

## Homework 13

1. In this problem you will implement a neural network to solve a classification problem. To keep things simple, the data will consist of covariates  $x^{(i)} \in \mathbb{R}^2$  and a response  $y_i \in \{0, 1\}$  for  $i = 1, 2, \dots, N$  (notice  $y$  takes on only two possible values). The classification problem involves fitting the model  $y \sim f(x)$  over functions  $f(x)$  that can be parameterized by our neural net, which is described below. The attached file `nn.txt` contains the samples. Each sample, corresponding to a row in the file, gives the three values  $(x_1^{(i)}, x_2^{(i)}, y_i)$ .

Your neural network should consist of three layers, as discussed in class. The input layer should contain  $X_1$  and  $X_2$  nodes, which will be the two coordinates for each of the samples  $x^{(i)}$  (i.e.  $X_1 = x_1^{(i)}$  and  $X_2 = x_2^{(i)}$ ). The middle (hidden) layer should contain  $m$  nodes,  $Z_j$  for  $j = 1, 2, \dots, m$ . And an output layer consisting of nodes  $T_1, T_2$ . Then, the probability that the class of  $x^{(i)}$  is 1 given by,

$$P(y = 1 \mid x^{(i)}, \alpha) = \frac{\exp[T_1]}{\exp[T_1] + \exp[T_2]}, \quad (1)$$

where  $\alpha$  is the vector of parameters of the neural net and  $T_1, T_2$  are computed using the neural net with input  $x^{(i)}$ . To repeat what we mentioned in class, each  $Z_j$  is parameterized as follows:

$$Z_j = \sigma(\beta_0^{(j)} + \beta^{(j)} \cdot x), \quad (2)$$

where  $x = (X_1, X_2)$ ,  $\beta_0^{(j)} \in \mathbb{R}$ ,  $\beta^{(j)} \in \mathbb{R}^2$ , and  $\sigma(w) = 1/(1 + \exp(-w))$ . The node  $T_j$  is parameterized as follows:

$$T_j = \sigma(\gamma_0^{(j)} + \gamma^{(j)} \cdot z), \quad (3)$$

where  $z = (Z_1, Z_2, \dots, Z_m)$ ,  $\gamma_0^{(j)} \in \mathbb{R}$ ,  $\gamma^{(j)} \in \mathbb{R}^m$ . Then  $\alpha$  is the concatenation of all the parameters:  $\beta_0^{(j)}, \beta^{(j)}$  for  $j = 1, 2, \dots, m$  and  $\gamma_0^{(j)}, \gamma^{(j)}$  for  $j = 1, 2$ .

- (a) Visualize the dataset by plotting it with different colors for the two classes of  $y$ .

- (b) What is the dimension of  $\alpha$  in terms of  $m$ ?
- (c) Write a function  $NN(x, \alpha, m)$  which takes a sample  $x \in \mathbb{R}^2$  and a choice for  $\alpha$  and returns the neural net estimate of  $P(y = 1 \mid x, \alpha)$ . (Hint: It may be helpful to write functions such as `get_beta(alpha i)`, which given  $\alpha$  and  $i$  returns  $\beta^{(i)}$ , and `get_beta_0(eta, i)`, which given  $\alpha$  and  $i$  returns  $\beta_0^{(i)}$ . Using such functions will greatly simplify your code.)
- (d) Explain why the log likelihood function  $\log L(\eta)$  for the neural net is given by

$$\log L(\eta) = \sum_{i=1}^N (1-y_i) \log \left( \frac{\exp[T_1]}{\exp[T_1] + \exp[T_2]} \right) + y_i \log \left( 1 - \frac{\exp[T_1]}{\exp[T_1] + \exp[T_2]} \right). \quad (4)$$

Write a function that computes  $\log L(\alpha)$  (you will need to pass the data to the function).

- (e) Write a function that uses finite difference to compute the stochastic gradient of  $\log L(\alpha)$  based on a single or small number of samples (you can pick whether to use one sample or a few).
- (f) Set  $m = 4$  and train your neural net by maximizing the  $\log L(\alpha)$  using **stochastic** steepest ascent.
- (g) Remember that a classifier in this case is a function  $F(x) : \mathbb{R}^2 \rightarrow \{0, 1\}$ , where  $x \in \mathbb{R}^2$ . Once you choose  $\alpha$  by computing the maximum likelihood in (e), choose a cut-off  $p \in [0, 1]$ . Set  $F$  by

$$F(x) = \begin{cases} 0 & \text{if } P(y = 1 \mid x, \alpha) > p \\ 1 & \text{if } P(y = 1 \mid x, \alpha) \leq p \end{cases} \quad (5)$$

Try different value of  $p$  and for each  $p$ , visualize your classifier. You can visualize your classifier in any way you like, but here is one way. You can generate random coordinates within  $[-2, 2]$ , which is roughly where all the data points lie, using

```
x1 <- 4*runif(10000) - 2
x2 <- 4*runif(10000) - 2
```

Then plot each pair  $x1[i]$ ,  $x2[i]$  and vary the color of the point depending on whether the classifier predicts 1 or 0.