(\frac{1}{2\sigma_\psi^q} j + \frac{\mu_\psi^q}{2(\sigma_\psi^{q^2})^{3/2}} \right) \phi \left(\frac{\mu_\psi^q}{\sigma_\psi^q} - \sigma_\psi^q j \right) \exp \left(\frac{\sigma_\psi^{q^2} j^2}{2} - \mu_\psi^q j \right) \\
\frac{\partial S_2}{\partial \mu_\psi^q} &= -\frac{1}{2} \frac{r_{q,\sigma}}{s_{q,\sigma}} \frac{r_{q,\tau}}{s_{q,\tau}} \left(\text{Tr}(\Sigma_\theta^q) + \mu_\theta^{q'} \mu_\theta^q \right) \sum_{j=1}^J \frac{\partial Q_j}{\partial \mu_\psi^q} - \frac{J(J+1)}{4\omega_0} \frac{\partial S_1}{\partial \mu_\psi^q} \\
\frac{\partial S_2}{\partial \sigma_\psi^{q^2}} &= -\frac{1}{2} \frac{r_{q,\sigma}}{s_{q,\sigma}} \frac{r_{q,\tau}}{s_{q,\tau}} \left(\text{Tr}(\Sigma_\theta^q) + \mu_\theta^{q'} \mu_\theta^q \right) \sum_{j=1}^J \frac{\partial Q_j}{\partial \sigma_\psi^{q^2}} - \frac{J(J+1)}{4\omega_0} \frac{\partial S_1}{\partial \sigma_\psi^{q^2}} \\
\sigma_\psi^{q^2} &\leftarrow -\frac{1}{2} \left\{ \frac{\partial S_1}{\partial \sigma_\psi^{q^2}} + \frac{\partial S_2}{\partial \sigma_\psi^{q^2}} \right\}^{-1} \\
\mu_\psi^q &\leftarrow \mu_\psi^q + \sigma_\psi^{q^2} \left\{ \frac{\partial S_1}{\partial \mu_\psi^q} + \frac{\partial S_2}{\partial \mu_\psi^q} \right\}
\end{aligned}$$

4 Probit: No restriction, with normal random effects

4.1 Model

$$\begin{aligned}
P(y_i = 1|f, \beta) &= \Phi(w_i^\top \beta + Zu + f(x_i)) \\
y_i^* &= w_i^\top \beta + Zu + f(x_i) + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, 1) \\
y_i &= \begin{cases} 1, & \text{if } y_i^* \geq 0 \\ 0, & \text{if } y_i^* < 0 \end{cases} \\
\theta_j | \sigma, \tau, \gamma &\sim \mathcal{N}(0, \sigma^2 \tau^2 \exp[-j\gamma]) \\
\tau^2 &\sim \text{IG}\left(\frac{r_{0,\tau}}{2}, \frac{s_{0,\tau}}{2}\right) \\
\sigma^2 &\sim \text{IG}\left(\frac{r_{0,\sigma}}{2}, \frac{s_{0,\sigma}}{2}\right) \\
\beta &\sim \mathcal{N}(\mu_\beta^0, \sigma^2 \Sigma_\beta^0) \quad (p \times 1) \\
u &\sim \mathcal{N}(\mu_u^0, \Sigma_u^0), \quad (s \times 1) \\
\gamma &\sim \text{Exp}(\omega_0) \\
|\psi| &= \gamma, \quad \psi \sim \text{DE}(0, \omega_0) \\
\varphi_j(x) &= \sqrt{2} \cos(\pi j x)
\end{aligned}$$

Joint density:

$$\begin{aligned}
p(y, y^*, \Theta) &= C \left\{ \prod_{j=1}^J \mathcal{N}(\theta_j | 0, \sigma^2 \tau^2 \exp[-j|\psi|]) \right\} \text{IG}\left(\tau^2 \middle| \frac{r_{0,\tau}}{2}, \frac{s_{0,\tau}}{2}\right) \text{IG}\left(\sigma^2 \middle| \frac{r_{0,\sigma}}{2}, \frac{s_{0,\sigma}}{2}\right) \mathcal{N}(\beta | \mu_\beta^0, \sigma^2 \Sigma_\beta^0) \\
&\quad \mathcal{N}(u | \mu_u^0, \Sigma_u^0) \text{DE}(\psi | 0, \omega_0) \left\{ \prod_{i=1}^n (1[y_i^* \geq 0] 1[y_i = 1] + 1[y_i^* < 0] 1[y_i = 0]) \phi(y_i^* - w_i' \beta - z_i' u - \varphi_i' \theta_J) \right\}
\end{aligned}$$

where C is the normalizing constant.

4.2 Lower Bound

4.2.1 LB: $E(\ln p(y^* | \text{rest})) + H(y^*)$

$$\begin{aligned}
E(\ln p(y^* | \text{rest})) + H(y^*) &= \sum_{i=1}^n E \left(\ln \phi(y_i^* - w_i' \beta - z_i' u - \varphi_i' \theta_J) - \ln \phi(y_i^* - w_i' \mu_\beta^q - z_i' \mu_u^q - \varphi_i' \mu_\theta^q) \right) \\
&\quad + \sum_{i=1}^n \ln \left(\left\{ \Phi(w_i' \mu_\beta^q + z_i' \mu_u^q + \varphi_i' \mu_\theta^q) \right\}^{y_i} \left\{ 1 - \Phi(w_i' \mu_\beta^q + z_i' \mu_u^q + \varphi_i' \mu_\theta^q) \right\}^{1-y_i} \right) \\
&= -\frac{1}{2} \left(\text{Tr}(W' W \Sigma_\beta^q) + \text{Tr}(Z' Z \Sigma_u^q) + \text{Tr}(\varphi_J' \varphi_J \Sigma_\theta^q) \right) \\
&\quad + \sum_{i=1}^n \ln \left(\left\{ \Phi(w_i' \mu_\beta^q + z_i' \mu_u^q + \varphi_i' \mu_\theta^q) \right\}^{y_i} \left\{ 1 - \Phi(w_i' \mu_\beta^q + z_i' \mu_u^q + \varphi_i' \mu_\theta^q) \right\}^{1-y_i} \right)
\end{aligned}$$

4.2.2 LB: $E(\ln p(u)) + H(u)$

$$E(\ln p(u)) + H(u) = \frac{1}{2} \ln \left| \Sigma_u^{0-1} \Sigma_u^q \right|$$

Everything else is the same as the one without random effects.

4.2.3 LB: $E[\ln p(\theta_j|\sigma, \tau, \psi)]$

$$\begin{aligned}
\sum_{j=1}^J E[\ln p(\theta_j|\sigma, \tau, \psi)] + H[\theta_J] &= \sum_{j=1}^J E \left[-\frac{1}{2} \ln(2\pi) + \frac{1}{2} \ln \frac{1}{\sigma^2} + \frac{1}{2} \ln \frac{1}{\tau^2} + \frac{j}{2} |\psi| - \frac{\theta_j^2 e^{j|\psi|}}{2\sigma^2 \tau^2} \right] + H[\theta_J] \\
&= -\frac{J}{2} \left\{ \ln(2\pi) - \left(\text{di} \left(\frac{r_{q,\sigma}}{2} \right) - \ln \left(\frac{s_{q,\sigma}}{2} \right) \right) - \left(\text{di} \left(\frac{r_{q,\tau}}{2} \right) - \ln \left(\frac{s_{q,\tau}}{2} \right) \right) \right\} \\
&\quad + \frac{J(J+1)}{4} \left\{ \sigma_\psi^q \sqrt{\frac{2}{\pi}} \exp \left(-\frac{\mu_\psi^{q^2}}{2\sigma_\psi^{q^2}} \right) + \mu_\psi^q \left(1 - 2\Phi \left(\frac{-\mu_\psi^q}{\sigma_\psi^q} \right) \right) \right\} \\
&\quad - \frac{1}{2} \frac{r_{q,\sigma}}{s_{q,\sigma}} \frac{r_{q,\tau}}{s_{q,\tau}} \left(\text{Tr}(\Sigma_\theta^q) + \mu_\theta^{q'} \mu_\theta^q \right) \sum_{j=1}^J Q_j(\mu_\psi^q, \sigma_\psi^{q^2}) + \frac{J}{2} (1 + \ln(2\pi)) + \frac{1}{2} \ln |\Sigma_\theta^q|
\end{aligned}$$

where

$$\begin{aligned}
Q_j(\mu_\psi^q, \sigma_\psi^{q^2}) &= E e^{j|\psi|} \\
&= \exp \left\{ \frac{\sigma_\psi^{q^2} j^2}{2} + \mu_\psi^q j \right\} \left[1 - \Phi \left(-\frac{\mu_\psi^q}{\sigma_\psi^q} - \sigma_\psi^q j \right) \right] + \exp \left\{ \frac{\sigma_\psi^{q^2} j^2}{2} - \mu_\psi^q j \right\} \left[1 - \Phi \left(\frac{\mu_\psi^q}{\sigma_\psi^q} - \sigma_\psi^q j \right) \right].
\end{aligned}$$

4.2.4 LB: $E[\ln p(\tau^2)] + H[\tau^2]$

$$\begin{aligned}
E[\ln p(\tau^2)] + H[\tau^2] &= \frac{r_{0,\tau}}{2} \ln \frac{s_{0,\tau}}{2} - \ln \Gamma \left(\frac{r_{0,\tau}}{2} \right) + \left(\frac{r_{0,\tau}}{2} + 1 \right) \left\{ \text{di} \left(\frac{r_{q,\tau}}{2} \right) - \ln \left(\frac{s_{q,\tau}}{2} \right) \right\} - \frac{s_{0,\tau}}{2} \frac{r_{q,\tau}}{s_{q,\tau}} \\
&\quad + \frac{r_{q,\tau}}{2} + \ln \frac{s_{q,\tau}}{2} + \ln \Gamma \left(\frac{r_{q,\tau}}{2} \right) - \left(1 + \frac{r_{q,\tau}}{2} \right) \text{di} \left(\frac{r_{q,\tau}}{2} \right)
\end{aligned}$$

4.2.5 LB: $E[\ln p(\sigma^2)] + H[\sigma^2]$

$$\begin{aligned}
E[\ln p(\sigma^2)] + H[\sigma^2] &= \frac{r_{0,\sigma}}{2} \ln \frac{s_{0,\sigma}}{2} - \ln \Gamma \left(\frac{r_{0,\sigma}}{2} \right) + \left(\frac{r_{0,\sigma}}{2} + 1 \right) \left\{ \text{di} \left(\frac{r_{q,\sigma}}{2} \right) - \ln \left(\frac{s_{q,\sigma}}{2} \right) \right\} - \frac{s_{0,\sigma}}{2} \frac{r_{q,\sigma}}{s_{q,\sigma}} \\
&\quad + \frac{r_{q,\sigma}}{2} + \ln \frac{s_{q,\sigma}}{2} + \ln \Gamma \left(\frac{r_{q,\sigma}}{2} \right) - \left(1 + \frac{r_{q,\sigma}}{2} \right) \text{di} \left(\frac{r_{q,\sigma}}{2} \right)
\end{aligned}$$

4.2.6 LB: $E[\ln p(\beta)] + H[\beta]$

$$\begin{aligned}
E[\ln p(\beta)] + H[\beta] &= \frac{p+1}{2} + \frac{1}{2} \left(\text{di} \left(\frac{r_{q,\sigma}}{2} \right) - \ln \left(\frac{s_{q,\sigma}}{2} \right) \right) + \frac{1}{2} \ln |\Sigma_\beta^{0^{-1}} \Sigma_\beta^q| \\
&\quad - \frac{1}{2} \frac{r_{q,\sigma}}{s_{q,\sigma}} \left\{ \text{Tr} \left(\Sigma_\beta^{0^{-1}} \Sigma_\beta^q \right) + \left(\mu_\beta^q - \mu_\beta^0 \right)' \Sigma_\beta^{0^{-1}} \left(\mu_\beta^q - \mu_\beta^0 \right) \right\}
\end{aligned}$$

4.2.7 LB: $E[\ln p(\psi)] + H[\psi]$

$$\begin{aligned}
E[\ln p(\psi)] + H[\psi] &= \ln \frac{\omega_0}{2} - \omega_0 \left\{ \sigma_\psi^q \sqrt{\frac{2}{\pi}} \exp \left(-\frac{\mu_\psi^{q^2}}{2\sigma_\psi^{q^2}} \right) + \mu_\psi^q \left(1 - 2\Phi \left(-\frac{\mu_\psi^q}{\sigma_\psi^q} \right) \right) \right\} \\
&\quad + \frac{1}{2} \ln \left(2\pi \sigma_\psi^{q^2} \right) - \frac{1}{2}
\end{aligned}$$

4.3 Update

4.3.1 u

$q(u) = \mathcal{N}(\mu_u^q, \Sigma_u^q)$ where

$$\begin{aligned}\Sigma_u^q &= \left(Z'Z + \Sigma_u^{0-1} \right)^{-1} \\ \mu_u^q &= \Sigma_u^q \left(\Sigma_u^{0-1} \mu_u^0 + Z' \left(\mu_{y^*}^q - W \mu_\beta^q - \varphi_J \mu_\theta^q \right) \right)\end{aligned}$$

4.3.2 y_i^*

$$q(y_i^*) = \mathcal{TN}(\mu_{y_i^*}, 1)$$

truncated at zero where

$$\mu_{y_i^*} = w_i' \mu_\beta^q + z_i' \mu_u^q + \varphi_i' \mu_\theta^q.$$

To distinguish $\mu_{y_i^*}$ which is the parameter of the variational distribution from the expected value, we will denote the expectation by $\mu_{y_i^*}^q$ where

$$\mathbb{E}(y_i^*) = \mu_{y_i^*}^q = \mu_{y_i^*} + \frac{\phi(\mu_{y_i^*})}{\Phi(\mu_{y_i^*})^{y_i} (\Phi(\mu_{y_i^*}) - 1)^{1-y_i}}$$

4.3.3 θ_j

$q(\theta_J) = \mathcal{N}(\mu_\theta^q, \Sigma_\theta^q)$ where

$$\begin{aligned}\Sigma_\theta^q &= \left(\frac{r_{q,\tau}}{s_{q,\tau}} \frac{r_{q,\sigma}}{s_{q,\sigma}} \text{Dg}(Q_{1:J}) + \varphi_J' \varphi_J \right)^{-1} \\ \mu_\theta^q &= \Sigma_\theta^q \varphi_J' \left(\mu_{y_i}^q - W \mu_\beta^q - Z \mu_u^q \right).\end{aligned}$$

4.3.4 β

$q(\beta) = \mathcal{N}(\mu_\beta^q, \Sigma_\beta^q)$ where

$$\begin{aligned}\Sigma_\beta^q &= \left(\frac{r_{q,\sigma}}{s_{q,\sigma}} \Sigma_\beta^{0-1} + W'W \right)^{-1} \\ \mu_\beta^q &= \Sigma_\beta^q \left(\Sigma_\beta^{0-1} \mu_\beta^0 + W' \left(\mu_{y^*}^q - Z \mu_u^q - \varphi_J \mu_\theta^q \right) \right).\end{aligned}$$

4.3.5 τ^2

$$\begin{aligned}r_{q,\tau} &\leftarrow r_{0,\tau} + J \\ s_{q,\tau} &\leftarrow s_{0,\tau} + \frac{r_{q,\sigma}}{s_{q,\sigma}} \sum_{j=1}^J \left(\Sigma_{\theta,jj}^q + \mu_{\theta,j}^q{}^2 \right) Q_j\end{aligned}$$

4.3.6 σ^2

$$\begin{aligned}r_{q,\sigma} &\leftarrow r_{0,\sigma} + J + p + 1 \\ s_{q,\sigma} &\leftarrow s_{0,\sigma} + \frac{r_{q,\tau}}{s_{q,\tau}} \sum_{j=1}^J \left(\Sigma_{\theta,jj}^q + \mu_{\theta,j}^q{}^2 \right) Q_j + \text{Tr} \left(\Sigma_\beta^{0-1} \Sigma_\beta^q \right) + \left(\mu_\beta^q - \mu_\beta^0 \right)' \Sigma_\beta^{0-1} \left(\mu_\beta^q - \mu_\beta^0 \right)\end{aligned}$$

5 Probit: Monotone Shape Restriction

5.1 Model

$$\begin{aligned}
P(y_i = 1 | \beta, \theta_J) &= \Phi(w'_i \beta + \delta \theta'_J \varphi_J^a(x_i) \theta_J) \\
y_i^* &= w'_i \beta + \delta \theta'_J \varphi_J^a(x_i) \theta_J + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, 1) \\
y_i &= \begin{cases} 1, & \text{if } y_i^* \geq 0 \\ 0, & \text{if } y_i^* < 0 \end{cases} \\
\theta_j | \sigma, \tau, \gamma &\sim \mathcal{N}(0, \sigma \tau^2 \exp[-j\gamma]), \quad \text{for } j \geq 2 \\
\theta_0 | \sigma &\sim \mathcal{N}(0, \sigma \sigma_0^2) \\
\tau^2 &\sim \text{IG}\left(\frac{r_{0,\tau}}{2}, \frac{s_{0,\tau}}{2}\right) \\
\sigma^2 &\sim \text{IG}\left(\frac{r_{0,\sigma}}{2}, \frac{s_{0,\sigma}}{2}\right) \\
\beta &\sim \mathcal{N}(\mu_\beta^0, \sigma^2 \Sigma_\beta^0) \quad (p \times 1) \\
\gamma &\sim \text{Exp}(\omega_0) \\
|\psi| &= \gamma, \quad \psi \sim \text{DE}(0, \omega_0) \\
\varphi_{0,0}^a(x) &= x - 0.5 \\
\varphi_{0,j}^a(x) &= \varphi_{j,0}^a(x) = \frac{\sqrt{2}}{\pi j} \sin(\pi j x) - \frac{\sqrt{2}}{(\pi j)^2} [1 - \cos(\pi j)] \quad \text{for } j \geq 1, \\
\varphi_{j,j}^a(x) &= \frac{\sin(2\pi j x)}{2\pi j} + x - 0.5 \quad \text{for } j \geq 1, \\
\varphi_{j,k}^a(x) &= \frac{\sin[\pi(j+k)x]}{\pi(j+k)} + \frac{\sin[\pi(j-k)x]}{\pi(j-k)} \\
&\quad - \frac{1 - \cos[\pi(j+k)]}{[\pi(j+k)]^2} - \frac{1 - \cos[\pi(j-k)]}{[\pi(j-k)]^2} \\
&\quad \text{for } j \neq k \text{ and } j, k \geq 1.
\end{aligned}$$

Joint density:

$$\begin{aligned}
p(y, y^*, \Theta) &\propto \mathcal{N}(\theta_0 | 0, \sigma \sigma_0^2) \left\{ \prod_{j=1}^J \mathcal{N}(\theta_j | 0, \sigma \tau^2 \exp[-j|\psi|]) \right\} \text{IG}\left(\tau^2 \middle| \frac{r_{0,\tau}}{2}, \frac{s_{0,\tau}}{2}\right) \text{IG}\left(\sigma^2 \middle| \frac{r_{0,\sigma}}{2}, \frac{s_{0,\sigma}}{2}\right) \mathcal{N}(\beta | \mu_\beta^0, \sigma^2 \Sigma_\beta^0) \\
&\quad \times \text{DE}(\psi | 0, \omega_0) \left\{ \prod_{i=1}^n (1[y_i^* \geq 0] 1[y_i = 1] + 1[y_i^* < 0] 1[y_i = 0]) \phi(y_i^* - w'_i \beta - \delta \theta'_J \varphi_J^a(x_i) \theta_J) \right\}
\end{aligned}$$

5.2 Update

5.2.1 y_i^*

$$\begin{aligned}
\ln q(y_i^*) &\propto -\frac{1}{2} \mathbb{E}_{-y_i^*} \left(y_i^{*2} - 2y_i^* (w_i' \beta + \delta \theta_J' \varphi_J^a(x_i) \theta_J) + (w_i' \beta + \delta \theta_J' \varphi_J^a(x_i) \theta_J)^2 \right) \\
&\propto -\frac{1}{2} \left(y_i^{*2} - 2y_i^* \left(w_i' \mu_\beta^q + \delta \left(\text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q) + \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \right) \right) \right. \\
&\quad + \text{Tr}(w_i w_i' \Sigma_\beta^q) + \mu_\beta^{q'} w_i w_i' \mu_\beta^q + 2\delta w_i' \mu_\beta^q \left(\text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q) + \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \right) \\
&\quad \left. + 2\delta^2 \text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q)^2 + 4\delta^2 \mu_\theta^{q'} \varphi_J^a(x_i) \Sigma_\theta^q \varphi_J^a(x_i) \mu_\theta^q + \delta^2 \left(\text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q) + \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \right)^2 \right) \\
&\propto -\frac{1}{2} \left(y_i^* - w_i' \mu_\beta^q - \delta \left(\text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q) + \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \right) \right)^2
\end{aligned}$$

Therefore,

$$q(y_i^*) \sim \mathcal{TN}(\mu_{y_i^*}, 1)$$

truncated at zero where

$$\mu_{y_i^*} = w_i' \mu_\beta^q + \delta \text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q) + \delta \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q.$$

To distinguish the mean of the normal distribution and the mean of the truncated normal distribution, the latter will be denoted $\mu_{y_i^*}^q$ where

$$\mathbb{E}(y_i^*) = \mu_{y_i^*}^q = \mu_{y_i^*} + \frac{\phi(\mu_{y_i^*})}{\Phi(\mu_{y_i^*})^{y_i} (\Phi(\mu_{y_i^*}) - 1)^{1-y_i}}.$$

5.2.2 θ

$$\begin{aligned}
S_1(\mu_\theta^q, \Sigma_\theta^q) &= \mathbb{E}(\ln p(\theta_J | \sigma^2, \sigma^2, \psi)) \\
&= -\frac{1}{2} \mathbb{E} \left(\frac{1}{\sigma} \right) \text{Tr} \left\{ \left(\Sigma_\theta^q + \mu_\theta^q \mu_\theta^{q'} \right) \text{Dg}(\mathbb{E}(\Upsilon^{-1})) \right\} \\
S_2(\mu_\theta^q, \Sigma_\theta^q) &= \mathbb{E}(\ln p(y^* | \beta, \theta_J, \sigma^2)) \\
&= -\frac{1}{2} \sum_{i=1}^n \left\{ \left(\mu_{y_i^*}^q - w_i' \mu_\beta^q - \delta \text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q) - \delta \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \right)^2 \right. \\
&\quad \left. + 2 \text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q \varphi_J^a(x_i) \Sigma_\theta^q) + 4 \mu_\theta^{q'} \varphi_J^a(x_i) \Sigma_\theta^q \varphi_J^a(x_i) \mu_\theta^q \right\}
\end{aligned}$$

Then by NCVMP introduced in Wand (2014),

$$\begin{aligned}
\Sigma_\theta^q &\leftarrow -\frac{1}{2} \left\{ \sum_{a=1}^2 \frac{\partial S_a(\mu_\theta^q, \Sigma_\theta^q)}{\partial \Sigma_\theta^q} \right\}^{-1} \\
\mu_\theta^q &\leftarrow \mu_\theta^q + \Sigma_\theta^q \left\{ \sum_{a=1}^2 \frac{\partial S_a(\mu_\theta^q, \Sigma_\theta^q)}{\partial \mu_\theta^q} \right\}.
\end{aligned}$$

By matrix differential calculus,

$$\begin{aligned}
\frac{\partial S_1}{\partial \Sigma_\theta^q} &= -\frac{1}{2} \mathbf{E} \left(\frac{1}{\sigma} \right) \text{Dg} \left(\mathbf{E} (\Upsilon^{-1}) \right) \\
\frac{\partial S_2}{\partial \Sigma_\theta^q} &= -\frac{1}{2} \sum_{i=1}^n \left\{ 4\varphi_J^a(x_i) \Sigma_\theta^q \varphi_J^a(x_i) + 4\varphi_J^a(x_i) \mu_\theta^q \mu_\theta^{q'} \varphi_J^a(x_i) \right. \\
&\quad \left. - 2\delta \left(\mu_{y_i^*}^q - w_i' \mu_\beta^q - \delta \text{Tr} (\Sigma_\theta^q \varphi_J^a(x_i)) - \delta \mu_\theta^{q'} \Sigma_\theta^q \mu_\theta^q \right) \varphi_J^a(x_i) \right\} \\
\frac{\partial S_1}{\partial \mu_\theta^q} &= -\mathbf{E} \left(\frac{1}{\sigma} \right) \text{Dg} \left(\mathbf{E} (\Upsilon^{-1}) \right) \mu_\theta^q \\
\frac{\partial S_2}{\partial \mu_\theta^q} &= -\frac{1}{2} \sum_{i=1}^n \left\{ 8\varphi_J^a(x_i) \Sigma_\theta^q \varphi_J^a(x_i) \mu_\theta^q - 4\delta \left(\mu_{y_i^*}^q - w_i' \mu_\beta^q - \delta \text{Tr} (\varphi_J^a(x_i) \Sigma_\theta^q) \right. \right. \\
&\quad \left. \left. - \delta \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \right) \varphi_J^a(x_i) \mu_\theta^q \right\}
\end{aligned}$$

5.2.3 β

$$\begin{aligned}
\ln q(\beta) &\propto \mathbf{E}_{-\beta} \left(-\frac{1}{2\sigma^2} (\beta - \mu_\beta^0)' \Sigma_\beta^{0^{-1}} (\beta - \mu_\beta^0) - \frac{1}{2} \sum_{i=1}^n (y_i^* - w_i' \beta - \delta \theta_J' \varphi_J^a(x_i) \theta_J)^2 \right) \\
&\propto -\frac{1}{2} \left(\beta' \left(\mathbf{E} \left(\frac{1}{\sigma^2} \right) \Sigma_\beta^{0^{-1}} + W'W \right) \beta \right. \\
&\quad \left. - 2 \left(\mathbf{E} \left(\frac{1}{\sigma^2} \right) \beta' \Sigma_\beta^{0^{-1}} \mu_\beta^0 + \beta' W' \mu_{y^*}^q - \beta' \delta \sum_{i=1}^n w_i \left(\text{Tr} (\varphi_J^a(x_i) \Sigma_\theta^q) + \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \right) \right) \right)
\end{aligned}$$

Therefore, $q(\beta) = \mathcal{N}(\mu_\beta^q, \Sigma_\beta^q)$ where

$$\begin{aligned}
\Sigma_\beta^q &\leftarrow \left(\mathbf{E} \left(\frac{1}{\sigma^2} \right) \Sigma_\beta^{0^{-1}} + W'W \right)^{-1} \\
\mu_\beta^q &\leftarrow \Sigma_\beta^q \left(\mathbf{E} \left(\frac{1}{\sigma^2} \right) \Sigma_\beta^{0^{-1}} \mu_\beta^0 + W' \mu_{y^*}^q - \delta \sum_{i=1}^n w_i \left(\text{Tr} (\varphi_J^a(x_i) \Sigma_\theta^q) + \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \right) \right)
\end{aligned}$$

5.2.4 τ^2

$$\begin{aligned}
r_{q,\tau} &\leftarrow r_{0,\tau} + J \\
s_{q,\tau} &\leftarrow s_{0,\tau} + \mathbf{E} \left(\frac{1}{\sigma} \right) \text{Tr} \left(\left(\Sigma_\theta^{q*} + \mu_\theta^{q*} \mu_\theta^{q*'} \right) \text{Dg} (Q_{1:J}) \right)
\end{aligned}$$

5.2.5 σ^2

$$\begin{aligned}
\ln q(\sigma^2) &\propto -\frac{1}{2} \ln \sigma - \frac{J}{2} \ln \sigma - \frac{1}{2} \frac{\theta_0^2}{\sigma_0^2} \frac{1}{\sigma} - \frac{1}{2} \sum_{j=1}^J \frac{r_{q,\tau}}{s_{q,\tau}} e^{j|\psi|} \theta_j^2 \frac{1}{\sigma} \\
&\quad + \left(\frac{r_{0,\sigma}}{2} + 1 \right) \ln \frac{1}{\sigma^2} - \frac{s_{0,\sigma}}{2} \frac{1}{\sigma^2} - \frac{p+1}{2} \ln \sigma^2 \\
&\quad - \frac{1}{2\sigma^2} \left\{ \left(\mu_\beta^q - \mu_\beta^0 \right)' \Sigma_\beta^{0^{-1}} \left(\mu_\beta^q - \mu_\beta^0 \right) + \text{Tr} \left(\Sigma_{\beta^0}^{-1} \Sigma_\beta^q \right) \right\} \\
&\propto \left(\frac{J+1}{4} + \frac{r_{0,\sigma} + p+1}{2} + 1 \right) \ln \frac{1}{\sigma^2} - \frac{1}{2} \frac{1}{\sigma} \text{Tr} \left\{ \left(\Sigma_\theta^q + \mu_\theta^q \mu_\theta^{q'} \right) \text{Dg} \left(\mathbf{E} \left(\Upsilon^{-1} \right) \right) \right\} \\
&\quad - \frac{1}{2} \frac{1}{\sigma^2} \left\{ s_{0,\sigma} + \left(\mu_\beta^q - \mu_\beta^0 \right)' \Sigma_\beta^{0^{-1}} \left(\mu_\beta^q - \mu_\beta^0 \right) + \text{Tr} \left(\Sigma_\beta^{0^{-1}} \Sigma_\beta^q \right) \right\} \\
q(\sigma^2) &\propto \left(\frac{1}{\sigma} \right)^{2a} \exp \left(\frac{b}{\sigma} - \frac{c}{\sigma^2} \right)
\end{aligned}$$

where

$$\begin{aligned}
a &\leftarrow \frac{J+1}{4} + \frac{r_{0,\sigma} + p+1}{2} + 1 \\
b &\leftarrow -\frac{1}{2} \text{Tr} \left\{ \left(\Sigma_\theta^q + \mu_\theta^q \mu_\theta^{q'} \right) \text{Dg} \left(\mathbf{E} \left(\Upsilon^{-1} \right) \right) \right\} \\
c &\leftarrow \frac{1}{2} \left\{ s_{0,\sigma} + \left(\mu_\beta^q - \mu_\beta^0 \right)' \Sigma_\beta^{0^{-1}} \left(\mu_\beta^q - \mu_\beta^0 \right) + \text{Tr} \left(\Sigma_\beta^{0^{-1}} \Sigma_\beta^q \right) \right\}
\end{aligned}$$

and $\Upsilon = (\sigma_0^2, \tau^2 e^{-\gamma}, \dots, \tau^2 e^{-J\gamma})'$ which gives $\mathbf{E}(\Upsilon^{-1}) = (1/\sigma_0^2, r_{q,\tau}/s_{q,\tau} \mathbf{E}(\Gamma^{-1}))$. Lastly, $\mathbf{E}(\Gamma^{-1}) = Q_{1:J}$.

5.2.6 ψ

Same as before except that $r_{q,\sigma}/s_{q,\sigma}$ in $S_2(\mu_\psi^q, \sigma_\psi^{q2})$ is replaced by $\mathbf{E}(1/\sigma)$.

5.3 Lower Bound

5.3.1 $E(\ln p(y^*|\text{rest})) + H(y^*)$

$$\begin{aligned}
E(\ln p(y^*|\text{rest})) + H(y^*) &= \sum_{i=1}^n E(\ln \phi(y_i^* - w_i' \beta - \delta \theta_J' \varphi_J^a(x_i) \theta_J) - \ln \phi(y_i^* - \mu_{y_i^*})) \\
&\quad + \sum_{i=1}^n \ln \left(\Phi(\mu_{y_i^*})^{y_i} (1 - \Phi(\mu_{y_i^*}))^{1-y_i} \right) \\
&= -\frac{1}{2} \sum_{i=1}^n \left[-2\mu_{y_i^*}^q \left(w_i' \mu_\beta^q + \delta \text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q) + \delta \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \right) \right. \\
&\quad + \text{Tr} \left(w_i w_i' \Sigma_\beta^q \right) + \mu_\beta^{q'} w_i w_i' \mu_\beta^q + 2w_i' \mu_\beta^q \left(\delta \text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q) + \delta \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \right) \\
&\quad + \delta^2 \left\{ 2 \text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q)^2 + 4\mu_\theta^{q'} \varphi_J^a(x_i) \Sigma_\theta^q \varphi_J^a(x_i) \mu_\theta^q + \left(\text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q) + \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \right)^2 \right\} \\
&\quad \left. + 2\mu_{y_i^*}^q \mu_{y_i^*} - \mu_{y_i^*}^2 \right] + \sum_{i=1}^n \ln \left(\Phi(\mu_{y_i^*})^{y_i} (1 - \Phi(\mu_{y_i^*}))^{1-y_i} \right) \\
&= -\frac{1}{2} \sum_{i=1}^n \left[\text{Tr} \left(w_i w_i' \Sigma_\beta^q \right) + \delta^2 \left\{ 2 \text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q)^2 + 4\mu_\theta^{q'} \varphi_J^a(x_i) \Sigma_\theta^q \varphi_J^a(x_i) \mu_\theta^q \right\} \right] \\
&\quad + \sum_{i=1}^n \ln \left(\Phi(\mu_{y_i^*})^{y_i} (1 - \Phi(\mu_{y_i^*}))^{1-y_i} \right)
\end{aligned}$$

Note that $\sum_{i=1}^n \text{Tr} \left(w_i w_i' \Sigma_\beta^q \right) = \text{Tr} \left(W' W \Sigma_\beta^q \right)$.

5.3.2 $E(\ln p(\theta)) + H(\theta)$

$$E(\ln p(\theta|\text{rest})) + H(\theta) = -\frac{J+1}{2} E(\ln \sigma) - \frac{1}{2} E \left(\frac{1}{\sigma} \right) \text{Tr} \left\{ \left(\Sigma_\theta^q + \mu_\theta^q \mu_\theta^{q'} \right) \text{Dg} \left(E(\Upsilon^{-1}) \right) \right\} + \frac{1}{2} \ln |\Sigma_\theta^q|$$

5.3.3 $E(\ln p(\beta)) + H(\beta)$

$$E(\ln p(\beta|\text{rest})) + H(\beta) = -\frac{p+1}{2} E(\ln \sigma^2) - \frac{1}{2} E \left(\frac{1}{\sigma^2} \right) \left\{ \left(\mu_\beta^q - \mu_\beta^0 \right)' \Sigma_\beta^{0-1} \left(\mu_\beta^q - \mu_\beta^0 \right) + \text{Tr} \left(\Sigma_\beta^{0-1} \Sigma_\beta^q \right) \right\} + \frac{1}{2} \ln |\Sigma_\beta^q|$$

5.3.4 $E(\ln p(\tau^2)) + H(\tau^2)$

$$\begin{aligned}
E(\ln p(\tau^2|\text{rest})) + H(\tau^2) &= -\frac{r_{0,\tau}}{2} \ln \left(\frac{s_{q,\tau}}{2} \right) + \left(\frac{r_{0,\tau}}{2} - \frac{r_{q,\tau}}{2} \right) \text{di} \left(\frac{r_{q,\tau}}{2} \right) + \left(1 - \frac{s_{0,\tau}}{s_{q,\tau}} \right) \frac{r_{q,\tau}}{2} + \ln \Gamma \left(\frac{r_{q,\tau}}{2} \right) \\
&\quad + \frac{r_{0,\tau}}{2} \ln \frac{s_{0,\tau}}{2} - \ln \Gamma \left(\frac{r_{0,\tau}}{2} \right)
\end{aligned}$$

5.3.5 $E(\ln p(\sigma^2)) + H(\sigma^2)$

$$\begin{aligned}
E(\ln p(\sigma^2|\text{rest})) + H(\sigma^2) &= \frac{r_{0,\sigma}}{2} \ln \left(\frac{s_{0,\sigma}}{2} \right) - \ln \Gamma \left(\frac{r_{0,\sigma}}{2} \right) - \left(\frac{r_{0,\sigma}}{2} + 1 \right) E(\ln \sigma^2) - \frac{s_{0,\sigma}}{2} E \left(\frac{1}{\sigma^2} \right) \\
&\quad + 2a E(\ln \sigma) - b E \left(\frac{1}{\sigma} \right) + c E \left(\frac{1}{\sigma^2} \right)
\end{aligned}$$

5.3.6 $E(\ln p(\psi)) + H(\psi)$

$$E(\ln p(\psi)) + H(\psi) = \ln\left(\frac{\omega_0}{2}\right) + S_1\left(\mu_\psi^q, \sigma_\psi^{q^2}\right) + \frac{1}{2} \ln\left(2\pi\sigma_\psi^{q^2}\right) - \frac{1}{2}$$

5.3.7 LB

$$\begin{aligned} \mathcal{L} = & -\frac{1}{2} \left\{ \text{Tr}\left(W'W\Sigma_\beta^q\right) + \delta^2 \sum_{i=1}^n \left(2 \text{Tr}\left(\varphi_J^a(x_i) \Sigma_\theta^q\right)^2 + 4\mu_\theta^{q'} \varphi_J^a(x_i) \Sigma_\theta^q \varphi_J^a(x_i) \mu_\theta^q\right) \right\} \\ & + \sum_{i=1}^n \left\{ \ln\left(\Phi\left(\mu_{y_i^*}\right)^{y_i} \left(1 - \Phi\left(\mu_{y_i^*}\right)\right)^{1-y_i}\right) \right\} \\ & - \frac{1}{2} E\left(\frac{1}{\sigma}\right) \text{Tr}\left\{\left(\Sigma_\theta^q + \mu_\theta^q \mu_\theta^{q'}\right) \text{Dg}\left(E\left(\Upsilon^{-1}\right)\right)\right\} + \frac{1}{2} \ln\left|\Sigma_\theta^q\right| \\ & - \frac{1}{2} E\left(\frac{1}{\sigma^2}\right) \left\{\left(\mu_\beta^q - \mu_\beta^0\right)' \Sigma_\beta^{0^{-1}} \left(\mu_\beta^q - \mu_\beta^0\right) + \text{Tr}\left(\Sigma_\beta^{0^{-1}} \Sigma_\beta^q\right)\right\} + \frac{1}{2} \ln\left|\Sigma_\beta^q\right| \\ & + \frac{r_{0,\sigma}}{2} \ln\left(\frac{s_{0,\sigma}}{2}\right) - \ln \Gamma\left(\frac{r_{0,\sigma}}{2}\right) - \frac{s_{0,\sigma}}{2} E\left(\frac{1}{\sigma^2}\right) - b E\left(\frac{1}{\sigma}\right) + c E\left(\frac{1}{\sigma^2}\right) \\ & - \frac{r_{0,\tau}}{2} \ln\left(\frac{s_{q,\tau}}{2}\right) + \left(\frac{r_{0,\tau}}{2} - \frac{r_{q,\tau}}{2}\right) \text{di}\left(\frac{r_{q,\tau}}{2}\right) + \left(1 - \frac{s_{0,\tau}}{s_{q,\tau}}\right) \frac{r_{q,\tau}}{2} + \ln \Gamma\left(\frac{r_{q,\tau}}{2}\right) \\ & + \ln\left(\frac{\omega_0}{2}\right) + S_1\left(\mu_\psi^q, \sigma_\psi^{q^2}\right) + \frac{1}{2} \ln\left(2\pi\sigma_\psi^{q^2}\right) - \frac{1}{2} \end{aligned}$$

5.4 Some Calculation

5.4.1 $E(1/\sigma)$

As we were going through the variational approximation for the monotone shape restriction model, we have seen the term $E(1/\sigma)$ and $E(1/\sigma^2)$ several times and did not mention how to compute the integral. We give the mathematical consideration. Wolfram Alpha gives

$$\int_0^\infty x^p \exp(qx - rx^2) dx = \frac{1}{2} r^{-p/2-1} \left(q \Gamma\left(\frac{p}{2} + 1\right) {}_1F_1\left(\frac{p}{2} + 1; \frac{3}{2}; \frac{q^2}{4r}\right) + \sqrt{r} \Gamma\left(\frac{p+1}{2}\right) {}_1F_1\left(\frac{p+1}{2}; \frac{1}{2}; \frac{q^2}{4r}\right) \right)$$

for $\text{Re}(r) > 0 \wedge \text{Re}(p) > -1$. Note that ${}_1F_1(a; b; x)$ is the *Kummer confluent hypergeometric function*. R package **fAsianOptions** provides the function `kummerM(x, a, b)` for ${}_1F_1(a; b; x)$.

However, since the variable is not x but rather the reciprocal $1/\sigma$, care must be taken in that the parameters should be changed accordingly. Let $x = 1/\sigma$. Then the differential is $dx = -d\sigma/\sigma^2$ and as $x \rightarrow 0$, $\sigma \rightarrow \infty$; as $x \rightarrow \infty$, $\sigma \rightarrow 0$. Therefore,

$$\begin{aligned} \int_0^\infty x^p \exp(qx - rx^2) dx &= \int_\infty^0 -\left(\frac{1}{\sigma}\right)^p \exp\left(\frac{q}{\sigma} - \frac{r}{\sigma^2}\right) \cdot \frac{1}{\sigma^2} d\sigma \\ &= \int_0^\infty \left(\frac{1}{\sigma}\right)^{p+2} \exp\left(\frac{q}{\sigma} - \frac{r}{\sigma^2}\right) d\sigma. \end{aligned}$$

Now we can compute the expectations.

$$\begin{aligned} E\left(\frac{1}{\sigma}\right) &= \frac{\int_0^\infty \left(\frac{1}{\sigma}\right)^{p+3} \exp\left(\frac{q}{\sigma} - \frac{r}{\sigma^2}\right) d\sigma}{\int_0^\infty \left(\frac{1}{\sigma}\right)^{p+2} \exp\left(\frac{q}{\sigma} - \frac{r}{\sigma^2}\right) d\sigma} \\ E\left(\frac{1}{\sigma^2}\right) &= \frac{\int_0^\infty \left(\frac{1}{\sigma}\right)^{p+4} \exp\left(\frac{q}{\sigma} - \frac{r}{\sigma^2}\right) d\sigma}{\int_0^\infty \left(\frac{1}{\sigma}\right)^{p+2} \exp\left(\frac{q}{\sigma} - \frac{r}{\sigma^2}\right) d\sigma} \end{aligned}$$

5.4.2 $\phi(x)/\Phi(x)$ when x is very small

In the variational parameter update section, we encounter the following evaluation:

$$\begin{aligned} E(y_i^*) &= \mu_{y_i^*} + \frac{\phi(\mu_{y_i^*})}{\Phi(\mu_{y_i^*})^{y_i} (\Phi(\mu_{y_i^*}) - 1)^{1-y_i}} \\ \mu_{y_i^*} &= w'_i \mu_\beta^q + \delta \text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q) + \delta \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \end{aligned}$$

However, we must note that the expectation behaves extremely pathologically. For example,

$$\lim_{t \rightarrow -\infty} \frac{\exp(-t^2/2)}{\int_{-\infty}^t \exp(-x^2/2) dx} = \infty.$$

Even though this does not transpire quite often for in actual computations since we do not deal with infinity in real life. However, we must not simply code `dnorm(x)/pnorm(x)` since `pnorm(x)` returns zero for even as reasonably small a value as -40 , notwithstanding the true value of the quotient being $\phi(-40)/\Phi(-40) = 40.02496884$. Therefore, we should use the following identity:

$$\frac{\phi(x)}{\Phi(x)} = \frac{(2/\pi)^{1/2} \exp(-x^2/2)}{\text{erf}(x/\sqrt{2}) + 1}.$$

The problem is, even the RHS of the identity fails if x is -9 . We thus turn to the Laurent series of $\phi(t)/\Phi(t)$:

$$\frac{\exp(-t^2/2)}{\int_{-\infty}^t \exp(-x^2/2) dx} = -t - \frac{1}{t} + \frac{2}{t^3} - \frac{10}{t^5} + \mathcal{O}\left(\left(\frac{1}{t}\right)^6\right) \quad \text{at } t = -\infty$$

for values smaller than -8 .

5.4.3 $\phi(x)/(\Phi(x) - 1)$

This is much better than the previous one.

$$\lim_{t \rightarrow \infty} \frac{\exp(-t^2/2)}{\int_{-\infty}^t \exp(-x^2/2) dx - 1} = 0.$$

The only problem for this calculation is that when we code the expression, we will be relying on `pnorm` which will give 1 for quite large values, immediately rendering the whole expression indefinite since it makes the denominator zero. Therefore, we again come up with another identity:

$$\frac{\phi(x)}{\Phi(x) - 1} = \frac{\exp(-x^2/2)}{(\pi/2)^{1/2} (\text{erf}(x/\sqrt{2}) + 1) - 1}.$$

Unlike the identity in the previous subsection, we do not have to consider large values since it will tend to zero as x grows larger.

5.5 Corrections

5.5.1 Original Paper: Linear model

There are some mistakes in the original paper so I provide the calculation. $S_2(\mu_\theta^q, \Sigma_\theta^q) = E(\ln p(y|\beta, \theta_J, \sigma^2))$. Let's do this.

$$\begin{aligned} S_2(\mu_\theta^q, \Sigma_\theta^q) &= -\frac{1}{2} E\left(\frac{1}{\sigma^2}\right) \sum_{i=1}^n E\left((y_i - w'_i \beta - \delta \theta'_J \varphi_J^a(x_i) \theta_J)^2\right) \\ &= -\frac{1}{2} E\left(\frac{1}{\sigma^2}\right) \sum_{i=1}^n E\left(y_i^2 - 2 \underbrace{y_i (w'_i \beta + \delta \theta'_J \varphi_J^a(x_i) \theta_J)}_{T_1} + \underbrace{(w'_i \beta + \delta \theta'_J \varphi_J^a(x_i) \theta_J)^2}_{T_2}\right) \end{aligned}$$

where

$$\begin{aligned}
E(T_1) &= y_i \left(w'_i \mu_\beta^q + \delta \left(\text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q) + \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \right) \right) \\
E(T_2) &= E \left((w'_i \beta)^2 \right) + 2\delta \left(w'_i \mu_\beta^q \left(\text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q) + \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \right) \right) + E \left((\theta'_J \varphi_J^a(x_i) \theta_J) \right) \\
&= \mu_\beta^{q'} w_i w'_i \mu_\beta^q + \text{Tr} \left(w_i w'_i \Sigma_\beta^q \right) + 2\delta \left(w'_i \mu_\beta^q \left(\text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q) + \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \right) \right) \\
&\quad + \delta^2 \left(3 \text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q)^2 + 6 \mu_\theta^{q'} \varphi_J^a(x_i) \Sigma_\theta^q \varphi_J^a(x_i) \mu_\theta^q + \left(\mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \right)^2 \right)
\end{aligned}$$

Arranging the terms,

$$\begin{aligned}
S_2(\mu_\theta^q, \Sigma_\theta^q) &= -\frac{1}{2} E \left(\frac{1}{\sigma^2} \right) \sum_{i=1}^n \underbrace{\left(y_i - w'_i \mu_\beta^q - \delta \left(\text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q) + \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \right) \right)^2}_{T_3} \\
&\quad + \delta^2 \left(\underbrace{2 \text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q)^2 + 4 \mu_\theta^{q'} \varphi_J^a(x_i) \Sigma_\theta^q \varphi_J^a(x_i) \mu_\theta^q}_{T_4} \right) + \text{Tr} \left(w_i w'_i \Sigma_\beta^q \right).
\end{aligned}$$

We have represented S_2 with regards to the squared term for the sake of succinctness. However, for matrix differentiation, let's expand it again.

$$\begin{aligned}
T_3 &= y_i^2 - 2y_i \left(w'_i \mu_\beta^q + \delta \left(\text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q) + \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \right) \right) + 2\delta w'_i \mu_\beta^q \left(\text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q) + \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \right) \\
&\quad + \delta^2 \left(\text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q)^2 + 2 \text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q) \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q + \left(\mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \right)^2 \right)
\end{aligned}$$

$$\frac{\partial T_3}{\partial \Sigma_\theta^q} = -2\delta y_i \varphi_J^a(x_i) + 2\delta w'_i \mu_\beta^q \varphi_J^a(x_i) + 2\delta^2 \varphi_J^a(x_i) \Sigma_\theta^q \varphi_J^a(x_i) + 2\delta^2 \mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q \varphi_J^a(x_i)$$

$$\frac{\partial T_4}{\partial \Sigma_\theta^q} = 4\varphi_J^a(x_i) \Sigma_\theta^q \varphi_J^a(x_i) + 4\varphi_J^a(x_i) \mu_\theta^q \mu_\theta^{q'} \varphi_J^a(x_i)$$

The original paper gives the following derivative:

$$\begin{aligned}
\frac{\partial S_2}{\partial \Sigma_\theta^q} &= -\frac{1}{2} E \left(\frac{1}{\sigma^2} \right) \sum_{i=1}^n \left\{ 4\varphi_J^a(x_i) \Sigma_\theta^q \varphi_J^a(x_i) + 4\varphi_J^a(x_i) \mu_\theta^q \mu_\theta^{q'} \varphi_J^a(x_i) \right. \\
&\quad \left. - 2\delta \left(y_i - w'_i \mu_\beta^q - \delta \underbrace{\text{Tr}(\Sigma_\theta^q \varphi_J^a(x_i))}_{(1)} - \delta \underbrace{\mu_\theta^{q'} \Sigma_\theta^q \mu_\theta^q}_{(2)} \right) \varphi_J^a(x_i) \right\}
\end{aligned}$$

First, where did (1) come from? Second, (2) should be $\mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q$.

(1) is supposed to be $\varphi_J^a(x_i) \Sigma_\theta^q \varphi_J^a(x_i)$ because the derivative of $\text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q)^2$ is missing. Let $f = \text{Tr}(\varphi_J^a(x_i) \Sigma_\theta^q)^2 = \varphi \Sigma : \varphi \Sigma$.

$$\begin{aligned}
f &= \varphi \Sigma : \varphi \Sigma \\
\partial f &= 2(\varphi \Sigma : \varphi \partial \Sigma) \\
&= 2\varphi \Sigma \varphi : \partial \Sigma \\
\frac{\partial f}{\partial \Sigma} &= 2\varphi \Sigma \varphi.
\end{aligned}$$

Therefore, the derivative should be as follows:

$$\frac{\partial S_2}{\partial \Sigma_\theta^q} = -\frac{1}{2} \text{E} \left(\frac{1}{\sigma^2} \right) \sum_{i=1}^n \left\{ \underbrace{6}_{(1)} \varphi_J^a(x_i) \Sigma_\theta^q \varphi_J^a(x_i) + 4 \varphi_J^a(x_i) \mu_\theta^q \mu_\theta^{q'} \varphi_J^a(x_i) \right. \\ \left. - 2\delta \left(y_i - w_i' \mu_\beta^q - \delta \underbrace{\mu_\theta^{q'} \varphi_J^a(x_i) \mu_\theta^q}_{(2)} \right) \varphi_J^a(x_i) \right\}$$

6 Probit: Monotone Convex/Concave Shape Restriction

6.1 Model