

Maximum A Posteriori Estimation

Nipun Batra

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IIT Gandhinagar

Agenda

Revision

Coin Toss Problem

Univariate Normal Distribution

MAP for Linear Regression

MAP for Logistic Regression

Revision

Bayes Rule

$$P(\theta|D) = \frac{P(D|\theta) \cdot P(\theta)}{P(D)}$$

- $P(\theta|D)$ is called the posterior
- $P(D|\theta)$ is called the likelihood
- $P(\theta)$ is called the prior
- $P(D)$ is called the evidence

Maximum Likelihood Estimation

$$P(\theta|D) = \frac{P(D|\theta) \cdot P(\theta)}{P(D)} = \frac{P(D|\theta) \cdot P(\theta)}{\int_{\theta} P(D|\theta) \cdot P(\theta) d\theta}$$

Given a dataset D , find the parameters θ that maximize the likelihood of the data.

$$\theta_{\text{MLE}} = \arg \max_{\theta} P(D|\theta)$$

For example, given a linear regression problem setup, we set the likelihood as normal distribution and find the parameters θ that maximize the likelihood of the data.

Maximum A Posteriori Estimation

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Given a dataset D , find the parameters θ that maximize the posterior of θ considering both the likelihood and the prior.

$$\theta_{\text{MAP}} = \arg \max_{\theta} P(\theta|D) = \arg \max_{\theta} P(D|\theta) \cdot P(\theta)$$

Maximum A Posteriori Estimation

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- **MLE:** Given N observations, obtain best θ estimate (or θ_{MLE})
- What if we have prior knowledge about θ ?
- **MAP:** Given N observations and prior knowledge, obtain best θ estimate (or θ_{MAP})
- When do we need prior knowledge?
 - When the dataset is not a good representation of the true distribution.
 - Can be a data quality and/or quantity issue.

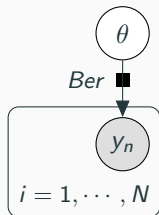
Coin Toss Problem

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- Assuming $y_i \sim \text{Bernoulli}(\theta)$, $P(y_i|\theta) = \theta^{y_i}(1 - \theta)^{1-y_i}$



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- Rewrite, $\theta_{MLE} = \frac{n_H}{n_H + n_T}$
- Suppose 10 tosses yield 9 heads and 1 tail. $\theta_{MLE} = 0.9$
- What if we have prior knowledge that the coin is fair?

Incorporating Prior Information

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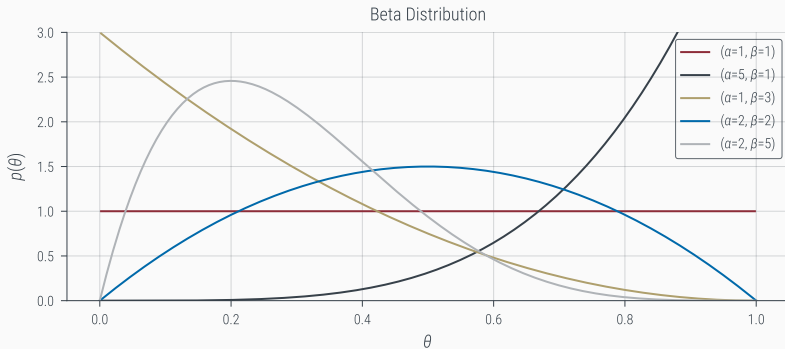
- A reasonable choice for prior is the Beta distribution.

$$\implies P(\theta|\alpha, \beta) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \cdot \theta^{\alpha-1}(1 - \theta)^{\beta-1}$$

where,

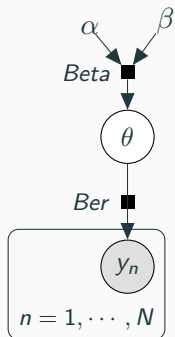
$$\Gamma(x) = \int_0^{\infty} t^{x-1} e^{-t} dt \quad (\text{Gamma Function})$$

Beta Distribution



Notebook

Coin Toss Problem with Prior



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$$\begin{aligned} \log P(\theta|D) = & \sum_{i=1}^N y_i \log \theta + (1 - y_i) \log(1 - \theta) + \\ & (\alpha - 1) \log \theta + (\beta - 1) \log(1 - \theta) \end{aligned}$$

$$\frac{\partial \log P(\theta|D)}{\partial \theta} = \frac{\sum_{i=1}^N y_i}{\theta} - \frac{\sum_{i=1}^N (1 - y_i)}{1 - \theta} + \frac{\alpha - 1}{\theta} - \frac{\beta - 1}{1 - \theta} = 0$$

$$\implies (1 - \theta) \sum_{i=1}^N y_i + \theta \sum_{i=1}^N (1 - y_i) + (1 - \theta)(\alpha - 1) - \theta(\beta - 1) = 0$$

$$\implies \sum_{i=1}^N y_i - \theta \sum_{i=1}^N y_i - N\theta + \theta \sum_{i=1}^N y_i + \alpha - 1 - \theta\alpha + \theta - \theta\beta + \theta = 0$$

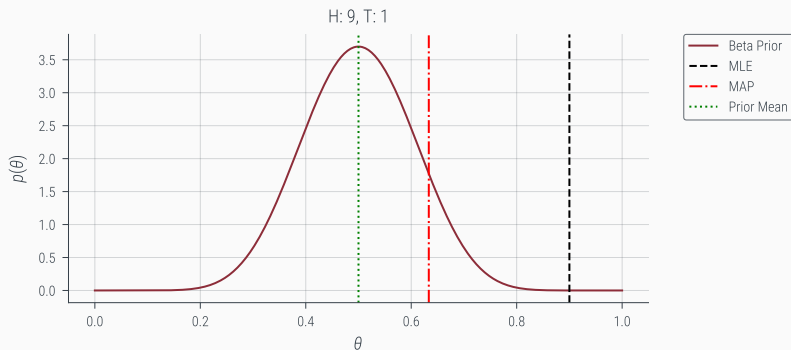
$$\Rightarrow \sum_{i=1}^N y_i + \alpha - 1 - \theta(N + \alpha + \beta - 2) = 0$$

$$\Rightarrow \theta_{MAP} = \frac{\sum_{i=1}^N y_i + \alpha - 1}{N + \alpha + \beta - 2}$$

Deriving θ_{MAP} (Coin toss context)

- Total number of tosses = N
- Number of heads = n_H
- Number of tails = n_T

Coin Toss Problem with Prior



Notebook

Univariate Normal Distribution

MAP for Normal Distribution

To estimate MAP for Normal Distribution, we can have the following 3 cases:

1. unknown μ , known σ^2
2. known μ , unknown σ^2
3. unknown μ , unknown σ^2

- Consider a sequence of independent N observations,
 $D = \{x_1, \dots, x_N\}$ drawn from $\mathcal{N}(x_i|\mu, \sigma^2)$

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 $D = \{x_1, \dots, x_N\}$ drawn from $\mathcal{N}(x_i|\mu, \sigma^2)$
- Likelihood is given by (Note: only μ is a random variable, σ^2 is known and assumed fixed)

$$P(D|\mu, \sigma^2) = \mathcal{L}(\mu) = \prod_{i=1}^N \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x_i - \mu)^2}{2\sigma^2}\right)$$

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- Log-Likelihood is given by

$$\log P(D|\mu, \sigma^2) = \mathcal{LL}(\mu) = \sum_{i=1}^N \left(-\frac{1}{2} \log(2\pi\sigma^2) - \frac{(x_i - \mu)^2}{2\sigma^2} \right)$$

$$\implies \mathcal{LL}(\mu) = -\frac{N}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^N (x_i - \mu)^2$$

- For MLE for μ , we set

$$\frac{\partial \mathcal{L}(\mu)}{\partial \mu} = 0 - \left(-\frac{1}{2\sigma^2} \sum_{i=1}^N 2(x_i - \mu) \right) = \frac{1}{\sigma^2} \left(\sum_{i=1}^N x_i - N\mu \right) = 0$$

or

$$\mu_{MLE} = \frac{\sum_{i=1}^N x_i}{N}$$

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$$\mu_{MLE} = \frac{\sum_{i=1}^N x_i}{N}$$

- However, similar to Coin Toss problem, this is prone to overfit.

Incorporating Prior Information

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- The Posterior for μ is given by

$$P(\mu|D) \propto P(D|\mu)P(\mu) \propto \prod_{i=1}^N \exp\left(-\frac{(x_i - \mu)^2}{2\sigma^2}\right) \exp\left(-\frac{(\mu - \mu_0)^2}{2\sigma_0^2}\right)$$

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- Simplifying, we get

$$P(\mu|D) \propto \exp\left(-\frac{(\mu - \mu_N)^2}{2\sigma_N^2}\right)$$

where,

$$(\mu_N, \sigma_N) = \left(\frac{\frac{\sigma^2}{N}}{\sigma_0 + \frac{\sigma^2}{N}} + \frac{\sigma_0^2}{\sigma_0 + \frac{\sigma^2}{N}} \frac{\sum_{i=1}^N x_i}{N}, \left(\frac{1}{\sigma_0^2} + \frac{N}{\sigma^2} \right)^{-1} \right)$$

Obtaining MAP

- For MAP, we set

$$\frac{\partial \log P(\mu|D)}{\partial \mu} = -\frac{1}{2\sigma^2} \sum_{i=1}^N -2(x_i - \mu) - \frac{1}{2\sigma_0^2} \sum_{i=1}^N 2(\mu - \mu_0) = 0$$

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$$\begin{aligned} \implies \frac{1}{\sigma^2} \left(\sum_{i=1}^N x_i - N\mu \right) - \frac{N}{\sigma_0^2} (\mu - \mu_0) = \\ \mu \left(-\frac{N}{\sigma^2} - \frac{N}{\sigma_0^2} \right) + \frac{\sum_{i=1}^N x_i}{\sigma^2} + \frac{N\mu_0}{\sigma_0^2} = 0 \end{aligned}$$

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$$\mu \left(-\frac{N}{\sigma^2} - \frac{N}{\sigma_0^2} \right) + \frac{\sum_{i=1}^N x_i}{\sigma^2} + \frac{N\mu_0}{\sigma_0^2} = 0$$

$$\mu_{MAP} = \frac{\frac{\mu_0}{\sigma_0^2} + \frac{\frac{\sum_{i=1}^N x_i}{N}}{\sigma^2}}{\frac{1}{\sigma_0^2} + \frac{1}{\sigma^2}} = \frac{\sigma^2 \mu_0 + \sigma_0^2 \frac{\sum_{i=1}^N x_i}{N}}{\sigma_0^2 + \sigma^2}$$

Assuuming μ is known, the conjugate prior for σ^2 is Inverse Gamma(α_0, β_0) which gives,

$$P(\sigma^2|\alpha_0, \beta_0) \propto \frac{1}{(\sigma^2)^{\alpha_0+1}} \exp\left(-\frac{\beta_0}{\sigma^2}\right)$$

\therefore The posterior is given by,

$$P(\sigma^2|D; \alpha_0, \beta_0) \sim \text{Inverse Gamma}\left(\alpha_0 + \frac{n}{2}, \beta_0 + \frac{\sum_{i=1}^n (x_i - \mu)^2}{2}\right)$$

unknown μ , unknown σ^2

Assuuming both μ and σ^2 are unknown, the conjugate prior for μ and σ^2 (or Precision $\tau = \frac{1}{\sigma^2}$) is as follows,

$$\begin{aligned}D|\mu, \tau &\sim \mathcal{N}(\mu, \tau^{-1}) \\ \mu|\tau &\sim \mathcal{N}(\mu_0, (\kappa_0\tau)^{-1}) \\ \tau &\sim \text{Gamma}(\alpha_0, \beta_0)\end{aligned}$$

\therefore The posterior is given by,

$$\begin{aligned}\mu|D, \tau &\sim \mathcal{N}\left(\frac{\kappa_0\mu_0 + n\bar{x}}{\kappa_0 + n}, (\kappa_0 + n)^{-1}\right) \\ \tau|D &\sim \text{Gamma}\left(\alpha_0 + \frac{n}{2}, \beta_0 + \frac{1}{2} \sum_{i=1}^n (x_i - \mu)^2 + \frac{\kappa_0 n (\bar{x} - \mu_0)^2}{2(\kappa_0 + n)}\right)\end{aligned}$$

MAP for Linear Regression

MLE for Linear Regression

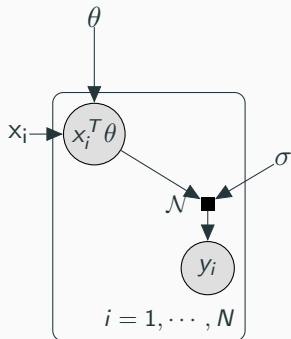
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- Suppose the data is generated from a linear model with additive Gaussian noise, i.e., $y_i = \theta^T x_i + \epsilon_i$ where $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$.

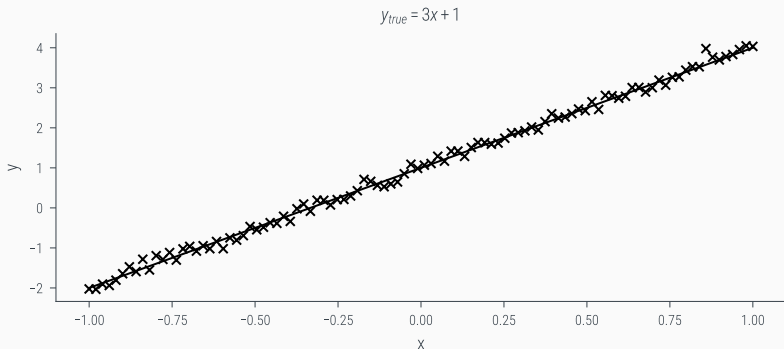
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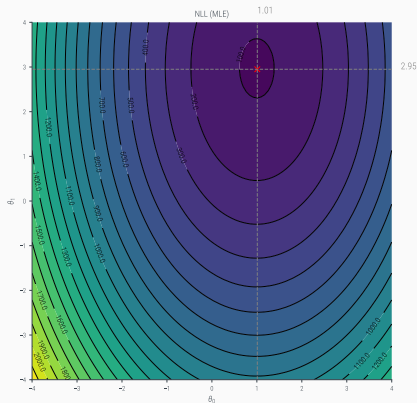
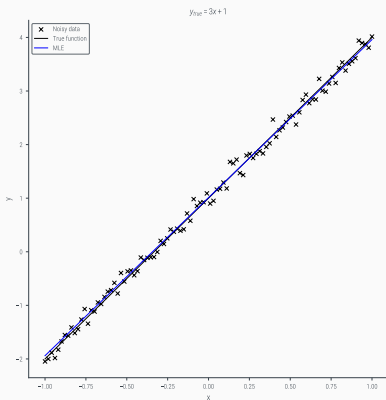
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MLE for Linear Regression

- The likelihood is given by, $P(y_i|x_i, \theta) = \mathcal{N}(y_i|\theta^T x_i, \sigma^2)$
- **Recall:** The negative log-likelihood is given by,
$$\mathcal{NLL}(\theta) = \frac{1}{2\sigma^2} (y - X\theta)^T (y - X\theta)$$
- **Recall:** The MLE is given by,
$$\theta_{MLE} = \arg \min_{\theta} \mathcal{NLL}(\theta) = (X^T X)^{-1} X^T y$$

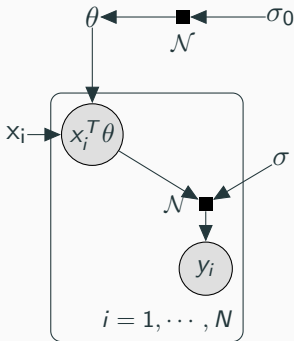


Using zero-mean Gaussian prior

Considering a zero-mean Gaussian prior on the weights, i.e., $P(\theta) = \mathcal{N}(\theta|0, \sigma_0^2)$, we have

$$P(\theta|D) \propto P(D|\theta)P(\theta)$$

$$\theta_{MAP} = \arg \min \log P(\theta|D) = \arg \min \mathcal{NLL}(\theta) + \log P(\theta)$$



Using zero-mean Gaussian prior

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We get

$$\theta_{MAP} = \arg \min \frac{1}{2\sigma^2} (y - X\theta)^T (y - X\theta) + \frac{1}{\sigma_0^2} \theta^T \theta$$

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We get

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Question

What does this expression remind you of?

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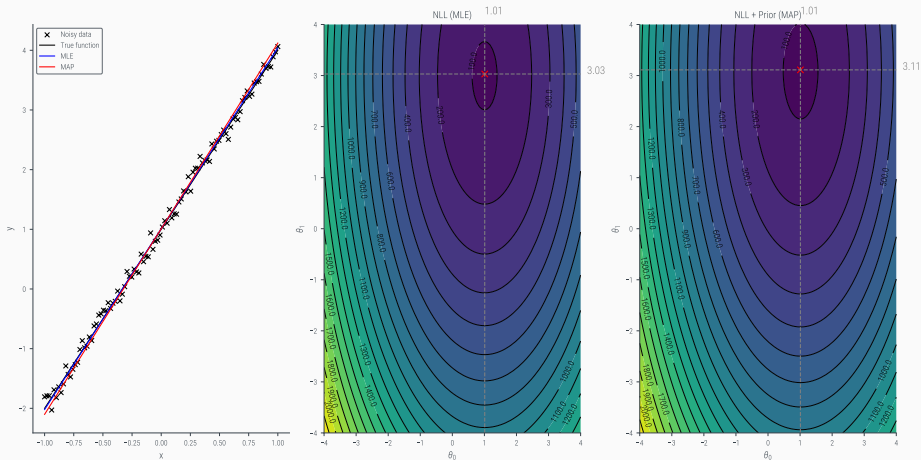
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Question

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Answer: Ridge Regression

Using zero-mean Gaussian prior

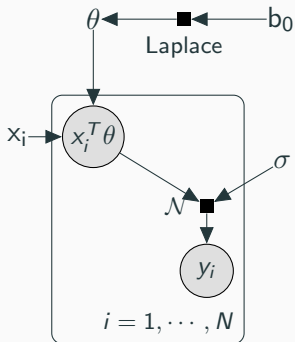


Notebook

Using Laplace prior

We can also use a Laplace prior on the weights, i.e.,

$$P(\theta) = \frac{1}{2b_0} \exp\left(-\frac{|x - \mu|}{b_0}\right)$$



The MAP takes the form,

$$\theta_{MAP} = \arg \min \frac{1}{2\sigma^2} (y - X\theta)^T (y - X\theta) + \frac{1}{b_0} |\theta_i|$$

Using Laplace prior

The MAP takes the form,

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Using Laplace prior

The MAP takes the form,

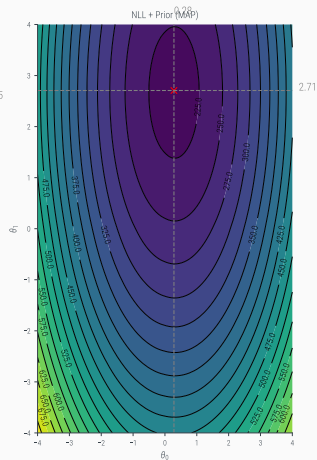
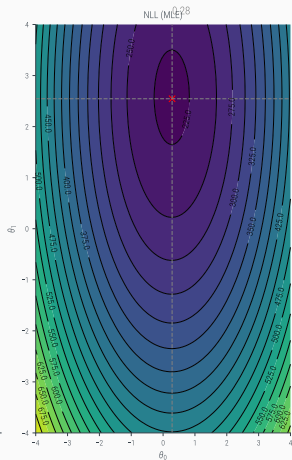
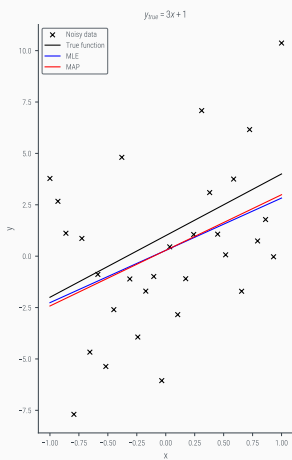
$$\theta_{MAP} = \arg \min \frac{1}{2\sigma^2} (y - X\theta)^T (y - X\theta) + \frac{1}{b_0} |\theta_i|$$

Question

What does this expression remind you of?

Answer: **Lasso Regression**

Using Laplace prior



Notebook

MAP for Logistic Regression

MLE for Logistic Regression

Consider a dataset $D = \{(x_1, y_1) \dots (x_N, y_N)\}$, where $x_i \in \mathbb{R}^d$ and $y_i \in \{0, 1\}$ such that

$$P(y = 1|x) = \hat{y} = \frac{1}{1 + \exp(-X^T \theta)} = \sigma(X^T \theta)$$

Take $y \sim \text{Bernoulli}(\sigma(X^T \theta))$

MLE for Logistic Regression

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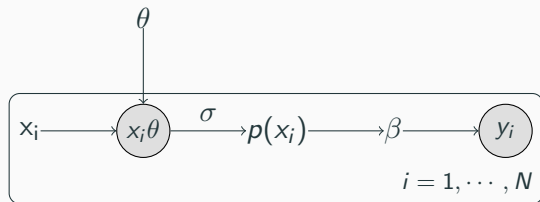
Take $y \sim \text{Bernoulli}(\sigma(X^T \theta))$

The likelihood is given by

$$\mathcal{L}(\theta) = \prod_{i=1}^N \hat{y}_i^{y_i} (1 - \hat{y}_i)^{1-y_i}$$

$$\implies \mathcal{LL}(\theta) = \sum_{i=1}^N y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i)$$

MLE for Logistic Regression



Binary Classification:

$$P(Y = 1|X) = \frac{1}{1 + e^{-(\theta_0 + \theta_1 X)}}$$

$$\therefore \mathcal{LL}(\theta) = \sum_{i=1}^N y_i \log p(x_i) + (1 - y_i) \log(1 - p(x_i))$$

Using zero-mean Gaussian prior

Considering a zero-mean Gaussian prior on the weights, i.e., $P(\theta) = \mathcal{N}(\theta|0, \sigma_0^2)$, the MAP is given by,

$$\theta_{MAP} = \arg \min \log(1 + \exp(-\theta^T X)) + \frac{1}{\sigma_0^2} \theta^T \theta$$

Considering a Laplace prior on the weights, i.e.,

$P(\theta) = \prod_D \text{Laplace}(\theta_i | 0, b_0) \propto \prod_D \exp(-\frac{1}{b_0} |\theta_i|)$, the MAP is given by,

$$\theta_{MAP} = \arg \min \log(1 + \exp(-\theta^T X)) + \frac{1}{b_0} |\theta|$$

Self-Study: Modify the code for Linear Regression to implement MAP for Logistic Regression.