CSCI 5622: Machine Learning
Assignment Q3 Bias Variance Derivation
Laksh Advani

September 15, 2017

- Derive the bias-variance decomposition for k-NN regression in class. Specifically assuming the training set is fixed $S = (x_1, y_1), ..., (x_n, y_n)$, where the data are generated from the process $y = f(x) + \epsilon, E(\epsilon) = 0, Var(\epsilon) = \sigma^2$. k-NN regression algorithm predict the value for x_0 as $h_s = 1/k\sum_{l=1}^{k} y(l)$ where $x_(l)$ is the l-th nearest neighbor to x_0. $Err(x_0)$ is defined as $E((y_0 - h_s(x_0))^2)$.

  Prove that

  $Err(x_0) = (\sigma_\epsilon)^2 + [f(x_0) - 1/k\sum_{l=1}^{k} f(x_{(l)})]^2 + (\sigma_\epsilon)^2/k$

  Answer: We have the error $Err(x_0)$ given as: $Err(x_0) = E((y - h(x_0))^2)$

$$Err(x_0) = E(f(x) + \epsilon - h(x_0))^2$$

$$Err(x_0) = f(x_0)^2 + \epsilon^2 + h(x_0)^2 + 2f(x_0).\epsilon - 2\epsilon.h(x_0) - 2f(x_0).h(x_0)$$

$$Err(x_0) = E(\epsilon^2 + 2\epsilon(f(x_0) - h(x_0))) + ((f(x_0) - h(x_0))^2)$$

$$Err(x_0) = E\epsilon^2 + 2E\epsilon * E(f(x_0) - h(x_0))) + E((f(x_0) - h(x_0))^2$$

The second term in the equation above will become '0' since $E\epsilon$ is zero.

$$2E\epsilon * E(f(x_0) - h(x_0))) = 0$$

$$Err(x_0) = (\sum \epsilon^2) + E(f(x_0) - h(x_0))^2$$

$$Err(x_0) = (\sigma_\epsilon^2) + (f(x_0) - E(h(x_0)))^2 + var(h(x_0))$$

Let us look at the $bias^2$, $((f(x_0) - Eh(x_0))^2)$
Here we replace $(h(x_0))$ with its value $1/k\sum_{l=1}^{k} y(l)$

We can move the terms around since the $bias^2$ is made up of squared terms.

$$bias^2 = ((f(x_0) - 1/k\sum_{l=1}^{k} y(l)))^2$$

Which is:

$$bias^2 = [(f(x_0) - 1/k\sum_{l=1}^{k} f(x_{(l)})]^2$$

Given that the set S is fixed, if we take the expectation of the bias over the test samples we will see that all the ϵ values disappear because the test sample has zero mean, so the value $E.1/k\sum_{l=1}^{k} y(l)))^2 = 1/k\sum_{l=1}^{k} f(x_{(l)}))^2$.
Now we will work on the variance section:

$$variance = var(h(x_0))$$

Here we will substitute the value of $h(x_0)$ with $1/k\sum_{l=1}^{k} y(l)$

$$variance = var(1/k\sum_{l=1}^{k} y(l))$$

$$variance = var(1/k\sum_{l=1}^{k} f(x_(l)) + \epsilon)$$

Here, we will use the following identity, $Var(aX) = a^2 Var(X)$

$$variance = 1/(k^2)\sum_{l=1}^{k} var(f(x_l) + \epsilon)$$

$$variance = 1/(k^2)\sum_{l=1}^{k} var(f(x_l)) + var(\epsilon)$$

$$variance = 1/(k^2)\sum_{l=1}^{k} var(f(x_l)) + var(\epsilon)$$

Given that set S is fixed, the neighbors have no variance, which implies that:
$var(f(x_l)) = 0$

Hence, we get:

$$variance = 1/(k^2)\sum_{l=1}^{k} var(\epsilon)$$

$$variance = (1/(k^2))k(\sigma_\epsilon^2)$$

$$variance = (1/(k))(\sigma_\epsilon^2)$$

Now we have the following:

$variance = (1/(k))(\sigma_\epsilon^2)$

$bias^2 = [(f(x_0) - 1/k \sum_{l=1}^{k} f(x_{(l)})]^2$

Now when we substitute the values of $bias^2$ and variance we get our intended equation:

$$Err(x_0) = (\sigma_\epsilon)^2 + [f(x_0) - 1/k \sum_{l=1}^{k} f(x_{(l)})]^2 + (\sigma_\epsilon)^2/k$$