CS 391L	Machine Learning WB	Spring 2025

Homework 2

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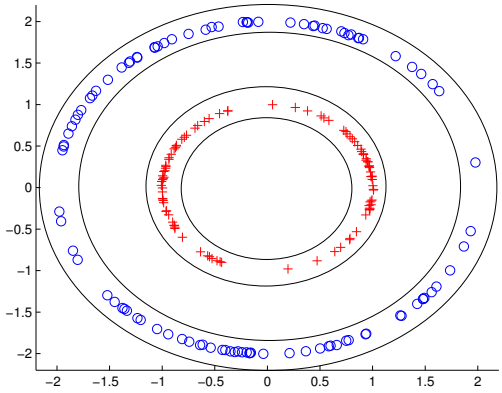
Keywords: *Classification, Gaussian Modeling, Neural Networks, PyTorch*

1. Suppose we have 2-dimensional data from two classes as shown in the figure below. The 'o' class lies in the tube $\{x = (x_1, x_2) \in \mathbb{R}^2 \mid 3.9 \leq \|x\|_2^2 \leq 4.1\}$ while the '+' class lies in the tube $\{x = (x_1, x_2) \in \mathbb{R}^2 \mid 0.9 \leq \|x\|_2^2 \leq 1.1\}$.



   (a) Can the classes be separated by a linear surface? Write down the equation of a quadratic surface that completely separates the two classes.

   (b) Recall the probability density function of a multivariate Gaussian with mean μ and covariance Σ:

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

   In class, we saw that by modeling the data in the classes as multivariate Gaussians with different covariance matrices, and then applying Bayes decision theory, we can obtain a quadratic decision surface. Consider modeling the two classes using two multivariate Gaussians $\Sigma_1 = \sigma_1^2 I$ and $\Sigma_2 = \sigma_2^2 I$, and means at the origin (i.e. $\mu_1 = \mu_2 = (0, 0)$). Write down the equation of the resulting decision surface. Can this strategy give good classification accuracy on the above data set?

   (c) What is the general condition required to get a circular decision surface for 2-dimensional data when modeling the classes as Gaussians? Explain your answer.

2. **Softmax Logistic Regression** Consider a classification problem with K classes, where the label y takes values in $\{1, 2, \ldots, K\}$. For a given observation $x \in \mathbb{R}^d$, the model assumes that the probability of class k is given by the softmax function:

$$P(y = k \mid x; W) = \frac{\exp(w_k^T x)}{\sum_{j=1}^K \exp(w_j^T x)},$$

   where $W = [w_1, w_2, \ldots, w_K]$ is the weight matrix with each $w_k \in \mathbb{R}^d$.

(a) Write down the likelihood function $L(W)$ (i.e. probability of the dataset given by our softmax logistic model) for a dataset

$$\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{N}.$$

Hint: Express your answer as product of probabilities, using indicator function $\mathbb{I}(y_i = k)$ which is 1 if $y_i = k$ and 0 otherwise.

(b) Starting from the likelihood (or log-likelihood) obtained in the previous part, derive the gradient of the log-likelihood with respect to the weight matrix W. More specifically, show that the gradient with respect to the weight vector w_k (the k-th column of W) is given by:

$$\nabla_{w_k} \ell(W) = \sum_{i=1}^{N} \left[\mathbb{I}(y_i = k) - P(y_i = k \mid x_i; W)\right] x_i.$$

(c) Consider now the special case when $K = 2$.

i. Show that the softmax formulation reduces to the standard logistic regression model. In particular, demonstrate that the softmax probability for one of the classes can be expressed as the logistic sigmoid function.

ii. Discuss any differences in parameterization or interpretation between the two formulations, and explain why logistic regression is essentially a special case of softmax regression when there are only two classes.

3. **CIFAR-10 Classification** For this problem, you will work on the CIFAR-10 dataset. The CIFAR-10 dataset is a widely used benchmark dataset for image classification tasks in the field of computer vision. It consists of 60,000 (50,000 training and 10,000 test) 32×32 color images in 10 classes, with 6,000 (5,000 for training and 1,000 for test) images per class. The 10 classes are: airplane, automobile, bird, cat, deer, dog, frog, horse, ship, and truck.

(a) Develop a 2-layer Multi-Layer Perceptron (MLP) based neural network using PyTorch to classify the CIFAR-10 dataset. The network should have 100 neurons in the hidden layer with sigmoid non-linearity and 10 neurons in the output layer (one for each class). The loss function to be used is the softmax cross-entropy loss. Use stochastic gradient descent with mini-batch size = 32.

Steps to solve the problem:

- Load the CIFAR-10 dataset into PyTorch using the available dataset loader.
- Create a two-layer MLP neural network in PyTorch with 100 neurons in the hidden layer and 10 neurons in the output layer.
- Write the forward propagation equations for the network.
- Define the loss function (softmax cross-entropy).
- Train the neural network for 10 epochs using the training dataset with the defined loss function and stochastic gradient descent optimizer.
- Experiment with different learning rates and report learning rate vs validation set accuracy for learning rates in $\{10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 10^{0}\}$. Also report the optimal learning rate and validation accuracy.
- Evaluate and report the performance of the trained model using the test dataset accuracy.
- (Optional) Experiment with the network architectures (e.g., more hidden layers, different activation functions) to improve accuracy.

(b) Now implement the same neural network and training code from scratch by using only numpy (i.e., without relying on any deep learning libraries such as PyTorch). For this question, you'll be implementing the backpropagation algorithm and stochastic gradient descent weight updates for training the neural network. Feel free to use PyTorch for debugging your numpy implementation (for e.g., to check if you are getting correct gradients).

Steps to solve the problem:

- Preprocess the dataset by normalizing the pixel values between -1 and 1 and reshaping the images into 1D arrays.
- Initialize the weights and biases for the two-layer MLP neural network randomly.
- Implement the forward pass of the neural network by computing the output probabilities of each class for a given input.
- Implement the backward pass of the neural network using the backpropagation algorithm to compute the gradients of the weights and biases.
- Update the weights and biases using the computed gradients and a specified learning rate.
- Train the neural network using the training dataset by iterating over multiple epochs and updating the weights and biases for each batch of inputs.
- Experiment with different learning rates and report learning rate vs validation set accuracy for learning rates in $\{10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 10^{0}\}$. Also report the optimal learning rate and validation accuracy.
- Evaluate and report the performance of the trained model using the test dataset by computing accuracy.

(c) Try changing the initializations of your neural network weight matrices to following options: (i) random values in $[-0.1, 0.1]$, (ii) random values in $[-10, 10]$, (iii) all zero values. Train the neural network using the training dataset and report the final test accuracies using different initializations. Explain your observations. How can we robustly initialize the weights of a neural network?