Bayesian Linear Models

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- Ingredients of a linear model include an $n \times 1$ response vector $\mathbf{y} = (y_1, \ldots, y_n)^T$ and an $n \times p$ design matrix (e.g. including regressors) $X = [\mathbf{x}_1, \ldots, \mathbf{x}_p]$, assumed to have been observed without error. The linear model:

$$\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\epsilon};\ \boldsymbol{\epsilon} \sim N(\mathbf{0}, \sigma^2 I)$$

- The linear model is the most fundamental of all serious statistical models encompassing:
  - ANOVA: $\mathbf{y}$ is continuous, $\mathbf{x}_i$'s are categorical
  - REGRESSION: $\mathbf{y}$ is continuous, $\mathbf{x}_i$'s are continuous
  - ANCOVA: $\mathbf{y}$ is continuous, some $\mathbf{x}_i$'s are continuous, some categorical.
- Unknown parameters include the regression parameters $\boldsymbol{\beta}$ and the variance σ^2. We assume X is observed without error and all inference is conditional on X.

- The classical unbiased estimates of the regression parameter $\boldsymbol{\beta}$ and σ^2 are

$$\hat{\boldsymbol{\beta}} = (X^TX)^{-1}X^T\mathbf{y};$$
$$\hat{\sigma}^2 = \frac{1}{n-p}(\mathbf{y} - X\hat{\boldsymbol{\beta}})^T(\mathbf{y} - X\hat{\boldsymbol{\beta}}).$$

- The above estimate of $\boldsymbol{\beta}$ is also a least-squares estimate. The *predicted* value of $\mathbf{y}$ is given by

$$\hat{\mathbf{y}} = X\hat{\boldsymbol{\beta}} = P_X\mathbf{y} \text{ where } P_X = X(X^TX)^{-1}X^T.$$

- P_X is called the *projector* of X. It projects any vector to the space spanned by the columns of X.
- The model residual is estimated as:

$$\hat{\mathbf{e}} = (\mathbf{y} - X\hat{\boldsymbol{\beta}})^T(\mathbf{y} - X\hat{\boldsymbol{\beta}}) = \mathbf{y}^T(I - P_X)\mathbf{y}.$$

- For Bayesian analysis, we will need to specify priors for the unknown regression parameters $\boldsymbol{\beta}$ and the variance σ^2.
- Consider independent flat priors on $\boldsymbol{\beta}$ and $\log\sigma^2$:

$$p(\boldsymbol{\beta}) \propto 1;\ p(\log(\sigma^2)) \propto 1 \text{ or equivalently } p(\boldsymbol{\beta}, \sigma^2) \propto \frac{1}{\sigma^2}.$$

- None of the above two "distributions" are valid probabilities (they do not integrate to any finite number). So why is it that we are even discussing them?
- It turns out that even if the priors are *improper* (that's what we call them), as long as the resulting posterior distributions are valid we can still conduct legitimate statistical inference on them.

- With a flat prior on $\boldsymbol{\beta}$ we obtain, after some algebra, the *conditional posterior* distribution:

$$p(\boldsymbol{\beta}\,|\,\sigma^2, \mathbf{y}) = N(\boldsymbol{\beta}\,|\,(X^TX)^{-1}X^T\mathbf{y},\ \sigma^2(X^TX)^{-1}).$$

- The conditional posterior distribution of $\boldsymbol{\beta}$ would have been the desired posterior distribution had σ^2 been known.
- Since that is not the case, we need to obtain the *marginal posterior* distribution by integrating out σ^2 as:

$$p(\boldsymbol{\beta} \mid \mathbf{y}) = \int p(\boldsymbol{\beta} \mid \sigma^2, \mathbf{y})p(\sigma^2 \mid \mathbf{y})d\sigma^2$$

- Can we solve this integration using composition sampling? YES: if we can generate samples from $p(\sigma^2\,|\,\mathbf{y})$!

- So, we need to find the marginal posterior distribution of σ^2. With the choice of the flat prior we obtain:

$$p(\sigma^2\,|\,\mathbf{y}) \propto \frac{1}{(\sigma^2)^{(n-p)/2+1}}\exp\left(-\frac{(n-p)s^2}{2\sigma^2}\right)$$
$$= IG\left(\sigma^2\,|\,\frac{n-p}{2}, \frac{(n-p)s^2}{2}\right),$$

where $s^2 = \hat{\sigma}^2 = \frac{1}{n-p}\mathbf{y}^T(I - P_X)\mathbf{y}$.

- This is known as an *inverted Gamma* distribution (also called a *scaled chi-square* distribution) $IG(\sigma^2\,|\,(n-p)/2, (n-p)s^2/2)$.
- In other words: $[(n-p)s^2/\sigma^2\,|\,\mathbf{y}] \sim \chi^2_{n-p}$ (with $n-p$ degrees of freedom). A striking similarity with the classical result: The distribution of $\hat{\sigma}^2$ is also characterized as $(n-p)s^2/\sigma^2$ following a chi-square distribution.

- Now we are ready to carry out compositting sampling from $p(\boldsymbol{\beta}, \sigma^2 \,|\, \mathbf{y})$ as follows:
  - Draw M samples from $p(\sigma^2 \,|\, \mathbf{y})$:
  $$\sigma^{2(j)} \sim IG\left(\frac{n-p}{2}, \frac{(n-p)s^2}{2}(n-p)\right),\ j = 1, \ldots M$$
  - For $j = 1, \ldots, M$, draw from $p(\boldsymbol{\beta} \,|\, \sigma^{2(j)}, \mathbf{y})$:
  $$\boldsymbol{\beta}^{(j)} \sim N\left((X^T X)^{-1} X^T \mathbf{y},\ \sigma^{2(j)}(X^T X)^{-1}\right)$$
- The resulting samples $\{\boldsymbol{\beta}^{(j)}, \sigma^{2(j)}\}_{j=1}^M$ represent M samples from $p(\boldsymbol{\beta}, \sigma^2 \,|\, \mathbf{y})$.
- $\{\boldsymbol{\beta}^{(j)}\}_{j=1}^M$ are samples from the marginal posterior distribution $p(\boldsymbol{\beta} \,|\, \mathbf{y})$. This is a *multivariate t* density:

$$p(\boldsymbol{\beta} \,|\, \mathbf{y}) = \frac{\Gamma(n/2)}{(\pi(n-p))^{p/2}\Gamma((n-p)/2)|s^2(X^T X)^{-1}|}\left[1 + \frac{(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})^T (X^T X)(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})}{(n-p)s^2}\right]^{-n/2}.$$

- The marginal distribution of each individual regression parameter β_j is a non-central univariate t_{n-p} distribution. In fact,
$$\frac{\beta_j - \hat{\beta}_j}{s\sqrt{(X^T X)^{-1}_{jj}}} \sim t_{n-p}.$$
The 95% credible intervals for each β_j are constructed from the quantiles of the t-distribution. The credible intervals exactly coicide with the 95% classical confidence intervals, but the intepretation is direct: the probability of β_j falling in that interval, given the observed data, is 0.95.
- Note: an intercept only linear model reduces to the simple univariate $N(\bar{y} \,|\, \mu, \sigma^2/n)$ likelihood, for which the marginal posterior of μ is:
$$\frac{\mu - \bar{y}}{s/\sqrt{n}} \sim t_{n-1}.$$

- Suppose we have observed the new predictors $\tilde{X}$, and we wish to predict the outcome $\tilde{\mathbf{y}}$. We specify $p(\tilde{\mathbf{y}}, \mathbf{y} \,|\, \boldsymbol{\theta})$ to be a normal distribution:
$$\begin{pmatrix} \mathbf{y} \\ \tilde{\mathbf{y}} \end{pmatrix} \sim N\left(\begin{bmatrix} X \\ \tilde{X} \end{bmatrix} \boldsymbol{\beta}, \sigma^2 I\right)$$
- Note $p(\tilde{\mathbf{y}} \,|\, \mathbf{y}, \boldsymbol{\beta}, \sigma^2) = p(\tilde{\mathbf{y}} \,|\, \boldsymbol{\beta}, \sigma^2) = N(\tilde{\mathbf{y}} \,|\, \tilde{X}\boldsymbol{\beta}, \sigma^2 I)$.
- The *posterior predictive* distribution:
$$\begin{aligned} p(\tilde{\mathbf{y}} \,|\, \mathbf{y}) &= \int p(\tilde{\mathbf{y}} \,|\, \mathbf{y}, \boldsymbol{\beta}, \sigma^2) p(\boldsymbol{\beta},\ \sigma^2 \,|\, \mathbf{y}) d\boldsymbol{\beta} d\sigma^2 \\ &= \int p(\tilde{\mathbf{y}} \,|\, \boldsymbol{\beta}, \sigma^2) p(\boldsymbol{\beta},\ \sigma^2 \,|\, \mathbf{y}) d\boldsymbol{\beta} d\sigma^2. \end{aligned}$$
- By now we are comfortable evaluating such integrals:
  - First obtain: $(\boldsymbol{\beta}^{(j)}, \sigma^{2(j)}) \sim p(\boldsymbol{\beta}, \sigma^2 \,|\, \mathbf{y})$, $j = 1, \ldots, M$
  - Next draw: $\tilde{\mathbf{y}}^{(j)} \sim N(\tilde{X}\boldsymbol{\beta}^{(j)}, \sigma^{2(j)} I)$.

- Suppose that $\boldsymbol{\theta} = (\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ and we seek the posterior distribution $p(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2 \,|\, \mathbf{y})$.
- For many interesting hierarchical models, we have access to *full conditional distributions* $p(\boldsymbol{\theta}_1 \,|\, \boldsymbol{\theta}_2, \mathbf{y})$ and $p(\boldsymbol{\theta}_1 \,|\, \boldsymbol{\theta}_2, \mathbf{y})$.
- The *Gibbs sampler* proposes the following sampling scheme. Set starting values $\boldsymbol{\theta}^{(0)} = (\boldsymbol{\theta}_1^{(0)}, \boldsymbol{\theta}_2^{(0)})$ For $j = 1, \ldots, M$
  - Draw $\boldsymbol{\theta}_1^{(j)} \sim p(\boldsymbol{\theta}_1 \,|\, \boldsymbol{\theta}_2^{(j-1)}, \mathbf{y})$
  - Draw $\boldsymbol{\theta}_2^{(j)} \sim p(\boldsymbol{\theta}_2 \,|\, \boldsymbol{\theta}_1^{(j)}, \mathbf{y})$
- This constructs a *Markov Chain* and, after an initial "burn-in" period when the chains are trying to find their way, the above algorithm guarantees that $\{\boldsymbol{\theta}_1^{(j)}, \boldsymbol{\theta}_2^{(j)}\}_{j=M_0+1}^M$ will be samples from $p(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2 \,|\, \mathbf{y})$, where M_0 is the burn-in period..

- More generally, if $\boldsymbol{\theta} = (\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_p)$ are the parameters in our model, we provide a set of initial values $\boldsymbol{\theta}^{(0)} = (\boldsymbol{\theta}_1^{(0)}, \ldots, \boldsymbol{\theta}_p^{(0)})$ and then performs the j-th iteration, say for $j = 1, \ldots, M$, by updating successively from the *full conditional* distributions:

$$\begin{aligned} &\boldsymbol{\theta}_1^{(j)} \sim p(\boldsymbol{\theta}_1^{(j)} \,|\, \boldsymbol{\theta}_2^{(j-1)}, \ldots, \boldsymbol{\theta}_p^{(j-1)}, \mathbf{y}) \\ &\boldsymbol{\theta}_2^{(j)} \sim p(\boldsymbol{\theta}_2 \,|\, \boldsymbol{\theta}_1^{(j)}, \boldsymbol{\theta}_3^{(j)}, \ldots, \boldsymbol{\theta}_p^{(j-1)}, \mathbf{y}) \\ &\ldots \\ &\text{(the generic } k^{th} \text{ element)} \\ &\boldsymbol{\theta}_k^{(j)} \sim p(\boldsymbol{\theta}_k | \boldsymbol{\theta}_1^{(j)}, \ldots, \boldsymbol{\theta}_{k-1}^{(j)}, \boldsymbol{\theta}_{k+1}^{(j)}, \ldots, \boldsymbol{\theta}_p^{(j-1)}, \mathbf{y}) \\ &\ldots \\ &\boldsymbol{\theta}_p^{(j)} \sim p(\boldsymbol{\theta}_p \,|\, \boldsymbol{\theta}_1^{(j)}, \ldots, \boldsymbol{\theta}_{p-1}^{(j)}, \mathbf{y}) \end{aligned}$$

- Example: Consider the linear model. Suppose we set $p(\sigma^2) = IG(\sigma^2 \,|\, a, b)$ and $p(\boldsymbol{\beta}) \propto 1$.
- The full conditional distributions are:
$$p(\boldsymbol{\beta} \,|\, \mathbf{y}, \sigma^2) = N(\boldsymbol{\beta} \,|\, (X^T X)^{-1} X^T \mathbf{y}, \sigma^2 (X^T X)^{-1})$$
$$p(\sigma^2 \,|\, \mathbf{y}, \boldsymbol{\beta}) = IG\left(\sigma^2 \,|\, a + n/2, b + \frac{1}{2}(\mathbf{y} - X\boldsymbol{\beta})^T(\mathbf{y} - X\boldsymbol{\beta})\right).$$
- Thus, the Gibbs sampler will initialize $(\boldsymbol{\beta}^{(0)}, \sigma^{2(0)})$ and draw, for $j = 1, \ldots, M$:
  - Draw $\boldsymbol{\beta}^{(j)} \sim N((X^T X)^{-1} X^T \mathbf{y}, \sigma^{2(j-1)}(X^T X)^{-1})$
  - Draw $\sigma^{2(j)} \sim IG\left(a + n/2, b + \frac{1}{2}(\mathbf{y} - X\boldsymbol{\beta}^{(j)})^T(\mathbf{y} - X\boldsymbol{\beta}^{(j)})\right)$

- 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.

- The Metropolis-Hastings algorithm: Start with a initial value for $\boldsymbol{\theta} = \boldsymbol{\theta}^{(0)}$. Select a *candidate* or *proposal* distribution from which to propose a value of $\boldsymbol{\theta}$ at the j-th iteration: $\boldsymbol{\theta}^{(j)} \sim q(\boldsymbol{\theta}^{(j-1)}, \nu)$. For example, $q(\boldsymbol{\theta}^{(j-1)}, \nu) = N(\boldsymbol{\theta}^{(j-1)}, \nu)$ with ν fixed.
- Compute
$$r = \frac{p(\boldsymbol{\theta}^* \mid \mathbf{y}) q(\boldsymbol{\theta}^{(j-1)} \mid \boldsymbol{\theta}^*, \nu)}{p(\boldsymbol{\theta}^{(j-1)} \mid \mathbf{y}) q(\boldsymbol{\theta}^* \mid \boldsymbol{\theta}^{(j-1)} \nu)}$$
- If $r \geq 1$ then set $\boldsymbol{\theta}^{(j)} = \boldsymbol{\theta}^*$. If $r \leq 1$ then draw $U \sim (0, 1)$. If $U \leq r$ then $\boldsymbol{\theta}^{(j)} = \boldsymbol{\theta}^*$. Otherwise, $\boldsymbol{\theta}^{(j)} = \boldsymbol{\theta}^{(j-1)}$.
- Repeat for $j = 1, \ldots M$. This yields $\boldsymbol{\theta}^{(1)}, \ldots, \boldsymbol{\theta}^{(M)}$, 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 $(\boldsymbol{\beta}, \sigma^2)$. We write $\boldsymbol{\theta} = (\boldsymbol{\beta}, \log(\sigma^2))$ and, at the j-th iteration, propose $\boldsymbol{\theta}^* \sim N(\theta^{(j-1)}, \Sigma)$. The log transformation on σ^2 ensures that all components of $\boldsymbol{\theta}$ 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 $p(\boldsymbol{\beta}, \log(\sigma^2))$.
- Let $z = \log(\sigma^2)$ and assume $p(\boldsymbol{\beta}, z) = p(\boldsymbol{\beta})p(z)$. 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 $p(\boldsymbol{\beta}) = 1$ and an $p(\sigma^2) = IG(\sigma^2 \mid a, b)$. Then log-posterior is:
$$-(a + n/2 + 1)z + z - \frac{1}{e^z}\{b + \frac{1}{2}(Y - X\boldsymbol{\beta})^T(Y - X\boldsymbol{\beta})\}.$$
- A symmetric proposal distribution, say $q(\boldsymbol{\theta}^* | \boldsymbol{\theta}^{(j-1)}, \Sigma) = N(\boldsymbol{\theta}^{(j-1)}, \Sigma)$, cancels out in r. In practice it is better to compute $\log(r)$: $\log(r) = \log(p(\boldsymbol{\theta}^* \mid \mathbf{y}) - \log(p(\boldsymbol{\theta}^{(j-1)} \mid \mathbf{y}))$. For the proposal, $N(\boldsymbol{\theta}^{(j-1)}, \Sigma)$, Σ is a $d \times d$ variance-covariance matrix, and $d = \dim(\boldsymbol{\theta}) = p + 1$.
- If $\log r \geq 0$ then set $\boldsymbol{\theta}^{(j)} = \boldsymbol{\theta}^*$. If $\log r \leq 0$ then draw $U \sim (0, 1)$. If $U \leq r$ (or $\log U \leq \log r$) then $\boldsymbol{\theta}^{(j)} = \boldsymbol{\theta}^*$. Otherwise, $\boldsymbol{\theta}^{(j)} = \boldsymbol{\theta}^{(j-1)}$.
- Repeat the above procedure for $j = 1, \ldots M$ to obtain samples $\boldsymbol{\theta}^{(1)}, \ldots, \boldsymbol{\theta}^{(M)}$.