

# Bayesian Linear Regression

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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  $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$  from a dataset  $d$ .
- The response variable  $\mathbf{y}$  is again modeled with a Gaussian distribution:  
 $y_i \sim N(\mu_i, \sigma^2)$ .
- We also maintain the assumption that each attribute has a linear relationship to the mean of the outcome.

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

- 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:

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

# Bayesian Linear Models

- The Bayesian linear regression 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 parameters of the model are  $\beta_0, \beta_1, \dots, \beta_b$  and  $\sigma$  but not  $\mu_i$ .
- This is because  $\mu_i$  it is determined deterministically from the linear model's coefficients.
- In order to build our posterior we need to define a likelihood function:

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

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

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

# Bayesian Linear Models

- Now we need a joint prior density:

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

- And the posterior gets specified as follows:

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

- The evidence is expressed by a multiple integral:

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

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

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

# 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:

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

- Parameters  $\beta_0$  and  $\beta_1$  are the intercept and the slope of our linear model.
- The parameter  $\sigma$  is the standard deviation of all the heights.
- Note that we are setting the same  $\sigma$  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  $\beta_0$  (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  $\beta_1$  (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  $\beta_1$ .<sup>1</sup>
  - 3 The uniform prior for the standard deviation  $\sigma$  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.

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<sup>1</sup>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  $\Sigma \in \mathcal{R}^{d \times d}$ ,
- 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  $\Sigma_{i,j}$ :

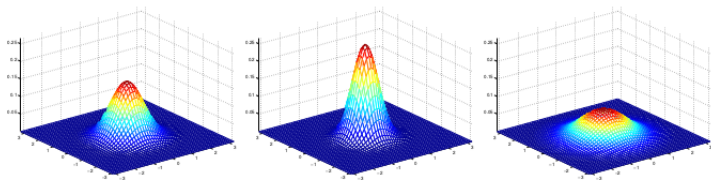
$$\text{Cov}(X) = \Sigma$$

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



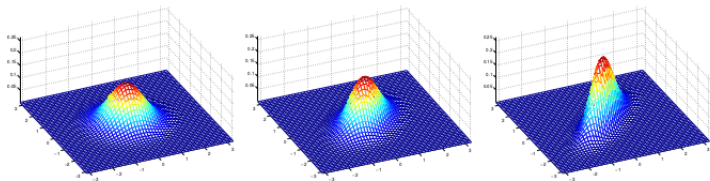
# The multivariate Gaussian distribution

- 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  $2 \times 1$  zero-vector) and covariance matrix  $\Sigma = I$  (the  $2 \times 2$  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  $\Sigma$  becomes larger, the Gaussian becomes more “spread-out”, and as it becomes smaller, the distribution becomes more “compressed”.

# The multivariate Gaussian distribution



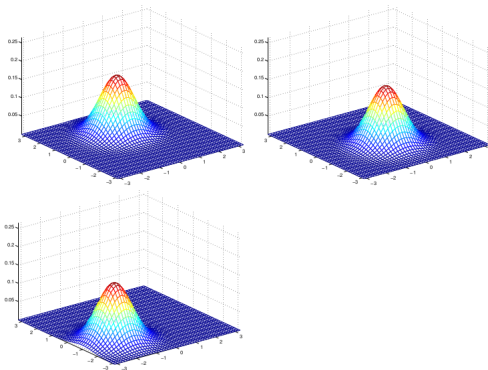
- The figures above show Gaussians with mean 0, and with covariance matrices respectively

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

- The leftmost figure shows the familiar standard normal distribution, and we see that as we increase the off-diagonal entry in  $\Sigma$ , 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  $f(\theta_1, \dots, \theta_n) = N(\vec{\mu}, \Sigma)$ .
- This approximation is convenient for unimodal and roughly symmetric posterior distributions [Gelman et al., 2013].
- The Bayesian asymptotic theory 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):

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

- These is done using numeric optimization techniques.

# Laplace approximation

- The values of  $\Sigma$  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  $\Sigma$  can be calculated from the unnormalized posterior  $f(d|\theta) * f(\theta)$
- We don't need to calculate the evidence  $f(d)$  to perform Laplace approximation [?].

# Fitting the Model

- Laplace approximation is implemented in the **quap** function from the **rethinking** package.
- The model for height defined above can be implemented as follows:

```
library(rethinking)
data(Howell1)
d <- Howell1
d2 <- d[ d$age >= 18 , ]

b.reg1 <- quap(
  alist(
    height ~ dnorm( b0 + b1*weight, sigma ),
    b0 ~ dnorm( 100 , 100 ) ,
    b1 ~ dnorm( 0 , 1) ,
    sigma ~ dunif( 0 , 50 )
  ) , data=d2 )
```

# Fitting the Model

- We can summarize this posterior with the command **precis**:

```
> precis( b.reg1, prob=0.95 )  
              mean      sd    2.5%   97.5%  
b0      113.95  1.90  110.21  117.68  
b1         0.90  0.04    0.82    0.99  
sigma    5.07  0.19    4.70    5.45
```

- These numbers provide Gaussian approximations for each parameter's marginal posterior distribution.
- This is the distribution of any parameter  $\theta_j$  regardless of the values of the others.
- In mathematical terms this is obtained, after integrating (averaging) over  $\theta_j \forall j \neq i$ :

$$f(\theta_i|d) = \int \cdots \int f(\theta_1, \dots, \theta_n|d) d\theta_1, \dots, d\theta_{i-1}, d\theta_{i+1}, \dots, d\theta_n$$

- We can compare the mean and standard deviation of  $\beta_0$  and  $\beta_1$  with what we obtained using least squares in previous lecture.
- The values are almost the same!

# Conclusions

- Blabla



# References I



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