

## Homework 2: Classification and Bias-Variance Trade-offs

**Introduction**

This homework is about classification and bias-variance trade-offs. In lecture we have primarily focused on binary classifiers trained to discriminate between two classes. In multiclass classification, we discriminate between three or more classes. We encourage you to read CS181 Textbook's Chapter 3 for more information on linear classification, gradient descent, classification in the discriminative setting (covers multiclass logistic regression and softmax), and classification in the generative setting. Read Chapter 2.8 for more information on the trade-offs between bias and variance.

As a general note, for classification problems we imagine that we have the input matrix  $\mathbf{X} \in \mathbb{R}^{n \times m}$  (or perhaps they have been mapped to some basis  $\Phi$ , without loss of generality) with outputs now "one-hot encoded." This means that if there are  $c$  output classes, rather than representing the output label  $y$  as an integer  $1, 2, \dots, c$ , we represent  $\mathbf{y}$  as a "one-hot" vector of length  $c$ . A "one-hot" vector is defined as having every component equal to 0 except for a single component which has value equal to 1. For example, if there are  $c = 7$  classes and a particular data point belongs to class 3, then the target vector for this data point would be  $\mathbf{y} = [0, 0, 1, 0, 0, 0, 0]$ . We will define  $C_1$  to be the one-hot vector for the 1st class,  $C_2$  for the 2nd class, etc. Thus, in the previous example  $\mathbf{y} = C_3$ . If there are  $c$  total classes, then the set of possible labels is  $\{C_1 \dots C_c\} = \{C_k\}_{k=1}^c$ . Throughout the assignment we will assume that each label  $\mathbf{y} \in \{C_k\}_{k=1}^c$ .

In problems 1 and 3, you may use `numpy` or `scipy`, but not `scipy.optimize` or `sklearn`. Example code given is in Python 3.

Please type your solutions after the corresponding problems using this  $\text{\LaTeX}$  template, and start each problem on a new page.

Please submit the **writeup PDF to the Gradescope assignment 'HW2'**. Remember to assign pages for each question.

Please submit your  **$\text{\LaTeX}$  file and code files to the Gradescope assignment 'HW2 - Supplemental'**.

You can use a **maximum of 2 late days** on this assignment. Late days will be counted based on the latest of the two submissions.

**Problem 1** (Exploring Bias and Variance, 10 pts)

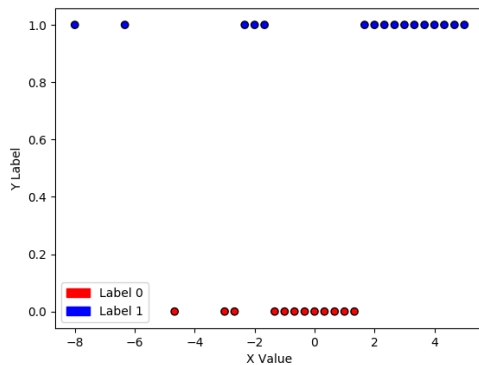
In this problem, we will explore the bias and variance of a couple of different model classes when it comes to classification.

The data have one-dimensional inputs  $x$  and binary outputs  $y$ .

```
x, y
-8, 1
-3, 0
-2, 1
-1, 0
0, 0
1, 0
2, 1
3, 1
4, 1
5, 1
```

1. Fit a linear classifier based off the value of  $\text{sigmoid}(w^T \phi)$  (using a decision threshold of 0.5) with the bases  $\phi_1(x) = [1, x]$ ,  $\phi_2(x) = [1, x, x^2]$ ,  $\phi_3(x) = [1, x, x^2, x^3, x^4, x^5, x^6]$  and a logistic loss with gradient descent. Note that the classes are represented with 0's and 1's. Repeat your gradient descent 25 times for each basis option, with different random starting values of  $w$ . Use  $\eta = 0.001$  and take 10000 steps for each run, and make sure to average the gradient over the data points (for each step). These parameters, while not perfect, will ensure your code runs in a reasonable amount of time. The emphasis of this problem is on capturing the bias-variance trend, so don't worry the exact details of the models as long as this trend is captured. Hint: if you run into  $\log(0)$  issues in the logistic loss function, you can use a small  $\epsilon = 0.000001$  to take care of it.
2. Create three plots, one for each basis. On each plot, first plot the the data points as given above, then plot the prediction functions of the top 10 runs (in terms of loss) of gradient descent. Explicitly, the prediction function of a given model is essentially plotting  $\text{sigmoid}(w^T \phi(x)) > 0.5$  for all  $x$ 's (seen in the starter code with a random  $w$  that you will need to change). While unlikely, in case all 25 runs were poor, you may need to rerun your code.
3. Explain what you see in terms of the bias-variance trade-off.
4. If we were to have "triple" the data, as in add in  $(-6.33, 1)$ ,  $(-4.67, 0)$ ,  $(-2.67, 0)$ ,  $(-2.33, 1)$  ...  $(4.33, 1)$ ,  $(4.66, 1)$ , how would the variance change (no need to rerun your code, just answer this as a conceptual question)? Why do you think that may be the case? See graph below for reference.

If we had triple the data:



## Solution

**Problem 2** (Matrix calculus, 15pts)

Consider now a generative  $c$ -class model. We adopt class prior  $p(\mathbf{y} = C_k; \boldsymbol{\pi}) = \pi_k$  for all  $k \in \{1, \dots, c\}$  (where  $\pi_k$  is a parameter of the prior). Let  $p(\mathbf{x}|\mathbf{y} = C_k)$  denote the class-conditional density of features  $\mathbf{x}$  (in this case for class  $C_k$ ). Consider the data set  $D = \{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^n$  where as above  $\mathbf{y}_i \in \{C_k\}_{k=1}^c$  is encoded as a one-hot target vector and the data are independent.

1. Write out the negative log-likelihood of the data set,  $-\ln p(D; \boldsymbol{\pi})$ .
2. Since the prior forms a distribution, it has the constraint that  $\sum_k \pi_k - 1 = 0$ . Using the hint on Lagrange multipliers below, give the expression for the maximum-likelihood estimator for the prior class-membership probabilities, i.e.  $\hat{\pi}_k$ . Make sure to write out the intermediary equation you need to solve to obtain this estimator. Double-check your answer: the final result should be very intuitive!

For the remaining questions, let the class-conditional probabilities be Gaussian distributions with the same covariance matrix

$$p(\mathbf{x}|\mathbf{y} = C_k) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}), \text{ for } k \in \{1, \dots, c\}$$

and different means  $\boldsymbol{\mu}_k$  for each class.

3. Derive the gradient of the negative log-likelihood with respect to vector  $\boldsymbol{\mu}_k$ . Write the expression in matrix form as a function of the variables defined throughout this exercise. Simplify as much as possible for full credit.
4. Derive the maximum-likelihood estimator  $\hat{\boldsymbol{\mu}}_k$  for vector  $\boldsymbol{\mu}_k$ . Once again, your final answer should seem intuitive.
5. Derive the gradient for the negative log-likelihood with respect to the covariance matrix  $\boldsymbol{\Sigma}$  (i.e., looking to find an MLE for the covariance). Since you are differentiating with respect to a *matrix*, the resulting expression should be a matrix!
6. Derive the maximum likelihood estimator  $\hat{\boldsymbol{\Sigma}}$  of the covariance matrix.

**Hint: Lagrange Multipliers.** Lagrange Multipliers are a method for optimizing a function  $f$  with respect to an equality constraint, i.e.

$$\min_{\mathbf{x}} f(\mathbf{x}) \text{ s.t. } g(\mathbf{x}) = 0.$$

This can be turned into an unconstrained problem by introducing a Lagrange multiplier  $\lambda$  and constructing the Lagrangian function,

$$L(\mathbf{x}, \lambda) = f(\mathbf{x}) + \lambda g(\mathbf{x}).$$

It can be shown that it is a necessary condition that the optimum is a critical point of this new function. We can find this point by solving two equations:

$$\frac{\partial L(\mathbf{x}, \lambda)}{\partial \mathbf{x}} = 0 \quad \text{and} \quad \frac{\partial L(\mathbf{x}, \lambda)}{\partial \lambda} = 0$$

**Cookbook formulas.** Here are some formulas you might want to consider using to compute difficult gradients. You can use them in the homework without proof. If you are looking to hone your matrix calculus skills, try to find different ways to prove these formulas yourself (will not be part of the evaluation of this homework). In general, you can use any formula from the matrix cookbook, as long as you cite it. We opt for the following common notation:  $\mathbf{X}^{-\top} := (\mathbf{X}^{\top})^{-1}$

$$\frac{\partial \mathbf{a}^{\top} \mathbf{X}^{-1} \mathbf{b}}{\partial \mathbf{X}} = -\mathbf{X}^{-\top} \mathbf{a} \mathbf{b}^{\top} \mathbf{X}^{-\top}$$

$$\frac{\partial \ln |\det(\mathbf{X})|}{\partial \mathbf{X}} = \mathbf{X}^{-\top}$$

## Solution

### Problem 3 (Classifying Stars, 15pts)

You're tasked with classifying three different kinds of stars, based on their magnitudes and temperatures. See `star.png` for a plot of the data, adapted from [http://astrosci.scimuze.com/stellar\\_data.htm](http://astrosci.scimuze.com/stellar_data.htm) and available as `data/hr.csv`, which you will find in the Github repository.

The CSV file has three columns: type, magnitude, and temperature. The first few lines look like this:

```
Type,Magnitude,Temperature
Dwarf,-5.8,-0.35
Dwarf,-4.1,-0.31
...
```

In this problem, you will code up 4 different classifiers for this task:

- A three-class generalization of logistic regression**, also known as softmax regression. You will do this by implementing gradient descent on the negative log-likelihood. You will need to find good values for the learning rate  $\eta$  (`self.eta`) and regularization strength  $\lambda$  (`self.lam`). Make sure to include a bias term and to use L2 regularization. See CS181 Textbook's Chapter 3.6 for more details on multi-class logistic regression and softmax.
- A generative classifier with Gaussian class-conditional densities with a *shared covariance matrix*** across all classes. Feel free to re-use your Problem 2 results.
- Another generative classifier with Gaussian class-conditional densities, but now with a *separate covariance matrix*** learned for each class. (Note: The staff implementation can switch between the two Gaussian generative classifiers with just a few lines of code.)
- A kNN classifier** in which you classify based on the  $k = 1, 3, 5$  nearest neighbors and the following distance function:  $\text{dist}(\text{star}_1, \text{star}_2) = ((\text{mag}_1 - \text{mag}_2)/3)^2 + (\text{temp}_1 - \text{temp}_2)^2$  (where nearest neighbors are those with the smallest distances from a given point).

Note: because we are predicting over a continuous space (not just the training data), we omit the step of making each training point ignore itself when selecting neighbors).

After implementing the above classifiers, complete the following exercises:

- Plot the decision boundaries generated by each classifier for the dataset. Include them in your PDF. Identify the similarities and differences among the classifiers. What explains the differences?
- For logistic regression only, make a plot with "Number of Iterations" on the x-axis and "Negative Log-Likelihood Loss" on the y-axis for several configurations of hyperparameters. Note which configuration yields the best final loss. What are your final choices of learning rate ( $\eta$ ) and regularization strength ( $\lambda$ ), and why are they reasonable? How does altering these hyperparameters affect the ability to converge and the rate of convergence (a qualitative description is sufficient)?
- For both Gaussian generative models, report the negative log-likelihood loss. Which model has a lower loss, and why? For the separate covariance model, be sure to use the covariance matrix that matches the true class of each data point.
- Consider a star with Magnitude 6 and Temperature 2. To what class does each classifier assign this star? Do the classifiers give any indication as to whether or not you should trust them?

**Implementation notes:** Run the controller file, `T2_P3.py`, to test your code. Write the actual implementations in the `GaussianGenerativeModel`, `LogisticRegression`, and `KNNModel` classes, which are defined in the three `T2_P3.ModelName.py` files. These classes follow the same interface pattern as `sklearn`. Their code currently outputs nonsense predictions just to show the high-level interface, so you should replace their `predict()` implementations. You'll also need to modify the hyperparameter values in `T2_P3.py` for logistic regression.

**Solution**

**Name**

**Collaborators and Resources**

Whom did you work with, and did you use any resources beyond cs181-textbook and your notes?

**Calibration**

Approximately how long did this homework take you to complete (in hours)?