Variational Inference Masterclass: Variational Message Passing

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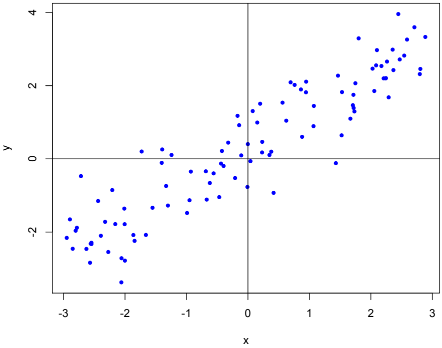
8 November 2022

Part I

Introduction and Motivation

Consider the following data:



In a typical regression problem we solve using:

$$\hat{\beta} = \underset{\beta \in \mathbb{R}^2}{\operatorname{argmin}} \|\boldsymbol{y} - \boldsymbol{X}\beta\|_2$$

Linear Regression

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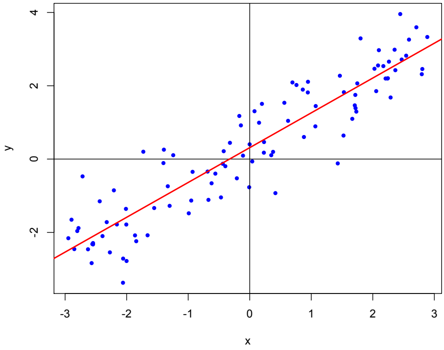

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$$\hat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta} \in \mathbb{R}^2}{\operatorname{argmin}} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}\|_2$$

Mean Field Variational Bayes

Tractable Bayesian inference is achieved by introducing a latent variable (Gelman, 2006; Huang and Wand, 2013):

$$
\begin{aligned}
y_i | x_i, \boldsymbol{\beta}, \sigma^2 &\overset{\text{ind.}}{\sim} N(\beta_0 + \beta_1 x_i, \sigma^2) \quad i = 1, \ldots, n \\
\boldsymbol{\beta} &\sim N(\mathbf{0}, \Sigma_0) \\
\sigma^2 | a &\sim \text{Inverse} - \chi^2(1, 1/a) \\
a &\sim \text{Inverse} - \chi^2(1, 1/A^2)
\end{aligned}
$$

Note that if

$$\sigma^2 | a \sim \text{Inverse} - \chi^2(1, 1/a) \quad \text{and} \quad a \sim \text{Inverse} - \chi^2(1, 1/A^2)$$

We use the mean field assumption (Menictas and Wand, 2013):

$$\{\boldsymbol{\beta}, a\} \perp\!\!\!\perp \sigma^2$$

That is,

$$p(\boldsymbol{\beta}, \sigma^2, a | \boldsymbol{y}) \approx p(\boldsymbol{\beta}, a | \boldsymbol{y}) p(\sigma^2 | \boldsymbol{y})$$

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Mean Field Variational Bayes

In variational inference, we approximate the posterior density function $p(\boldsymbol{\beta},\sigma^2,a|\boldsymbol{y})$ by another density function $q(\boldsymbol{\beta},\sigma^2,a)$.

The "best" approximate density function $q^*(\boldsymbol{\beta},\sigma^2,a)$ is the one that is "closest" to the true posterior density function $p(\boldsymbol{\beta},\sigma^2,a|\boldsymbol{y})$:

$$q^*(\boldsymbol{\beta},\sigma^2,a) = \underset{q\in\mathcal{Q}}{\operatorname{argmin}}\, D_{\text{KL}}\left\{q(\boldsymbol{\beta},\sigma^2,a)\|p(\boldsymbol{\beta},\sigma^2,a|\boldsymbol{y})\right\}$$

Our mean field assumption combined with results from Graph Theory, see Chapter 8 of Bishop (2006), allow us to enforce the product form:

$$p(\boldsymbol{\beta},\sigma^2,a|\boldsymbol{y}) \approx q(\boldsymbol{\beta},\sigma^2,a) = q(\boldsymbol{\beta},a)q(\sigma^2) = q(\boldsymbol{\beta})q(\sigma^2)q(a)$$

For $\boldsymbol{\beta}$, the optimisation problem has the following solution:

$$\begin{aligned} q^*(\boldsymbol{\beta}) &= C_1 \exp\left[\mathbb{E}_{-q(\boldsymbol{\beta})} \log\left\{p(\boldsymbol{y},\boldsymbol{\beta},\sigma^2,a)\right\}\right] \\ &= C_2 \exp\left[\mathbb{E}_{-q(\boldsymbol{\beta})} \log\left\{p(\boldsymbol{y}|\boldsymbol{\beta},\sigma^2,a)p(\boldsymbol{\beta})\right\}\right] \end{aligned}$$

where

$$\mathbb{E}_{-q(\boldsymbol{\beta})} f(\boldsymbol{y},\boldsymbol{\beta},\sigma^2,a) \equiv \int\int f(\boldsymbol{y},\boldsymbol{\beta},\sigma^2,a)q(\sigma^2)q(a)\,da\,d\sigma^2$$

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Mean Field Variational Bayes

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\begin{aligned}
&\mathbb{E}_{-q(\boldsymbol{\beta})} \log\left\{p(\boldsymbol{y}|\boldsymbol{\beta},\sigma^2)p(\boldsymbol{\beta})\right\} \\
&\qquad = \mathbb{E}_{-q(\boldsymbol{\beta})} \log p(\boldsymbol{y}|\boldsymbol{\beta},\sigma^2) + \log p(\boldsymbol{\beta}) \\
&\qquad = \mathbb{E}_{-q(\boldsymbol{\beta})} \left\{-\frac{1}{2\sigma^2}(\boldsymbol{y}-\boldsymbol{X\beta})^T(\boldsymbol{y}-\boldsymbol{X\beta})\right\} - \frac{1}{2}\boldsymbol{\beta}^T\Sigma_0^{-1}\boldsymbol{\beta} + \text{const.} \\
&\qquad = -\frac{1}{2}\,\mathbb{E}_q\left(\frac{1}{\sigma^2}\right)(\boldsymbol{y}-\boldsymbol{X\beta})^T(\boldsymbol{y}-\boldsymbol{X\beta}) - \frac{1}{2}\boldsymbol{\beta}^T\Sigma_0^{-1}\boldsymbol{\beta} + \text{const.} \\
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\end{aligned}
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Remember that $q^*(\boldsymbol{\beta}) \propto \exp\left[\mathbb{E}_{-q(\boldsymbol{\beta})} \log\left\{p(\boldsymbol{y}|\boldsymbol{\beta},\sigma^2)p(\boldsymbol{\beta})\right\}\right]$

That is, $q^*(\boldsymbol{\beta})$ is a normal density function.

Similar arguments can be used to show that $q^*(\sigma^2)$ and $q^*(a)$ are inverse chi-squared density functions.

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Mean Field Variational Bayes

$q^*(\boldsymbol{\beta})$ is the $N(\boldsymbol{\mu}_{q(\boldsymbol{\beta})}, \Sigma_{q(\boldsymbol{\beta})})$ density function, where

$$\Sigma_{q(\boldsymbol{\beta})} \longleftarrow \left\{ \left(\frac{N+1}{\lambda_{q(\sigma^2)}} \right) \boldsymbol{X}^T \boldsymbol{X} + \Sigma_0^{-1} \right\}^{-1}$$

$$\text{and} \quad \boldsymbol{\mu}_{q(\boldsymbol{\beta})} \longleftarrow \left(\frac{N+1}{\lambda_{q(\sigma^2)}} \right) \Sigma_{q(\boldsymbol{\beta})} \boldsymbol{X}^T \boldsymbol{y}$$

$q^*(\sigma^2)$ is the Inverse $-\chi^2(N+1, \lambda_{q(\sigma^2)})$ density function, where

$$\lambda_{q(\sigma^2)} \longleftarrow \boldsymbol{y}^T \boldsymbol{y} - 2\boldsymbol{\mu}_{q(\boldsymbol{\beta})} \boldsymbol{X}^T \boldsymbol{y} + \operatorname{tr}\left\{ \boldsymbol{X}^T \boldsymbol{X} (\Sigma_{q(\boldsymbol{\beta})} + \boldsymbol{\mu}_{q(\boldsymbol{\beta})} \boldsymbol{\mu}_{q(\boldsymbol{\beta})}^T) \right\} + \frac{2}{\lambda_{q(a)}}$$

$q^*(a)$ is the Inverse $-\chi^2(2, \lambda_{q(a)})$ density function, where

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MFVB for the Bayesian linear regression model

1. Initialise all optimal posterior density functions
2. Cycle:

$$q^*(a) \propto \exp\left\{\mathbb{E}_{-q^*(a)} \log p(\boldsymbol{y}, \boldsymbol{\beta}, \sigma^2, a)\right\}$$
$$q^*(\sigma^2) \propto \exp\left\{\mathbb{E}_{-q^*(\sigma^2)} \log p(\boldsymbol{y}, \boldsymbol{\beta}, \sigma^2, a)\right\}$$
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3. Stop: $D_{\text{KL}}\left\{q(\boldsymbol{\beta}, \sigma^2, a) \| p(\boldsymbol{\beta}, \sigma^2, a | \boldsymbol{y})\right\}$ converges.

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Limitations of MFVB

The advantage of MFVB over Monte Carlo alternatives is that it is a much faster algorithm

However, for Bayesian inference on more complex models, we have to re-do all the derivations.

Take for example, the Bayesian Gaussian-response linear mixed model:

$$
\begin{aligned}
&\boldsymbol{y}_i \mid \boldsymbol{\beta}, \boldsymbol{u}_i, \sigma^2 \sim N(\boldsymbol{X}_i\boldsymbol{\beta} + \boldsymbol{X}_i\boldsymbol{u}_i, \sigma^2\boldsymbol{I}), \qquad \boldsymbol{u}_i \mid \Sigma \sim N(\boldsymbol{0}, \Sigma), \quad \text{for } 1 \le i \le m \\
&\boldsymbol{\beta} \sim N(\boldsymbol{0}, \sigma_\beta^2\boldsymbol{I}); \qquad \sigma^2 \mid a \sim \text{Inverse} - \chi^2(1, 1/a) \\
&a \sim \text{Inverse} - \chi^2(1, 1/2), \quad \Sigma|\boldsymbol{A} \sim \text{Inverse G-Wishart}(G_{\text{full}}, 2q, \boldsymbol{A}^{-1}) \\
&\boldsymbol{A} \sim \text{Inverse G-Wishart}(G_{\text{diag}}, 1, \tfrac{1}{2}\boldsymbol{I})
\end{aligned}
$$

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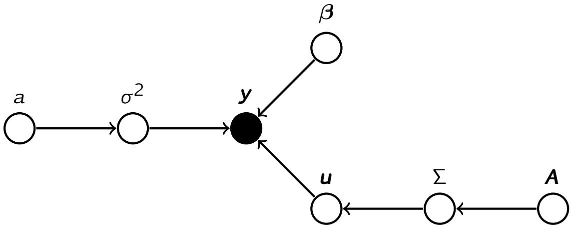

Variational Message Passing

Prof. Matt Wand
Distinguished professor of statistics, University of Technology Sydney
Fast Approximate Inference for Arbitrarily Large Semiparametric Regression Models via Message Passing, Journal of the American Statistical Association, 2017, VOL. 112, NO. 517, 137–168, Theory and Methods

Steps Towards Message Passing Algorithms

Let's reconsider the Bayesian linear regression model:

$$y_i | x_i, \boldsymbol{\beta}, \sigma^2 \stackrel{\text{ind.}}{\sim} N(\beta_0 + \beta_1 x_i, \sigma^2) \quad i = 1, \ldots, n, \quad \boldsymbol{\beta} \sim N(\mathbf{0}, \Sigma_0)$$

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We showed that the optimal posterior density function for $\boldsymbol{\beta}$ is

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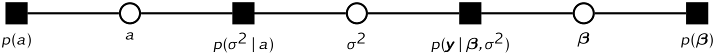

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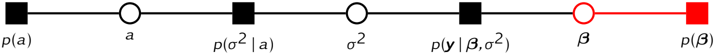

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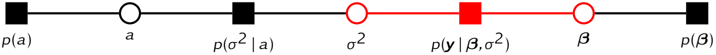

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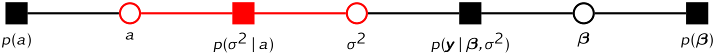

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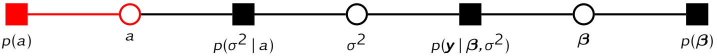

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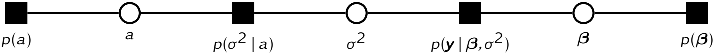

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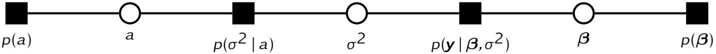

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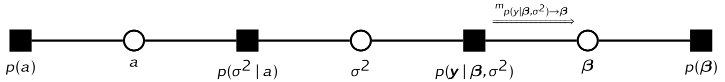

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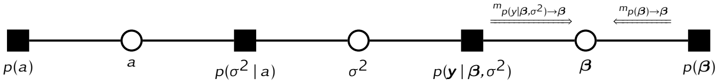

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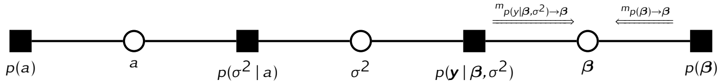

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$$\sigma^2|a \sim \text{Inverse} - \chi^2(1, 1/a) \quad a \sim \text{Inverse} - \chi^2(1, 1/A^2)$$

We showed that the optimal posterior density function for $\boldsymbol{\beta}$ is

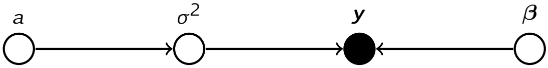
$$q^*(\boldsymbol{\beta}) = C\exp\left\{-\frac{1}{2}\,\mathbb{E}_q(1/\sigma^2)\boldsymbol{\beta}^T\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{\beta} + \mathbb{E}_q(1/\sigma^2)\boldsymbol{\beta}^T\boldsymbol{X}^T\boldsymbol{y}\right\}\exp\left\{-\frac{1}{2}\boldsymbol{\beta}^T\Sigma_0^{-1}\boldsymbol{\beta}\right\}$$

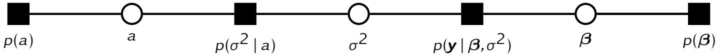
We define the messages as

$$m_{p(y|\boldsymbol{\beta},\sigma^2)\to\boldsymbol{\beta}}(\boldsymbol{\beta}) \equiv \exp\left\{-\frac{1}{2}\,\mathbb{E}_q(1/\sigma^2)\boldsymbol{\beta}^T\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{\beta} + \mathbb{E}_q(1/\sigma^2)\boldsymbol{\beta}^T\boldsymbol{X}^T\boldsymbol{y}\right\}$$

$$m_{p(\boldsymbol{\beta})\to\boldsymbol{\beta}}(\boldsymbol{\beta}) \equiv \exp\left\{-\frac{1}{2}\boldsymbol{\beta}^T\Sigma_0^{-1}\boldsymbol{\beta}\right\}$$

The representation via a directed acyclic graph does not facilitate this factorised form:





The message passed from a factor f to its neighbouring parameter $\boldsymbol{\theta}$ is

$$m_{f\to\boldsymbol{\theta}}(\boldsymbol{\theta}) \propto \exp\Big\{\mathbb{E}_{-q(\boldsymbol{\theta})}(\log f)\Big\}$$

For example, the message from the Gaussian likelihood factor $p(\boldsymbol{y}|\boldsymbol{\beta}, \sigma^2)$ to the parameter $\boldsymbol{\beta}$ is

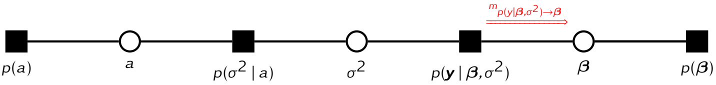
$$m_{p(\boldsymbol{y}|\boldsymbol{\beta},\sigma^2)\to\boldsymbol{\beta}}(\boldsymbol{\beta}) \propto \exp\Big[\mathbb{E}_{-q(\boldsymbol{\beta})}\{\log p(\boldsymbol{y}|\boldsymbol{\beta},\sigma^2)\}\Big]$$

The message that $\boldsymbol{\theta}$ will pass on to another neighbouring factor is simply the message that it received from the factor f. For example, the message that $\boldsymbol{\beta}$ passes on to $p(\boldsymbol{\beta})$ is

$$m_{\boldsymbol{\beta}\to p(\boldsymbol{\beta})}(\boldsymbol{\beta}) = m_{p(\boldsymbol{y}|\boldsymbol{\beta},\sigma^2)\to\boldsymbol{\beta}}(\boldsymbol{\beta})$$

The approximate q-density function for a parameter $\boldsymbol{\theta}$ is the product of all messages that it received. For example, $q(\boldsymbol{\beta})$ is

$$q(\boldsymbol{\beta}) = m_{p(\boldsymbol{y}|\boldsymbol{\beta},\sigma^2)\to\boldsymbol{\beta}}(\boldsymbol{\beta}) \times m_{\boldsymbol{\beta}\to p(\boldsymbol{\beta})}(\boldsymbol{\beta})$$



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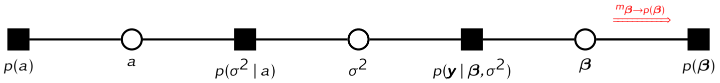
General Message Passing Rules



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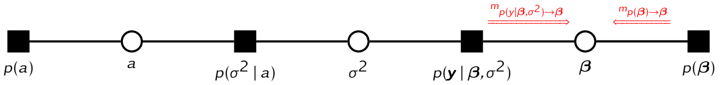

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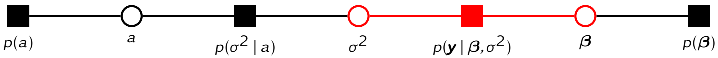
The Gaussian Likelihood Fragment



The message from the likelihood specification to the parameter $\boldsymbol{\beta}$ is

$$m_{p(\boldsymbol{y}|\boldsymbol{\beta},\sigma^2)\to\boldsymbol{\beta}}(\boldsymbol{\beta}) \propto \exp\left\{\begin{bmatrix}\boldsymbol{\beta}\\ \text{vec}(\boldsymbol{\beta}\boldsymbol{\beta}^T)\end{bmatrix}^T \begin{bmatrix}\mathbb{E}_q(1/\sigma^2)\boldsymbol{X}^T\boldsymbol{y}\\ -\frac{1}{2}\,\mathbb{E}_q(1/\sigma^2)\,\text{vec}(\boldsymbol{X}^T\boldsymbol{X})\end{bmatrix}\right\}$$

That is, $m_{p(\boldsymbol{y}|\boldsymbol{\beta},\sigma^2)\to\boldsymbol{\beta}}(\boldsymbol{\beta})$ is a multivariate normal density function in exponential family form:

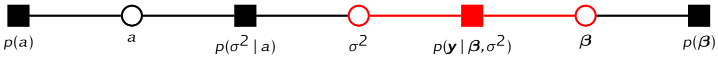
$$p(\boldsymbol{x}) = C\exp\{\boldsymbol{T}(\boldsymbol{x})^T\boldsymbol{\eta}\}.$$

The message to σ^2 is

$$m_{p(\boldsymbol{y}|\boldsymbol{\beta},\sigma^2)\to\sigma^2}(\sigma^2) = \exp\left\{\begin{bmatrix}\log(\sigma^2)\\ 1/\sigma^2\end{bmatrix}^T \begin{bmatrix}-n/2\\ -\frac{1}{2}\,\mathbb{E}_q(\|\boldsymbol{y}-\boldsymbol{X}\boldsymbol{\beta}\|^2)\end{bmatrix}\right\},$$

which is an inverse chi-squared density function in exponential family form.

The Gaussian Likelihood Fragment



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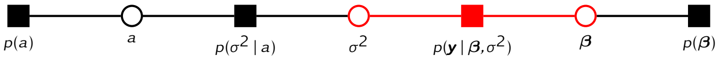
The Gaussian Likelihood Fragment



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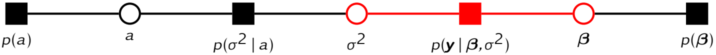
The Gaussian Likelihood Fragment



By restricting the form of the messages passing updates to distributions in the exponential family form, we can completely characterise these message updates by their natural parameter vectors:

$$\boldsymbol{\eta}_{p(\boldsymbol{y}|\boldsymbol{\beta},\sigma^2)\to\boldsymbol{\beta}} = \begin{bmatrix} \mathbb{E}_q(1/\sigma^2)\boldsymbol{X}^T\boldsymbol{y} \\ -\frac{1}{2}\,\mathbb{E}_q(1/\sigma^2)\operatorname{vec}(\boldsymbol{X}^T\boldsymbol{X}) \end{bmatrix}$$

$$\boldsymbol{\eta}_{p(\boldsymbol{y}|\boldsymbol{\beta},\sigma^2)\to\sigma^2} = \begin{bmatrix} -n/2 \\ -\frac{1}{2}\,\mathbb{E}_q(\|\boldsymbol{y}-\boldsymbol{X}\beta\|^2) \end{bmatrix}$$

Gaussian Density Function in Exponential Family Form

$$\boldsymbol{x}|\boldsymbol{\mu},\Sigma \sim \mathrm{N}(\boldsymbol{\mu},\Sigma)$$

The density function in exponential family form is:

$$p(\boldsymbol{x}|\boldsymbol{\mu},\Sigma) = C\exp\left\{\begin{bmatrix}\boldsymbol{\beta}\\ \mathrm{vec}(\boldsymbol{\beta}\boldsymbol{\beta}^{\mathsf{T}})\end{bmatrix}^{\mathsf{T}}\boldsymbol{\eta}\right\},\quad \boldsymbol{\eta}=\begin{bmatrix}\boldsymbol{\eta}_1\\ \boldsymbol{\eta}_2\end{bmatrix}=\begin{bmatrix}\Sigma^{-1}\boldsymbol{\mu}\\ -\frac{1}{2}\,\mathrm{vec}(\Sigma^{-1})\end{bmatrix}$$

The transformation back to the common parameters is

$$\Sigma = -\frac{1}{2}\{\mathrm{vec}^{-1}(\boldsymbol{\eta}_2)\}^{-1},\quad \boldsymbol{\mu}=\Sigma\boldsymbol{\eta}_1$$

Inverse Wishart Density Function in Exponential Family Form

$$\Sigma|\kappa, \boldsymbol{\Lambda} \sim \text{Inverse Wishart}(\kappa, \boldsymbol{\Lambda})$$

The density function in exponential family form is:

$$p(\Sigma|\kappa, \boldsymbol{\Lambda}) = C \exp\left\{\begin{bmatrix} \log|\Sigma| \\ \text{vec}(\Sigma^{-1}) \end{bmatrix}^{\mathsf{T}} \boldsymbol{\eta}\right\}, \quad \boldsymbol{\eta} = \begin{bmatrix} \boldsymbol{\eta}_1 \\ \boldsymbol{\eta}_2 \end{bmatrix} = \begin{bmatrix} -\frac{1}{2}(\kappa + 2) \\ -\frac{1}{2}\,\text{vec}(\boldsymbol{\Lambda}) \end{bmatrix}$$

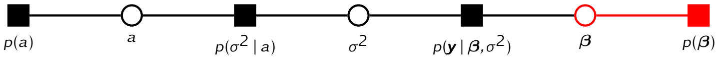
The transformation back to the common parameters is

$$\kappa = -2\eta_1 - 2, \quad \boldsymbol{\Lambda} = -2\,\text{vec}^{-1}(\boldsymbol{\eta}_2)$$

For variational inference, we require:

$$\mathbb{E}(\boldsymbol{\Sigma}^{-1}) = \begin{cases} \{\eta_1 + \frac{1}{2}(d+1)\}\{\text{vec}^{-1}(\boldsymbol{\eta}_2)\}^{-1}, & \text{if } \Sigma \text{ is a complete matrix} \\ \{\eta_1 + 1\}\{\text{vec}^{-1}(\boldsymbol{\eta}_2)\}^{-1}, & \text{if } \Sigma \text{ is a diagonal; matrix} \end{cases}$$

Fragments



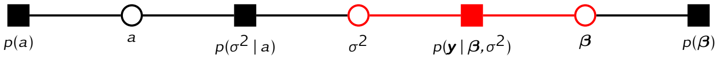
Gaussian prior fragment (Wand, 2017)

Gaussian likelihood fragment (Wand, 2017)

Iterated inverse Wishart fragment (Maestrini and Wand, 2020)

Inverse Wishart prior fragment (Maestrini and Wand, 2020)

Fragments



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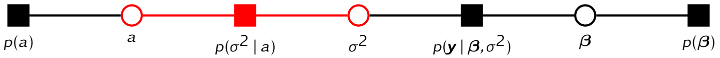

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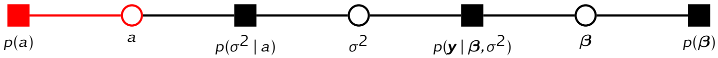

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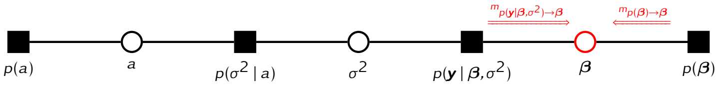
q-Density Functions



Recall that the approximate q-density function for each parameter is the product of all the messages that it received.

The computation for $q(\boldsymbol{\beta})$ is

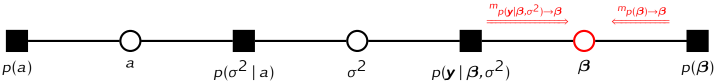
$$q(\boldsymbol{\beta}) = m_{p(\mathbf{y}|\boldsymbol{\beta},\sigma^2)\rightarrow\boldsymbol{\beta}}(\boldsymbol{\beta}) \times m_{p(\boldsymbol{\beta})\rightarrow\boldsymbol{\beta}}(\boldsymbol{\beta})$$

$$= \exp\left\{ \begin{bmatrix} \boldsymbol{\beta} \\ \mathrm{vec}(\boldsymbol{\beta}\boldsymbol{\beta}^T) \end{bmatrix}^T \left(\boldsymbol{\eta}_{p(\mathbf{y}|\boldsymbol{\beta},\sigma^2)\rightarrow\boldsymbol{\beta}} + \boldsymbol{\eta}_{p(\boldsymbol{\beta})\rightarrow\boldsymbol{\beta}} \right) \right\}$$

So the q-density function is also in the exponential family of density functions with natural parameter vector:

$$\boldsymbol{\eta}_{q^*(\boldsymbol{\beta})} = \boldsymbol{\eta}_{p(\mathbf{y}|\boldsymbol{\beta},\sigma^2)\rightarrow\boldsymbol{\beta}} + \boldsymbol{\eta}_{p(\boldsymbol{\beta})\rightarrow\boldsymbol{\beta}}$$

q-Density Functions



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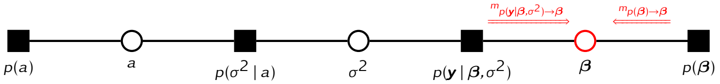

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$$\begin{aligned} q(\boldsymbol{\beta}) &= m_{p(\boldsymbol{y}|\boldsymbol{\beta},\sigma^2)\rightarrow\boldsymbol{\beta}}(\boldsymbol{\beta}) \times m_{p(\boldsymbol{\beta})\rightarrow\boldsymbol{\beta}}(\boldsymbol{\beta}) \\ &= \exp\left\{\begin{bmatrix} \boldsymbol{\beta} \\ \text{vec}(\boldsymbol{\beta}\boldsymbol{\beta}^T) \end{bmatrix}^T \left(\boldsymbol{\eta}_{p(\boldsymbol{y}|\boldsymbol{\beta},\sigma^2)\rightarrow\boldsymbol{\beta}} + \boldsymbol{\eta}_{p(\boldsymbol{\beta})\rightarrow\boldsymbol{\beta}}\right)\right\} \end{aligned}$$

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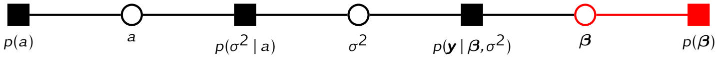
The Gaussian Prior Fragment



$$\boldsymbol{\beta} \sim N(\mathbf{0}, \sigma_\beta^2 \boldsymbol{I})$$

Inputs:

$$\sigma_\beta^2$$

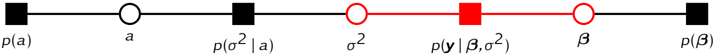
Updates:

$$\boldsymbol{\eta}_{p(\boldsymbol{\beta}) \to \boldsymbol{\beta}} = \begin{bmatrix} \mathbf{0} \\ -\frac{1}{2\sigma_\beta^2}\,\mathrm{vec}(\boldsymbol{I}) \end{bmatrix}$$

Outputs:

$$\boldsymbol{\eta}_{p(\boldsymbol{\beta}) \to \boldsymbol{\beta}}$$

The Gaussian Likelihood Fragment



$$\boldsymbol{y}|\boldsymbol{\beta},\sigma^2 \sim N(\boldsymbol{X}\boldsymbol{\beta},\sigma^2\boldsymbol{I})$$

Inputs:

$$\boldsymbol{\eta}_{q^*(\boldsymbol{\beta})}, \quad \boldsymbol{\eta}_{q^*(\sigma^2)}$$

Updates:

$$\text{Cov}_q(\boldsymbol{\beta}) = -\frac{1}{2}\{\text{vec}^{-1}(\boldsymbol{\eta}_{q^*(\boldsymbol{\beta})})_2\}^{-1}, \quad \mathbb{E}_q(\boldsymbol{\beta}) = \text{Cov}_q(\boldsymbol{\beta})(\boldsymbol{\eta}_{q^*(\boldsymbol{\beta})})_1,$$

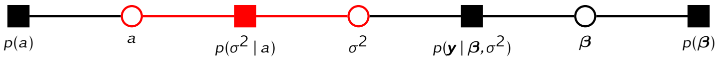
$$\mathbb{E}_q(1/\sigma^2) = \frac{(\boldsymbol{\eta}_{q^*(\sigma^2)})_1 + 1}{(\boldsymbol{\eta}_{q^*(\sigma^2)})_2}$$

$$\boldsymbol{\eta}_{p(\boldsymbol{y}|\boldsymbol{\beta},\sigma^2)\to\boldsymbol{\beta}} = \begin{bmatrix} \mathbb{E}_q(1/\sigma^2)\boldsymbol{X}^T\boldsymbol{y} \\ -\frac{1}{2}\,\mathbb{E}_q(1/\sigma^2)\text{vec}(\boldsymbol{X}^T\boldsymbol{X}) \end{bmatrix}, \quad \boldsymbol{\eta}_{p(\boldsymbol{y}|\boldsymbol{\beta},\sigma^2)\to\sigma^2} = \begin{bmatrix} -n/2 \\ -\frac{1}{2}\,\mathbb{E}_q(\|\boldsymbol{y}-\boldsymbol{X}\boldsymbol{\beta}\|^2) \end{bmatrix}$$

Outputs:

$$\boldsymbol{\eta}_{p(\boldsymbol{y}|\boldsymbol{\beta},\sigma^2)\to\boldsymbol{\beta}}, \quad \boldsymbol{\eta}_{p(\boldsymbol{y}|\boldsymbol{\beta},\sigma^2)\to\sigma^2}$$

Iterated Inverse Wishart Fragment



$$\Sigma | \boldsymbol{A} \sim \text{Inverse-Wishart}(\kappa, \boldsymbol{A}^{-1})$$

Inputs:

$$\boldsymbol{\eta}_{q^*(\Sigma)}, \quad \boldsymbol{\eta}_{q^*(\boldsymbol{A})}$$

Updates:

$$\mathbb{E}_q(\Sigma) = \{(\boldsymbol{\eta}_{q^*(\Sigma)})_1 + 1\}\{\text{vec}^{-1}(\boldsymbol{\eta}_{q^*(\Sigma)})_2\}^{-1},$$

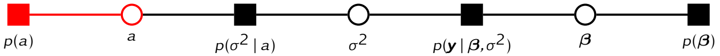
$$\mathbb{E}_q(\boldsymbol{A}) = \{(\boldsymbol{\eta}_{q^*(\boldsymbol{A})})_1 + 1\}\{\text{vec}^{-1}(\boldsymbol{\eta}_{q^*(\boldsymbol{A})})_2\}^{-1},$$

$$\boldsymbol{\eta}_{p(\Sigma|\boldsymbol{A})\to\Sigma} = \begin{bmatrix} -\frac{1}{2}(\kappa + d + 1) \\ -\frac{1}{2}\{\text{vec}\,\mathbb{E}_q(\boldsymbol{A}^{-1})\} \end{bmatrix}, \quad \boldsymbol{\eta}_{p(\Sigma|\boldsymbol{A})\to\boldsymbol{A}} = \begin{bmatrix} -\kappa/2 \\ -\frac{1}{2}\{\text{vec}\,\mathbb{E}_q(\Sigma^{-1})\} \end{bmatrix}$$

Outputs:

$$\boldsymbol{\eta}_{p(\Sigma|\boldsymbol{A})\to\Sigma}, \quad \boldsymbol{\eta}_{p(\Sigma|\boldsymbol{A})\to\boldsymbol{A}}$$

Inverse Wishart Prior Fragment



$$\boldsymbol{A} \sim \text{Inverse-Wishart}(\kappa, \boldsymbol{\Lambda})$$

Inputs:

$$\kappa, \boldsymbol{\Lambda}$$

Updates:

$$\boldsymbol{\eta}_{p(\boldsymbol{A}) \to \boldsymbol{A}} = \begin{bmatrix} -\frac{1}{2}(\kappa + d + 1) \\ -\frac{1}{2}\,\text{vec}(\boldsymbol{\Lambda}) \end{bmatrix}$$

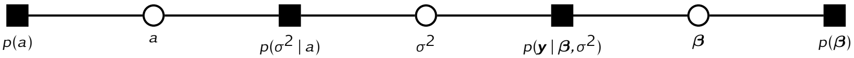
Outputs:

$$\boldsymbol{\eta}_{p(\boldsymbol{A}) \to \boldsymbol{A}}$$

Variational Message Passing

VMP for the Bayesian linear regression model

1. Initialise all messages from stochastic nodes to factors
2. Cycle:
   - (i) Update all messages from factors to stochastic nodes
   - (ii) Update all messages from stochastic nodes to factors
   - (iii) Update all optimal posterior density functions
3. Stop: $D_{\mathrm{KL}}\left\{q(\boldsymbol{\beta},\sigma^2,a)\|p(\boldsymbol{\beta},\sigma^2,a|\mathbf{y})\right\}$ converges.



VMP for the Bayesian linear regression model

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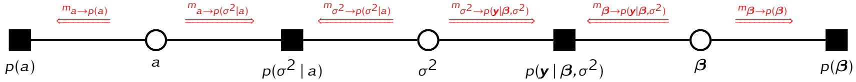

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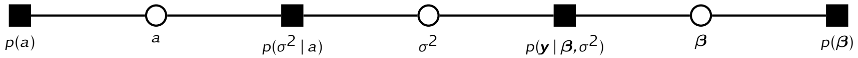

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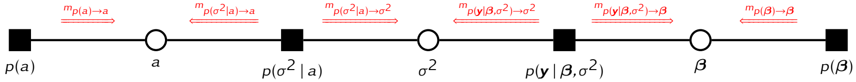

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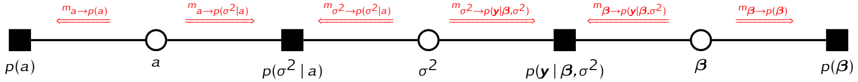

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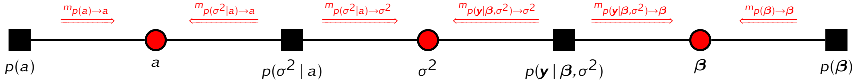

Variational Message Passing

VMP for the Bayesian linear regression model

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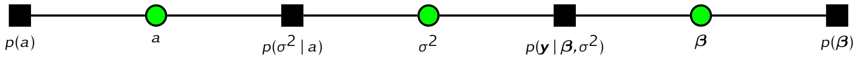
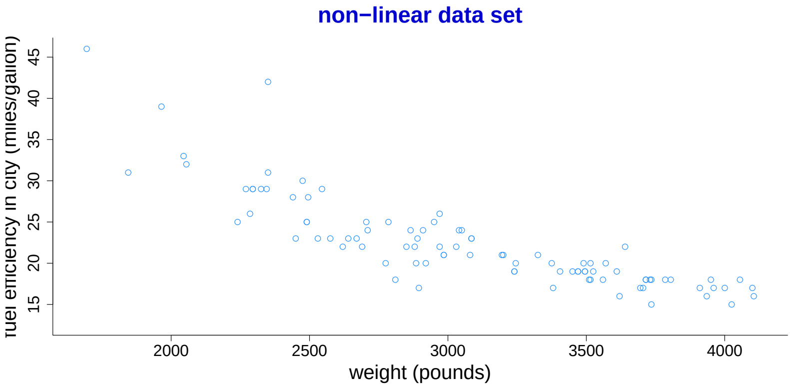


Part II

Building Model Complexity

Nonlinear Data



We can address nonlinear data sets using semiparametric regression techniques

Let x_i be the ith vehicle weight and y_i be its corresponding fuel efficiency score. The corresponding vectors are $\boldsymbol{x}$ and $\boldsymbol{y}$.

We construct a fixed effects matrix

$$\boldsymbol{X} = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}$$

Nonlinear effects are incorporated through a random effects matrix

$$\boldsymbol{Z} = \begin{bmatrix} z_1(x_1) & \dots & z_K(x_1) \\ \vdots & \ddots & \vdots \\ z_1(x_N) & \dots & z_K(x_N) \end{bmatrix},$$

where $\{z_k\}_{k=1}^{K}$ is a suitable spline basis – see Wand and Ormerod (2008) for a description of canonical cubic O'Sullivan penalised splines.

Bayesian Semiparametric Regression

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Bayesian Semiparametric Regression

A fundamental ingredient, which facilitates the incorporation of nonlinear predictor effects, is that of mixed model-based penalized splines:

$$f(x) = \beta_0 + \beta_1 x + \sum_{k=1}^{K} u_k z_k(x), \quad u_k|\sigma_u \overset{\text{ind.}}{\sim} \mathrm{N}(0, \sigma_u^2), \quad k = 1, \ldots, K.$$

The Bayesian semiparametric regression model is

$$\boldsymbol{y}|\boldsymbol{\beta}, \sigma^2 \sim \mathrm{N}(\boldsymbol{X\beta} + \boldsymbol{Zu}, \sigma^2 \boldsymbol{I}), \quad \boldsymbol{\beta} \sim \mathrm{N}(\boldsymbol{0}, \sigma_\beta^2 \boldsymbol{I}_2)$$

$$\boldsymbol{u}|\sigma_u^2 \sim \mathrm{N}(\boldsymbol{0}, \sigma_u^2 \boldsymbol{I}_K)$$

$$\sigma_u^2|a_u \sim \text{Inverse-}\chi^2(1, 1/a_u), \quad a_u \sim \text{inverse-}\chi^2(1, 1/A^2)$$

$$\sigma^2|a \sim \text{Inverse-}\chi^2(1, 1/a), \quad a \sim \text{inverse-}\chi^2(1, 1/A^2)$$

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$$y|\boldsymbol{\beta},\boldsymbol{u},\sigma^2 \sim \mathrm{N}(\boldsymbol{X}\boldsymbol{\beta}+\boldsymbol{Z}\boldsymbol{u},\sigma^2\boldsymbol{I}),\quad \begin{bmatrix}\boldsymbol{\beta}\\ \boldsymbol{u}\end{bmatrix}\Bigg|\ \sigma_u^2 \sim \mathrm{N}\left(\begin{bmatrix}\boldsymbol{0}\\ \boldsymbol{0}\end{bmatrix},\begin{bmatrix}\sigma_\beta^2\boldsymbol{I}_2 & \boldsymbol{O}^T\\ \boldsymbol{O} & \sigma_u^2\boldsymbol{I}_m\end{bmatrix}\right)$$

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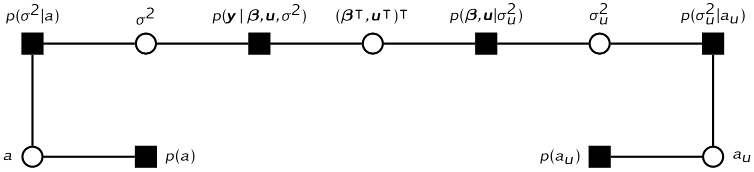

Gaussian likelihood fragment

Gaussian penalization fragment (Wand, 2017)

Iterated inverse Wishart fragment

Inverse Wishart prior fragment

$$y|\boldsymbol{\beta},\boldsymbol{u},\sigma^2 \sim \mathrm{N}(\boldsymbol{X}\boldsymbol{\beta}+\boldsymbol{Z}\boldsymbol{u},\sigma^2\boldsymbol{I}), \quad \left.\begin{bmatrix}\boldsymbol{\beta}\\ \boldsymbol{u}\end{bmatrix}\right|\sigma_u^2 \sim \mathrm{N}\left(\begin{bmatrix}0\\0\end{bmatrix},\begin{bmatrix}\sigma_\beta^2\boldsymbol{I}_2 & \boldsymbol{O}^T\\ \boldsymbol{O} & \sigma_u^2\boldsymbol{I}_m\end{bmatrix}\right)$$

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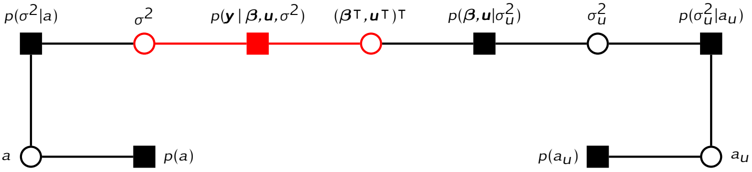

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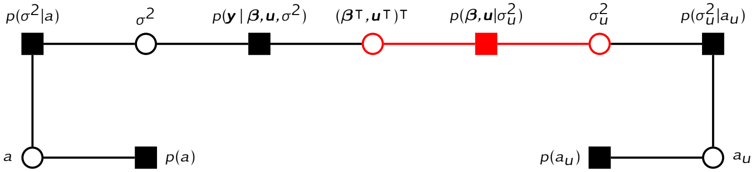

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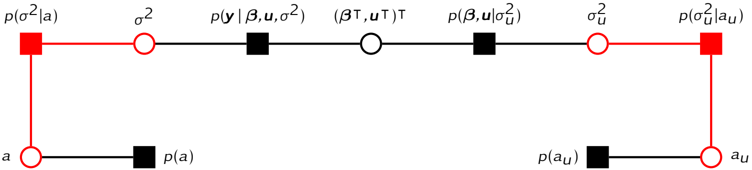

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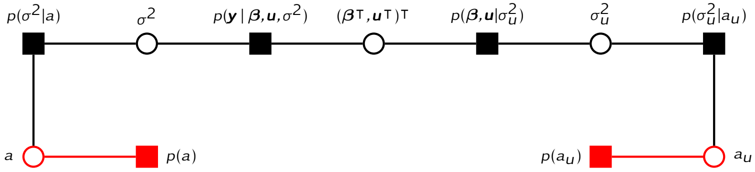

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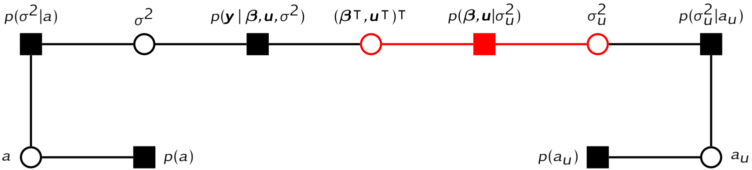

$$\begin{bmatrix}\boldsymbol{\beta}\\ \boldsymbol{u}\end{bmatrix}\Bigg|\ \Sigma_u \sim \mathrm{N}\left(\begin{bmatrix}0\\0\end{bmatrix},\begin{bmatrix}\sigma^2_\beta \boldsymbol{I}_2 & \boldsymbol{O}^T\\ \boldsymbol{O} & \Sigma_u\end{bmatrix}\right)$$

Inputs:

$$\boldsymbol{\eta}_{q^*(\boldsymbol{\beta},\boldsymbol{u})},\quad \boldsymbol{\eta}_{q^*(\Sigma_u)}$$

Updates:

$$\mathrm{Cov}_q\{(\boldsymbol{\beta}^\top,\boldsymbol{u}^\top)^\top\} = -\tfrac{1}{2}\{\mathrm{vec}^{-1}(\boldsymbol{\eta}_{q^*(\boldsymbol{\beta},\boldsymbol{u})})_2\}^{-1},\quad \mathbb{E}_q\{(\boldsymbol{\beta}^\top,\boldsymbol{u}^\top)^\top\} = \mathrm{Cov}_q\{(\boldsymbol{\beta}^\top,\boldsymbol{u}^\top)^\top\}(\boldsymbol{\eta}_{q^*(\boldsymbol{\beta},\boldsymbol{u})})_1,$$

$$\mathbb{E}_q(\Sigma_u^{-1}) = \{(\boldsymbol{\eta}_{q^*(\Sigma_u)})_1 + 1\}\left\{\mathrm{vec}^{-1}(\boldsymbol{\eta}_{q^*(\sigma^2_u)})_2\right\}^{-1},$$

$$\boldsymbol{\eta}_{p(\boldsymbol{\beta},\boldsymbol{u}|\Sigma_u)\to(\boldsymbol{\beta},\boldsymbol{u})} = \begin{bmatrix}\boldsymbol{0}_{K+2}\\ -\frac{1}{2}\,\mathrm{vec}\left(\begin{bmatrix}(1/\sigma^2_\beta)\boldsymbol{I}_2 & \boldsymbol{O}\\ \boldsymbol{O} & \mathbb{E}_q(\Sigma_u^{-1})\end{bmatrix}\right)\end{bmatrix},\quad \boldsymbol{\eta}_{p(\boldsymbol{\beta},\boldsymbol{u}|\Sigma_u)\to(\Sigma_u)} = \begin{bmatrix}-K/2\\ -\frac{1}{2}\,\mathrm{vec}\{\mathbb{E}_q(\boldsymbol{u}\boldsymbol{u}^\top)\}\end{bmatrix}$$

Outputs:

$$\boldsymbol{\eta}_{p(\boldsymbol{\beta},\boldsymbol{u}|\Sigma_u)\to(\boldsymbol{\beta},\boldsymbol{u})},\quad \boldsymbol{\eta}_{p(\boldsymbol{\beta},\boldsymbol{u}|\Sigma_u)\to(\Sigma_u)}$$

VMP for the Bayesian semiparametric regression model

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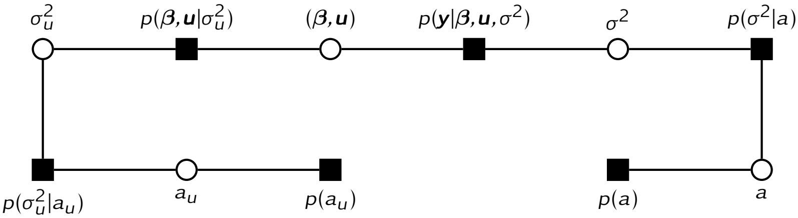

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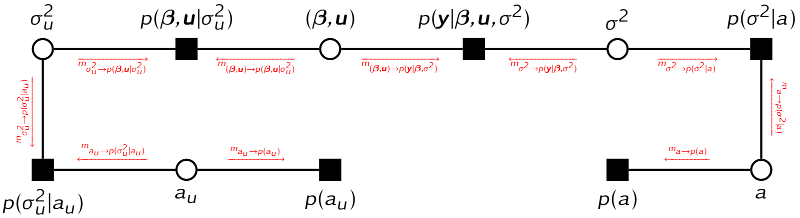

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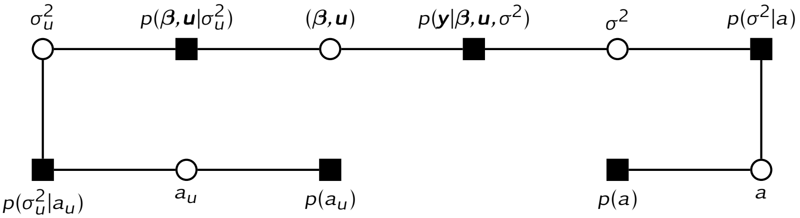

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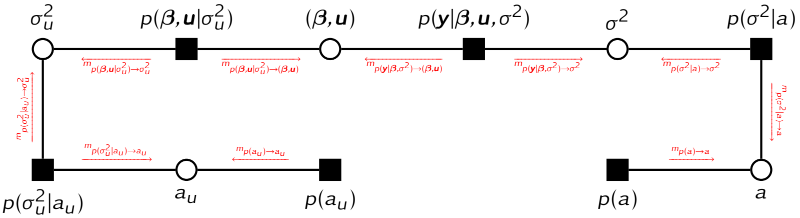

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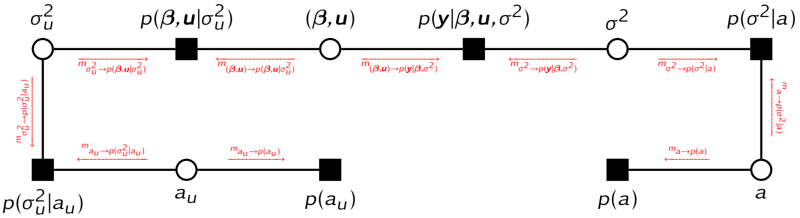

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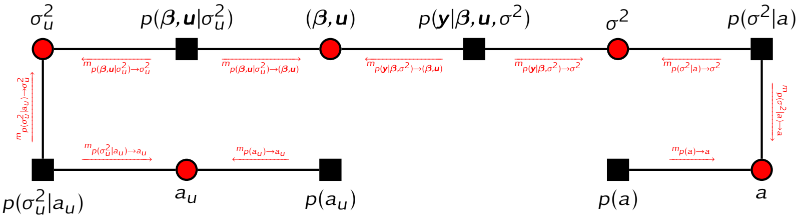

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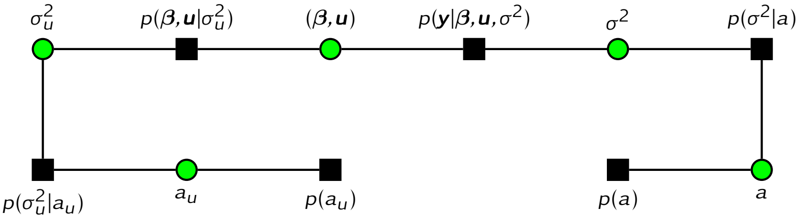
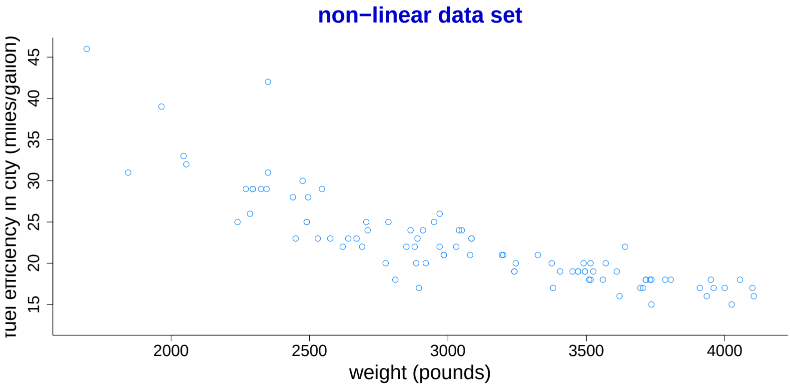
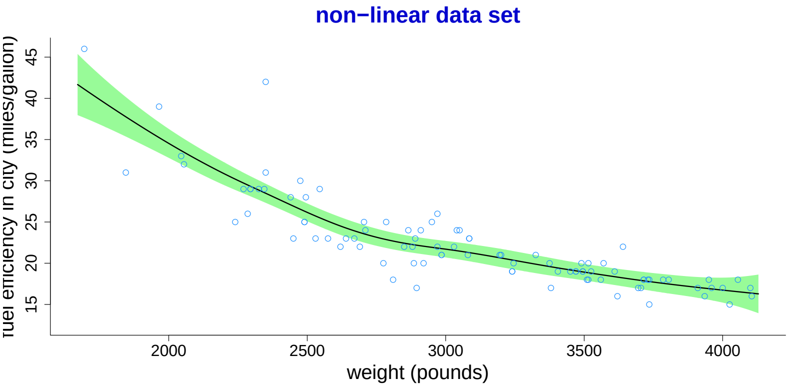



non−linear data set
fuel efficiency in city (miles/gallon)
15
20
25
30
35
40
45
2000
2500
3000
3500
4000
weight (pounds)


non−linear data set
fuel efficiency in city (miles/gallon)
15
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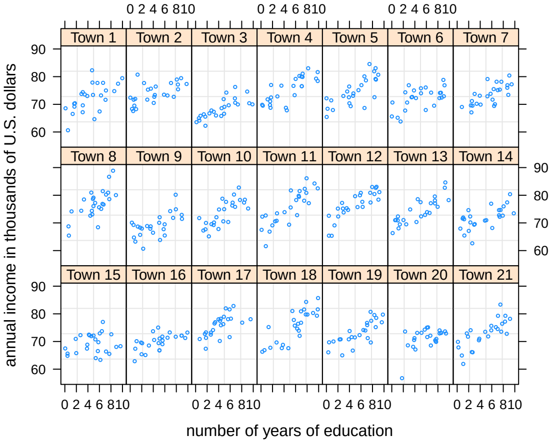
3500
4000
weight (pounds)

Multilevel Data



Multilevel Data

Suppose we have m groups and n_i subjects in the ith group.

Let x_{ij} be the predictor for the jth subject in the ith, and let y_{ij} be the corresponding observation.

A Gaussian response linear mixed model for such data consists of

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Bayesian Multilevel Data Model

$$\boldsymbol{y}_i|\boldsymbol{\beta},\boldsymbol{u}_i,\sigma^2 \sim \mathrm{N}(\boldsymbol{X}_i\boldsymbol{\beta}+\boldsymbol{X}_i\boldsymbol{u}_i,\sigma^2\boldsymbol{I}), \quad \left.\begin{bmatrix}\boldsymbol{\beta}\\ \boldsymbol{u}_i\end{bmatrix}\right| \Sigma_u \overset{\text{ind.}}{\sim} \mathrm{N}\left(\begin{bmatrix}\boldsymbol{0}\\ \boldsymbol{0}\end{bmatrix},\begin{bmatrix}\sigma_\beta^2\boldsymbol{I}_2 & \boldsymbol{O}^T\\ \boldsymbol{O} & \Sigma_u\end{bmatrix}\right)$$

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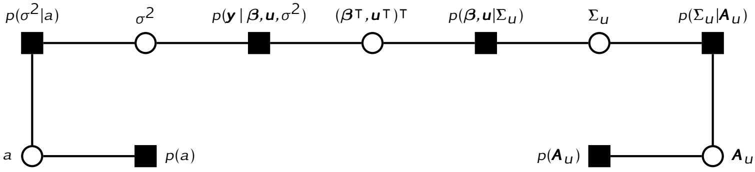

Gaussian likelihood fragment

Gaussian penalization fragment

Iterated inverse Wishart fragment

Inverse Wishart prior fragment

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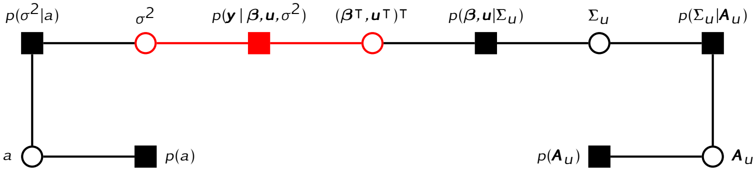

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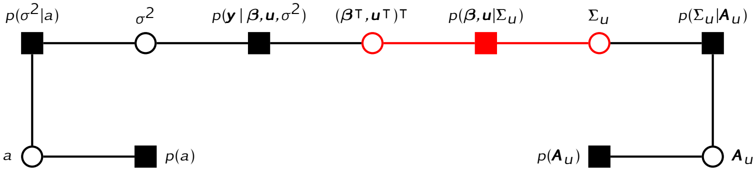

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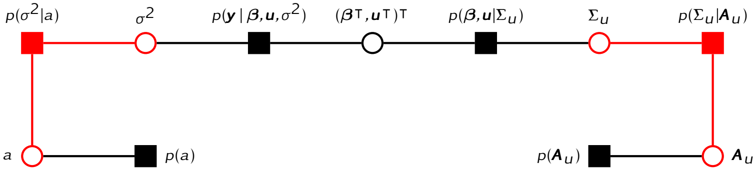

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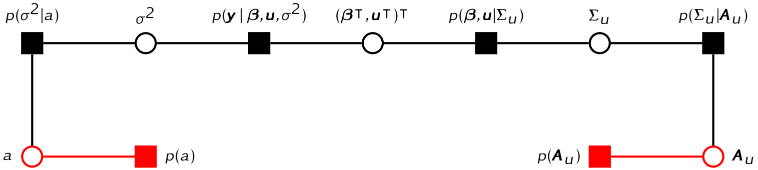

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The parameters for the posterior of $\boldsymbol{\nu} \equiv (\boldsymbol{\beta}^\top, \boldsymbol{u}^\top)^\top$ take the form - Lee and Wand (2016):

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where $\boldsymbol{A}$ and $\boldsymbol{a}$ are known

The posterior of σ^2 also depends on norms and determinants involving $\boldsymbol{A}$.

What is the issue with $\boldsymbol{A}$?

Consider our fictitious model of income against number of years of education for 21 towns.

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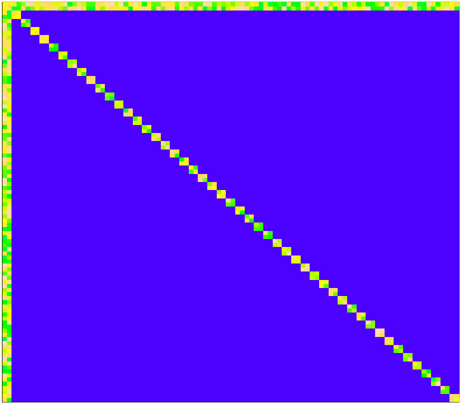
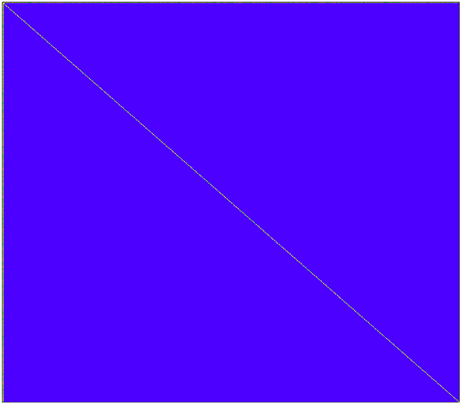
Multilevel Model (21 Towns)

$\boldsymbol{A} =$ 

$\boldsymbol{A} =$ 

The solution comes from a simple observation:

$$\mathrm{Cov}_q(\boldsymbol{\nu}) = \boldsymbol{A}^{-1} \implies \boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) = \boldsymbol{I}$$

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Matrices and vectors are partitioned as:

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Matrices and vectors are partitioned as:

$$\boldsymbol{A} \equiv \begin{bmatrix} \boldsymbol{A}_{11} & \boldsymbol{A}_{12,1} & \boldsymbol{A}_{12,2} & \boldsymbol{A}_{12,3} \\ \boldsymbol{A}_{12,1}^T & \boldsymbol{A}_{22,1} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{A}_{12,2}^T & \boldsymbol{O} & \boldsymbol{A}_{22,2} & \boldsymbol{O} \\ \boldsymbol{A}_{12,3}^T & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{A}_{22,3} \end{bmatrix} \quad \mathrm{Cov}_q(\boldsymbol{\nu}) \equiv \begin{bmatrix} \mathrm{Cov}_q(\boldsymbol{\beta}) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3) \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1)^T & \mathrm{Cov}_q(\boldsymbol{u}_1) & \times & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2)^T & \times & \mathrm{Cov}_q(\boldsymbol{u}_2) & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3)^T & \times & \times & \mathrm{Cov}_q(\boldsymbol{u}_3) \end{bmatrix}$$

$$\mathbb{E}_q(\boldsymbol{\nu}) \equiv \begin{bmatrix} \mathbb{E}_q(\boldsymbol{\beta}) \\ \mathbb{E}_q(\boldsymbol{u}_1) \\ \mathbb{E}_q(\boldsymbol{u}_2) \\ \mathbb{E}_q(\boldsymbol{u}_3) \end{bmatrix} \quad \boldsymbol{a} \equiv \begin{bmatrix} \boldsymbol{a}_1 \\ \boldsymbol{a}_{2,1} \\ \boldsymbol{a}_{2,2} \\ \boldsymbol{a}_{2,3} \end{bmatrix}$$

The solution comes from a simple observation:

$$\mathrm{Cov}_q(\boldsymbol{\nu}) = \boldsymbol{A}^{-1} \implies \boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) = \boldsymbol{I}$$
$$\mathbb{E}_q(\boldsymbol{\nu}) = \boldsymbol{A}^{-1}\boldsymbol{a} \implies \boldsymbol{A}\,\mathbb{E}_q(\boldsymbol{\nu}) = \boldsymbol{a}$$

where $\boldsymbol{A}$ and $\boldsymbol{a}$ are known.

Matrices and vectors are partitioned as:

$$\boldsymbol{A} \equiv \begin{bmatrix} \boldsymbol{A}_{11} & \boldsymbol{A}_{12,1} & \boldsymbol{A}_{12,2} & \boldsymbol{A}_{12,3} \\ \boldsymbol{A}_{12,1}^T & \boldsymbol{A}_{22,1} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{A}_{12,2}^T & \boldsymbol{O} & \boldsymbol{A}_{22,2} & \boldsymbol{O} \\ \boldsymbol{A}_{12,3}^T & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{A}_{22,3} \end{bmatrix} \quad \mathrm{Cov}_q(\boldsymbol{\nu}) \equiv \begin{bmatrix} \mathrm{Cov}_q(\boldsymbol{\beta}) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3) \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1)^T & \mathrm{Cov}_q(\boldsymbol{u}_1) & \times & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2)^T & \times & \mathrm{Cov}_q(\boldsymbol{u}_2) & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3)^T & \times & \times & \mathrm{Cov}_q(\boldsymbol{u}_3) \end{bmatrix}$$

$$\mathbb{E}_q(\boldsymbol{\nu}) \equiv \begin{bmatrix} \mathbb{E}_q(\boldsymbol{\beta}) \\ \mathbb{E}_q(\boldsymbol{u}_1) \\ \mathbb{E}_q(\boldsymbol{u}_2) \\ \mathbb{E}_q(\boldsymbol{u}_3) \end{bmatrix} \quad \boldsymbol{a} \equiv \begin{bmatrix} \boldsymbol{a}_1 \\ \boldsymbol{a}_{2,1} \\ \boldsymbol{a}_{2,2} \\ \boldsymbol{a}_{2,3} \end{bmatrix}$$

Multilevel Model ($\boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) = \boldsymbol{I}$)

$$
\begin{aligned}
\boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) &= \begin{bmatrix} \boldsymbol{A}_{11} & \boldsymbol{A}_{12,1} & \boldsymbol{A}_{12,2} & \boldsymbol{A}_{12,3} \\ \boldsymbol{A}_{12,1}^T & \boldsymbol{A}_{22,1} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{A}_{12,2}^T & \boldsymbol{O} & \boldsymbol{A}_{22,2} & \boldsymbol{O} \\ \boldsymbol{A}_{12,3}^T & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{A}_{22,3} \end{bmatrix}
\begin{bmatrix} \mathrm{Cov}_q(\boldsymbol{\beta}) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3) \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1)^T & \mathrm{Cov}_q(\boldsymbol{u}_1) & \times & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2)^T & \times & \mathrm{Cov}_q(\boldsymbol{u}_2) & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3)^T & \times & \times & \mathrm{Cov}_q(\boldsymbol{u}_3) \end{bmatrix} \\
&= \begin{bmatrix} \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{I} \end{bmatrix}
\end{aligned}
$$

$$\boldsymbol{A}_{11}\mathrm{Cov}_q(\boldsymbol{\beta}) + \textstyle\sum_{i=1}^{3} \boldsymbol{A}_{12,i}\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = \boldsymbol{I}$$

$$\boldsymbol{A}_{12,i}^T\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) + \boldsymbol{A}_{22,i}\mathrm{Cov}_q(\boldsymbol{u}_i) = \boldsymbol{I}, \quad i = 1, 2, 3$$

$$\boldsymbol{A}_{12,i}^T\mathrm{Cov}_q(\boldsymbol{\beta}) + \boldsymbol{A}_{22,i}\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = \boldsymbol{O}, \quad i = 1, 2, 3$$

Multilevel Model ($\boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) = \boldsymbol{I}$)

$$\boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) = \begin{bmatrix} \boldsymbol{A}_{11} & \boldsymbol{A}_{12,1} & \boldsymbol{A}_{12,2} & \boldsymbol{A}_{12,3} \\ \boldsymbol{A}_{12,1}^T & \boldsymbol{A}_{22,1} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{A}_{12,2}^T & \boldsymbol{O} & \boldsymbol{A}_{22,2} & \boldsymbol{O} \\ \boldsymbol{A}_{12,3}^T & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{A}_{22,3} \end{bmatrix} \begin{bmatrix} \mathrm{Cov}_q(\boldsymbol{\beta}) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3) \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1)^T & \mathrm{Cov}_q(\boldsymbol{u}_1) & \times & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2)^T & \times & \mathrm{Cov}_q(\boldsymbol{u}_2) & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3)^T & \times & \times & \mathrm{Cov}_q(\boldsymbol{u}_3) \end{bmatrix}$$

$$= \begin{bmatrix} \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{I} \end{bmatrix}$$

$$\boldsymbol{A}_{11}\mathrm{Cov}_q(\boldsymbol{\beta}) + \textstyle\sum_{i=1}^{3} \boldsymbol{A}_{12,i}\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = \boldsymbol{I}$$

$$\boldsymbol{A}_{12,i}^T\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) + \boldsymbol{A}_{22,i}\mathrm{Cov}_q(\boldsymbol{u}_i) = \boldsymbol{I}, \quad i = 1,2,3$$

$$\boldsymbol{A}_{12,i}^T\mathrm{Cov}_q(\boldsymbol{\beta}) + \boldsymbol{A}_{22,i}\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = \boldsymbol{O}, \quad i = 1,2,3$$

Multilevel Model ($\boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) = \boldsymbol{I}$)

$$\boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) = \begin{bmatrix} \boldsymbol{A}_{11} & \boldsymbol{A}_{12,1} & \boldsymbol{A}_{12,2} & \boldsymbol{A}_{12,3} \\ \boldsymbol{A}_{12,1}^T & \boldsymbol{A}_{22,1} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{A}_{12,2}^T & \boldsymbol{O} & \boldsymbol{A}_{22,2} & \boldsymbol{O} \\ \boldsymbol{A}_{12,3}^T & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{A}_{22,3} \end{bmatrix} \begin{bmatrix} \mathrm{Cov}_q(\boldsymbol{\beta}) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3) \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1)^T & \mathrm{Cov}_q(\boldsymbol{u}_1) & \times & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2)^T & \times & \mathrm{Cov}_q(\boldsymbol{u}_2) & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3)^T & \times & \times & \mathrm{Cov}_q(\boldsymbol{u}_3) \end{bmatrix}$$

$$= \begin{bmatrix} \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{I} \end{bmatrix}$$

$$\boldsymbol{A}_{11}\mathrm{Cov}_q(\boldsymbol{\beta}) + \textstyle\sum_{i=1}^3 \boldsymbol{A}_{12,i}\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = \boldsymbol{I}$$

$$\boldsymbol{A}_{12,i}^T\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) + \boldsymbol{A}_{22,i}\mathrm{Cov}_q(\boldsymbol{u}_i) = \boldsymbol{I}, \quad i = 1,2,3$$

$$\boldsymbol{A}_{12,i}^T\mathrm{Cov}_q(\boldsymbol{\beta}) + \boldsymbol{A}_{22,i}\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = \boldsymbol{O}, \quad i = 1,2,3$$

Multilevel Model ($\boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) = \boldsymbol{I}$)

$$\boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) = \begin{bmatrix} \boldsymbol{A}_{11} & \boldsymbol{A}_{12,1} & \boldsymbol{A}_{12,2} & \boldsymbol{A}_{12,3} \\ \boldsymbol{A}_{12,1}^T & \boldsymbol{A}_{22,1} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{A}_{12,2}^T & \boldsymbol{O} & \boldsymbol{A}_{22,2} & \boldsymbol{O} \\ \boldsymbol{A}_{12,3}^T & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{A}_{22,3} \end{bmatrix} \begin{bmatrix} \mathrm{Cov}_q(\boldsymbol{\beta}) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3) \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1)^T & \mathrm{Cov}_q(\boldsymbol{u}_1) & \times & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2)^T & \times & \mathrm{Cov}_q(\boldsymbol{u}_2) & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3)^T & \times & \times & \mathrm{Cov}_q(\boldsymbol{u}_3) \end{bmatrix}$$

$$= \begin{bmatrix} \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{I} \end{bmatrix}$$

$$\boldsymbol{A}_{11}\mathrm{Cov}_q(\boldsymbol{\beta}) + \textstyle\sum_{i=1}^{3} \boldsymbol{A}_{12,i}\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = \boldsymbol{I}$$

$$\boldsymbol{A}_{12,i}^T\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) + \boldsymbol{A}_{22,i}\mathrm{Cov}_q(\boldsymbol{u}_i) = \boldsymbol{I}, \quad i = 1, 2, 3$$

$$\boldsymbol{A}_{12,i}^T\mathrm{Cov}_q(\boldsymbol{\beta}) + \boldsymbol{A}_{22,i}\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = \boldsymbol{O}, \quad i = 1, 2, 3$$

Multilevel Model ($\boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) = \boldsymbol{I}$)

$$
\boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) = \begin{bmatrix} \boldsymbol{A}_{11} & \boldsymbol{A}_{12,1} & \boldsymbol{A}_{12,2} & \boldsymbol{A}_{12,3} \\ \boldsymbol{A}_{12,1}^T & \boldsymbol{A}_{22,1} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{A}_{12,2}^T & \boldsymbol{O} & \boldsymbol{A}_{22,2} & \boldsymbol{O} \\ \boldsymbol{A}_{12,3}^T & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{A}_{22,3} \end{bmatrix} \begin{bmatrix} \mathrm{Cov}_q(\boldsymbol{\beta}) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3) \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1)^T & \mathrm{Cov}_q(\boldsymbol{u}_1) & \times & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2)^T & \times & \mathrm{Cov}_q(\boldsymbol{u}_2) & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3)^T & \times & \times & \mathrm{Cov}_q(\boldsymbol{u}_3) \end{bmatrix}
$$

$$
= \begin{bmatrix} \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{I} \end{bmatrix}
$$

$$\boldsymbol{A}_{11}\mathrm{Cov}_q(\boldsymbol{\beta}) + \textstyle\sum_{i=1}^{3} \boldsymbol{A}_{12,i}\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = \boldsymbol{I}$$

$$\boldsymbol{A}_{12,i}^T\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) + \boldsymbol{A}_{22,i}\mathrm{Cov}_q(\boldsymbol{u}_i) = \boldsymbol{I}, \quad i = 1, 2, 3$$

$$\boldsymbol{A}_{12,i}^T\mathrm{Cov}_q(\boldsymbol{\beta}) + \boldsymbol{A}_{22,i}\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = \boldsymbol{O}, \quad i = 1, 2, 3$$

Multilevel Model ($\boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) = \boldsymbol{I}$)

$$\boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) = \begin{bmatrix} \boldsymbol{A}_{11} & \boldsymbol{A}_{12,1} & \boldsymbol{A}_{12,2} & \boldsymbol{A}_{12,3} \\ \boldsymbol{A}_{12,1}^T & \boldsymbol{A}_{22,1} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{A}_{12,2}^T & \boldsymbol{O} & \boldsymbol{A}_{22,2} & \boldsymbol{O} \\ \boldsymbol{A}_{12,3}^T & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{A}_{22,3} \end{bmatrix} \begin{bmatrix} \mathrm{Cov}_q(\boldsymbol{\beta}) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3) \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1)^T & \mathrm{Cov}_q(\boldsymbol{u}_1) & \times & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2)^T & \times & \mathrm{Cov}_q(\boldsymbol{u}_2) & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3)^T & \times & \times & \mathrm{Cov}_q(\boldsymbol{u}_3) \end{bmatrix}$$

$$= \begin{bmatrix} \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{I} \end{bmatrix}$$

$$\boldsymbol{A}_{11}\mathrm{Cov}_q(\boldsymbol{\beta}) + \textstyle\sum_{i=1}^{3} \boldsymbol{A}_{12,i}\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = \boldsymbol{I}$$

$$\boldsymbol{A}_{12,i}^T\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) + \boldsymbol{A}_{22,i}\mathrm{Cov}_q(\boldsymbol{u}_i) = \boldsymbol{I}, \quad i = 1,2,3$$

$$\boldsymbol{A}_{12,i}^T\mathrm{Cov}_q(\boldsymbol{\beta}) + \boldsymbol{A}_{22,i}\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = \boldsymbol{O}, \quad i = 1,2,3$$

Multilevel Model ($\boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) = \boldsymbol{I}$)

$$\boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) = \begin{bmatrix} \boldsymbol{A}_{11} & \boldsymbol{A}_{12,1} & \boldsymbol{A}_{12,2} & \boldsymbol{A}_{12,3} \\ \boldsymbol{A}_{12,1}^T & \boldsymbol{A}_{22,1} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{A}_{12,2}^T & \boldsymbol{O} & \boldsymbol{A}_{22,2} & \boldsymbol{O} \\ \boldsymbol{A}_{12,3}^T & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{A}_{22,3} \end{bmatrix} \begin{bmatrix} \mathrm{Cov}_q(\boldsymbol{\beta}) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3) \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1)^T & \mathrm{Cov}_q(\boldsymbol{u}_1) & \times & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2)^T & \times & \mathrm{Cov}_q(\boldsymbol{u}_2) & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3)^T & \times & \times & \mathrm{Cov}_q(\boldsymbol{u}_3) \end{bmatrix}$$

$$= \begin{bmatrix} \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{I} \end{bmatrix}$$

$$\boldsymbol{A}_{11}\mathrm{Cov}_q(\boldsymbol{\beta}) + \textstyle\sum_{i=1}^{3} \boldsymbol{A}_{12,i}\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = \boldsymbol{I}$$

$$\boldsymbol{A}_{12,i}^T\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) + \boldsymbol{A}_{22,i}\mathrm{Cov}_q(\boldsymbol{u}_i) = \boldsymbol{I}, \quad i = 1, 2, 3$$

$$\boldsymbol{A}_{12,i}^T\mathrm{Cov}_q(\boldsymbol{\beta}) + \boldsymbol{A}_{22,i}\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = \boldsymbol{O}, \quad i = 1, 2, 3$$

Multilevel Model ($\boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) = \boldsymbol{I}$)

$$\boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) = \begin{bmatrix} \boldsymbol{A}_{11} & \boldsymbol{A}_{12,1} & \boldsymbol{A}_{12,2} & \boldsymbol{A}_{12,3} \\ \boldsymbol{A}_{12,1}^T & \boldsymbol{A}_{22,1} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{A}_{12,2}^T & \boldsymbol{O} & \boldsymbol{A}_{22,2} & \boldsymbol{O} \\ \boldsymbol{A}_{12,3}^T & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{A}_{22,3} \end{bmatrix} \begin{bmatrix} \mathrm{Cov}_q(\boldsymbol{\beta}) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3) \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1)^T & \mathrm{Cov}_q(\boldsymbol{u}_1) & \times & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2)^T & \times & \mathrm{Cov}_q(\boldsymbol{u}_2) & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3)^T & \times & \times & \mathrm{Cov}_q(\boldsymbol{u}_3) \end{bmatrix}$$

$$= \begin{bmatrix} \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{I} \end{bmatrix}$$

$$\boldsymbol{A}_{11}\mathrm{Cov}_q(\boldsymbol{\beta}) + \textstyle\sum_{i=1}^{3} \boldsymbol{A}_{12,i}\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = \boldsymbol{I}$$

$$\boldsymbol{A}_{12,i}^T\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) + \boldsymbol{A}_{22,i}\mathrm{Cov}_q(\boldsymbol{u}_i) = \boldsymbol{I}, \quad i = 1,2,3$$

$$\boldsymbol{A}_{12,i}^T\mathrm{Cov}_q(\boldsymbol{\beta}) + \boldsymbol{A}_{22,i}\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = \boldsymbol{O}, \quad i = 1,2,3$$

$$\boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) = \begin{bmatrix} \boldsymbol{A}_{11} & \boldsymbol{A}_{12,1} & \boldsymbol{A}_{12,2} & \boldsymbol{A}_{12,3} \\ \boldsymbol{A}_{12,1}^T & \boldsymbol{A}_{22,1} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{A}_{12,2}^T & \boldsymbol{O} & \boldsymbol{A}_{22,2} & \boldsymbol{O} \\ \boldsymbol{A}_{12,3}^T & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{A}_{22,3} \end{bmatrix} \begin{bmatrix} \mathrm{Cov}_q(\boldsymbol{\beta}) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3) \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1)^T & \mathrm{Cov}_q(\boldsymbol{u}_1) & \times & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2)^T & \times & \mathrm{Cov}_q(\boldsymbol{u}_2) & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3)^T & \times & \times & \mathrm{Cov}_q(\boldsymbol{u}_3) \end{bmatrix}$$

$$= \begin{bmatrix} \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{I} \end{bmatrix}$$

$$\boldsymbol{A}_{11}\mathrm{Cov}_q(\boldsymbol{\beta}) + \textstyle\sum_{i=1}^{3} \boldsymbol{A}_{12,i}\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = \boldsymbol{I}$$

$$\boldsymbol{A}_{12,i}^T\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) + \boldsymbol{A}_{22,i}\mathrm{Cov}_q(\boldsymbol{u}_i) = \boldsymbol{I}, \quad i = 1,2,3$$

$$\boldsymbol{A}_{12,i}^T\mathrm{Cov}_q(\boldsymbol{\beta}) + \boldsymbol{A}_{22,i}\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = \boldsymbol{O}, \quad i = 1,2,3$$

Multilevel Model ($\boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) = \boldsymbol{I}$)

$$
\boldsymbol{A}\,\mathrm{Cov}_q(\boldsymbol{\nu}) = \begin{bmatrix} \boldsymbol{A}_{11} & \boldsymbol{A}_{12,1} & \boldsymbol{A}_{12,2} & \boldsymbol{A}_{12,3} \\ \boldsymbol{A}_{12,1}^T & \boldsymbol{A}_{22,1} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{A}_{12,2}^T & \boldsymbol{O} & \boldsymbol{A}_{22,2} & \boldsymbol{O} \\ \boldsymbol{A}_{12,3}^T & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{A}_{22,3} \end{bmatrix} \begin{bmatrix} \mathrm{Cov}_q(\boldsymbol{\beta}) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2) & \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3) \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_1)^T & \mathrm{Cov}_q(\boldsymbol{u}_1) & \times & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_2)^T & \times & \mathrm{Cov}_q(\boldsymbol{u}_2) & \times \\ \mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_3)^T & \times & \times & \mathrm{Cov}_q(\boldsymbol{u}_3) \end{bmatrix}
$$

$$
= \begin{bmatrix} \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{I} & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{I} \end{bmatrix}
$$

$$\boldsymbol{A}_{11}\mathrm{Cov}_q(\boldsymbol{\beta}) + \textstyle\sum_{i=1}^{3} \boldsymbol{A}_{12,i}\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = \boldsymbol{I}$$

$$\boldsymbol{A}_{12,i}^T\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) + \boldsymbol{A}_{22,i}\mathrm{Cov}_q(\boldsymbol{u}_i) = \boldsymbol{I}, \quad i = 1,2,3$$

$$\boldsymbol{A}_{12,i}^T\mathrm{Cov}_q(\boldsymbol{\beta}) + \boldsymbol{A}_{22,i}\mathrm{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = \boldsymbol{O}, \quad i = 1,2,3$$

$$\boldsymbol{A}\,\mathbb{E}_q(\boldsymbol{\nu}) = \begin{bmatrix} \boldsymbol{A}_{11} & \boldsymbol{A}_{12,1} & \boldsymbol{A}_{12,2} & \boldsymbol{A}_{12,3} \\ \boldsymbol{A}_{12,1}^T & \boldsymbol{A}_{22,1} & \boldsymbol{O} & \boldsymbol{O} \\ \boldsymbol{A}_{12,2}^T & \boldsymbol{O} & \boldsymbol{A}_{22,2} & \boldsymbol{O} \\ \boldsymbol{A}_{12,3}^T & \boldsymbol{O} & \boldsymbol{O} & \boldsymbol{A}_{22,3} \end{bmatrix} \begin{bmatrix} \mathbb{E}_q(\boldsymbol{\beta}) \\ \mathbb{E}_q(\boldsymbol{u}_1) \\ \mathbb{E}_q(\boldsymbol{u}_2) \\ \mathbb{E}_q(\boldsymbol{u}_3) \end{bmatrix} = \begin{bmatrix} \boldsymbol{a}_1 \\ \boldsymbol{a}_{2,1} \\ \boldsymbol{a}_{2,2} \\ \boldsymbol{a}_{2,3} \end{bmatrix}$$

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Theorem: Nolan and Wand (2020)

For the two-level mean field variational Bayes model, the solutions for the required sub-blocks of $\mathrm{Cov}_q(\boldsymbol{\nu})$ are

$$\mathrm{Cov}_q(\boldsymbol{\beta}) = \left(\boldsymbol{A}_{11} - \sum_{i=1}^{m} \boldsymbol{A}_{12,i}\boldsymbol{A}_{22,i}^{-1}\boldsymbol{A}_{12,i}^T\right)^{-1}$$

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The determinant of $\mathrm{Cov}_q(\boldsymbol{\nu})$ is

$$|\mathrm{Cov}_q(\boldsymbol{\nu})| = \left|\mathrm{Cov}_q(\boldsymbol{\beta})\right| \prod_{i=1}^{m} \left|\mathrm{Cov}_q(\boldsymbol{u}_i)\right|.$$

The solutions for the sub-vectors of $\boldsymbol{\mu}_{q(\boldsymbol{\beta},\boldsymbol{u})}$ are

$$\mathbb{E}_q(\boldsymbol{\beta}) = \mathrm{Cov}_q(\boldsymbol{\beta})\left(\boldsymbol{a}_1 - \sum_{i=1}^{m}\boldsymbol{A}_{12,i}\boldsymbol{A}_{22,i}^{-1}\boldsymbol{a}_{2,i}\right) \quad \text{and} \quad \mathbb{E}_q(\boldsymbol{u}_i) = \boldsymbol{A}_{22,i}^{-1}(\boldsymbol{a}_{2,i} - \boldsymbol{A}_{12,i}^T\,\mathbb{E}_q(\boldsymbol{\beta})).$$

Streamlined Multilevel Computations

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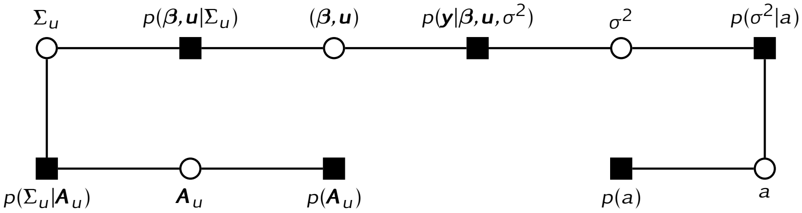
VMP for the Bayesian multilevel data model

1. Initialise all messages from stochastic nodes to factors
2. Cycle:
   (i) Update all messages from factors to stochastic nodes
   (ii) Update all messages from stochastic nodes to factors
   (iii) Update all optimal posterior density functions
3. Stop: $D_{\text{KL}}\left\{q(\boldsymbol{\beta},\boldsymbol{u},\sigma^2,\Sigma_u,a,\boldsymbol{A}_u)\|p(\boldsymbol{\beta},\boldsymbol{u},\sigma^2,\Sigma_u,a,\boldsymbol{A}_u|\boldsymbol{y})\right\}$ converges.



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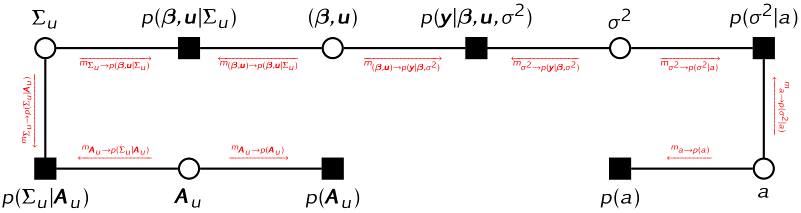

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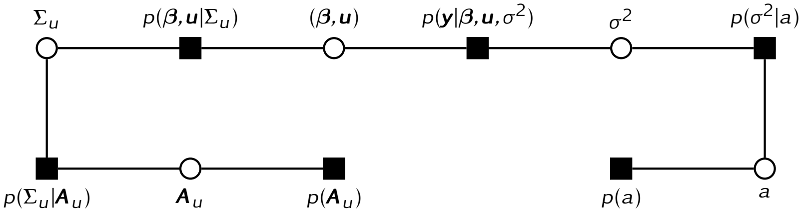

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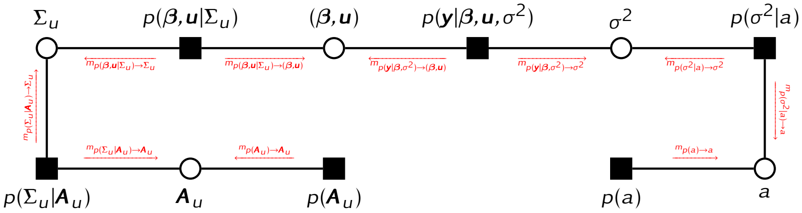

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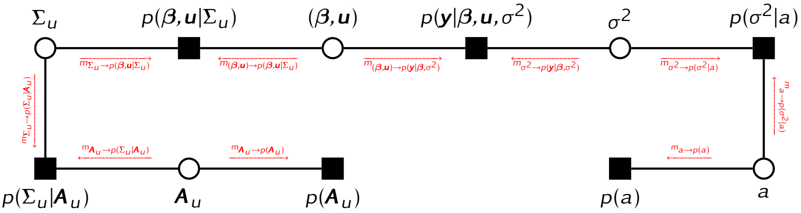

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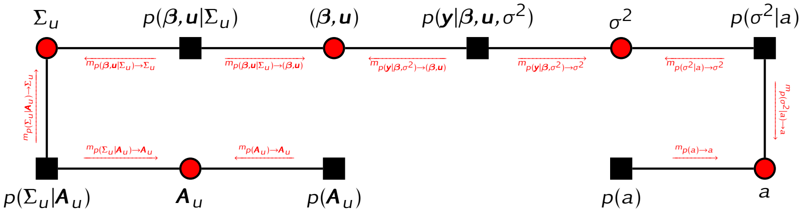

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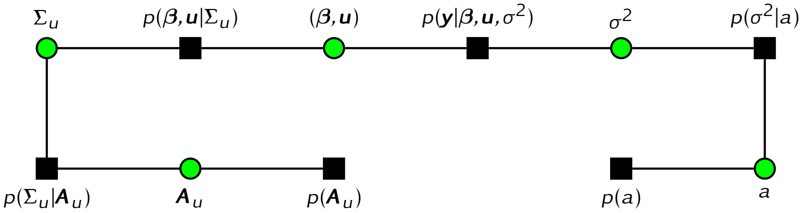
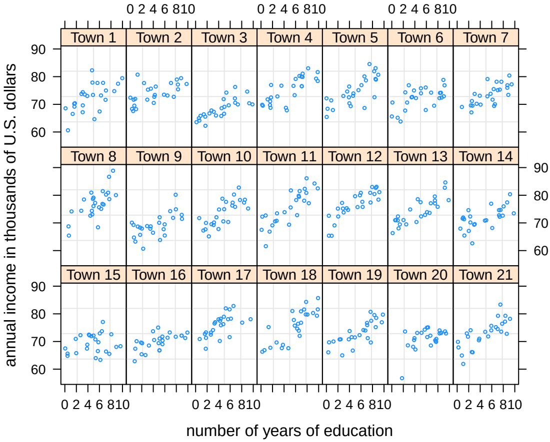


Multilevel Data



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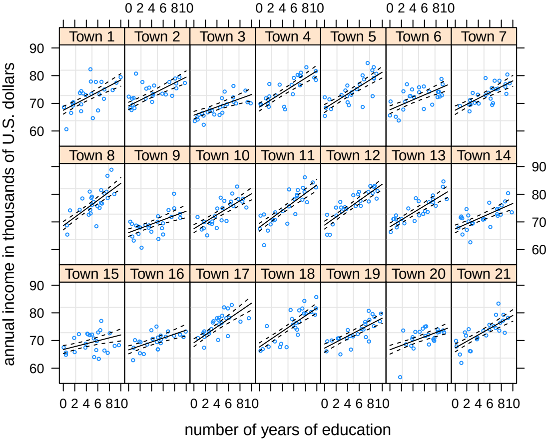
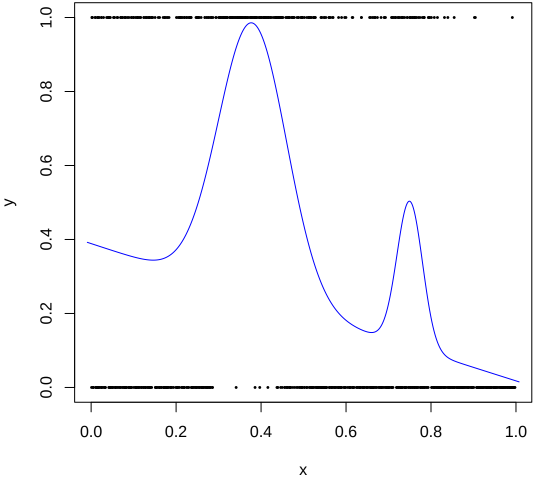


Part III

Nonconjugate Models

Binary Response Data



Bayesian Logistic Regression Model

Consider the Bayesian logistic regression model:

$$\boldsymbol{y} \mid \boldsymbol{\beta} \sim \text{Bernoulli}\left\{\left[1+\exp\{-\boldsymbol{X}\boldsymbol{\beta}\}\right]^{-1}\right\}$$
$$\boldsymbol{\beta} \sim N(\boldsymbol{0}, \sigma_\beta^2 \boldsymbol{I})$$

The factor graph is

Gaussian Prior Fragment

Logistic Likelihood Fragment (Nolan and Wand, 2017)

The message takes the form:

$$m_{p(\boldsymbol{y}|\boldsymbol{\beta})\to\boldsymbol{\beta}}(\boldsymbol{\beta}) \longleftarrow \exp\left\{\boldsymbol{y}^T\boldsymbol{X}\boldsymbol{\beta} - \boldsymbol{1}^T\mathbb{E}_q \log\left[\boldsymbol{1}+\exp(\boldsymbol{X}\boldsymbol{\beta})\right]\right\}$$

The messages that are typically passed to $\boldsymbol{\beta}$ from other fragments are Gaussian density messages.

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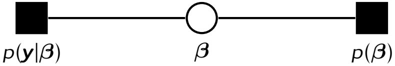

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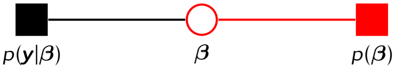

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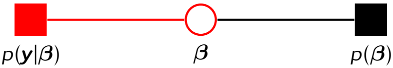

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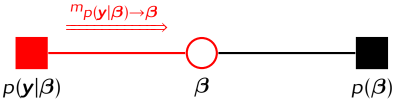


Gaussian Prior Fragment

Logistic Likelihood Fragment (Nolan and Wand, 2017)

The message takes the form:

$$m_{p(\boldsymbol{y}|\boldsymbol{\beta})\rightarrow\boldsymbol{\beta}}(\boldsymbol{\beta}) \longleftarrow \exp\left\{ \boldsymbol{y}^T \boldsymbol{X}\boldsymbol{\beta} - \boldsymbol{1}^T \mathbb{E}_q \log\left[\boldsymbol{1} + \exp(\boldsymbol{X}\boldsymbol{\beta}) \right] \right\}$$

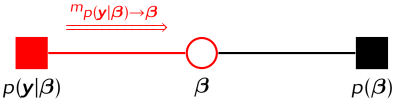
The messages that are typically passed to $\boldsymbol{\beta}$ from other fragments are Gaussian density messages.

Bayesian Logistic Regression Model

Consider the Bayesian logistic regression model:

$$\boldsymbol{y} \mid \boldsymbol{\beta} \sim \text{Bernoulli}\left\{[1+\exp\{-\boldsymbol{X}\boldsymbol{\beta}\}]^{-1}\right\}$$
$$\boldsymbol{\beta} \sim N(\boldsymbol{0}, \sigma_{\beta}^2 \boldsymbol{I})$$

The factor graph is



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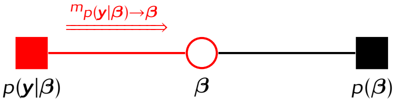

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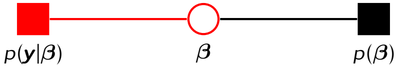

A fixed point iterative scheme for $\boldsymbol{\eta}_{p(\boldsymbol{y}|\boldsymbol{\beta})\to\boldsymbol{\beta}}$ (Wand, 2014):

$$\boldsymbol{\mu} = \boldsymbol{X}\,\mathbb{E}_q(\boldsymbol{\beta}), \quad \boldsymbol{\sigma}^2 = \text{diagonal}\left\{\boldsymbol{X}\text{Cov}_q(\boldsymbol{\beta})\boldsymbol{X}^T\right\}$$

$$\boldsymbol{\eta}_{p(\boldsymbol{y}|\boldsymbol{\beta})\to\boldsymbol{\beta}} = \begin{bmatrix} \boldsymbol{X}^T\left\{\boldsymbol{y} - \mathcal{B}_0(\boldsymbol{\mu},\boldsymbol{\sigma}^2) + \mathcal{B}_1(\boldsymbol{\mu},\boldsymbol{\sigma}^2)\odot\frac{\boldsymbol{\mu}}{\boldsymbol{\sigma}}\right\} \\ -\frac{1}{2}\,\text{vec}\left\{\boldsymbol{X}^T\,\text{diag}(\omega_2)\boldsymbol{X}\right\} \end{bmatrix}$$

where

$$\mathcal{B}_r(\mu,\sigma^2) \equiv \int_{-\infty}^{\infty} x^r \frac{d}{d\mu}\log\{1+\exp(\mu+\sigma x)\}\,\phi(x)\,dx, \quad \text{for } r = 0, 1$$

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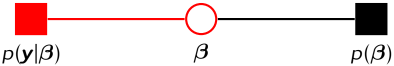

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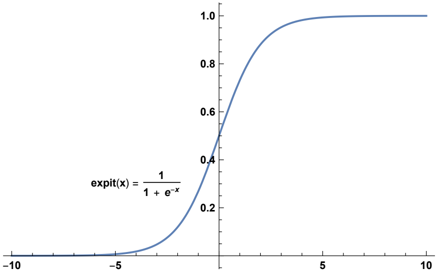

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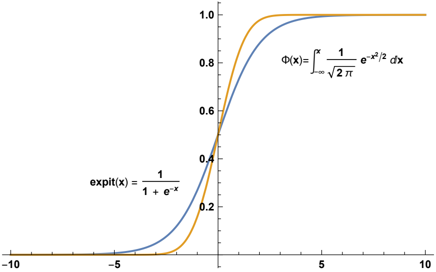

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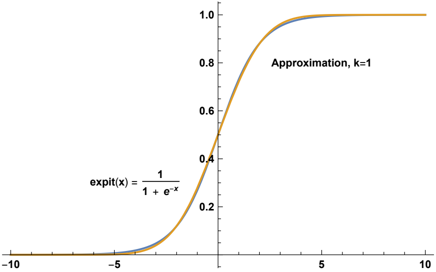

p	s
1.00000	0.58763

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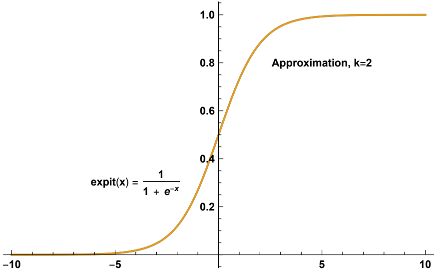

p	s
0.56442	0.76862
0.43557	0.43525

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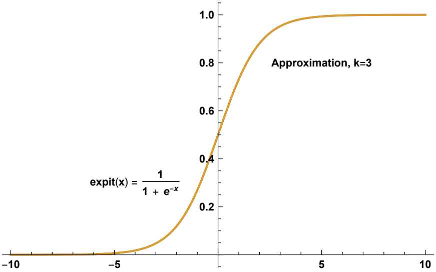

p	s
0.25220	0.90793
0.58522	0.57778
0.16257	0.36403

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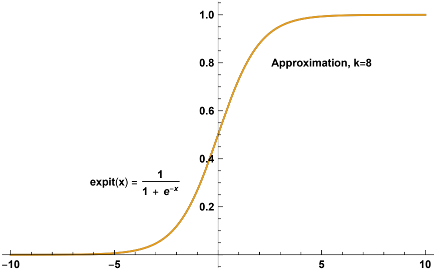
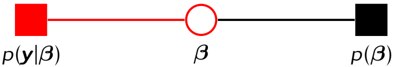


p	s
0.00324	1.36534
0.05151	1.05952
0.19507	0.83079
0.31556	0.65073
0.27414	0.50813
0.13107	0.39631
0.02791	0.30890
0.00144	0.23821

Logistic Likelihood Fragment



$$\boldsymbol{y}|\boldsymbol{\beta} \sim \text{Bernoulli}\left[\{\mathbf{1} + \exp(-\boldsymbol{X}\boldsymbol{\beta})\}^{-1}\right]$$

Inputs:

$$\boldsymbol{\eta}_{q^*(\boldsymbol{\beta})}$$

Updates:

$$\text{Cov}_q\{(\boldsymbol{\beta})\} = -\tfrac{1}{2}\{\text{vec}^{-1}(\boldsymbol{\eta}_{q^*(\boldsymbol{\beta})})_2\}^{-1}, \quad \mathbb{E}_q\{(\boldsymbol{\beta})\} = \text{Cov}_q\{(\boldsymbol{\beta})\}(\boldsymbol{\eta}_{q^*(\boldsymbol{\beta})})_1,$$

$$\boldsymbol{\mu} = \boldsymbol{X}\,\mathbb{E}_q(\boldsymbol{\beta}), \quad \boldsymbol{\sigma}^2 = \text{diagonal}\left\{\boldsymbol{X}\text{Cov}_q(\boldsymbol{\beta})\boldsymbol{X}^T\right\},$$

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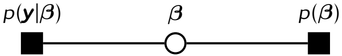
Outputs:

$$\boldsymbol{\eta}_{p(\boldsymbol{y}|\boldsymbol{\beta})\to\boldsymbol{\beta}}$$

Bayesian Logistic Regression

VMP for the Bayesian logistic regression model

1. Initialise all messages from stochastic nodes to factors
2. Cycle:
   - (i) Update all messages from factors to stochastic nodes
   - (ii) Update all messages from stochastic nodes to factors
   - (iii) Update all optimal posterior density functions
3. Stop: $D_{\mathrm{KL}}\{q(\boldsymbol{\beta})||p(\boldsymbol{\beta}|\boldsymbol{y})\}$ converges.



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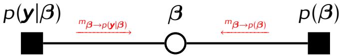

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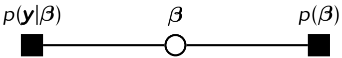

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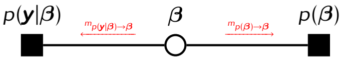

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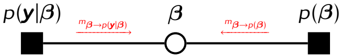

Bayesian Logistic Regression

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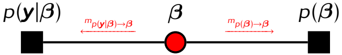

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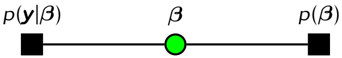
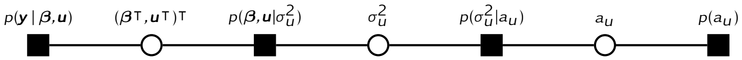


$$\boldsymbol{y}\,|\,\boldsymbol{\beta},\boldsymbol{u} \sim \text{Bernoulli}\Big\{\big[1+\exp\{-(\boldsymbol{X}\boldsymbol{\beta}+\boldsymbol{X}\boldsymbol{u})\}\big]^{-1}\Big\}, \quad \left.\begin{bmatrix}\boldsymbol{\beta}\\ \boldsymbol{u}\end{bmatrix}\right|\, \sigma_u^2 \sim \text{N}\left(\begin{bmatrix}\boldsymbol{0}\\ \boldsymbol{0}\end{bmatrix}, \begin{bmatrix}\sigma_\beta^2 \boldsymbol{I}_2 & \boldsymbol{O}^T\\ \boldsymbol{O} & \sigma_u^2\, \boldsymbol{I}_m\end{bmatrix}\right)$$

$$\sigma_u^2|a_u \sim \text{Inverse-}\chi^2(1, 1/a_u), \quad a_u \sim \text{Inverse-}\chi^2(1, 1/A^2)$$



Logistic likelihood fragment

Gaussian penalization fragment (Wand, 2017)

Iterated inverse Wishart fragment

Inverse Wishart prior fragment

Bayesian Logistic Semiparametric Regression

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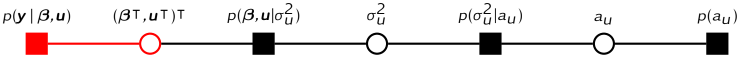

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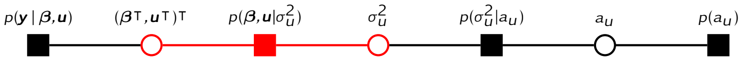

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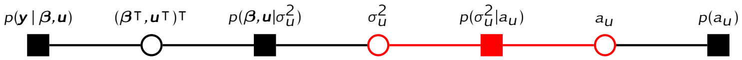

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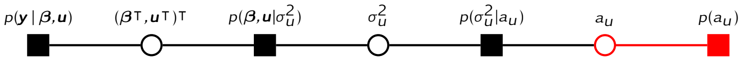
$$\boldsymbol{y}\,|\,\boldsymbol{\beta},\boldsymbol{u} \sim \text{Bernoulli}\Big\{\big[1+\exp\{-(\boldsymbol{X}\boldsymbol{\beta}+\boldsymbol{X}\boldsymbol{u})\}\big]^{-1}\Big\}, \quad \left.\begin{bmatrix}\boldsymbol{\beta}\\ \boldsymbol{u}\end{bmatrix}\right|\, \sigma_u^2 \sim \text{N}\left(\begin{bmatrix}\boldsymbol{0}\\ \boldsymbol{0}\end{bmatrix}, \begin{bmatrix}\sigma_\beta^2\boldsymbol{I}_2 & \boldsymbol{O}^T\\ \boldsymbol{O} & \sigma_u^2\,\boldsymbol{I}_m\end{bmatrix}\right)$$

$$\sigma_u^2|a_u \sim \text{Inverse-}\chi^2(1,1/a_u), \quad a_u \sim \text{Inverse-}\chi^2(1,1/A^2)$$



Logistic likelihood fragment

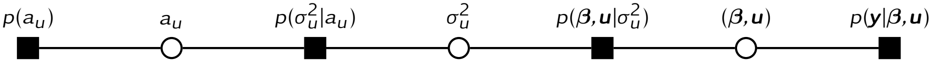
Gaussian penalization fragment (Wand, 2017)

Iterated inverse Wishart fragment

Inverse Wishart prior fragment

VMP for the Bayesian logistic semiparametric regression model

1. Initialise all messages from stochastic nodes to factors
2. Cycle:
   (i) Update all messages from factors to stochastic nodes
   (ii) Update all messages from stochastic nodes to factors
   (iii) Update all optimal posterior density functions
3. Stop: $D_{\mathrm{KL}}\left\{q(\boldsymbol{\beta},\boldsymbol{u},\sigma_u^2,a_u)\|p(\boldsymbol{\beta},\boldsymbol{u},\sigma_u^2,a_u|\boldsymbol{y})\right\}$ converges.



VMP for the Bayesian logistic semiparametric regression model

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2. Cycle:
   (i) Update all messages from factors to stochastic nodes
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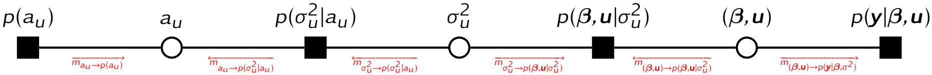
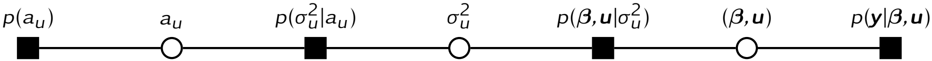


Bayesian Logistic Semiparametric Regression

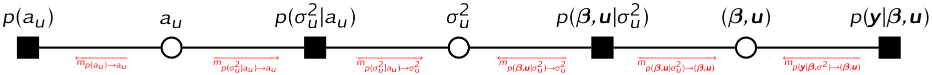
VMP for the Bayesian logistic semiparametric regression model

1. Initialise all messages from stochastic nodes to factors
2. Cycle:
   (i) Update all messages from factors to stochastic nodes
   (ii) Update all messages from stochastic nodes to factors
   (iii) Update all optimal posterior density functions
3. Stop: $D_{\mathrm{KL}}\left\{q(\boldsymbol{\beta},\boldsymbol{u},\sigma_u^2,a_u)\|p(\boldsymbol{\beta},\boldsymbol{u},\sigma_u^2,a_u|\boldsymbol{y})\right\}$ converges.



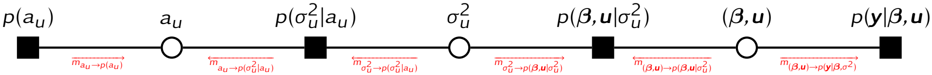
VMP for the Bayesian logistic semiparametric regression model

1. Initialise all messages from stochastic nodes to factors
2. Cycle:
   (i) Update all messages from factors to stochastic nodes
   (ii) Update all messages from stochastic nodes to factors
   (iii) Update all optimal posterior density functions
3. Stop: $D_{\mathrm{KL}}\left\{q(\boldsymbol{\beta},\boldsymbol{u},\sigma_u^2,a_u)\|p(\boldsymbol{\beta},\boldsymbol{u},\sigma_u^2,a_u|\boldsymbol{y})\right\}$ converges.



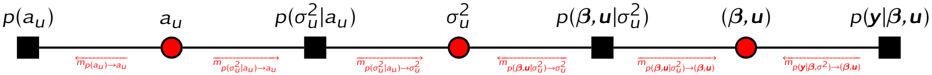
VMP for the Bayesian logistic semiparametric regression model

1. Initialise all messages from stochastic nodes to factors
2. Cycle:
   - (i) Update all messages from factors to stochastic nodes
   - (ii) Update all messages from stochastic nodes to factors
   - (iii) Update all optimal posterior density functions
3. Stop: $D_{\text{KL}}\left\{q(\boldsymbol{\beta},\boldsymbol{u},\sigma_u^2,a_u)\|p(\boldsymbol{\beta},\boldsymbol{u},\sigma_u^2,a_u|\boldsymbol{y})\right\}$ converges.



VMP for the Bayesian logistic semiparametric regression model

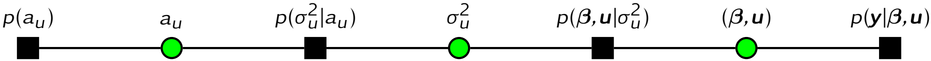
1. Initialise all messages from stochastic nodes to factors
2. Cycle:
   - (i) Update all messages from factors to stochastic nodes
   - (ii) Update all messages from stochastic nodes to factors
   - (iii) Update all optimal posterior density functions
3. Stop: $D_{\mathrm{KL}}\left\{q(\boldsymbol{\beta},\boldsymbol{u},\sigma_u^2,a_u)\|p(\boldsymbol{\beta},\boldsymbol{u},\sigma_u^2,a_u|\boldsymbol{y})\right\}$ converges.



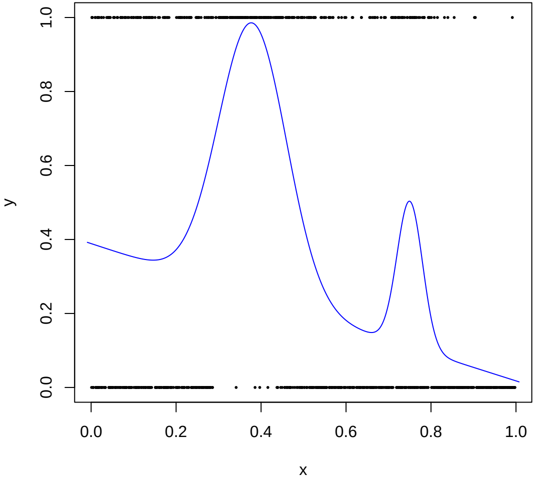
Bayesian Logistic Semiparametric Regression

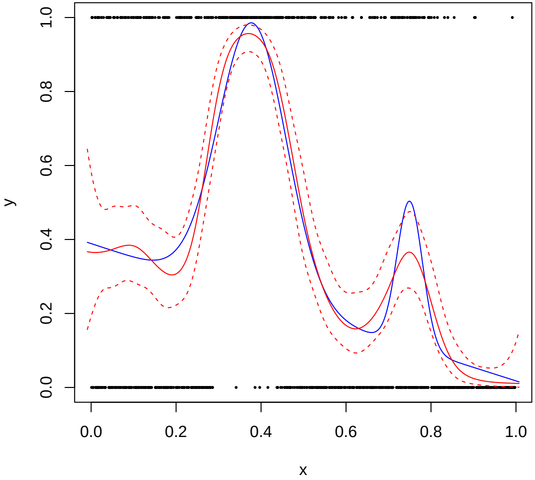
VMP for the Bayesian logistic semiparametric regression model

1. Initialise all messages from stochastic nodes to factors
2. Cycle:
   (i) Update all messages from factors to stochastic nodes
   (ii) Update all messages from stochastic nodes to factors
   (iii) Update all optimal posterior density functions
3. Stop: $D_{\text{KL}}\left\{q(\boldsymbol{\beta},\boldsymbol{u},\sigma_u^2,a_u)\|p(\boldsymbol{\beta},\boldsymbol{u},\sigma_u^2,a_u|\boldsymbol{y})\right\}$ converges.



Binary Response Data





y
x
0.0
0.2
0.4
0.6
0.8
1.0

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