ML Notes

Somnath Sikdar

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Chapter 1

Bias-Variance Decomposition

The bias-variance decomposition is the decomposotion of the generalization error of a predictor into the sum of the bias, the variance and an irreducible error term.

Consider a setting where a response variable Y is related to a set of predictor variables $X \in \mathbf{R}^p$ as follows: $Y = f(X) + \varepsilon$, where $f\colon \mathbf{R}^p \to \mathbf{R}$ is some deterministic function and ε is white noise. That is, $\mathbf{E}\left[\varepsilon | X = x\right] = 0$ and $\mathrm{Var}(\varepsilon | X = x) = \sigma^2$, for some variance σ^2. Let us assume that there is an underlying data distribution $\mathscr{D}(X, Y)$ which is unknown to us. We have an algorithm that, given an n-sized training set $S = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ sampled iid from this distribution $\mathscr{D}$, yields $\hat{f}_S$, which is an approximation to the true function f. We assume that the algorithm itself is deterministic: that is, given the same n-sized sample S, it produces the same output $\hat{f}_S$.

What is the expected generalization error of this algorithm? This is defined as:

$$\mathbf{E}_{S \sim \mathscr{D}^n, (X,Y) \sim \mathscr{D}} \left[(Y - f_S\hat{(X)})^2 \right]. \tag{1.1}$$

We may write this as:

$$\mathbf{E}_{S \sim \mathscr{D}^n, (X,Y) \sim \mathscr{D}} \left[(Y - \hat{f}_S(X))^2 \right] = \int \mathbf{E}_{(X,Y) \sim \mathscr{D}} \left[(Y - \hat{f}_S(X))^2 \mid S \right] \cdot \mathbf{Pr}_{\mathscr{D}^n} \left\{ S \right\} \mathrm{d}S. \tag{1.2}$$

We will first work with the expectation term on the right-hand side of the above equation. That is, we will assume that the sample S is fixed and then calculate the expected error wrt the approximation $\hat{f}_S$. In order to implify our notation a bit, we will index the expectation operator with the random variable to indicate which distribution is being referred to.

Let us write $(Y - \hat{f}_S(X))^2$ as $(Y - f(X) + f(X) - \hat{f}_S(X))^2$. Expanding, we get:

$$\begin{aligned} \mathbf{E}_{(X,Y)} \left[(Y - \hat{f}_S(X))^2 | S \right] = {} & \mathbf{E}_{(X,Y)} \left[(f(X) - \hat{f}_S(X))^2 | S \right] + \\ & \mathbf{E}_{(X,Y)} \left[(Y - f(X))^2 | S \right] + \\ & \mathbf{E}_{(X,Y)} \left[2(Y - f(X))(f(X) - \hat{f}_S(X)) | S \right] \end{aligned} \tag{1.3}$$

Consider the last term on the right-hand side. We claim that this is 0. Indeed, we may write $\mathbf{E}_{(X,Y)}\left[2(Y-f(X))(f(X)-\hat{f}_S(X))|S\right]$ as

$$
\begin{aligned}
&= \iint 2\cdot(y-f(x))\cdot(f(x)-\hat{f}_S(x))\cdot p_{X,Y}(x,y)\mathrm{d}y\,\mathrm{d}x\\
&= \iint 2\cdot(y-f(x))\cdot(f(x)-\hat{f}_S(x))\cdot p_{Y|X}(y|x)\cdot p_X(x)\mathrm{d}y\,\mathrm{d}x\\
&= \int 2\cdot(f(x)-\hat{f}_S(x))\cdot\mathbf{E}_{Y|X}\left[Y-f(x)|X=x\right]\cdot p_X(x)\mathrm{d}x.
\end{aligned}
$$

Now we know that $\mathbf{E}_{Y|X}\left[Y-f(x)|X=x\right]=\mathbf{E}_{Y|X}\left[\varepsilon|X=x\right]=0$. Hence this whole expression evaluates to 0 as claimed.

Next consider the second term $\mathbf{E}_{(X,Y)}\left[(Y-f(X))^2|S\right]$ of Equation (1.3). Since the term $(Y-f(X))^2$ does not depend on the sample S that is chosen, this further simplifies to $\mathbf{E}_{(X,Y)}\left[(Y-f(X))^2\right]$. This is simply the variance of the error term and is equal to σ^2. Finally, consider the first term of Equation (1.3) which is $\mathbf{E}_{(X,Y)}\left[(f(X)-\hat{f}_S(X))^2|S\right]$. We use the trick of adding and subtracting as before. This time around, we add and subtract the term $g(X) \coloneqq \mathbf{E}_S\left[\hat{f}_S(X)\right]$ to obtain:

$$
\begin{aligned}
(f(X)-g(X)+g(X)-\hat{f}_S(X))^2 = (f(X)-g(X))^2+(g(X)-\hat{f}_S(X))^2+\\
2\cdot(f(X)-g(X))\cdot(g(X)-\hat{f}_S(X)).
\end{aligned}
\tag{1.4}
$$

We will evaluate each of these terms by directly plugging them in the expression in Equation (1.2). Let's examine the first term $(f(X)-g(X))^2$. Plugging this in the said expression, we see that we have to evaluate:

$$
\begin{aligned}
\int \mathbf{E}_{(X,Y)}\left[(f(X)-g(X))^2|S\right]\mathbf{Pr}_{S\sim\mathscr{D}^n}\left\{S\right\}\mathrm{d}S &= \mathbf{E}_{(X,Y)}\left[(f(X)-g(X))^2\right]\int \mathbf{Pr}_{S\sim\mathscr{D}^n}\left\{S\right\}\mathrm{d}S\\
&= \mathbf{E}_{(X,Y)}\left[(f(X)-g(X))^2\right].
\end{aligned}
\tag{1.5}
$$

The first equality holds because neither $f(X)$ nor $g(X)$ depends on the sample S chosen. The resulting expression is the expected squared bias of the estimator $\hat{f}_S$.

Forging ahead, we evaluate the next term which is $(g(X)-\hat{f}_S(X))^2$.

$$
\int \mathbf{E}_{(X,Y)}\left[(g(X)-\hat{f}_S(X))^2|S\right]\mathbf{Pr}_{S\sim\mathscr{D}^n}\left\{S\right\}\mathrm{d}S = \mathbf{E}_{S,(X,Y)}\left[(g(X)-\hat{f}_S(X))^2\right].
\tag{1.6}
$$

This term is the variance of the estimator $\hat{f}_S$ obtained by our algorithm.

Finally, we evaluate the term $2\cdot(f(X)-g(X))\cdot(g(X)-\hat{f}_S(X))$. We now have to evaluate this integral:

$$
\int \mathbf{E}_{(X,Y)}\left[2\cdot(f(X)-g(X))\cdot(g(X)-\hat{f}_S(X))|S\right]\mathbf{Pr}_{S\sim\mathscr{D}^n}\left\{S\right\}\mathrm{d}S
\tag{1.7}
$$

This may be written as:

$$
\iint \mathbf{E}_S\left[2\cdot(f(x)-g(x))\cdot(g(x)-\hat{f}_S(x))|X=x,Y=y\right]p_{X,Y}(x,y)\mathrm{d}y\,\mathrm{d}x.
\tag{1.8}
$$

Now the term $f(x) - g(x)$ does not depend on S and $\mathbf{E}_S\left[g(x) - \hat{f}_S(x)\right] = 0$ and hence the above integral evaluates to 0.

To summarize, we may write the expected generalization error of our algorithm as:

$$\begin{aligned}
\mathbf{E}_{S\sim\mathscr{D}^n,(X,Y)\sim\mathscr{D}}\left[(Y - \hat{f}_S(X))^2\right] &= \underbrace{\mathbf{E}_{(X,Y)}\left[(\mathbf{E}_S\left[\hat{f}_S(X)\right] - f(X))^2\right]}_{\text{expected squared bias}} \\
&\quad + \underbrace{\mathbf{E}_{S,(X,Y)}\left[(\hat{f}_S(X) - \mathbf{E}_S\left[\hat{f}_S(X)\right])^2\right]}_{\text{variance}} \\
&\quad + \underbrace{\sigma^2}_{\text{irreducible error}} .
\end{aligned}$$