Introduction to Machine Learning (67577)

Exercise V – Validation, Feature Selection and Regularization

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**Theoretical Questions**

**Validation**

1. Bounding the generalization error using the *standard method*

From Hoeffding’s inequality we know that , therefore, . If we set we have . Inverting the signs . Using Hoeffding’s yet again while adding to the , we have

This is true for every , therefore using Union bound over all we get

So, inverting the probabilities yet again - for every we have . Let us concentrate in the inner section of the probability, and for

is better than any , so

Substituting again:

This is true , therefore we can substitute with . Consequently, we have that with probability at least ,

1. Bounding the generalization error using *model selection*

Using section (A) with , the validation set of size and is of size , therefore we have

Denote the best in as , so with probability we have

the training set, on the other hand, is of size , and for every we have

If so, with probability we have

in total the probability of the two independent events is at least , and specifically is at least

1. The first case would be when the model selection is better than the standard method – this can be achieved if the best index is smaller than , that is . for such if we take the size of to be for every and for some constant c

For the standard model -

For the model selection -

From here it is understood that the standard model error is increasing with magnitude , that is, linear in though the model selection increases with , so for large the error for the model selection would be smaller.

If than for the standard method we have and for the model selection we get . From here we understand that the standard method is preferred because

Since the second element is nonnegative, we can consider the first element and see that

Now since the first element is greater than 1, and the second element is greater than . In other words, the model selection’s error is greater than the standard model.

**Orthogonal Design**

1. Prove :

We have seen that . Using the fact that we have

1. Prove :

We know that the error, given some weights vector , is . Since we want to minimize the loss, we can multiply by without worrying that the result will change:

Substituting the above to the subset selection problem we have

From here we understand that if for some , then , which in turn means that . This in correlation to the definition of . If on the other hand , we get . In other words, we have

**Regularization**

1. starting with , We know that is given by (this is the solution with no regularization) therefore . We have seen in class that this form is exactly , so we are done.
2. We will show that

Since we are given with a constant , the expectancy of is simply

Now, if would have been , then would be . But since we have , therefore , as needed.

1. Show that :

Using the hint, we have

1. Similar to what we have seen in class, let us denote as the true hypothesis, as the expectancy and as the estimation. Under those definitions we can write . This is because and .

The true hypothesis is the expectancy of (with no regularization terms), that is . Furthermore, our estimator (with regularization) is therefore also . We can now calculate the needed values:

For the variance, we have

For simplicity let us denote , so and

Now, deriving the variance in terms of (Trace is a linear operation; hence it commutes with the derivative)

Now deriving in terms of :

Which is a negative value.

And for the bias

If so,

Or in terms of

Again, deriving (and using summation syntax)

So, the MSE is given by

And the derivative is the sum of derivatives, which is , simply because the derivative of the bias squared is zero, and the derivative of the variance is negative.

1. We know that the linear model with no regularization is the case where . Now, since we have found in (3.D) that for some , , we conclude that such satisfies . In other words, using regularization we have decreased the error – which is awesome.

**Practical Questions**

**k-Fold Cross Validation on Polynomial Fitting**



A,B,C & D: code

E. The first graph is for 2-Fold (where each data point was only used once, either for training or for validation):

Chart, line chart

Description automatically generated



**k-Fold and Regularization**