# Variational Inference Masterclass: Variational Message Passing

https://github.com/tui-nolan/Variational-Inference-Masterclass

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# Outline

Part I: Message Passing for Variational Inference



Part II: Efficient Model Extensions

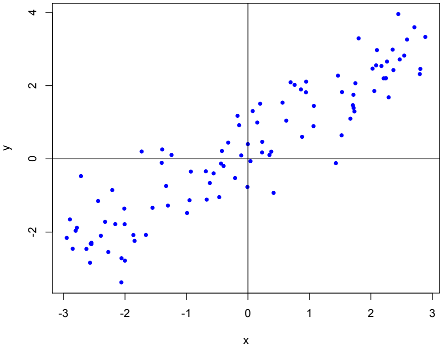


Part III: Nonconjugate Models

Part I

# Introduction and Motivation

Consider the following data:




In a typical regression problem we solve using:

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

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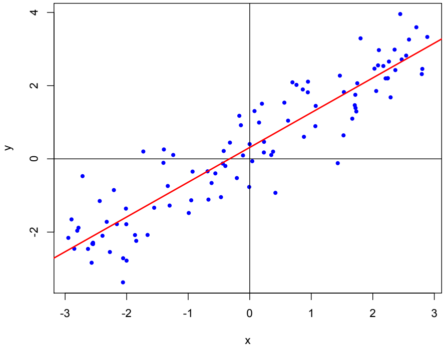


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$$\hat{\boldsymbol{\beta}} = \operatorname*{argmin}_{\boldsymbol{\beta} \in \mathbb{R}^2} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}\|_2$$

# Mean Field Variational Bayes

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

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

where

$$x \sim \text{Inverse} - \chi^2(\kappa, \lambda) \quad \text{if and only if} \quad x \sim \text{Inverse-Gamma}(\kappa/2, \lambda/2)$$

Note that (Gelman, 2006) if

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

then

$$\sigma \sim \text{Half-Cauchy}(A)$$

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:

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

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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

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

$q^*(a)$ 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:

$$q^*(a) \propto \exp\left\{\mathbb{E}_{-q^*(a)} \log p(\boldsymbol{y}, \boldsymbol{\beta}, \sigma^2, a)\right\}$$
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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.

# 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:

$$\boldsymbol{y}_i \mid \boldsymbol{\beta}, \boldsymbol{u}_i, \sigma^2 \sim N(\boldsymbol{X}_i\boldsymbol{\beta} + \boldsymbol{X}_i\boldsymbol{u}_i, \sigma^2\boldsymbol{I}), \qquad \boldsymbol{u}_i \mid \Sigma \sim N(\boldsymbol{0}, \Sigma), \quad \text{for } 1 \le i \le m$$

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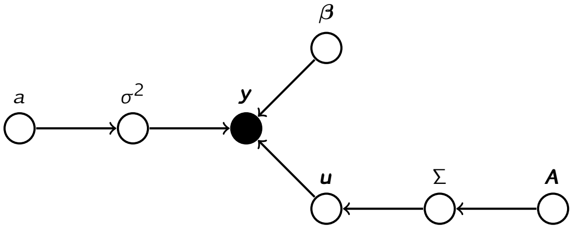

Prof. Matt Wand
Distinguished professor of statistics, University of Technology Sydney
*Fast Approximate Inference for Arbitrarily Large Semiparametric Regression Models via Message Passing, Journal of the American Statistical Association, 2017, VOL. 112, NO. 517, 137–168, Theory and Methods*

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Let's reconsider the Bayesian linear regression model:

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

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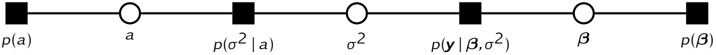


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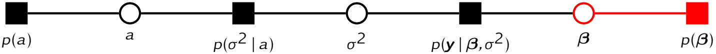


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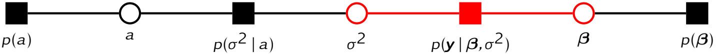


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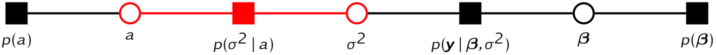


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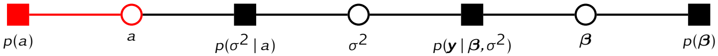


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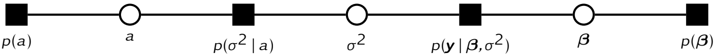


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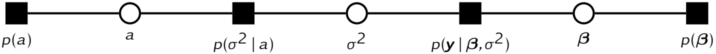


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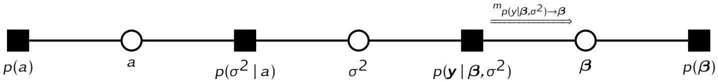


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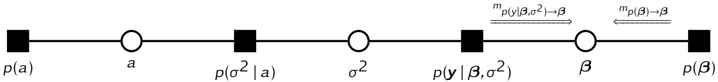


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$$q^*(\boldsymbol{\beta}) = C\exp\left\{-\frac{1}{2}\,\mathbb{E}_q(1/\sigma^2)\boldsymbol{\beta}^T\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{\beta}+\mathbb{E}_q(1/\sigma^2)\boldsymbol{\beta}^T\boldsymbol{X}^T\boldsymbol{y}\right\}\exp\left\{-\frac{1}{2}\boldsymbol{\beta}^T\Sigma_0^{-1}\boldsymbol{\beta}\right\}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

We define the messages as

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

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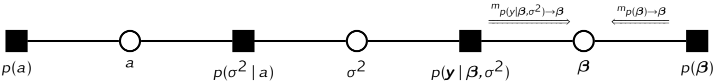
The representation via a directed acyclic graph does not facilitate this factorised form:

# Steps Towards Message Passing Algorithms

This factorised approach is key to the message passing infrastructure:




$$\boldsymbol{y}|\boldsymbol{\beta},\sigma^2 \sim N(\boldsymbol{X}\boldsymbol{\beta},\sigma^2\boldsymbol{I}_n), \quad \boldsymbol{\beta} \sim N(\boldsymbol{0},\Sigma_0)$$

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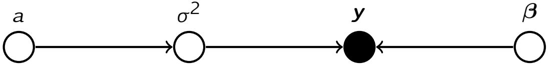
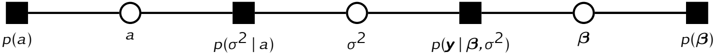


# General Message Passing Rules




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

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

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

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

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

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

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

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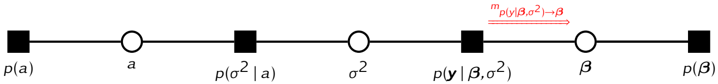


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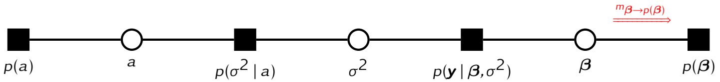


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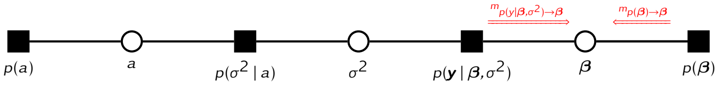


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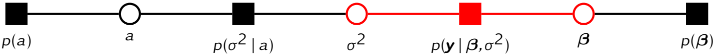
# The Gaussian Likelihood Fragment




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

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

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 $\sigma^2$ 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.

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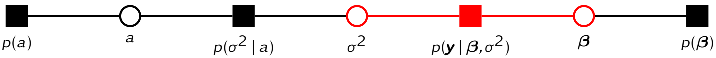


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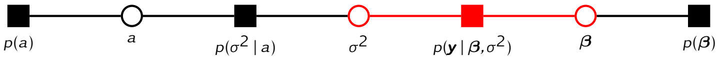


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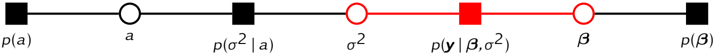



By restricting the form of the messages passing updates to distributions in the exponential family form, we can completely characterise these message updates by their natural parameter vectors:

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

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

# 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-$\chi^2$ Density Function in Exponential Family Form

$$x|\kappa, \lambda \sim \text{Inverse} - \chi^2(\kappa, \lambda)$$

The density function in exponential family form is:

$$p(x|\kappa,\lambda) = C \exp\left\{ \begin{bmatrix} \log|x| \\ 1/x \end{bmatrix}^{\mathsf{T}} \boldsymbol{\eta} \right\}, \quad \boldsymbol{\eta} = \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix} = \begin{bmatrix} -\frac{1}{2}(\kappa+2) \\ -\frac{\lambda}{2} \end{bmatrix}$$

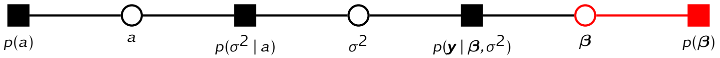
The transformation back to the common parameters is

$$\kappa = -2\eta_1 - 2, \quad \lambda = -2\eta_2$$

For variational inference, we require:

$$\mathbb{E}(1/\sigma^2) = \frac{\eta_1 + 1}{\eta_2}$$

# Fragments




Gaussian prior fragment (Wand, 2017)

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Iterated inverse chi-squared fragment (Maestrini and Wand, 2020)

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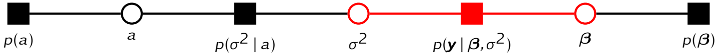


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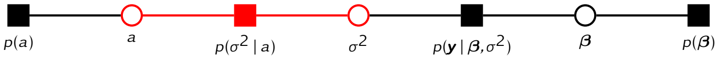


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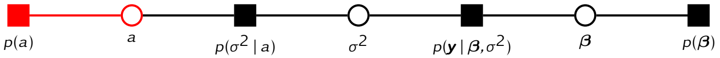


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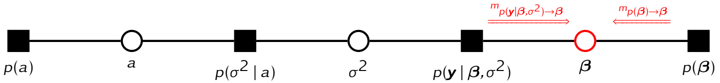
# $q$-Density Functions




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

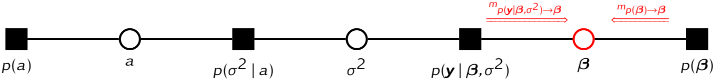
$$q(\boldsymbol{\beta}) = m_{p(\boldsymbol{y}|\boldsymbol{\beta},\sigma^2)\to\boldsymbol{\beta}}(\boldsymbol{\beta}) \times m_{p(\boldsymbol{\beta})\to\boldsymbol{\beta}}(\boldsymbol{\beta})$$

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

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

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

# $q$-Density Functions

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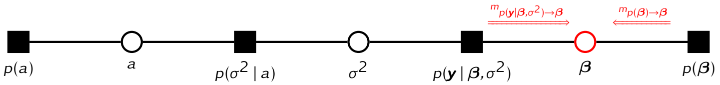


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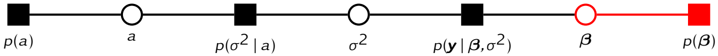
# The Gaussian Prior Fragment




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

Inputs:

$$\sigma_\beta^2$$

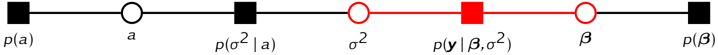
Updates:

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

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:

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

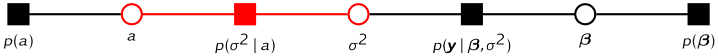
$$\mathbb{E}_q(1/\sigma^2) = \frac{(\boldsymbol{\eta}_{q^*(\sigma^2)})_1 + 1}{(\boldsymbol{\eta}_{q^*(\sigma^2)})_2}$$

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

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-$\chi^2$ Fragment




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

Inputs:

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

Updates:

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

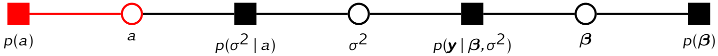
$$\mathbb{E}_q(1/a) = \frac{(\boldsymbol{\eta}_{q^*(a)})_1 + 1}{(\boldsymbol{\eta}_{q^*(a)})_2},$$

$$\boldsymbol{\eta}_{p(\sigma^2|a)\to\sigma^2} = \begin{bmatrix} -\frac{3}{2} \\ -\frac{1}{2}\,\mathbb{E}_q(1/a) \end{bmatrix}, \quad \boldsymbol{\eta}_{p(\sigma^2|a)\to a} = \begin{bmatrix} -\frac{1}{2} \\ -\frac{1}{2}\{\text{vec}\,\mathbb{E}_q(1/\sigma^2)\} \end{bmatrix}$$

Outputs:

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

# Inverse-$\chi^2$ Prior Fragment




$$a \sim \text{Inverse-}\chi^2(\kappa, \lambda)$$

Inputs:

$$\kappa, \lambda$$

Updates:

$$\boldsymbol{\eta}_{p(a)\to a} = \begin{bmatrix} -\frac{1}{2}(\kappa+2) \\ -\frac{\lambda}{2} \end{bmatrix}$$

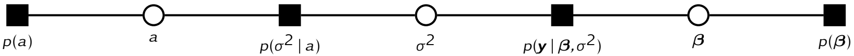
Outputs:

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

# 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: $D_{\mathrm{KL}}\left\{q(\boldsymbol{\beta},\sigma^2,a)\|p(\boldsymbol{\beta},\sigma^2,a|\boldsymbol{y})\right\}$ converges.



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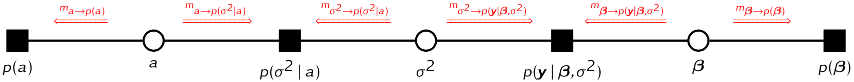

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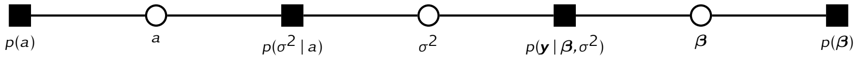

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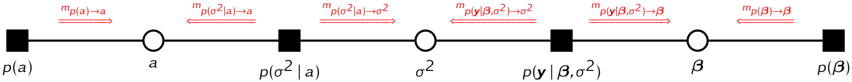

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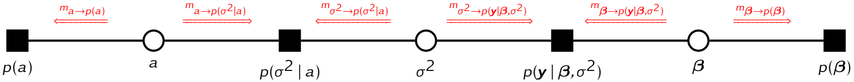

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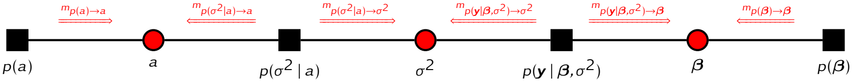

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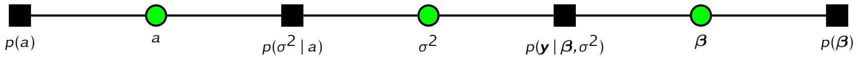
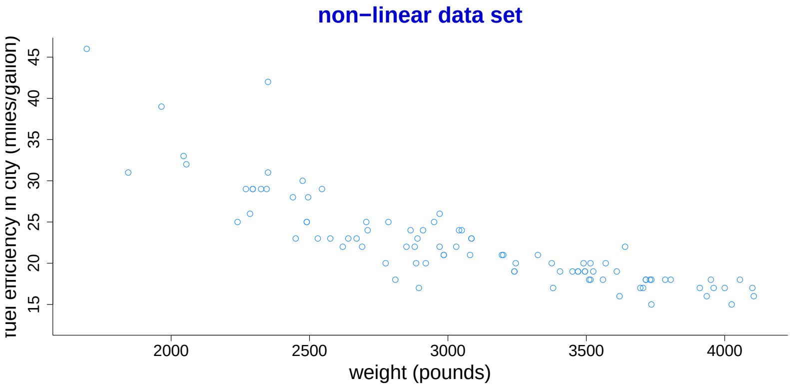


Part II

# Building Model Complexity

# Nonlinear Data



We can address nonlinear data sets using semiparametric regression techniques

Let $x_i$ be the $i$th 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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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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# Bayesian Semiparametric Regression

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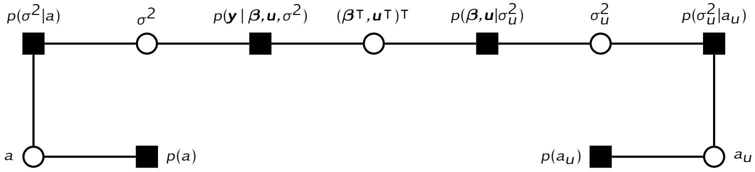


Gaussian likelihood fragment

Gaussian penalization fragment (Wand, 2017)

Iterated inverse Wishart fragment

Inverse Wishart prior fragment

# Bayesian Semiparametric Regression

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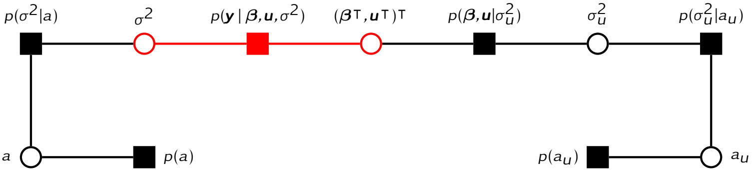


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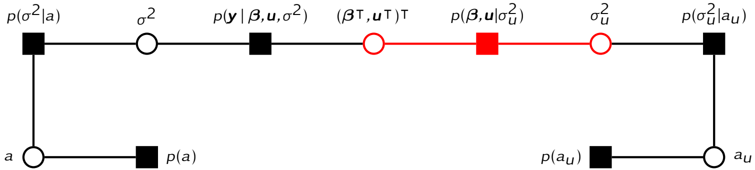


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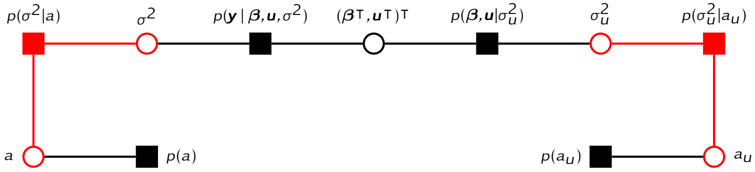


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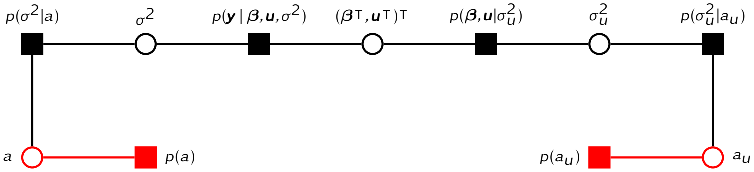


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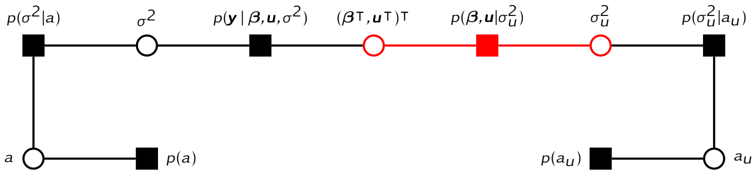
# Gaussian Penalization Fragment




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

Inputs:

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

Updates:

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

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

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

Outputs:

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

## VMP for the Bayesian semiparametric regression model

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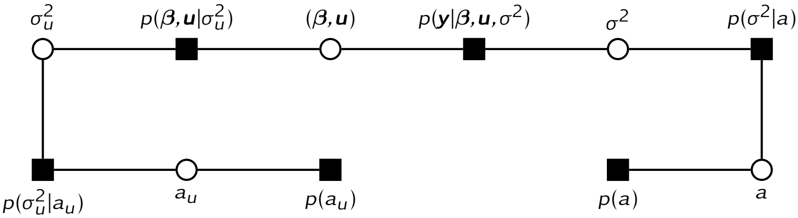

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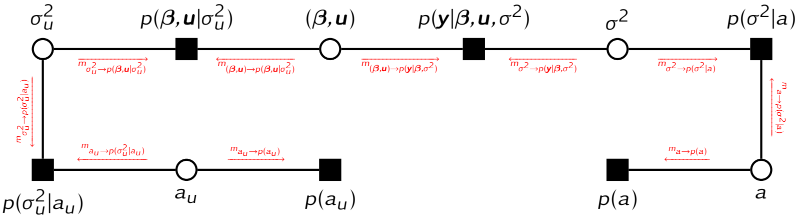

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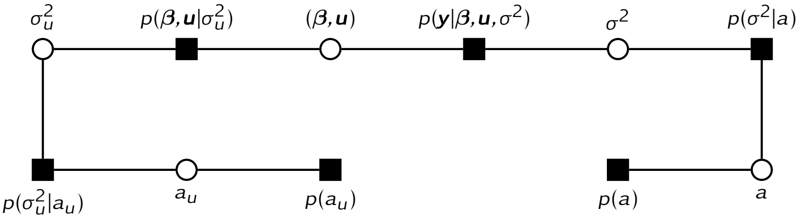

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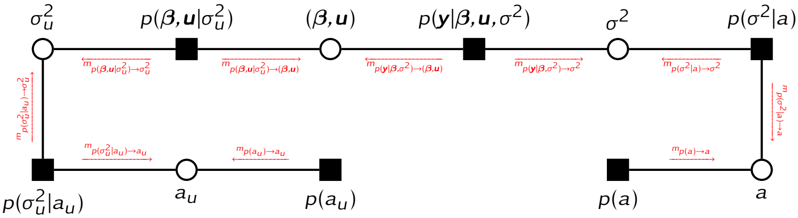

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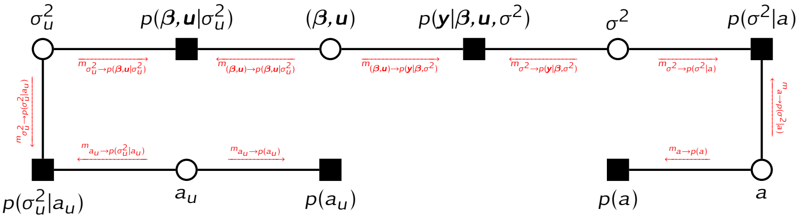

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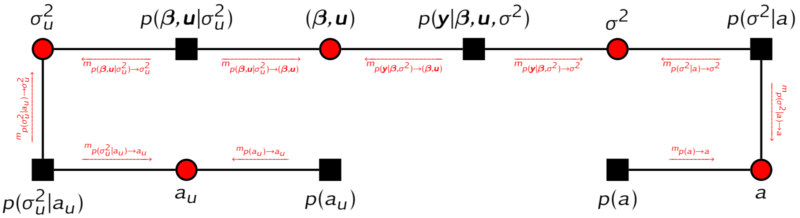

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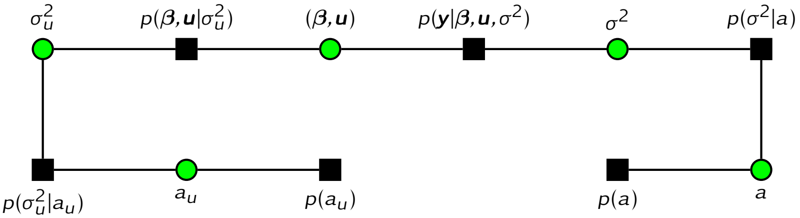
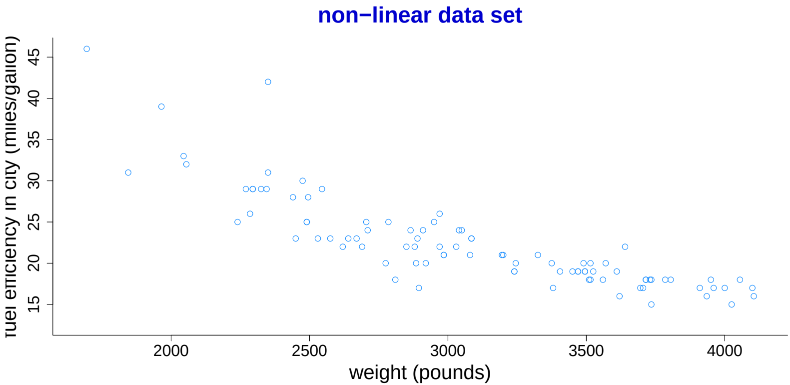
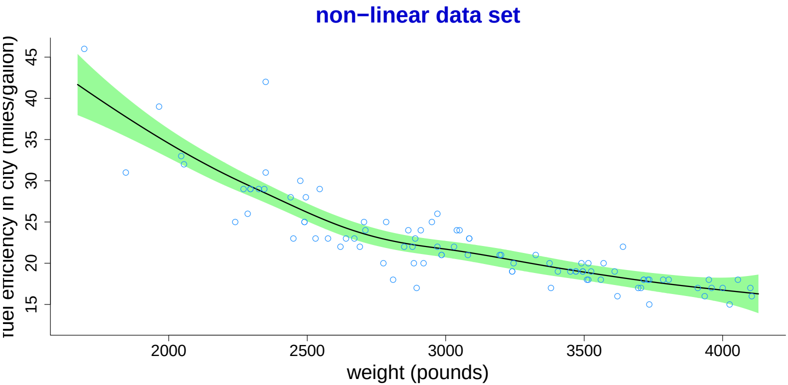



non−linear data set
fuel efficiency in city (miles/gallon)
15
20
25
30
35
40
45
2000
2500
3000
3500
4000
weight (pounds)


non−linear data set
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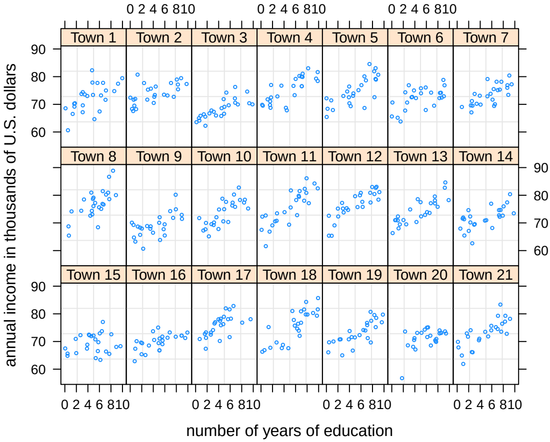
20
25
30
35
40
45
2000
2500
3000
3500
4000
weight (pounds)

# Multilevel Data



# Multilevel Data

Suppose we have $m$ groups and $n_i$ subjects in the $i$th group.

Let $x_{ij}$ be the predictor for the $j$th subject in the $i$th, and let $y_{ij}$ be the corresponding observation.

A Gaussian response linear mixed model for such data consists of

$$y_{ij} = \beta_0 + \beta_1 x_{ij} + u_{i1} + u_{i2} x_{ij} + \epsilon_{ij}, \quad \begin{bmatrix} u_{i1} \\ u_{i2} \end{bmatrix} \overset{\text{ind.}}{\sim} \mathrm{N}(\mathbf{0}_2, \Sigma_u),$$

$$\epsilon_{ij} \overset{\text{ind.}}{\sim} \mathrm{N}(0, \sigma^2), \quad j = 1, \ldots, n_i, \quad i = 1, \ldots, m.$$

Next, set

$$\boldsymbol{y}_i \equiv \begin{bmatrix} y_{i1} \\ \vdots \\ y_{in_i} \end{bmatrix}, \quad \boldsymbol{x}_i \equiv \begin{bmatrix} x_{i1} \\ \vdots \\ x_{in_i} \end{bmatrix}, \quad \boldsymbol{X}_i \equiv \begin{bmatrix} \mathbf{1}_{n_i} & \boldsymbol{x}_i \end{bmatrix} \quad \text{and} \quad \boldsymbol{u}_i \equiv \begin{bmatrix} u_{i1} \\ u_{i2} \end{bmatrix}.$$

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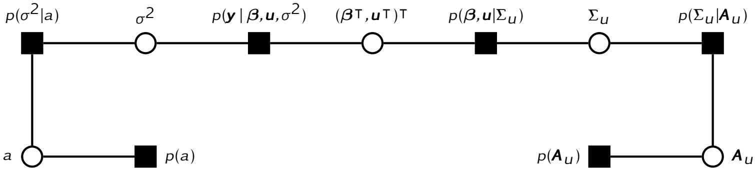
# Bayesian Multilevel Data Model

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

$$\Sigma_u|\boldsymbol{A}_u \sim \text{Inverse Wishart}(1,\boldsymbol{A}_u^{-1}), \quad \boldsymbol{A}_u \sim \text{Inverse Wishart}\left(1,\frac{1}{A^2}\boldsymbol{I}\right)$$

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




Gaussian likelihood fragment

Gaussian penalization fragment

Iterated inverse Wishart fragment

Inverse Wishart prior fragment

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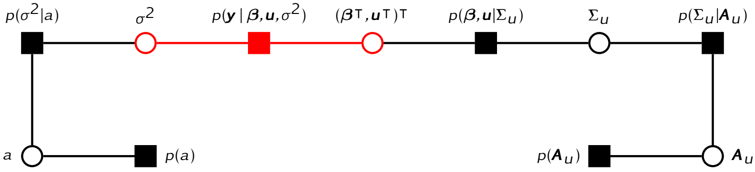


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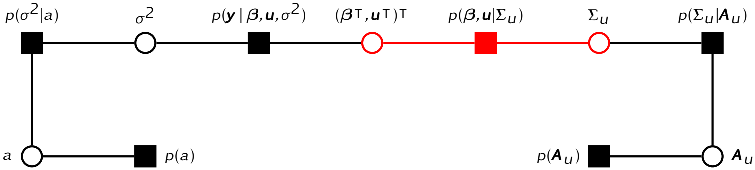


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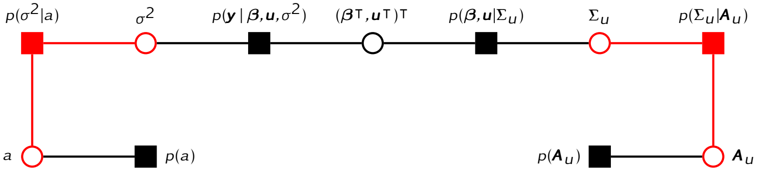


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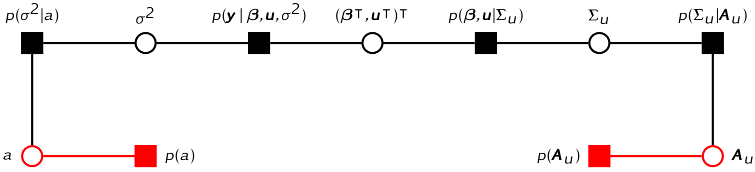


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The parameters for the posterior of $\boldsymbol{\nu} \equiv (\boldsymbol{\beta}^{\top}, \boldsymbol{u}^{\top})^{\top}$ take the form - Lee and Wand (2016):

$$\mathbb{E}_q(\boldsymbol{\nu}) \equiv \boldsymbol{A}^{-1}\boldsymbol{a}, \quad \text{Cov}_q(\boldsymbol{\nu}) \equiv \boldsymbol{A}^{-1}$$

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

The posterior of $\sigma^2$ 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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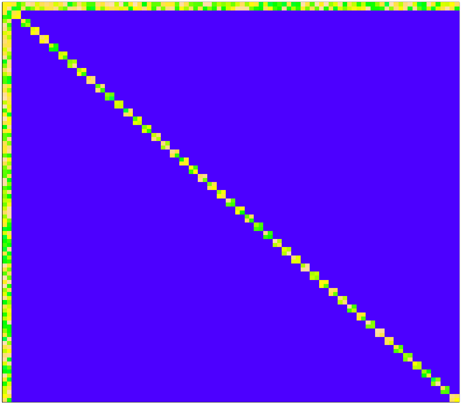
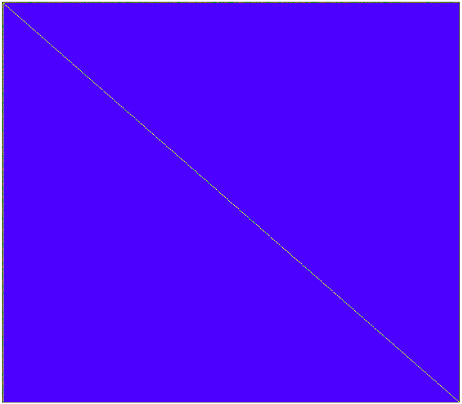
# Multilevel Model (21 Towns)

$\boldsymbol{A} =$ 

# Multilevel Model (1000 Towns)

$A =$ 

# Multilevel Model

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

Matrices and vectors are partitioned as:

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

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

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

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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

# 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 ($\boldsymbol{A}\,\mathbb{E}_q(\boldsymbol{\nu}) = \boldsymbol{a}$)

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

$$\boldsymbol{A}_{11}\,\mathbb{E}_q(\boldsymbol{\beta}) + \sum_{i=1}^{3} \boldsymbol{A}_{12,i}\,\mathbb{E}_q(\boldsymbol{u}_i) = \boldsymbol{a}_1$$

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

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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 $\text{Cov}_q(\boldsymbol{\nu})$ are

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

$$\text{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i) = -(\boldsymbol{A}_{22,i}^{-1}\boldsymbol{A}_{12,i}^{T}\text{Cov}_q(\boldsymbol{\beta}))^{T}, \quad \text{Cov}_q(\boldsymbol{u}_i) = \boldsymbol{A}_{22,i}^{-1}(\boldsymbol{I} - \boldsymbol{A}_{12.i}^{T}\text{Cov}_q(\boldsymbol{\beta},\boldsymbol{u}_i)), \quad 1 \le i \le m.$$

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

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

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

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

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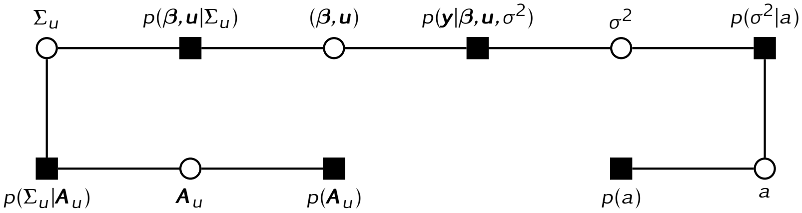
## VMP for the Bayesian multilevel data model

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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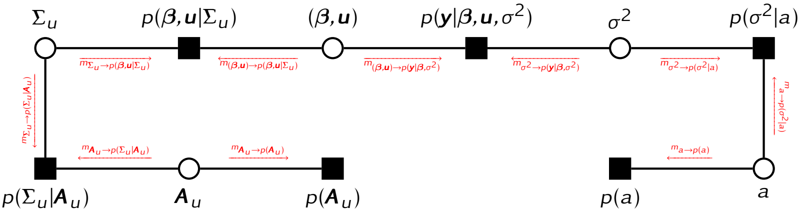

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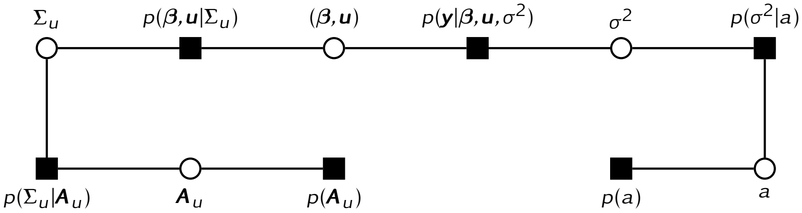

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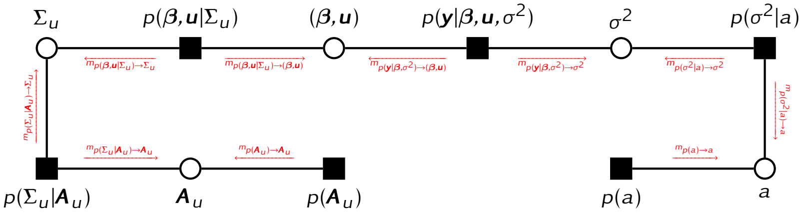

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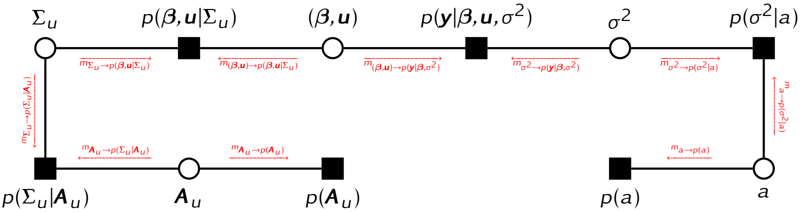

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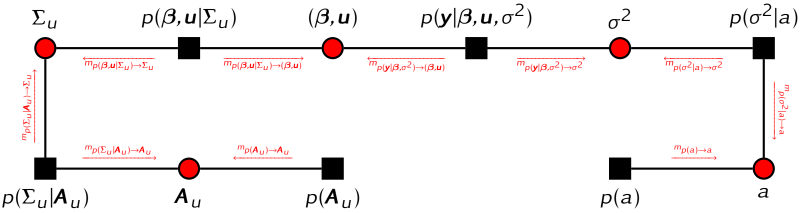

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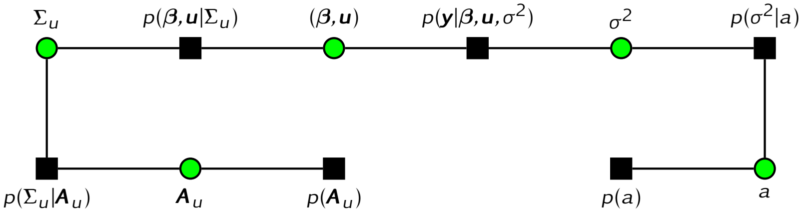
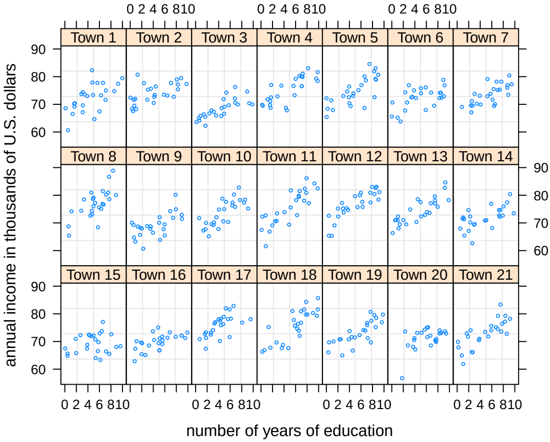
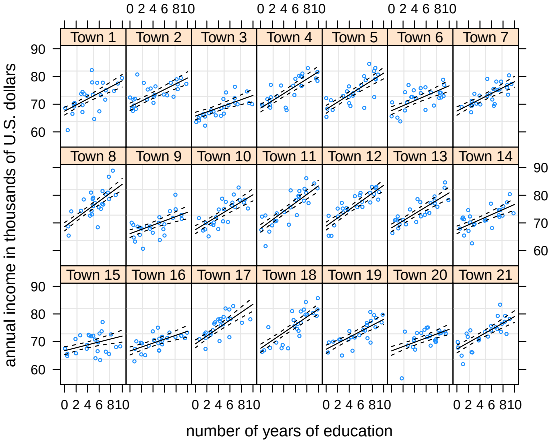


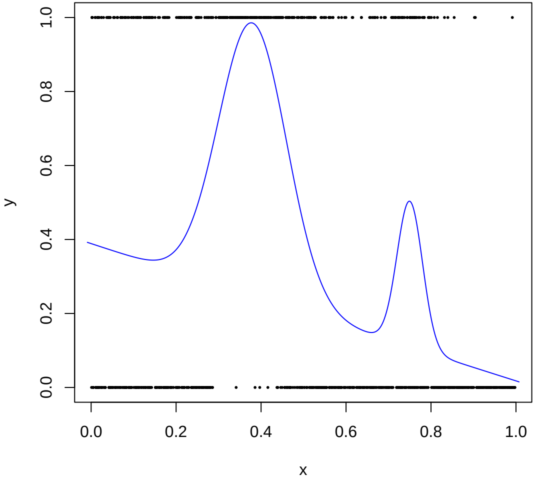

Town 1
Town 2
Town 3
Town 4
Town 5
Town 6
Town 7
Town 8
Town 9
Town 10
Town 11
Town 12
Town 13
Town 14
Town 15
Town 16
Town 17
Town 18
Town 19
Town 20
Town 21
0 2 4 6 810
60
70
80
90
annual income in thousands of U.S. dollars
number of years of education

# Multilevel Data



Part III

# Non-conjugate Models


y
x
0.0
0.2
0.4
0.6
0.8
1.0

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




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.

# Bayesian Logistic Regression Model

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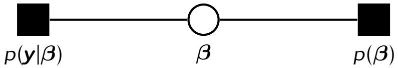


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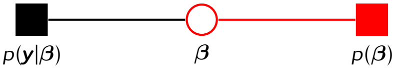
The factor graph is




Gaussian Prior Fragment

Logistic Likelihood Fragment (Nolan and Wand, 2017)

The message takes the form:

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

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

Consider the Bayesian logistic regression model:

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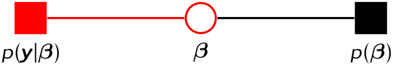


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# Bayesian Logistic Regression Model

Consider the Bayesian logistic regression model:

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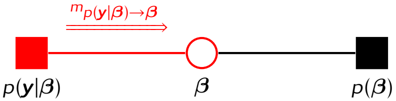


Gaussian Prior Fragment

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The message takes the form:

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

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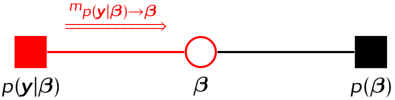


Gaussian Prior Fragment

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The message takes the form:

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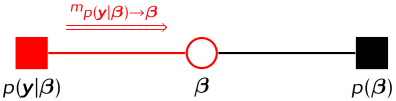


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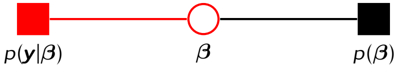


A fixed point iterative scheme for $\boldsymbol{\eta}_{p(\boldsymbol{y}|\boldsymbol{\beta})\to\boldsymbol{\beta}}$ (Wand, 2014):

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

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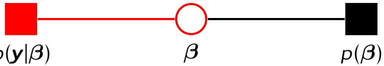
where

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

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A fixed point iterative scheme for $q(\boldsymbol{\beta})$ - Wand (2014):

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$$\Downarrow \text{ Monahan and Stefanski (1992)}$$

$$\mathcal{B}_r(\mu,\sigma) \approx \int_{-\infty}^{\infty} x^r \sum_{i=1}^{k} p_i \Phi\left(s_i \frac{x-\mu}{\sigma}\right)\phi(x)dx, \quad \text{for } r = 0,1$$

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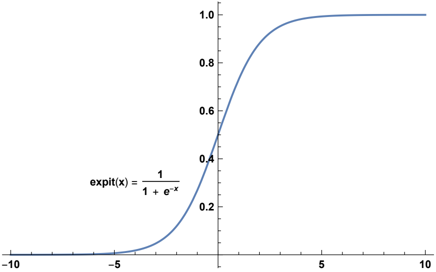

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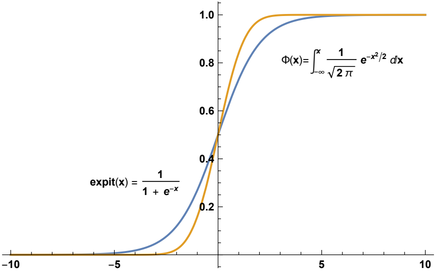

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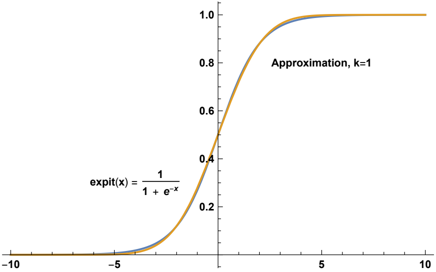


| $p$ | $s$ |
|---|---|
| 1.00000 | 0.58763 |

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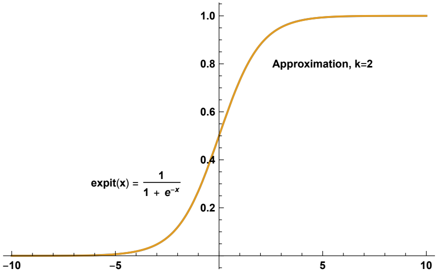


| $p$ | $s$ |
|---|---|
| 0.56442 | 0.76862 |
| 0.43557 | 0.43525 |

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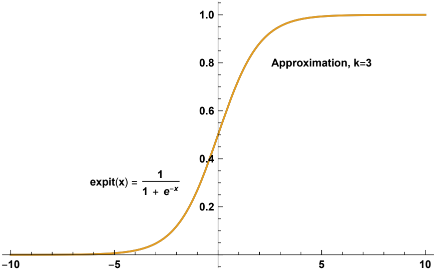


| $p$ | $s$ |
|---|---|
| 0.25220 | 0.90793 |
| 0.58522 | 0.57778 |
| 0.16257 | 0.36403 |

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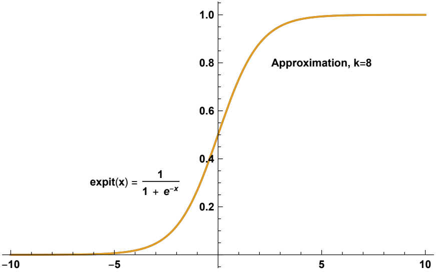
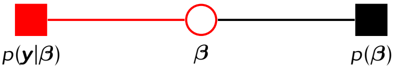



| p | s |
|---|---|
| 0.00324 | 1.36534 |
| 0.05151 | 1.05952 |
| 0.19507 | 0.83079 |
| 0.31556 | 0.65073 |
| 0.27414 | 0.50813 |
| 0.13107 | 0.39631 |
| 0.02791 | 0.30890 |
| 0.00144 | 0.23821 |

# 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:

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

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

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

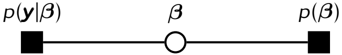
Outputs:

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

# 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: $D_{\mathrm{KL}}\left\{q(\boldsymbol{\beta})||p(\boldsymbol{\beta}|\boldsymbol{y})\right\}$ converges.



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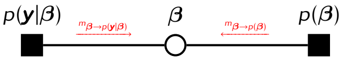

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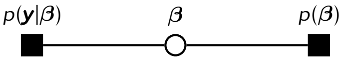

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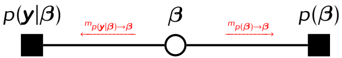

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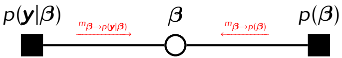

# Bayesian Logistic Regression

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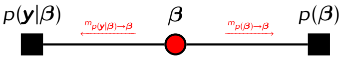

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1. Initialise all messages from stochastic nodes to factors
2. Cycle:
   (i) Update all messages from factors to stochastic nodes
   (ii) Update all messages from stochastic nodes to factors
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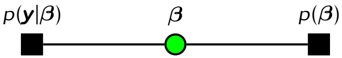
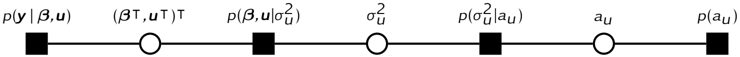


# Bayesian Logistic Semiparametric Regression

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

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




Logistic likelihood fragment

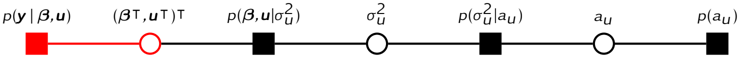
Gaussian penalization fragment (Wand, 2017)

Iterated inverse Wishart fragment

Inverse Wishart prior fragment

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

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

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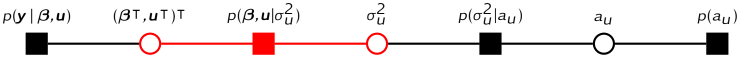
Inverse Wishart prior fragment

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

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




Logistic likelihood fragment

Gaussian penalization fragment (Wand, 2017)

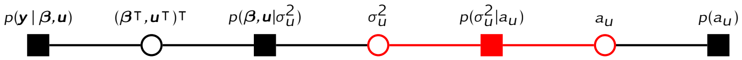
Iterated inverse Wishart fragment

Inverse Wishart prior fragment

# Bayesian Logistic Semiparametric Regression

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

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




Logistic likelihood fragment

Gaussian penalization fragment (Wand, 2017)

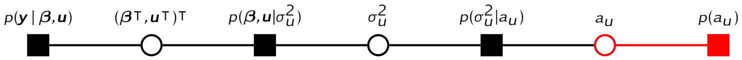
Iterated inverse Wishart fragment

Inverse Wishart prior fragment

# Bayesian Logistic Semiparametric Regression

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

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




Logistic likelihood fragment

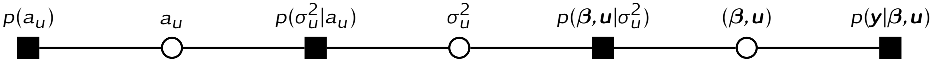
Gaussian penalization fragment (Wand, 2017)

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.



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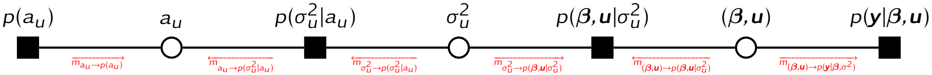

## VMP for the Bayesian logistic semiparametric regression model

1. Initialise all messages from stochastic nodes to factors
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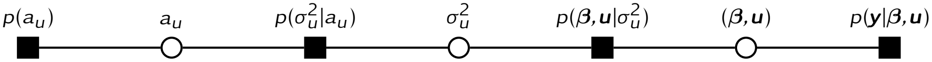

# Bayesian Logistic Semiparametric Regression

## VMP for the Bayesian logistic semiparametric regression model

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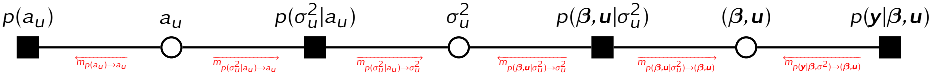
3. Stop: $D_{\text{KL}}\left\{q(\boldsymbol{\beta},\boldsymbol{u},\sigma_u^2,a_u)||p(\boldsymbol{\beta},\boldsymbol{u},\sigma_u^2,a_u|\boldsymbol{y})\right\}$ converges.



## VMP for the Bayesian logistic semiparametric regression model

1. Initialise all messages from stochastic nodes to factors
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   - (i) Update all messages from factors to stochastic nodes
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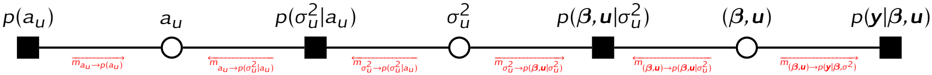

## VMP for the Bayesian logistic semiparametric regression model

1. Initialise all messages from stochastic nodes to factors
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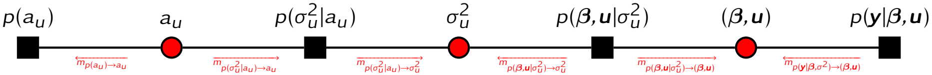

## VMP for the Bayesian logistic semiparametric regression model

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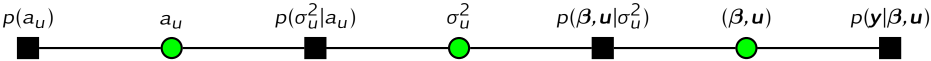
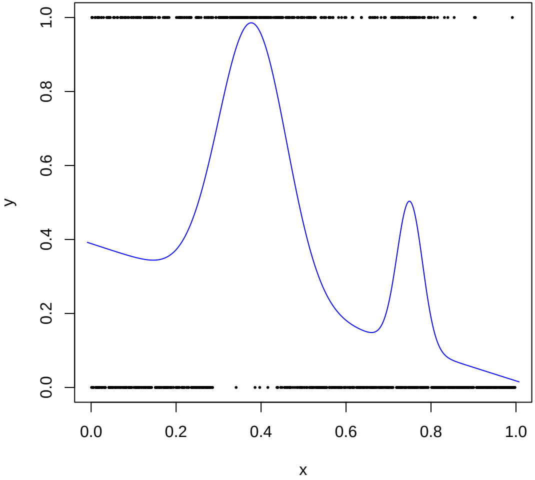
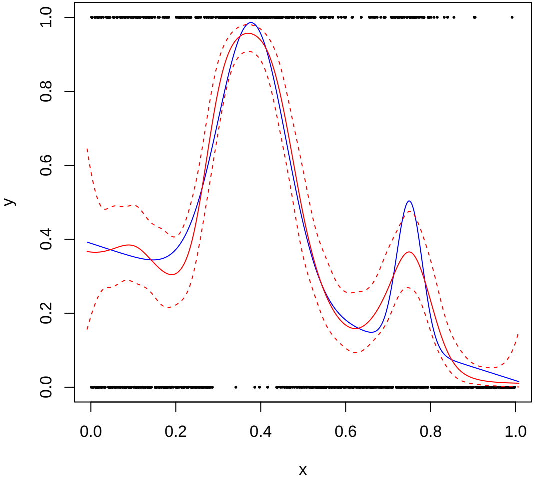


# Binary Response Data



# Binary Response Data



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