

CSE546 Machine Learning HW1 - A

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1 A.0

1.1 In your own words, describe what bias and variance are? What is bias-variance trade-off?

In class, we have derived that the total variability is composed by three parts: irreducible error, bias and variance. Irreducible error is the lowest error that our model can get. Bias is how much our model is deviated from the true model. When the model is too simple, it is more likely to deviate largely from the model. When the model is too complex and fits all training data points. There would not be any bias at all. Variance is basically the variance of the model, when model is a horizontal line, there is no variance at all. But if the model is too complex, the geometry representation of the model becoming too zigzag, and this is where the variance tends to be very big. The bias-variance trade-off is saying that we need to find a balance point where testing error is at the lowest point. Testing error is presented as an u shape, so ideally we want to find the model that produces the testing error at the bottom of the u shape curve.

1.2 What happens to bias and variance when the model complexity increases/decreases?

When complexity increase, bias decrease, variance increase. When complexity decrease, bias increase, variance decrease. Bias will be monotonically decrease and finally fits all training data points. Variance will be monotonically increase.

1.3 True or False: The bias of a model increases as the amount of training data available increases.

False, bias does not depend on the amount of training data points.

1.4 True or False: The variance of a model decreases as the amount of training data available increases.

True, the variance does depend on the amount of training data.

1.5 True or False: A learning algorithm will generalize better if we use less features to represent our data.

False, we want enough useful and good predictors in the model. The quality of predictor and coefficients determined how good our model might be. And less feature will not be better to present the ground truth model.

1.6 To get better generalization, should we use the train set or the test set to tune our hyper-parameters?

We should use train set to train the model and get hyper-parameters. We must not use any testing data in getting the hyper-parameters.

1.7 True or False: The training error of a function on the training set provides an overestimate of the true error of that function.

False, since we saw in both practice and theory that the training error is always lower than the testing error, in expectation. And when we train our model, our best model are generated by minimizing the error on training data. So it is an optimistic/underestimated estimation of the true function.

A.1

Use MLE to estimate λ in Poisson Distribution.

a.

$$\begin{aligned}P(x|\lambda) &= \frac{e^{-\lambda}\lambda^x}{x!} \\P(x_1, x_2, x_3, x_4, x_5|\lambda) &= \prod_{i=1}^n \frac{e^{-\lambda}\lambda^{x_i}}{x_i!} \text{ (Where } n = 5.) \\ \hat{\lambda}_{MLE} &= \arg \max_{\lambda} (P(x_1, x_2, x_3, x_4, x_5|\lambda)) \\ &= \arg \max_{\lambda} \left(\prod_{i=1}^n \frac{e^{-\lambda}\lambda^{x_i}}{x_i!} \right) \\ &= \arg \max_{\lambda} \ln \left(\prod_{i=1}^n \frac{e^{-\lambda}\lambda^{x_i}}{x_i!} \right) \\ &= \arg \max_{\lambda} \sum_{i=1}^n \ln \left(\frac{e^{-\lambda}\lambda^{x_i}}{x_i!} \right) \\ &= \arg \max_{\lambda} \sum_{i=1}^n (\ln e^{-\lambda} + \ln \lambda^{x_i} - \ln(x_i!)) \\ &= \arg \max_{\lambda} (-n\lambda + \ln \lambda * \sum_{i=1}^n x_i + \sum_{i=1}^n \ln(x_i!)) \\ \text{Then set the derivative to 0.} \\ 0 &= \frac{d}{d\lambda} (-n\lambda + \ln \lambda * \sum_{i=1}^n x_i + \sum_{i=1}^n \ln(x_i!)) \\ &= -n + \frac{1}{\lambda} \sum_{i=1}^n x_i + 0 \\ n &= \frac{1}{\lambda} \sum_{i=1}^n x_i \\ \hat{\lambda}_{MLE} &= \frac{1}{n} \sum_{i=1}^n x_i, n = 5.\end{aligned}$$

b.

$$\begin{aligned}\hat{\lambda}_{MLE} &= \arg \max_{\lambda} (P(\mathcal{D}|\lambda)) \\ &= \arg \max_{\lambda} (P(x_1, x_2, x_3, x_4, x_5, x_6|\lambda)) \\ &= \frac{1}{n} \sum_{i=1}^n x_i, n = 6.\end{aligned}$$

c.

For λ after 5, $\hat{\lambda}_{MLE} = (2 + 0 + 1 + 1 + 2)/5 = \frac{6}{5}$.

For λ after 6, $\hat{\lambda}_{MLE} = (2 + 0 + 1 + 1 + 2 + 4)/6 = \frac{5}{3}$.

So, we can see the result that the outlier has a big effect on the estimation.

A.2 German tank problem

From the problem, we know that the serial of number came from a uniform distribution with $[0, \theta]$.

$$f(x_i) = \begin{cases} \frac{1}{\theta} & \text{for } 0 \leq x_i \leq \theta. \\ 0 & \text{Otherwise.} \end{cases}$$

We can derive the MLE with uniform distribution.

$$\begin{aligned} \hat{\theta}_{MLE} &= \arg \max_{\theta} (P(\mathcal{D}|\theta)) \\ &= \arg \max_{\theta} \left(\prod_{i=1}^n \frac{1}{\theta} \right) \\ &= \arg \max_{\theta} \ln \left(\prod_{i=1}^n \frac{1}{\theta} \right) \\ &= \arg \max_{\theta} \ln \left(\frac{1}{\theta^n} \right) \\ &= \arg \max_{\theta} -n \ln(\theta) \\ \frac{d(\ln(L(\theta)))}{d\theta} &= -n/\theta \end{aligned}$$

We can not set the derivative to zero in this particular problem since θ is impossible to be infinity. So here, the only thing we can do is let θ to be as large as it could be. We can not arbitrage assign value to θ . What we can do is to assign the biggest X we have observed to θ .

$$\hat{\theta} = \max(x_1, \dots, x_n)$$

A.3

a.

$$E_{train}[\hat{\epsilon}_{train}(f)] = E\left[\frac{1}{N_{train}} \sum_{(x,y) \in S_{train}} (f(x) - y)^2\right]$$

$$E_{train}[\hat{\epsilon}_{train}(f)] = \frac{N_{train}}{N_{train}} E[(f(x) - y)^2]$$

$$E_{train}[\hat{\epsilon}_{train}(f)] = E[(f(x) - y)^2] = \epsilon(f)$$

Since data from train and test are draw iid, the expectation for $(f(x) - y)^2$ should be the same.

$$E_{test}[\hat{\epsilon}_{test}(f)] = \frac{N_{test}}{N_{test}} E[(f(x) - y)^2] = E[(f(x) - y)^2] = \epsilon(f)$$

So,

$$E_{train}[\hat{\epsilon}_{train}(f)] = E_{test}[\hat{\epsilon}_{test}(f)] = \epsilon(f)$$

b.

No, the equation is not generally true, because the estimator we got from training is by minimizing the training error. It is not able to be general enough to describe the true model.

c.

From the hint we know that,

$$E_{train,test}[\hat{\epsilon}_{test}(\hat{f}_{train})] = \sum_{f \in \mathcal{F}} E_{test}[\hat{\epsilon}_{test}(f)] \mathbb{P}_{train}(\hat{f}_{train} = f)$$

From a., we know that $E_{train}[\hat{\epsilon}_{train}(f)] = E_{test}[\hat{\epsilon}_{test}(f)]$.

So,

$$= \sum_{f \in \mathcal{F}} E_{train}[\hat{\epsilon}_{train}(f)] \mathbb{P}_{train}(\hat{f}_{train} = f)$$

Since $\hat{\epsilon}_{train}(\hat{f}) \leq \hat{\epsilon}_{train}(f)$:

$$\begin{aligned} \sum_{f \in \mathcal{F}} E_{train}[\hat{\epsilon}_{train}(\hat{f})] \mathbb{P}_{train}(\hat{f}_{train} = f) &\leq \sum_{f \in \mathcal{F}} E_{train}[\hat{\epsilon}_{train}(f)] \mathbb{P}_{train}(\hat{f}_{train} = f) \\ \sum_{f \in \mathcal{F}} E_{train}[\hat{\epsilon}_{train}(\hat{f})] \mathbb{P}_{train}(\hat{f}_{train} = f) &\leq E_{train,test}[\hat{\epsilon}_{test}(\hat{f}_{train})] \end{aligned}$$

Because $\sum_{f \in \mathcal{F}} \mathbb{P}_{train}(\hat{f}_{train} = f) = 1$:

$$E_{train}[\hat{\epsilon}_{train}(\hat{f})] \sum_{f \in \mathcal{F}} \mathbb{P}_{train}(\hat{f}_{train} = f) \leq E_{train,test}[\hat{\epsilon}_{test}(\hat{f}_{train})]$$

$$E_{train}[\hat{\epsilon}_{train}(\hat{f}_{train})] \leq E_{train,test}[\hat{\epsilon}_{test}(\hat{f}_{train})]$$

A.4

```

1  import numpy as np
2
3
4  #-----
5  #  Class PolynomialRegression
6  #-----
7
8  class PolynomialRegression:
9
10 def __init__(self, degree=1, reg_lambda=1E-8):
11     """
12     Constructor
13     """
14     self.theta = None
15     self.regLambda = reg_lambda
16     self.degree = degree
17     self.mean = None
18     self.std = None
19
20 def polyfeatures(self, X, degree):
21     """
22     Expands the given X into an n * d array of polynomial features of
23     degree d.
24
25     Returns:
26     A n-by-d numpy array, with each row comprising of
27     X, X * X, X ** 3, ... up to the dth power of X.
28     Note that the returned matrix will not include the zero-th power.
29
30     Arguments:

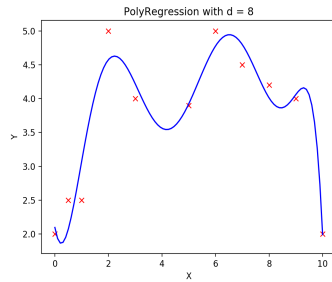
```

```

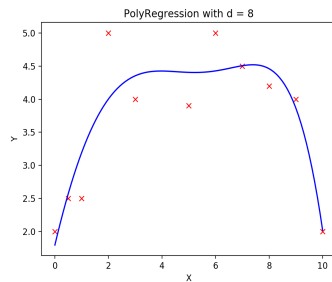
31 X is an n-by-1 column numpy array
32 degree is a positive integer
33 """
34 outputX = X[:]
35 for i in range(2, degree + 1):
36     outputX = np.hstack((outputX, X**i))
37 return outputX
38
39
40 def fit(self, X, y):
41     """
42     Trains the model
43     Arguments:
44     X is a n-by-1 array
45     y is an n-by-1 array
46     Returns:
47     No return value
48     Note:
49     You need to apply polynomial expansion and scaling
50     at first
51     """
52
53     X = self.polyfeatures(X, self.degree)
54     # standardization
55     self.mean = np.mean(X, axis=0)
56     self.std = np.std(X, axis=0)
57     X = (X - self.mean) / self.std
58     n = len(X)
59     # add 1s column
60     X_ = np.c_[np.ones([n, 1]), X]
61     n, d = X_.shape
62     reg_matrix = self.regLambda * np.identity(d )
63     reg_matrix[0, 0] = 0
64     self.theta = np.linalg.pinv((X_.T @ X_) + reg_matrix) @ (X_.T @ y)
65     print(self.theta)
66
67 def predict(self, X):
68     """
69     Use the trained model to predict values for each instance in X
70     Arguments:
71     X is a n-by-1 numpy array
72     Returns:
73     an n-by-1 numpy array of the predictions
74     """
75
76     n = len(X)
77     X = self.polyfeatures(X, self.degree)
78     X = (X - self.mean) / self.std
79     # add 1s column
80     X_ = np.c_[np.ones([n, 1]), X]
81     # predict
82     return X_ @ self.theta
83
84
85 #-----
86 # End of Class PolynomialRegression
87 #-----

```

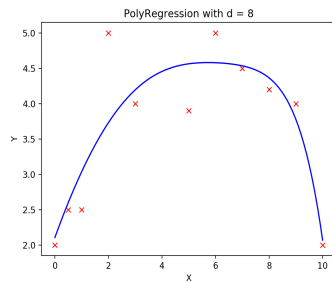
When lambda is 0:



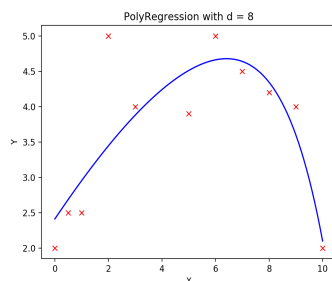
When lambda is 0.0001:



When lambda is 0.01:



When lambda is 0.1:



From the graph, we can see that when lambda increase our model gets smoother. And the model tends to be simpler. And the weight tends to be smaller.

A.5

```

1 def learningCurve(Xtrain, Ytrain, Xtest, Ytest, reg_lambda, degree):
2     """
3     Compute learning curve
4
5     Arguments:
6     Xtrain -- Training X, n-by-1 matrix
7     Ytrain -- Training y, n-by-1 matrix
8     Xtest  -- Testing X, m-by-1 matrix
9     Ytest  -- Testing Y, m-by-1 matrix
10    regLambda -- regularization factor
11    degree -- polynomial degree

```

12

13 *Returns:*14 *errorTrain* -- *errorTrain[i]* is the training accuracy using
15 *model* trained by *Xtrain[0:(i+1)]*16 *errorTest* -- *errorTrain[i]* is the testing accuracy using
17 *model* trained by *Xtrain[0:(i+1)]*

18

19 *Note:*20 *errorTrain[0:1]* and *errorTest[0:1]* won't actually matter, since we start displaying the learning curve
21 *""*22 `n = len(Xtrain)`

23

24 `errorTrain = np.zeros(n)`25 `errorTest = np.zeros(n)`

26

27 `for i in range(3, n+1):`28 `print("i = ", i, " Degree= ", degree, " lambda: ", reg_lambda)`29 `model = PolynomialRegression(degree, reg_lambda)`30 `model.fit(Xtrain[:i], Ytrain[:i])`

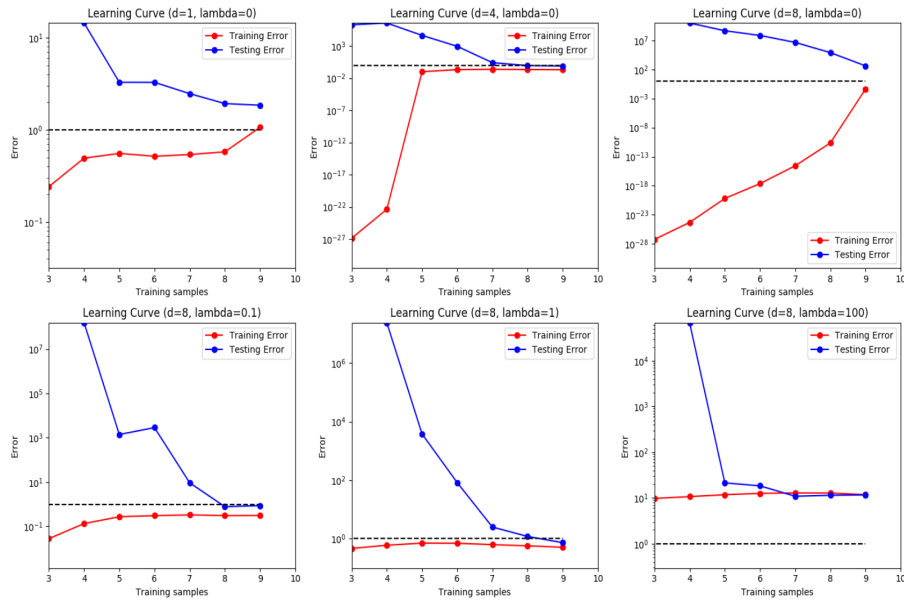
31

32 `trainPredicted = model.predict(Xtrain[:i])`33 `singleErrorFromTrain = np.mean((trainPredicted - Ytrain[:i])**2)`34 `errorTrain[i-1] = singleErrorFromTrain`

35

36 `test_predicted = model.predict(Xtest[:i])`37 `singleErrorFromTest = np.mean((test_predicted - Ytest[:i])**2)`38 `errorTest[i-1] = singleErrorFromTest`

39

40 `return errorTrain, errorTest`

A.6

a.

From the problem we know that:

$$\sum_{i=0}^n \|W^T x_i - y_i\|_2^2 + \lambda \|W\|_F^2 = \sum_{j=0}^k \left[\|X w_j - Y e_j\|^2 + \lambda \|w_j\|^2 \right]$$

Let:

$$A = \sum_{j=0}^k \left[\|Xw_j - Ye_j\|^2 + \lambda \|w_j\|^2 \right]$$

Take derivative:

$$\frac{\partial A}{\partial w_j} = \sum_{j=0}^k 2X^T [Xw_j - Ye_j] + 2\lambda w_j$$

Set derivative to 0 to find minimum,

$$0 = \sum_{j=0}^k 2X^T [Xw_j - Ye_j] + 2\lambda w_j$$

$$0 = \sum_{j=0}^k X^T Xw_j + \lambda w_j - X^T Ye_j$$

$$\sum_{j=0}^k (X^T X + \lambda I)w_j = \sum_{j=0}^k X^T Ye_j$$

Here, $X^T \in \mathbb{R}^{n \times d}$, $Y^T \in \mathbb{R}^{n \times k}$, $w_j \in \mathbb{R}^{d \times 1}$, $x_i \in \mathbb{R}^{d \times 1}$, $y_i \in \mathbb{R}^{k \times 1}$, $\lambda \in \mathbb{R}$, $e_j \in \mathbb{R}^{k \times 1}$, let's write it in matrix form:

$$(X^T X + \lambda I)\hat{W} = X^T Y$$

$$\hat{W} = (X^T X + \lambda I)^{-1} X^T Y$$

b.

```

1  import mnist
2  import numpy as np
3
4  mndata = mnist.MNIST("./python-mnist/data/")
5  X_train, labels_train = map(np.array, mndata.load_training())
6  X_test, labels_test = map(np.array, mndata.load_testing())
7  X_train = X_train/255.0
8  X_test = X_test/255.0
9
10 # Train function
11 def train(X,y,lam):
12     n, d = X.shape
13     y = np.eye(10)[y] # put y into a one hot encoding matrix
14     reg_matrix = self.regLambda * np.identity(d )
15     reg_matrix[0, 0] = 0
16     self.theta = np.linalg.pinv((X_.T @ X_) + reg_matrix) @ (X_.T @ y)
17     return W
18
19 def predict(W, X_new):
20     return (X_new @ W_hat).argmax(axis=1)
21
22 # Compute weights
23 W_hat = train(X_train, labels_train, lam = 0.00001)
24 # Computed predicted training label
25 predicted_train = predict(W=W_hat, X_new=X_train)
26 # Compute predicted testing label
27 predicted = predict(W=W_hat, X_new=X_test)
28 # Compute error rate for both training and testing
29 train_error_rate = 1 - (sum(predicted_train == labels_train) / len(labels_train))
30 test_error_rate = 1 - (sum(predicted == labels_test) / len(labels_test))
31 print("Training Accuracy is: ", train_error_rate)

```



```
32 print("Testing Error Rate is: ", test_error_rate)
33 #Training Error is:  0.14806666666666668
34 #Testing Error Rate is:  0.14659999999999995
```