STA 314: Statistical Methods for Machine Learning I

Lecture 3 - Bias-Variance Decomposition

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Today

- Expand a bit on Q3 and Q4 of the HW1.
- Today we will talk about the bias-variance decomposition, which is beginning to make more precise our discussion of overfitting and underfitting last class.

Q3, HW1

- Given any finite set $\{x_i\}_{i=1}^N$ of $x_i \in \mathbb{R}$, we can define the uniform random variable over $\{x_i\}_{i=1}^N$, which is any D such that

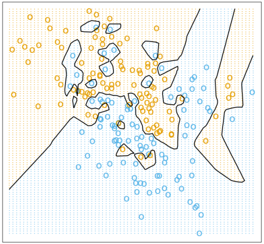
$$P(D = x_i) = \frac{1}{N}$$

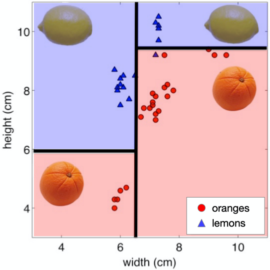
- Sampling from this random variable is easy: sample an integer $J \in \{1, \ldots, N\}$ uniformly at random and return x_J.
- For this distribution, we have

$$\mathbb{E}[D] = \sum_{i=1}^{N} P(D = x_i) x_i = \sum_{i=1}^{N} \frac{1}{N} x_i$$

Recall: supervised learning

- In supervised learning, our learning algorithms (k-NN, decision trees) produce predictions $\hat{y}^\star(\mathbf{x}) \approx t$ for a query point $\mathbf{x}$.





Recall: supervised learning

- We can think of this as picking a predictor function $\hat{y}^\star \in \mathcal{H}$ from a hypothesis class by minimizing the average loss on the training set

$$\hat{y}^\star = \arg\min_{y \in \mathcal{H}} \hat{\mathcal{R}}[y, \mathcal{D}^{train}]$$

- Then, we measure the average loss on an unseen test set to approximate how well $\hat{y}^\star$ does on the true data generating distribution,

$$\hat{\mathcal{R}}[\hat{y}^\star, \mathcal{D}_{test}] \approx \mathcal{R}[\hat{y}^\star]$$

Recall: supervised learning

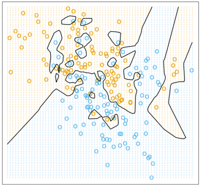
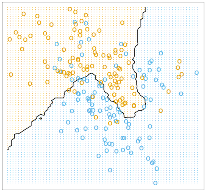
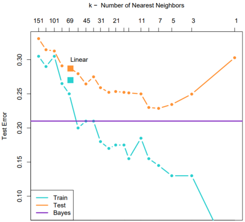
- This view of supervise learning is a very idealized view:
  - k-NN algorithm for $k > 1$ doesn't really select the predictor by minimizing a global loss.
  - Decision tree fitting does select $\hat{y}^\star$ based on training loss, but it is often greedy and sometimes does not find the global optimal $\hat{y}^\star$.
- Still, it's a very useful general model for supervised learning.

Q4, HW1

- Let's consider Q4 in HW1 as a way to review this supervised framewrok.

Bias-Variance Decomposition

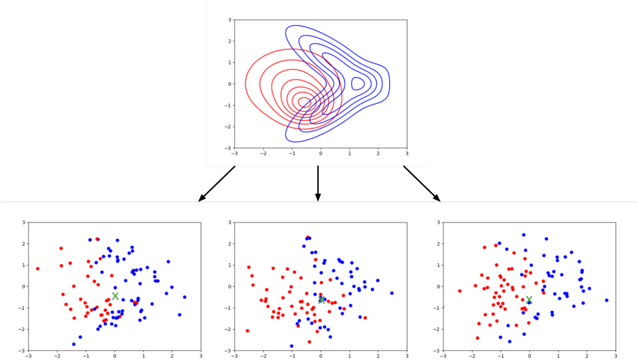
- Recall that overly simple hypothesis classes underfit the data, and overly complex ones overfit.

- Last lecture we talked about this intuitively.
- We can quantify this effect in terms of the bias-variance decomposition.
  - So far we've been talking about the training set as if it is fixed, but it makes more sense to think of it as random.
  - So, we'd like to understand how our learning algorithm is impacted by selecting a predictor on a finite, random, training set.

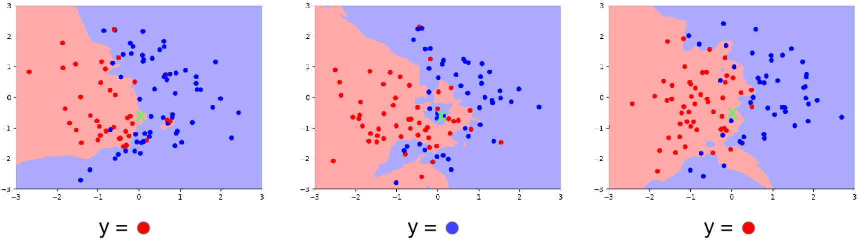
Bias-Variance Decomposition: Basic Setup

- Recall: the training set $\mathcal{D}^{train} = \{(\mathbf{x}^{(i)}, t^{(i)})\}_{i=1}^{N}$ contains N i.i.d. draws from a single data generating distribution p_{data}.
- Consider a fixed query point $\mathbf{x}$ (green $\mathbf{x}$ below).
- Consider sampling many training sets $\mathcal{D}_n^{train}$ independently from p_{data}.



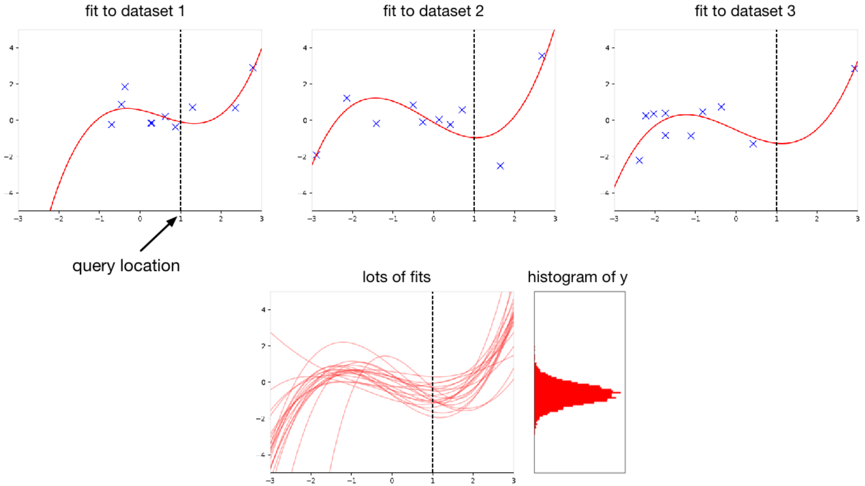
Bias-Variance Decomposition: Basic Setup

- For each training set $\mathcal{D}_n^{train}$, run learning alg. to get a predictor $\hat{y}_n^\star \in \mathcal{H}$.
- Compute the prediction $\hat{y}_n^\star(\mathbf{x})$ and compare it to a label t drawn from $p_{\text{data}}(t|\mathbf{x})$.
- We can view $\hat{y}_n^\star$ as a random variable, where the randomness comes from the choice of training set.



Bias-Variance Decomposition: Basic Setup

Here is the analogous setup for regression:



Bias-Variance Decomposition: Basic Setup

- Recap of basic setup:
  - Fix a query point $\mathbf{x}$.
  - Sample the (true) target t from the conditional distribution $p_{\text{data}}(t|\mathbf{x})$.
  - Repeat:
    - Sample a random training dataset $\mathcal{D}_n^{train}$ i.i.d. from the data generating distribution p_{data}.
    - Run the learning algorithm on $\mathcal{D}_n^{train}$ to get a prediction $\hat{y}_n^\star(\mathbf{x})$ from $\mathcal{H}$ at $\mathbf{x}$.
    - Compute the loss $L(\hat{y}_n^\star(\mathbf{x}), t)$.
  - Average the losses.
- Notice: y is independent of t given $\mathbf{x}$.
- This gives a distribution over the loss at $\mathbf{x}$, with expectation $\mathbb{E}[L(\hat{y}^\star(\mathbf{x}), t) \,|\, \mathbf{x}]$ taken over t and the *random* training set $\mathcal{D}^{train}$ where $\hat{y}^\star = \arg\min_{y \in \mathcal{H}} \hat{\mathcal{R}}[y, \mathcal{D}^{train}]$.
- For each query point $\mathbf{x}$, the expected loss is different. We are interested in minimizing the expectation of this with respect to $\mathbf{x} \sim p_{\text{data}}(\mathbf{x})$.

Bayes Optimality

- For now, focus on squared error loss, $L(y, t) = \frac{1}{2}(y - t)^2$ with $y, t \in \mathbb{R}$.
- A first step: suppose we knew the conditional distribution $p_{\mathrm{data}}(t \mid \mathbf{x})$. What is the best deterministic value $y(\mathbf{x}) \in \mathbb{R}$ should we predict?
  - Here, we are treating t as a random variable and choosing $y(\mathbf{x})$.
- **Claim:** $y^\star(\mathbf{x}) = \mathbb{E}[t \mid \mathbf{x}]$ is the best possible prediction.
- **Proof:** Consider a fixed $y \in \mathbb{R}$

$$\begin{aligned}
\mathbb{E}[(y - t)^2 \mid \mathbf{x}] &= \mathbb{E}[y^2 - 2yt + t^2 \mid \mathbf{x}] \\
&= y^2 - 2y\mathbb{E}[t \mid \mathbf{x}] + \mathbb{E}[t^2 \mid \mathbf{x}] \\
&= y^2 - 2y\mathbb{E}[t \mid \mathbf{x}] + \mathbb{E}[t \mid \mathbf{x}]^2 + \mathrm{Var}[t \mid \mathbf{x}] \\
&= y^2 - 2yy^\star(\mathbf{x}) + y^\star(\mathbf{x})^2 + \mathrm{Var}[t \mid \mathbf{x}] \\
&= (y - y^\star(\mathbf{x}))^2 + \mathrm{Var}[t \mid \mathbf{x}]
\end{aligned}$$

Bayes Optimality

$$\mathbb{E}[(y - t)^2 \mid \mathbf{x}] = (y - y^\star(\mathbf{x}))^2 + \mathrm{Var}[t \mid \mathbf{x}]$$

- The first term is nonnegative, and can be made 0 by setting $y = y^\star(\mathbf{x})$.
- The second term corresponds to the inherent unpredictability, or noise, of the targets, and is called the Bayes error.
  - This is the best we can ever hope to do with any learning algorithm. An algorithm that achieves it is Bayes optimal.
  - Notice that this term doesn't depend on y.
- This process of choosing a single value $y^\star(\mathbf{x})$ based on $p_{\mathrm{data}}(t \mid \mathbf{x})$ is an example of decision theory.

Bayes Optimality

- But, in practice, our prediction $\hat{y}^\star(\mathbf{x})$ is not $y^\star(\mathbf{x})$. Instead, it is a random variable (where the randomness comes from randomness of the training set) taking values in $\mathcal{H}$.
- We can decompose out the expected loss.
- Suppressing the dependence on $\mathbf{x}$ for clarity:

$$
\begin{aligned}
\mathbb{E}[(\hat{y}^\star - t)^2] &= \mathbb{E}[(\hat{y}^\star - y^\star)^2] + \mathrm{Var}(t) \\
&= \mathbb{E}[{y^\star}^2 - 2y^\star \hat{y}^\star + {\hat{y}^\star}{}^2] + \mathrm{Var}(t) \\
&= {y^\star}^2 - 2y^\star\, \mathbb{E}[\hat{y}^\star] + \mathbb{E}[{\hat{y}^\star}{}^2] + \mathrm{Var}(t) \\
&= {y^\star}^2 - 2y^\star\, \mathbb{E}[\hat{y}^\star] + \mathbb{E}[\hat{y}^\star]^2 + \mathrm{Var}(\hat{y}^\star) + \mathrm{Var}(t) \\
&= \underbrace{(y^\star - \mathbb{E}[\hat{y}^\star])^2}_{\text{bias}} + \underbrace{\mathrm{Var}(\hat{y}^\star)}_{\text{variance}} + \underbrace{\mathrm{Var}(t)}_{\text{Bayes error}}
\end{aligned}
$$

Bayes Optimality

- Let's step back and consider what we just did. First, recall:
  - Picking a predictor by minimizing the average loss on the training set

$$\hat{y}^\star = \arg\min_{y \in \mathcal{H}} \hat{\mathcal{R}}[y, \mathcal{D}^{train}]$$

    returns a random predictor $\hat{y}^\star$.
  - But, we're interested in our performance in terms of expected loss:

$$\mathcal{R}[\hat{y}^\star]$$

- In our case:

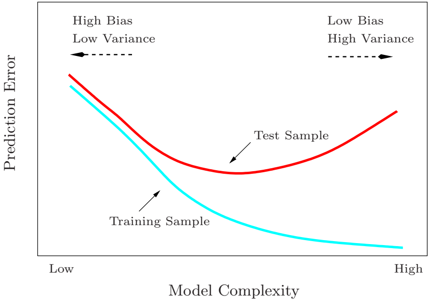
$$\mathcal{R}[\hat{y}^\star] = \mathbb{E}\left[\mathbb{E}[(\hat{y}^\star(\mathbf{x}) - t)^2 \mid \mathbf{x}]\right].$$

Bayes Optimality

$$\mathbb{E}\left[\mathbb{E}[(\hat{y}^\star(\mathbf{x}) - t)^2 \mid \mathbf{x}]\right] = \mathbb{E}\left[\underbrace{(y^\star(\mathbf{x}) - \mathbb{E}[\hat{y}^\star(\mathbf{x}) \mid \mathbf{x}])^2}_{\text{bias}} + \underbrace{\mathrm{Var}[\hat{y}^\star(\mathbf{x}) \mid \mathbf{x}]}_{\text{variance}} + \underbrace{\mathrm{Var}[t \mid \mathbf{x}]}_{\text{Bayes error}}\right]$$

- So, we just split the expected loss $\mathcal{R}[\hat{y}^\star]$ into three terms:
  - bias: how wrong the expected prediction is
  - variance: the amount of variability in the predictions
  - Bayes error: the inherent unpredictability of the targets
- How does our choice of $\mathcal{H}$ interact with this analysis?

Bayes Optimality

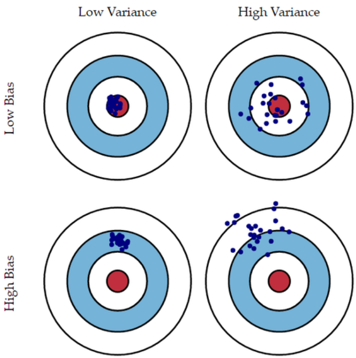


Source: ESL

- If $\mathcal{H}$ is large, then $\hat{y}^\star$ can get close $y^\star$, therefore reducing bias. It's also sensitive to the finite training set, therefore increasing variance.
- If $\mathcal{H}$ is small, then $\hat{y}^\star$ is typically from $y^\star$, therefore increasing bias. It's less sensitive to the finite training set, therefore reducing variance.
- Even though this analysis only applies to squared error, we often loosely use "bias" and "variance" as synonyms for "underfitting" and "overfitting".

Bias and Variance

- Throwing darts = predictions for each draw of a dataset

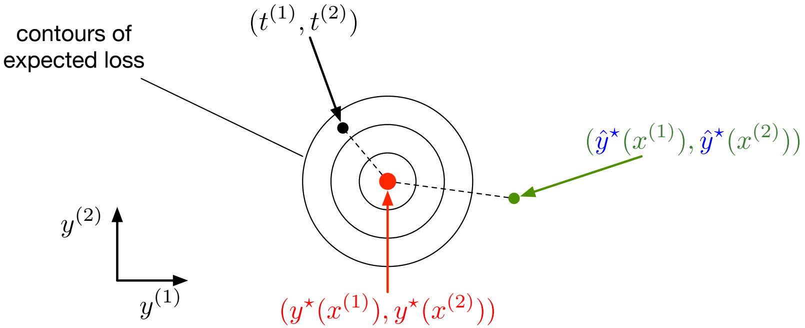


Source: ESL.

- Be careful, the expected loss averages over points **x** from the data distribution, so this produces its own type of variance.

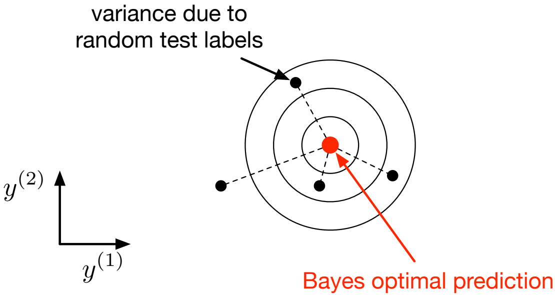
Bias/Variance Decomposition: Another Visualization

- In practice, measure the average loss $\hat{\mathcal{R}}[\hat{y}^\star, \mathcal{D}_{test}]$ on the test set instead of $\mathcal{R}[\hat{y}^\star]$.
- Let's visualize the bias-variance decomposition by plotting the space of predictions of the model, where each axis correspond to predictions on a two test examples $(\mathbf{x}^{(1)}, \mathbf{x}^{(2)})$.



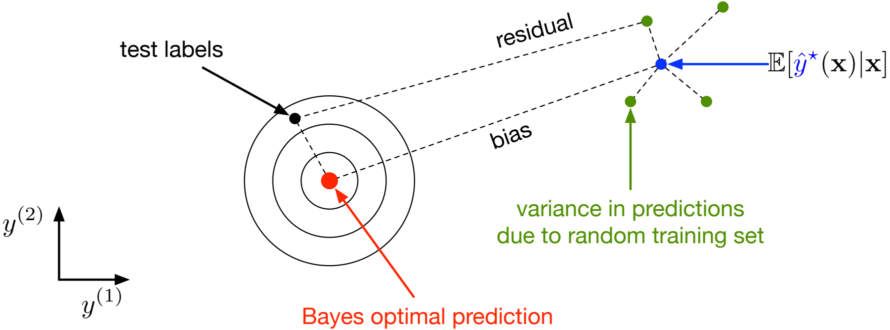
Bias/Variance Decomposition: Another Visualization

- The Bayes error is an irreducible error that comes from the randomness in $p_{\mathrm{data}}(t \mid \mathbf{x})$.



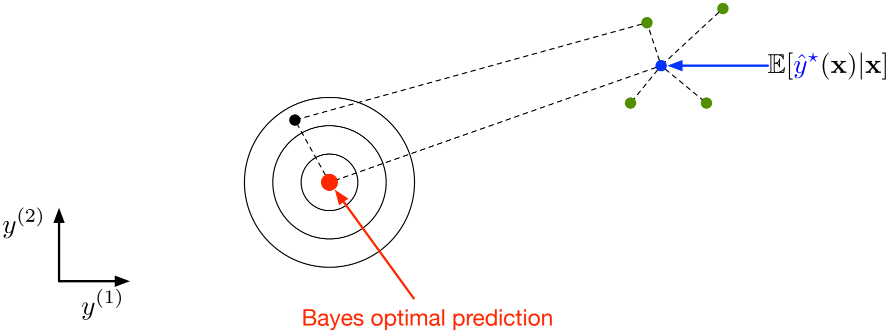
Bias/Variance Decomposition: Another Visualization

- Selecting a predictor $\hat{y}^\star \in \mathcal{H}$ from a training set comes with bias and variance.



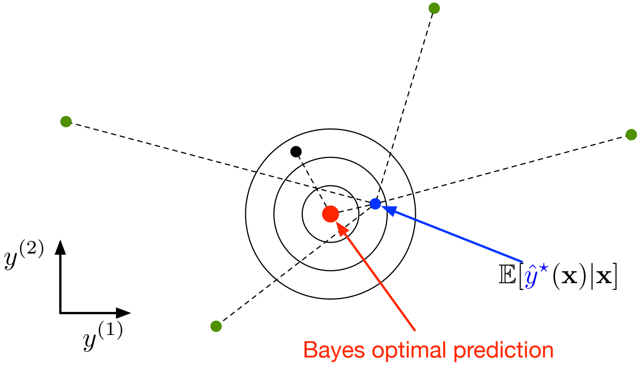
Bias/Variance Decomposition: Another Visualization

- An overly simple model (e.g. k-NN with large k) might have
  - high bias (too simplistic to capture the structure in the data)
  - low variance (there's enough data to get a stable estimate of the decision boundary)



Bias/Variance Decomposition: Another Visualization

- An overly complex model (e.g. KNN with $k = 1$) may have
  - low bias (since it learns all the relevant structure)
  - high variance (it fits the quirks of the data you happened to sample)



Validation

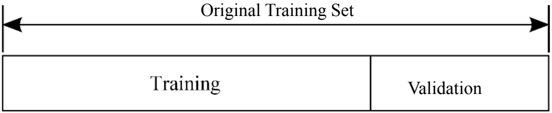
- Before we move on to bagging, it's a good time to mention validation.
- We may want to assess how likely a learning algorithm is to generalize before picking one and reporting the final test error.
- In other words, until now we've been picking predictors that optimize the training loss, but we want a technique for picking predictors that are likely to generalize as well.

Validation

- For example, we may want to assess the following types of choices:
  1. Hyper-parameters of the learning algorithm that lead to better generalization. Often there are parameters that cannot be fit on the training set, e.g., k in k-NN, because the training set would give meaningless answers about the best setting, i.e., $k = 1$ is always gives optimal training set loss for k-NN.
  2. Picking predictors that generalize better. E.g., should we use a decision tree or k-NN if we want to generalize?
- We make these choices using validation to avoid measuring test loss (then the test set would no longer be unseen data!).
- Suppose we are trying to estimate the generalization of two learning algorithms, e.g., a decision tree and a k-NN model.

Hold-out validation

- The most common method of validation is to hold-out a subset of the training set and use it to assess how likely we are to generalize to unseen data.



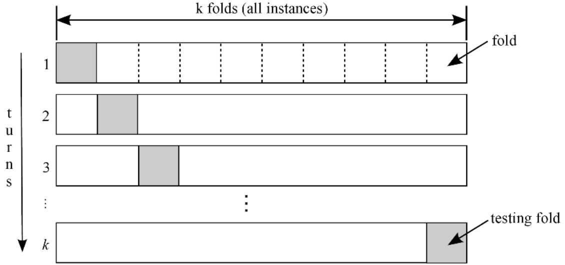
- In our example of deciding between a decision tree and k-NN in terms of generalization, we would fit $\hat{y}^{\star}_{k\text{NN}}$ and $\hat{y}^{\star}_{\text{d-tree}}$ on the training set and measure the average loss on the validation set

$$\hat{\mathcal{R}}[\hat{y}^{\star}_{k\text{NN}}, \mathcal{D}^{valid}] \text{ vs. } \hat{\mathcal{R}}[\hat{y}^{\star}_{\text{d-tree}}, \mathcal{D}^{valid}]$$

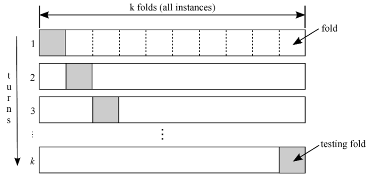
- We pick the predictor $\hat{y}^{\star}_{k\text{NN}}$ vs. $\hat{y}^{\star}_{\text{d-tree}}$ with lowest validation loss.
- Problem: this is usually a waste of data.

K-fold cross validation

- Second most common way: partition training data randomly into K equally sized subsets. For each "turn", use the first $K-1$ subsets (or "folds") as training data and the last subset as validation



K-fold cross validation



- In our running example: fit a new predictor using each learning algorithm on $K-1$ folds for each of the K turns, and measure the validation loss on the held-out fold, averaged over the turns:

$$\frac{1}{K}\sum_{i=1}^{K}\hat{\mathcal{R}}[\hat{y}^{\star}_{k\mathrm{NN},i}, \mathcal{D}_i^{valid}] \text{ vs. } \frac{1}{K}\sum_{i=1}^{K}\hat{\mathcal{R}}[\hat{y}^{\star}_{d-tree,i}, \mathcal{D}_i^{valid}]$$

  where $\hat{y}^{\star}_{A,i}$ is the predictor fit on the training subset of the ith turn using algorithm A and $\mathcal{D}_i^{valid}$ is the validation subset of the ith turn.

- We pick the learning algorithm, e.g., k-NN v. decision tree, with lowest validation loss averaged across the K turns.