Bayesian Linear Regression

Felipe José Bravo Márquez

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Bayesian Linear Regression

- In this class, which is mostly based on chapter 4 of [McElreath, 2020], we are going to revisit the linear regression model from a Bayesian point of view.
- The idea is the same: to model the relationship of a numerical dependent variable $\mathbf{y}$ with n independent variables $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ from a dataset d.
- The response vaiable $\mathbf{y}$ is again modeled with a Gaussian distribution: $y_i \sim N(\mu_i, \sigma^2)$.
- We also mantain the assumption that each attribute has a linear relationship to the mean of the outcome.

$$\mu_i = \beta_0 + \beta_1 x_i + \ldots \beta_n x_n$$

- However, we are not going to use least squares or maximum likelihood to obtain point estimates of the parameters.
- Instead, we are going to estimate the joint posterior distribution of all the parameters of the model:

$$f(\theta|d) = f(\beta_0, \beta_1, \ldots, \beta_n, \sigma|d)$$

Bayesian Linear Models

- The Bayesian linear regresion is more flexible than least squares as it allows incorporating prior information.
- It also allows to interpret the uncertainty of the model in a clearer way.
- Notice that the the parameters of the model are $\beta_0, \beta_1, \ldots, \beta_b$ and σ but not μ_i.
- This is because μ_i it is determined deterministically from the linear model's coefficients.
- In order to build our posterior we need to define a likelihood function:

$$f(d|\beta_0, \beta_1, \cdots, \beta_n, \sigma) = \prod_{i=1}^{m} f(d_i|\beta_0, \beta_1, \cdots, \beta_n, \sigma)$$

- Where d_i corresponds to each data point in the dataset containing values for y and $x_1, \ldots, x_n$ (IID assumption).
- The likelihood of each point is modeled with a Gaussian distribution:

$$f(d_i|\beta_0, \beta_1, \cdots, \beta_n, \sigma) = N(\mu_i, \sigma^2)$$

Bayesian Linear Models

- Now we need a joint prior density:

$$f(\theta) = f(\beta_0, \beta_1, \ldots, \beta_n, \sigma)$$

- And the posterior gets specified as follows:

$$f(\theta|d) = \frac{\prod_{i=1}^{m} f(d_i|\beta_0, \beta_1, \cdots, \beta_n, \sigma) * f(\beta_0, \beta_1, \ldots, \beta_n, \sigma)}{f(d)}$$

- The evidence is expressed by a multiple integral:

$$f(d) = \int \int \cdots \int \prod_{i=1}^{m} f(d_i|\beta_0, \beta_1, \cdots, \beta_n, \sigma) * f(\beta_0, \beta_1, \ldots, \beta_n, \sigma) d\beta_0 d\beta_1 \cdots d\beta_n d\sigma$$

- In most cases, the priors are specified independently for each parameter, which is equivalent to assuming:

$$f(\beta_0, \beta_1, \cdots, \beta_b, \sigma) = f(\beta_0) * f(\beta_1) * \cdots * f(\beta_n) * f(\sigma).$$

A model of height revisited

- To understand this more concretely, we will rebuild the linear model relating the height and weight of the !Kung San people using a Bayesian approach.
- We will refer to each person's height and weight as y_i and x_i respectively.
- Our probabilistic model specifying all components of a Bayesian model is defined as follows:

$$
\begin{array}{lr}
y_i \sim N(\mu_i, \sigma) & \text{[likelihood]} \\
\mu_i = \beta_0 + \beta_1 x_i & \text{[linear model]} \\
\beta_0 \sim N(100, 100) & [\beta_0 \text{ prior}] \\
\beta_1 \sim N(0, 1) & [\beta_1 \text{ prior}] \\
\sigma \sim \text{Uniform}(0, 50) & [\sigma \text{ prior}]
\end{array}
$$

- Parameters β_0 and β_1 are the intercept and the slope of our linear model.
- The parameter σ is the standard deviation of all the heights.
- Note that we are setting the same σ for all observations, which is equivalent to the Homoscedasticity property of the standard linear regression.

A model of height revisited

- Our priors were set independently for each parameter which implies that the joint prior density $f(\beta_0, \beta_1, \sigma)$ can be expressed as $f(\beta_0) * f(\beta_1) * f(\sigma)$.
- It should be kept in mind that the choice of priors is subjective and should be evaluated accordingly.
- Let's try to justify our choice a bit:

  1. The Gaussian prior for β_0 (intercept), centered on 100cm with a standard variation of 100, covers a huge range of plausible mean heights for human populations while giving very little chance for negative heights.
  2. The Gaussian prior for β_1 (slope), centered on 0 with a standard variation of 1, acts as a **regularizer** to prevent the model from **overfitting** the data by assigning extreme values to β_1.[1]
  3. The uniform prior for the standard deviation σ between 0 and 50 prohibits obtaining negative standard deviations. The upper bound (50 cm) would imply that 95% of individual heights lie within 100cm of the average height. That's a very large range.

[1] Regularization and overfitting will be discussed later in the course.

Fitting the Model

- Now we need to fit the model to the data to build the posterior distribution.
- Grid approximation is not a valid option, as setting up a grid for 3 parameters would be too computationally expensive.
- We will use Laplace approximation instead.
- In this approach we obtain the MAP estimates for each parameter using a hill-climbing **optimization** method.
- Then we fit a **multivariate Gaussian distribution** centered on these values.
- This distribution is the multidimensional extension to the standard Gaussian.

The multivariate Gaussian distribution

- The multivariate Gaussian distribution in d-dimensions defined by the following density function (PDF):

$$f_x = \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(\vec{x}-\vec{\mu})^T\Sigma^{-1}(\vec{x}-\mu)\right)$$

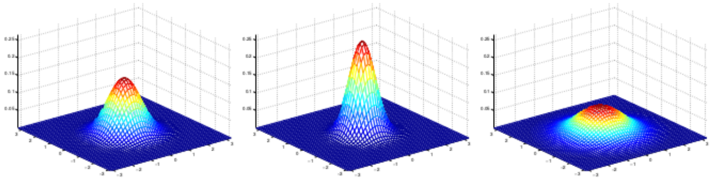
- This density function allows working with a d-dimensional vector of random variables $\vec{X}$.
- The first parameter of this distributions is a mean vector $\vec{\mu} \in \mathcal{R}^d$ with the mean value of each dimension.
- The second parameter is a covariance matrix $\Sigma \in R^{d\times d}$,
- This matrix contains the variance of each variable in the diagonal and the covariance of variables X_i and X_j in the other cells $\Sigma_{i,j}$:

$$Cov(X) = \Sigma$$

- The matrix Σ is symmetric and positive semi-definite.
- The multivariate Gaussian $N(\vec{\mu}, \Sigma)$ is a very convenient distribution for modeling multidimensional random variables.

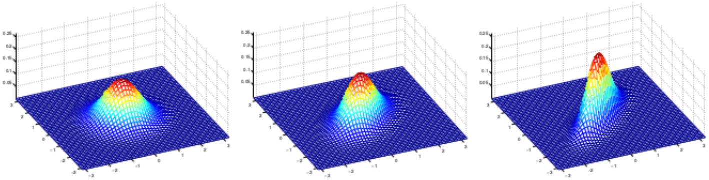
The multivariate Gaussian distribution

- Here are some examples taken from [Ng, 2008] of what the density of a multivariate Gaussian distribution looks like:



- The left-most figure shows a Gaussian with mean zero (that is, the 2x1 zero-vector) and covariance matrix $\Sigma = I$ (the 2×2 identity matrix).
- A Gaussian with zero mean and identity covariance is also called the standard normal distribution.
- The middle figure shows the density of a Gaussian with zero mean and $\Sigma = 0.6I$.
- The rightmost figure shows one with , $\Sigma = 2I$.
- We see that as Σ becomes larger, the Gaussian becomes more “spread-out”, and as it becomes smaller, the distribution becomes more “compressed”.

The multivariate Gaussian distribution



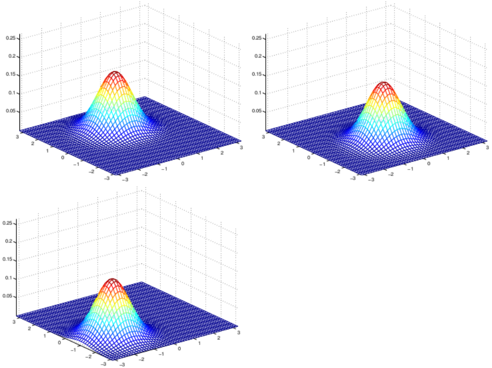
- The figures above show Gaussians with mean 0, and with covariance matrices respectively

$$\Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}; \ \Sigma = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}; \ \Sigma = \begin{bmatrix} 1 & 0.8 \\ 0.8 & 1 \end{bmatrix}.$$

- The leftmost figure shows the familiar standard normal distribution, and we see that as we increase the off-diagonal entry in Σ, the density becomes more "compressed" towards the 45· line (given by $x_1 = x_2$).

The multivariate Gaussian distribution

- As our last set of examples, fixing $\Sigma = I$, by varying $\vec{\mu}$ we can also move the mean of the density around.



- The figures above were generated using $\Sigma = I$, and respectively

$$\mu = \begin{bmatrix} 1 \\ 0 \end{bmatrix}; \quad \mu = \begin{bmatrix} -0.5 \\ 0 \end{bmatrix}; \quad \mu = \begin{bmatrix} -1 \\ -1.5 \end{bmatrix}.$$

Laplace approximation

- In Laplace approximation we assume that the joint posterior follows a multivariate Gaussian distribution $f(\theta_1, \ldots, \theta_n) = N(\vec{\mu}, \Sigma)$.
- This approximation is convenient for unimodal and roughly symmetric posterior distributions [Gelman et al., 2013].
- Moreover, there is Bayesian asymptotic theory that says that if the dataset is large enough, a posterior distribution can be approximated by a Gaussian [Gelman et al., 2013].
- The values of $\vec{\mu}$ are obtained from the posterior mode of each parameters (MAP):

$$\vec{\mu} = \vec{\theta}_{MAP}$$

- The values of Σ are obtained from the curvature near these values, which are obtained from the second derivatives of the posterior:

$$\Sigma = [I(\theta_{MAP})]^{-1}$$

where

$$I(\theta) = -\frac{d^2}{d\theta^2} \log f(\theta|d)$$

- Notice that both $\vec{\mu}$ and Σ can be calculated from the unnormalized posterior: $f(d|\theta) * f(\theta)$ because the evidence $f(d)$ is a constant that doesn't affect the maximum nor the curvature.

Conclusions

- Blabla

References I

Gelman, A., Carlin, J. B., Stern, H. S., Dunson, D. B., Vehtari, A., and Rubin, D. B. (2013).
Bayesian data analysis.
CRC press.

McElreath, R. (2020).
Statistical rethinking: A Bayesian course with examples in R and Stan.
CRC press.

Ng, A. (2008).
Generative learning algorithms.
Stanford Lecture Notes, 5(4).