Bayesian Linear Regression

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Linear regression models: a Bayesian perspective

Typically, we have a set of units or experimental subjects

\( i = 1, 2, \ldots, n \).

For each of these units we have measured an outcome \( y_i \) and a set of explanatory variables \( x'_i = (1, x_{i1}, x_{i2}, \ldots, x_{ip}) \).

The first element of \( x'_i \) 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:

\[
\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}, \quad \mathbf{X} = \begin{pmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1p} \\ 1 & x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{np} \end{pmatrix} = \begin{pmatrix} x'_1 \\ x'_2 \\ \vdots \\ x'_n \end{pmatrix}.
\]

The Bayesian or hierarchical linear model is given by:

\[
y_i \mid \mu_i, \sigma^2, \mathbf{X} \sim N(\mu_i, \sigma^2); \quad i = 1, 2, \ldots, n;
\mu_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} = \mathbf{x}'_i \beta; \quad \beta = (\beta_0, \beta_1, \ldots, \beta_p);
\beta, \sigma^2 \mid \mathbf{X} \sim p(\beta, \sigma^2 \mid \mathbf{X}).
\]

Unknown parameters include the regression parameters and the variance, i.e. \( \theta = \{\beta, \sigma^2\} \).

\( p(\beta, \sigma^2 \mid \mathbf{X}) \equiv p(\theta \mid \mathbf{X}) \) is the joint prior on the parameters.

We assume \( \mathbf{X} \) is observed without error and all inference is conditional on \( \mathbf{X} \).

We suppress dependence on \( \mathbf{X} \) in subsequent notation.

Linear regression is, perhaps, the most widely used statistical modelling tool.

It addresses the following question: How does a quantity of primary interest, \( y_i \), vary as (depend upon) another quantity, or set of quantities, \( x \)?

The quantity \( y_i \) 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 \( y_i \), given \( \mathbf{x} \), parametrized as \( p(y_i \mid \theta, \mathbf{x}) \).

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.

Specifying \( p(\beta, \sigma^2) \) completes the hierarchical model.

All inference proceeds from \( p(\beta, \sigma^2 \mid \mathbf{y}) \)

With no prior information, we specify

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

The above is NOT a probability density (they do not integrate to any finite number). So why is it that we are even discussing them?

Even if the priors are improper, as long as the resulting posterior distributions are valid we can still conduct legitimate statistical inference on them.
Bayesian regression with flat priors

Computing the posterior distribution

- Strategy: Factor the joint posterior distribution for \( \beta \) and \( \sigma^2 \) as:
  \[ p(\beta, \sigma^2 | y) = p(\beta | \sigma^2, y) \times p(\sigma^2 | y). \]
- The conditional posterior distribution of \( \beta \), given \( \sigma^2 \):
  \[ \beta | \sigma^2, y \sim N(\tilde{\beta}, \sigma^2 V_{\beta}), \]
  where, using some algebra, one finds
  \[ \tilde{\beta} = (X'X)^{-1}X'y \quad \text{and} \quad V_{\beta} = (X'X)^{-1}. \]

Algorithm for sampling from the posterior distribution

- We draw samples from \( p(\beta, \sigma^2 | y) \) by executing the following steps:
  - Step 1: Compute \( \tilde{\beta} \) and \( V_{\beta} \).
  - Step 2: Compute \( s^2 \).
  - Step 3: Draw \( M \) samples from \( p(\sigma^2 | y) \):
    \[ \sigma^2(j) \sim IG\left(\frac{n-k}{2}, \frac{(n-k)s^2}{2}\right), \quad j = 1, \ldots, M \]
  - Step 4: For \( j = 1, \ldots, M \), draw \( \beta^{(j)} \) from \( p(\beta | \sigma^2(j), y) \):
    \[ \beta^{(j)} \sim N\left(\tilde{\beta}, \sigma^2(j)V_{\beta}\right). \]

Bayesian predictions from the linear model

- Suppose we have observed the new predictors \( \tilde{X} \), and we wish to predict the outcome \( y \).
  - If \( \beta \) and \( \sigma^2 \) were known exactly, the random vector \( \tilde{y} \) would follow \( N(\tilde{X}\beta, \sigma^2 I) \).
  - But we do not know model parameters, which contribute to the uncertainty in predictions.
  - Predictions are carried out by sampling from the posterior predictive distribution, \( p(\tilde{y} | y) \):
    - Draw \( (\beta^{(1)}, \sigma^2(1)) \sim p(\beta, \sigma^2 | y) \), \( j = 1, 2, \ldots, M \)
    - Draw \( \tilde{y}^{(j)} \sim N(\tilde{X}\beta^{(j)}, \sigma^2(j)I), \quad j = 1, 2, \ldots, M \).
    - The marginal posterior distribution of \( \sigma^2 \): Let \( k = (p + 1) \) be the number of columns of \( X \).
      \[ \sigma^2 | y \sim IG\left(\frac{n-k}{2}, \frac{(n-k)s^2}{2}\right), \]
      where
      \[ s^2 = \frac{1}{n-k}(y - X\tilde{\beta})'(y - X\tilde{\beta}) \]
      is the classical unbiased estimate of \( \sigma^2 \) in the linear regression model.
    - The marginal posterior distribution \( p(\beta | y) \), averaging over \( \sigma^2 \), is multivariate \( t \) with \( n - k \) degrees of freedom. But we rarely use this fact in practice.
    - Instead, we sample from the posterior distribution.
Incorporating prior information

\[ y_i | \mu_i, \sigma^2 \overset{ind}{\sim} N(\mu_i, \sigma^2); \quad i = 1, 2, \ldots, n; \]
\[ \mu_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} = \mathbf{x}_i^\top \beta; \quad \beta = (\beta_0, \beta_1, \ldots, \beta_p); \]
\[ \beta | \sigma^2 \overset{\text{indep}}{\sim} N(\mu_0, \sigma^2 R); \quad \sigma^2 \sim IG(a_\sigma, b_\sigma), \]

where \( R \) is a fixed correlation matrix. Alternatively,

\[ y_i | \mu_i, \sigma^2 \overset{\text{indep}}{\sim} N(\mu_i, \sigma^2); \quad i = 1, 2, \ldots, n; \]
\[ \mu_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} = \mathbf{x}_i^\top \beta; \quad \beta = (\beta_0, \beta_1, \ldots, \beta_p); \]
\[ \beta | \Sigma_\beta \sim N(\mu_0, \Sigma_\beta) ; \quad \Sigma_\beta \sim IW(\nu, S); \quad \sigma^2 \sim IG(a_\sigma, b_\sigma), \]

where \( \Sigma_\beta \) is a random covariance matrix.

The Gibbs sampler

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.