

Problem Set #2: Supervised Learning II

Problem 1 Logistic Regression: Training stability

- (a) The most notable difference in training the logistic regression model on datasets A and B is that the algorithm does not converge on dataset B .
- (b) To investigate why the training procedure behaves unexpectedly on dataset B , but not on A , we print the value of θ after every 10000 iterations. We notice that for data set B , although the normalized $\frac{\theta}{\|\theta\|}$ almost stop changing after several tens of thousands of iterations, each component of the unnormalized θ keeps increasing. We also notice that dataset A is not linearly separable while dataset B is linearly separable.

From the code, we notice that the algorithm calculates the gradient of loss function as

$$\nabla_{\theta} J(\theta) = -\frac{1}{m} \sum_{i=1}^m \frac{y^{(i)} x^{(i)}}{1 + \exp(y^{(i)} \theta^T x^{(i)})}.$$

From this, we know that the algorithm uses gradient descent to minimize the loss function

$$J(\theta) = -\frac{1}{m} \sum_{i=1}^m \log \frac{1}{1 + \exp(-y^{(i)} \theta^T x^{(i)})}.$$

Hence, for a dataset that is linearly separable, that is, $y^{(i)} \theta^T x^{(i)} > 0$ for all i , a θ with larger norm always leads to a smaller loss, preventing the algorithm from converging. However, on a dataset that is not linearly separable, there exists i such that $y^{(i)} \theta^T x^{(i)} < 0$. By plotting $f(z) = \log(1 + e^{-z})$ in Figure 1, we notice that negative margin dominates when scaling θ to a larger norm. Hence, we cannot always increase θ to a larger norm while minimizing $J(\theta)$.

- (c) Consider the following modifications
- i. Using a different constant learning rate will not make the algorithm converge on dataset B , since scaling θ to larger norm still always decreases the loss.
 - ii. Decreasing the learning rate over time will make the algorithm converge for dataset B , since in this way the change of θ converge to 0.

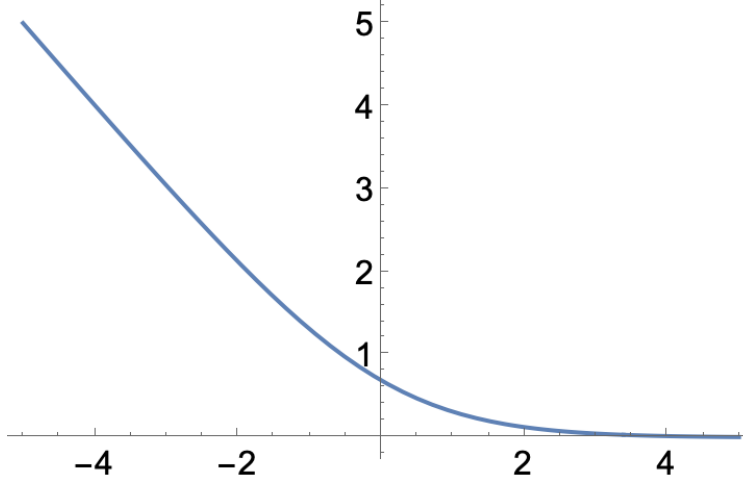


Figure 1: Plot of $f(z) = \log(1 + e^{-z})$ for $-5 \leq z \leq 5$.

- iii. Linear scaling the input features does not help, since it does not change the dataset's linear separability.
 - iv. Adding a regularization term $\|\theta\|_2^2$ helps, since now scaling θ to larger norm penalize the algorithm.
 - v. Adding zero-mean Gaussian noise to the training data or labels helps as long as it makes the dataset not linearly separable.
- (d) Support vector machines, which uses hinge loss, are not vulnerable to datasets like B . In SVM, geometric margin is considered, instead of functional margin considered here. In other words, θ is normalized, so for linearly separable datasets like B , the algorithm will still converge.

■

Problem 2 Model Calibration

Try to understand the output $h_\theta(x)$ of the hypothesis function of a logistic regression model, in particular why we might treat the output as a probability.

When probabilities outputted by a model match empirical observation, the model is *well-calibrated*. For example, if a set of examples $x^{(i)}$ for which $h_\theta(x^{(i)}) \approx 0.7$, around 70% of those examples should have positive labels. In a well-calibrated model, this property holds true at every probability value.

Suppose training set $\{x^{(i)}, y^{(i)}\}_{i=1}^m$ with $x^{(i)} \in \mathbb{R}^{n+1}$ and $y^{(i)} \in \{0, 1\}$. Assume we have an intercept term $x_0^{(i)} = 1$ for all i . Let θ be the maximum likelihood parameters learned after training logistic regression model. In order for model to be well-calibrated, given any range of probabilities (a, b) such that $0 \leq a < b \leq 1$, and training examples $x^{(i)}$ where the model outputs $h_\theta(x^{(i)})$ fall in the range (a, b) , the fraction of positives in that set of examples should be equal to the average of the model outputs for those examples. That is,

$$\frac{\sum_{i \in I_{a,b}} P(y^{(i)} = 1 \mid x^{(i)}; \theta)}{|\{i \in I_{a,b}\}|} = \frac{\sum_{i \in I_{a,b}} \mathbb{I}\{y^{(i)} = 1\}}{|\{i \in I_{a,b}\}|},$$

where $P(y^{(i)} = 1 \mid x; \theta) = h_\theta(x) = 1/(1 + \exp(-\theta^T x))$, $I_{a,b} = \{i : h_\theta(x^{(i)}) \in (a, b)\}$.

- (a) For the described logistic regression model over the range $(a, b) = (0, 1)$, we want to show the above equality holds. Recall the gradient of log-likelihood

$$\frac{\partial \ell}{\partial \theta_j} = \sum_{i=1}^m (y^{(i)} - h_\theta(x^{(i)})) x_j^{(i)}.$$

For a maximum likelihood estimation, $\frac{\partial \ell}{\partial \theta} = 0$. Hence $\frac{\partial \ell}{\partial \theta_0} = 0$. Since $x_0^{(i)} = 1$, we have

$$\sum_{i=1}^m y^{(i)} - h_\theta(x^{(i)}) = 0.$$

The desired equality follows immediately since $i \in I_{0,1}$ for all i .

- (b) A perfectly calibrated model — that is, the equality holds for any $(a, b) \subset [0, 1]$ — does not imply that the model achieves perfect accuracy. Consider $(a, b) = (\frac{1}{2}, 1)$, the above equality implies

$$\frac{\sum_{i \in I_{a,b}} P(y^{(i)} = 1 \mid x^{(i)}; \theta)}{|\{i \in I_{a,b}\}|} = \frac{\sum_{i \in I_{a,b}} \mathbb{I}\{y^{(i)} = 1\}}{|\{i \in I_{a,b}\}|} < 1.$$

This shows that the model does not have perfect accuracy.

For the converse direction, a perfect accuracy does not imply perfectly calibrated. Consider again $(a, b) = (\frac{1}{2}, 1)$, then we have

$$\frac{\sum_{i \in I_{a,b}} \mathbb{I}\{y^{(i)} = 1\}}{|\{i \in I_{a,b}\}|} = 1 > \frac{\sum_{i \in I_{a,b}} P(y^{(i)} = 1 \mid x^{(i)}; \theta)}{|\{i \in I_{a,b}\}|}.$$

- (c) Discuss what effect of L_2 regularization in the logistic regression objective has on model calibration. For L_2 regularization in logistic regression, the gradient becomes

$$\frac{\partial \ell}{\partial \theta_j} = \sum_{i=1}^m (y^{(i)} - h_{\theta}(x^{(i)})) x_j^{(i)} - 2C\theta_j = 0.$$

Hence, the equality does not hold unless $\theta_0 = 0$. ■

The interval $(0, 1)$ is the only range for which logistic regression is guaranteed to be calibrated. When GLM assumptions hold, all ranges $(a, b) \subset [0, 1]$ are well calibrated. In addition, when test set has same distribution and when model has not overfit or underfit, logistic regression are well-calibrated on test data as well. Thus logistic regression is popular when we are interested in level of uncertainty in the model output. △

Problem 3 Bayesian Interpretation of Regularization

In Bayesian statistics, almost every quantity is a random variable. Joint distribution of all the random variables are called *model* (e.g. $p(x, y, \theta)$). Every unknown quantity can be estimated by conditioning the model on all observed quantities. Such conditional distribution $p(\theta | x, y)$ is called *posterior distribution*. A consequence of this approach is that we are required to endow a *prior distribution* $p(\theta)$.

In purest Bayesian interpretation, we are required to keep the entire posterior distribution over the parameters all the way until prediction to come up with the *posterior predictive distribution*, and the final prediction will be the EV of the posterior predictive distribution. However, this is computationally very expensive.

The compromise is to estimate a point value of the parameters instead of the full distribution, which is the mode of the posterior distribution. Estimating the mode of posterior distribution is also called *maximum a posteriori estimation* (MAP). That is,

$$\theta_{\text{MAP}} = \underset{\theta}{\operatorname{argmax}} p(\theta | x, y).$$

Compare this to the *maximum likelihood estimation* (MLE):

$$\theta_{\text{MLE}} = \underset{\theta}{\operatorname{argmax}} p(y | x, \theta).$$

In this problem, explore connections between MAP estimation and common regularization techniques that are applied with MLE estimation. In particular, we will show how choice of prior distribution over θ is equivalent to different kinds of regularization.

- (a) Assume that $p(\theta) = p(\theta | x)$, we have

$$p(\theta | x, y) = \frac{p(y | \theta, x)p(\theta | x)}{p(y | x)} = \frac{p(y | \theta, x)p(\theta)}{p(y | x)}.$$

Since $p(y \mid x)$ does not depend on θ ,

$$\theta_{\text{MAP}} = \underset{\theta}{\operatorname{argmax}} p(y \mid \theta, x) p(\theta).$$

Note that the assumption $p(\theta) = p(\theta \mid x)$ will be valid for models such as linear regression where the input x are not explicitly modeled by θ . Note also that this means x and θ are marginally independent, but not conditionally independent when y is given.

- (b) Now we show that MAP estimation with a zero-mean Gaussian priori over θ , specifically $\theta \sim \mathcal{N}(0, \eta^2 I)$, is equivalent to applying L_2 regularization with MLE estimation. Specifically, we need to show

$$\theta_{\text{MAP}} = \underset{\theta}{\operatorname{argmin}} -\log p(y \mid x, \theta) + \lambda \|\theta\|_2^2.$$

Recall the definition of multivariate normal, we have

$$\begin{aligned} \theta_{\text{MAP}} &= \underset{\theta}{\operatorname{argmax}} p(\theta \mid x, y) \\ &= \underset{\theta}{\operatorname{argmax}} p(y \mid \theta, x) p(\theta) \\ &= \underset{\theta}{\operatorname{argmax}} p(y \mid \theta, x) \exp\left(-\frac{1}{2\eta^2} \|\theta\|_2^2\right), \end{aligned}$$

where we have ignored some of the constants. Taking the negative log on both sides, it follows that

$$\theta_{\text{MAP}} = \underset{\theta}{\operatorname{argmin}} -\log p(y \mid x, \theta) + \frac{1}{2\eta^2} \|\theta\|_2^2,$$

as desired, where $\lambda = \frac{1}{2\eta^2}$.

- (c) Now consider a specific instance, a linear regression model given by $y = \theta^T x + \varepsilon$, where $\varepsilon \sim \mathcal{N}(0, \sigma^2)$. Like before, assume a Gaussian prior on this model such that $\theta \sim \mathcal{N}(0, \eta^2 I)$. Let X be the design matrix of all training examples where each row is one example input, and y be the column vector of all the example outputs. We want to derive a closed form expression for θ_{MAP} .

For this model, the likelihood of an example $(x^{(i)}, y^{(i)})$ is

$$p(y^{(i)} \mid x^{(i)}, \theta) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2}\right).$$

Hence,

$$\log p(y^{(i)} \mid x^{(i)}, \theta) = -\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2} + C,$$

where C is some constant, and θ_{MAP} is given by

$$\begin{aligned}\theta_{\text{MAP}} &= \underset{\theta}{\operatorname{argmin}} \sum_{i=1}^m \frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2} + \frac{1}{2\eta^2} \|\theta\|_2^2 \\ &= \underset{\theta}{\operatorname{argmin}} \frac{1}{2\sigma^2} (y - X\theta)^T (y - X\theta) + \frac{1}{2\eta^2} \theta^T \theta.\end{aligned}$$

Set the gradient of the function to 0, we have

$$0 = -\frac{1}{\sigma^2} X^T (y - X\theta_{\text{MAP}}) + \frac{1}{\eta^2} \theta_{\text{MAP}}$$

It follows that

$$\theta_{\text{MAP}} = \eta^2 (\eta^2 X^T X + \sigma^2 I)^{-1} X^T y.$$

(d) Now consider the Laplace distribution, whose density

$$f(z \mid \mu, b) = \frac{1}{2b} \exp\left(-\frac{|z - \mu|}{b}\right).$$

As before, consider a linear regression model given by $y = \theta^T x + \varepsilon$ where $\varepsilon \sim \mathcal{N}(0, \sigma^2)$. Assume a Laplace prior on this model where $\theta \sim \mathcal{L}(0, bI)$. We want to show that θ_{MAP} in this case is equivalent to the solution of linear regression with L_1 regularization, whose loss is specified as

$$J(\theta) = \|X\theta - y\|_2^2 + \gamma \|\theta\|_1.$$

■