Approximation error versus variability

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**Theorem.** Assume $(X_1, Y_1), \ldots, (X_n, Y_n)$ (training data) and $(\bar{X}, Y)$ are IID random examples, and also assume the predictor $F$ only depends on the training data. For any feature vector $\bar{x}$,

\[
\begin{align*}
\mathbb{E}[(F(\bar{x}) - Y)^2 \mid \bar{X} = \bar{x}] &= \mathbb{E}[F(\bar{x})] - \eta(\bar{x})^2 \quad \text{("approximation error")}
\end{align*}
\]

where $\eta(\bar{x}) := \mathbb{E}[Y \mid \bar{X} = \bar{x}]$.

**Proof.** By assumption, $F(\bar{x})$ is independent of $(\bar{X}, Y)$. We shall use this fact a couple of times below.

Let us use the notation $\mathbb{E}_x[\cdot]$ for conditional expectation given $\bar{X} = \bar{x}$, i.e., $\mathbb{E}[\cdot \mid \bar{X} = \bar{x}]$. By the tower property of conditional expectation,

\[
\mathbb{E}_x[(F(\bar{x}) - Y)^2] = \mathbb{E}_x[\mathbb{E}_x[(F(\bar{x}) - Y)^2 \mid F(\bar{x})]] \tag{1}
\]

Let us first consider the “inner” conditional expectation ($\ast$). By the bias-variance decomposition,

\[
\begin{align*}
\mathbb{E}_x[(F(\bar{x}) - Y)^2 \mid F(\bar{x})] &= (F(\bar{x}) - \mathbb{E}_x[Y \mid F(\bar{x})])^2 \quad \text{("squared bias")}
\end{align*}
\]

where the second step uses the independence of $F(\bar{x})$ and $(\bar{X}, Y)$. Plugging this back into Equation (1), we obtain

\[
\begin{align*}
\mathbb{E}_x[(F(\bar{x}) - Y)^2] &= \mathbb{E}_x[(F(\bar{x}) - \eta(\bar{x}))^2] + \mathbb{E}_x[(Y - \eta(\bar{x}))^2]
\end{align*}
\]

where, again, the second step uses the independence of $F(\bar{x})$ and $(\bar{X}, Y)$. This first term on the right-hand side ($\ast\ast$) in Equation (2) can be written as

\[
\begin{align*}
\mathbb{E}[(F(\bar{x}) - \eta(\bar{x}))^2] &= (\mathbb{E}[F(\bar{x})] - \eta(\bar{x}))^2 \quad \text{("squared bias")}
\end{align*}
\]

by the bias-variance decomposition. Plugging this back into Equation (2) finally gives

\[
\begin{align*}
\mathbb{E}_x[(F(\bar{x}) - Y)^2] &= (\mathbb{E}[F(\bar{x})] - \eta(\bar{x}))^2 \\
&\quad + \mathbb{E}_x[(Y - \eta(\bar{x}))^2].
\end{align*}
\]

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