Bayesian Linear Models

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Linear Regression

- Linear regression is, perhaps, the most widely used statistical modeling tool.
- It addresses the following question: How does a quantity of primary interest, y, vary as (depend upon) another quantity, or set of quantities, x?
- The quantity y is called the response or outcome variable.
 Some people simply refer to it as the dependent variable.
- The variable(s) x are called *explanatory variables*, *covariates* or simply *independent variables*.
- In general, we are interested in the conditional distribution of y, given x, parametrized as $p(y | \theta, x)$.

- Typically, we have a set of *units* or *experimental subjects* i = 1, 2, ..., n.
- For each of these units we have measured an outcome y_i and a set of explanatory variables $\mathbf{x}_i^{\top} = (1, x_{i1}, x_{i2}, \dots, x_{ip})$.
- The first element of \mathbf{x}_i^{\top} is often taken as 1 to signify the presence of an "intercept".
- We collect the outcome and explanatory variables into an $n \times 1$ vector and an $n \times (p+1)$ matrix:

$$\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}; \quad \mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1p} \\ 1 & x_{21} & x_{22} & \dots & x_{2p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{np} \end{bmatrix} = \begin{pmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_n^\top \end{pmatrix}.$$

- The linear model is the most fundamental of all serious statistical models underpinning:
 - ANOVA: y_i is continuous, x_{ij} 's are all categorical
 - REGRESSION: y_i is continuous, x_{ij} 's are continuous
 - ANCOVA: y_i is continuous, x_{ij}'s are continuous for some j and categorical for others.

Conjugate Bayesian Linear Regression

A conjugate Bayesian linear model is given by:

$$y_i \mid \beta, \sigma^2, \mathbf{x}_i \stackrel{ind}{\sim} N(\mu_i, \sigma^2); \quad i = 1, 2, ..., n;$$

 $\mu_i = \beta_0 + \beta_1 x_{i1} + \dots + \beta_p x_{ip} = \mathbf{x}_i^\top \beta; \quad \beta = (\beta_0, \beta_1, \dots, \beta_p)^\top;$
 $\beta \mid \sigma^2 \sim N(\mu_\beta, \sigma^2 \mathbf{V}_\beta); \quad \sigma^2 \sim IG(a, b).$

- Unknown parameters include the regression parameters and the variance, i.e. $\theta = \{\beta, \sigma^2\}$.
- We assume X is observed without error and all inference is conditional on X.
- The above model is often written in terms of the posterior density $p(\theta \mid \mathbf{y}) \propto p(\theta, \mathbf{y})$:

$$IG(\sigma^2 \mid a, b) \times N(\beta \mid \boldsymbol{\mu}_{\beta}, \sigma^2 \mathbf{V}_{\beta}) \times \prod_{i=1}^{n} N(y_i \mid \mathbf{x}_i^{\top} \boldsymbol{\beta}, \sigma^2)$$
.

Conjugate Bayesian (General) Linear Regression

A more general conjugate Bayesian linear model is given by:

$$\mathbf{y} \mid \beta, \sigma^2, \mathbf{X} \sim N(\mathbf{X}\beta, \sigma^2 \mathbf{V}_y)$$

 $\beta \mid \sigma^2 \sim N(\mu_\beta, \sigma^2 \mathbf{V}_\beta)$;
 $\sigma^2 \sim IG(a, b)$.

- V_V , V_β and μ_β are assumed fixed.
- Unknown parameters include the regression parameters and the variance, i.e. $\theta = \{\beta, \sigma^2\}$.
- We assume X is observed without error and all inference is conditional on X.
- The posterior density $p(\theta \mid \mathbf{y}) \propto p(\theta, \mathbf{y})$:

$$IG(\sigma^2 \mid a, b) \times N(\beta \mid \mu_{\beta}, \sigma^2 \mathbf{V}_{\beta}) \times N(\mathbf{y} \mid \mathbf{X}\beta, \sigma^2 \mathbf{V}_{y})$$

■ The model on the previous slide is a special case with $\mathbf{V}_y = \mathbf{I}_n$ ($n \times n$ identity matrix).

Conjugate Bayesian (General) Linear Regression

The joint posterior density can be written as

$$p(\beta, \sigma^2 | \mathbf{y}) \propto \underbrace{\frac{IG(\sigma^2 | a^*, b^*)}{p(\sigma^2 | \mathbf{y})}}^{\times} \underbrace{\frac{N(\beta | \mathbf{Mm}, \sigma^2 \mathbf{M})}{p(\beta | \sigma^2, \mathbf{y})}}_{p(\beta | \sigma^2, \mathbf{y})}$$

where

$$a^* = a + \frac{n}{2}; \quad b^* = b + \frac{1}{2} \left(\mu_{\beta}^{\top} \mathbf{V}_{\beta}^{-1} \mu_{\beta} + \mathbf{y}^{\top} \mathbf{V}_{y}^{-1} \mathbf{y} - \mathbf{m}^{\top} \mathbf{M} \mathbf{m} \right);$$

$$\mathbf{m} = \mathbf{V}_{\beta}^{-1} \mu_{\beta} + \mathbf{X}^{\top} \mathbf{V}_{y}^{-1} \mathbf{y}; \quad \mathbf{M}^{-1} = \mathbf{V}_{\beta}^{-1} + \mathbf{X}^{\top} \mathbf{V}_{y}^{-1} \mathbf{X}.$$

- Exact posterior sampling from $p(\beta, \sigma^2 | \mathbf{y})$ will automatically yield samples from $p(\beta | \mathbf{y})$ and $p(\sigma^2 | \mathbf{y})$.
- For each j = 1, 2, ..., N do the following:
 - 1. Draw $\sigma_{(i)}^2 \sim IG(a^*, b^*)$
 - 2. Draw $\beta_{(j)} \sim N\left(\mathbf{Mm}, \sigma_{(j)}^2 \mathbf{M}\right)$
- The above is sometimes referred to as composition sampling.

Exact sampling from joint posterior distributions

Suppose we wish to draw samples from a joint posterior:

$$p(\theta_1, \theta_2 | \mathbf{y}) = p(\theta_1 | \mathbf{y}) \times p(\theta_2 | \theta_1, \mathbf{y}).$$

- In conjugate models, it is often easy to draw samples from $p(\theta_1 | \mathbf{y})$ and from $p(\theta_2 | \theta_1, \mathbf{y})$.
- We can draw N samples from $p(\theta_1, \theta_2 | \mathbf{y})$ as follows.
- For each j = 1, 2, ..., N do the following:
 - 1. Draw $\theta_{1(i)} \sim p(\theta_1 \mid \mathbf{y})$
 - 2. Draw $\theta_{2(j)} \sim p(\theta_2 \mid \theta_{1(j)}, \mathbf{y})$
- Remarkably, the $\theta_{2(j)}$'s drawn above have marginal distribution $p(\theta_2 | \mathbf{y})$ (see, Gelfand and Smith 1990).
- "Automatic Marginalization" we draw samples $p(\theta_1, \theta_2 \mid \mathbf{y})$ and automatically get samples from $p(\theta_1 \mid \mathbf{y})$ and $p(\theta_2 \mid \mathbf{y})$.

Bayesian predictions from linear regression

- Let $\tilde{\mathbf{y}}$ denote an $m \times 1$ vector of outcomes we seek to predict based upon predictors $\tilde{\mathbf{X}}$.
- We seek the posterior predictive density:

$$p(\tilde{\mathbf{y}} | \mathbf{y}) = \int p(\tilde{\mathbf{y}} | \boldsymbol{\theta}, \mathbf{y}) p(\boldsymbol{\theta} | \mathbf{y}) d\boldsymbol{\theta}.$$

- Posterior predictive inference: sample from $p(\tilde{\mathbf{y}} | \mathbf{y})$.
- For each j = 1, 2, ..., N do the following:
 - 1. Draw $heta_{(j)} \sim p(heta \, | \, \mathbf{y})$
 - 2. Draw $\tilde{\mathbf{y}}_{(j)} \sim p(\tilde{\mathbf{y}} \,|\, \boldsymbol{\theta}_{(j)}, \mathbf{y})$

Bayesian predictions from linear regression (cont'd)

- For legitimate probabilistic predictions (forecasting), the conditional distribution $p(\tilde{\mathbf{y}} | \boldsymbol{\theta}, \mathbf{y})$ must be well-defined.
- For example, consider the case with $V_y = I_n$. Specify the linear model:

$$\begin{bmatrix} \mathbf{y} \\ \tilde{\mathbf{y}} \end{bmatrix} = \begin{bmatrix} \mathbf{X} \\ \tilde{\mathbf{X}} \end{bmatrix} \boldsymbol{\beta} + \begin{bmatrix} \boldsymbol{\epsilon} \\ \tilde{\boldsymbol{\epsilon}} \end{bmatrix} \; ; \quad \begin{bmatrix} \boldsymbol{\epsilon} \\ \tilde{\boldsymbol{\epsilon}} \end{bmatrix} \sim N \left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \; \sigma^2 \begin{bmatrix} \mathbf{I}_n & O \\ O & \mathbf{I}_m \end{bmatrix} \right) \; .$$

Easy to derive the conditional density:

$$p(\tilde{\mathbf{y}} \mid \boldsymbol{\theta}, \mathbf{y}) = p(\tilde{\mathbf{y}} \mid \boldsymbol{\theta}) = N(\tilde{\mathbf{y}} \mid \tilde{\mathbf{X}} \boldsymbol{\beta}, \sigma^2 \mathbf{I}_m)$$

• Posterior predictive density:

$$p(\tilde{\mathbf{y}} | \mathbf{y}) = \int N(\tilde{\mathbf{y}} | \tilde{\mathbf{X}} \beta, \sigma^2 \mathbf{I}_m) p(\beta, \sigma^2 | \mathbf{y}) d\beta d\sigma^2.$$

- For each j = 1, 2, ..., N do the following:
 - 1. Draw $\{\beta_{(j)}, \sigma_{(j)}^2\} \sim p(\beta, \sigma^2 | \mathbf{y})$
 - 2. Draw $\tilde{\mathbf{y}}_{(i)} \sim N(\tilde{\mathbf{X}}\boldsymbol{\beta}_{(i)}, \sigma_{(i)}^2 \mathbf{I}_m)$

Bayesian predictions from general linear regression

• For example, consider the case with general V_y . Specify:

$$\begin{bmatrix} \mathbf{y} \\ \tilde{\mathbf{y}} \end{bmatrix} = \begin{bmatrix} \mathbf{X} \\ \tilde{\mathbf{X}} \end{bmatrix} \boldsymbol{\beta} + \begin{bmatrix} \boldsymbol{\epsilon} \\ \tilde{\boldsymbol{\epsilon}} \end{bmatrix} \; ; \quad \begin{bmatrix} \boldsymbol{\epsilon} \\ \tilde{\boldsymbol{\epsilon}} \end{bmatrix} \sim N \left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} , \; \sigma^2 \begin{bmatrix} \mathbf{V}_y & \mathbf{V}_{y\tilde{y}} \\ \mathbf{V}_{y\tilde{y}}^\top & \mathbf{V}_{\tilde{y}} \end{bmatrix} \right) \; .$$

Derive the conditional density

$$p(\tilde{\mathbf{y}} | \boldsymbol{\theta}, \mathbf{y}) = N(\tilde{\mathbf{y}} | \boldsymbol{\mu}_{\tilde{y}|y}, \sigma^2 \mathbf{V}_{\tilde{y}|y})$$
:

$$\boldsymbol{\mu}_{\tilde{\boldsymbol{y}}|\boldsymbol{y}} = \tilde{\mathbf{X}}\boldsymbol{\beta} + \mathbf{V}_{\boldsymbol{y}\tilde{\boldsymbol{y}}}^{\top}\mathbf{V}_{\boldsymbol{y}}^{-1}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) \; ; \quad \mathbf{V}_{\tilde{\boldsymbol{y}}|\boldsymbol{y}} = \mathbf{V}_{\tilde{\boldsymbol{y}}} - \mathbf{V}_{\boldsymbol{y}\tilde{\boldsymbol{y}}}^{\top}\mathbf{V}_{\boldsymbol{y}}^{-1}\mathbf{V}_{\boldsymbol{y}\tilde{\boldsymbol{y}}} \; .$$

Posterior predictive density:

$$p(\tilde{\mathbf{y}} | \mathbf{y}) = \int N\left(\tilde{\mathbf{y}} | \boldsymbol{\mu}_{\tilde{y}|y}, \sigma^2 \mathbf{V}_{\tilde{y}|y}\right) p(\boldsymbol{\beta}, \sigma^2 | \mathbf{y}) d\boldsymbol{\beta} d\sigma^2.$$

- For each j = 1, 2, ..., N do the following:
 - 1. Draw $\{\beta_{(j)}, \sigma_{(j)}^2\} \sim p(\beta, \sigma^2 \mid \mathbf{y})$
 - 2. Compute $\mu_{\tilde{y}|y}$ using $\beta_{(j)}$ and draw $\tilde{\mathbf{y}}_{(j)} \sim N(\mu_{\tilde{y}|y}, \sigma_{(j)}^2 \mathbf{V}_{\tilde{y}})$

Application to Bayesian Geostatistics

Consider the spatial regression model

$$y(s_i) = \mathbf{x}^{\top}(\mathbf{s}_i)\beta + w(\mathbf{s}_i) + \epsilon(\mathbf{s}_i),$$

where $w(\mathbf{s}_i)$'s are spatial random effects and $\epsilon(\mathbf{s}_i)$'s are unstructured errors ("white noise").

- $\mathbf{w} = (w(\mathbf{s}_1), w(\mathbf{s}_2), \dots, w(\mathbf{s}_n))^{\top} \sim N(\mathbf{0}, \sigma^2 \mathbf{R}(\phi))$
- $\epsilon = (\epsilon(\mathbf{s}_1), \epsilon(\mathbf{s}_2), \dots, \epsilon(\mathbf{s}_n))^{\top} \sim N(\mathbf{0}, \tau^2 \mathbf{I}_n)$
- Integrating out random effects leads to a Bayesian model:

$$\mathit{IG}(\sigma^2 \,|\, a,b) \times \mathit{N}(\beta \,|\, \mu_{\beta},\sigma^2 \mathbf{V}_{\beta}) \times \mathit{N}(\mathbf{y} \,|\, \mathbf{X}\beta,\sigma^2 \mathbf{V}_y)$$
 where $\mathbf{V}_y = \mathbf{R}(\phi) + \alpha \mathbf{I}_n$ and $\alpha = \tau^2/\sigma^2$.

- Fixing ϕ and α (e.g., from variogram or other EDA) yields a conjugate Bayesian model.
- Exact posterior sampling is easily achieved as before!

Inference on spatial random effects

Rewrite the model in terms of w as:

$$IG(\sigma^2 \mid a, b) \times N(\beta \mid \mu_{\beta}, \sigma^2 \mathbf{V}_{\beta}) \times N(\mathbf{w} \mid \mathbf{0}, \sigma^2 \mathbf{R}(\phi)) \times N(\mathbf{y} \mid \mathbf{X}\beta + \mathbf{w}, \tau^2 \mathbf{I}_n) .$$

Posterior distribution of spatial random effects w:

$$p(\mathbf{w} \,|\, \mathbf{y}) = \int \textit{N}(\mathbf{w} \,|\, \mathbf{Mm}, \sigma^2 \mathbf{M}) \times p(\beta, \sigma^2 \,|\, \mathbf{y}) \mathrm{d}\beta \mathrm{d}\sigma^2 \;,$$
 where $\mathbf{m} = (1/\alpha)(\mathbf{y} - \mathbf{X}\beta)$ and $\mathbf{M}^{-1} = \mathbf{R}^{-1}(\phi) + (1/\alpha)\mathbf{I}_p$.

- For each j = 1, 2, ..., N do the following:
 - 1. Draw $\{oldsymbol{eta}_{(j)}, \sigma_{(j)}^2\} \sim p(oldsymbol{eta}, \sigma^2 \,|\, \mathbf{y})$
 - 2. Compute **m** from $\beta_{(j)}$ and draw $\mathbf{w}_{(j)} \sim \mathcal{N}(\mathbf{Mm}, \sigma_{(j)}^2 \mathbf{M})$

Inference on the process

• Posterior distribution of $w(\mathbf{s}_0)$ at new location \mathbf{s}_0 :

$$p(w(\mathbf{s}_0) \,|\, \mathbf{y}) = \int N(w(\mathbf{s}_0) \,|\, \mu_{w(\mathbf{s}_0)|w}, \sigma^2_{w(\mathbf{s}_0)|w}) \times p(\sigma^2, \mathbf{w} \,|\, \mathbf{y}) \mathrm{d}\sigma^2 \mathrm{d}\mathbf{w} \;,$$

where

$$\begin{split} &\mu_{w(\mathbf{s}_0)|w} = \mathbf{r}^\top(\mathbf{s}_0;\phi)\mathbf{R}^{-1}(\phi)\mathbf{w}\;;\\ &\sigma^2_{w(\mathbf{s}_0)|w} = \sigma^2\{1-\mathbf{r}^\top(\mathbf{s}_0;\phi)\mathbf{R}^{-1}(\phi)\mathbf{r}(\mathbf{s}_0,\phi)\} \end{split}$$

- For each j = 1, 2, ..., N do the following:
 - 1. Compute $\mu_{w(\mathbf{s}_0)|w}$ and $\sigma^2_{w(\mathbf{s}_0)|w}$ from $\mathbf{w}_{(j)}$ and $\sigma^2_{(j)}$.
 - 2. Draw $w_{(j)}(\mathbf{s}_0) \sim N(\mu_{w(\mathbf{s}_0)|w}, \sigma^2_{w(\mathbf{s}_0)|w})$.

Bayesian "kriging" or prediction

■ Posterior predictive distribution at new location \mathbf{s}_0 is $p(y(\mathbf{s}_0) | \mathbf{y})$:

$$\int N(y(\mathbf{s}_0) | \mathbf{x}^{\top}(s_0)\beta + w(\mathbf{s}_0), \alpha\sigma^2) \times p(\beta, \sigma^2, \mathbf{w} | \mathbf{y}) d\beta d\sigma^2 d\mathbf{w},$$

- For each j = 1, 2, ..., N do the following:
 - 1. Draw $y_{(j)}(\mathbf{s}_0) \sim N(\mathbf{x}^{\top}(\mathbf{s}_0)\beta_{(j)} + w_{(j)}(\mathbf{s}_0), \alpha\sigma_{(j)}^2)$.

Non-conjugate models: The Gibbs Sampler

- Let $\theta = (\theta_1, \dots, \theta_p)$ be the parameters in our model.
- Initialize with starting values $\theta^{(0)} = (\theta_1^{(0)}, \dots, \theta_p^{(0)})$
- For j = 1, ..., N, update successively using the *full conditional* distributions:

$$\begin{split} & \theta_1^{(j)} \sim p(\theta_1^{(j)} \,|\, \theta_2^{(j-1)}, \dots, \theta_p^{(j-1)}, \mathbf{y}) \\ & \theta_2^{(j)} \sim p(\theta_2 \,|\, \theta_1^{(j)}, \theta_3^{(j-1)}, \dots, \theta_p^{(j-1)}, \mathbf{y}) \\ & \vdots \\ & \text{(the generic } k^{th} \text{ element)} \\ & \theta_k^{(j)} \sim p(\theta_k | \theta_1^{(j)}, \dots, \theta_{k-1}^{(j)}, \theta_{k+1}^{(j-1)}, \dots, \theta_p^{(j-1)}, \mathbf{y}) \\ & \vdots \\ & \theta_p^{(j)} \sim p(\theta_p \,|\, \theta_1^{(j)}, \dots, \theta_{p-1}^{(j)}, \mathbf{y}) \end{split}$$

- In principle, the Gibbs sampler will work for extremely complex hierarchical models. The only issue is sampling from the full conditionals. They may not be amenable to easy sampling – when these are not in closed form. A more general and extremely powerful - and often easier to code - algorithm is the Metropolis-Hastings (MH) algorithm.
- This algorithm also constructs a Markov chain, but does not necessarily care about full conditionals.
- Popular approach: Embed Metropolis steps within Gibbs to draw from full conditionals that are not accessible to directly generate from.

The Metropolis-Hastings Algorithm

- The Metropolis-Hastings algorithm: Start with a initial value for $\theta = \theta^{(0)}$. Select a *candidate* or *proposal* distribution from which to propose a value of θ at the j-th iteration: $\theta^{(j)} \sim q(\theta^{(j-1)}, \nu)$. For example, $q(\theta^{(j-1)}, \nu) = N(\theta^{(j-1)}, \nu)$ with ν fixed.
- Compute

$$r = \frac{p(\theta^* \mid y)q(\theta^{(j-1)} \mid \theta^*, \nu)}{p(\theta^{(j-1)} \mid y)q(\theta^* \mid \theta^{(j-1)} \nu)}$$

- If $r \ge 1$ then set $\theta^{(j)} = \theta^*$. If $r \le 1$ then draw $U \sim (0,1)$. If $U \le r$ then $\theta^{(j)} = \theta^*$. Otherwise, $\theta^{(j)} = \theta^{(j-1)}$.
- Repeat for $j=1,\ldots N$. This yields $\theta^{(1)},\ldots,\theta^{(N)}$, which, after a burn-in period, will be samples from the true posterior distribution. It is important to monitor the acceptance ratio r of the sampler through the iterations. Rough recommendations: for vector updates $r\approx 20\%$., for scalar updates $r\approx 40\%$. This can be controlled by "tuning" ν .
- Popular approach: Embed Metropolis steps within Gibbs to draw from full conditionals that are not accessible to directly generate from.

- Example: For the linear model, our parameters are (β, σ^2) . We write $\theta = (\beta, \log(\sigma^2))$ and, at the j-th iteration, propose $\theta^* \sim N(\theta^{(j-1)}, \Sigma)$. The log transformation on σ^2 ensures that all components of θ have support on the entire real line and can have meaningful proposed values from the multivariate normal. But we need to transform our prior to $p(\beta, \log(\sigma^2))$.
- Let $z = \log(\sigma^2)$ and assume $p(\beta, z) = p(\beta)p(z)$. Let us derive p(z). REMEMBER: we need to adjust for the jacobian. Then $p(z) = p(\sigma^2)|d\sigma^2/dz| = p(e^z)e^z$. The jacobian here is $e^z = \sigma^2$.
- Let $p(\beta) = 1$ and an $p(\sigma^2) = IG(\sigma^2 \mid a, b)$. Then log-posterior is:

$$-(a+n/2+1)z+z-\frac{1}{e^{z}}\{b+\frac{1}{2}(Y-X\beta)^{T}(Y-X\beta)\}.$$

- A symmetric proposal distribution, say $q(\theta^*|\theta^{(j-1)}, \Sigma) = N(\theta^{(j-1)}, \Sigma)$, cancels out in r. In practice it is better to compute $\log(r)$: $\log(r) = \log(p(\theta^*|y) \log(p(\theta^{(j-1)}|y))$. For the proposal, $N(\theta^{(j-1)}, \Sigma)$, Σ is a $d \times d$ variance-covariance matrix, and $d = \dim(\theta) = p + 1$.
- If $\log r \ge 0$ then set $\theta^{(j)} = \theta^*$. If $\log r \le 0$ then draw $U \sim (0,1)$. If $U \le r$ (or $\log U \le \log r$) then $\theta^{(j)} = \theta^*$. Otherwise, $\theta^{(j)} = \theta^{(j-1)}$.
- Repeat the above procedure for $j=1,\ldots N$ to obtain samples $\theta^{(1)},\ldots,\theta^{(N)}$.