CSC 411: Introduction to Machine Learning

Lecture 4: Ensemble I

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Overview

- We've seen two particular learning algorithms: k-NN and decision trees
- Next two lectures: **combine multiple models into an ensemble** which performs better than the individual members
  - Generic class of techniques that can be applied to almost any learning algorithms...
  - ... but are particularly well suited to decision trees
- Today
  - Understanding generalization using the **bias/variance decomposition**
  - Reducing variance using bagging
- Next lecture
  - Making a weak classifier stronger (i.e. reducing bias) using boosting

Ensemble methods: Overview

- An **ensemble** of predictors is a set of predictors whose individual decisions are combined in some way to predict new examples
  - E.g., (possibly weighted) majority vote
- For this to be nontrivial, the learned hypotheses must differ somehow, e.g.
  - Different algorithm
  - Different choice of hyperparameters
  - Trained on different data
  - Trained with different weighting of the training examples
- Ensembles are usually easy to implement. The hard part is deciding what kind of ensemble you want, based on your goals.

Agenda

- This lecture: **bagging**
  - Train classifiers independently on random subsets of the training data.
- Next lecture: **boosting**
  - Train classifiers sequentially, each time focusing on training examples that the previous ones got wrong.
- Bagging and boosting serve very different purposes. To understand this, we need to take a detour to understand the bias and variance of a learning algorithm.

Loss Functions

- A **loss function** $L(y, t)$ defines how bad it is if, for some example x, the algorithm predicts y, but the target is actually t.
- Example: **0-1 loss** for classification

$$L_{0-1}(y, t) = \begin{cases} 0 & \text{if } y = t \\ 1 & \text{if } y \neq t \end{cases}$$

  - Averaging the 0-1 loss over the training set gives the **training error rate**, and averaging over the test set gives the **test error rate**.

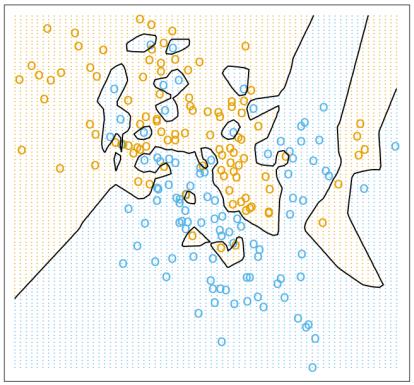
- Example: **squared error loss** for regression

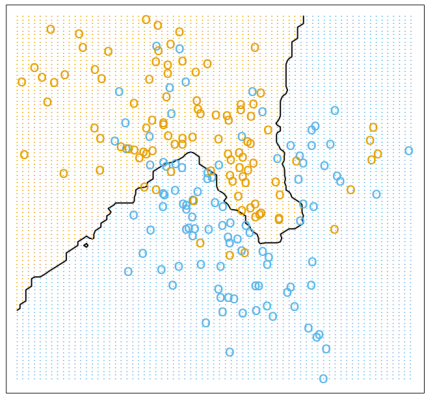
$$L_{\text{SE}}(y, t) = \frac{1}{2}(y - t)^2$$

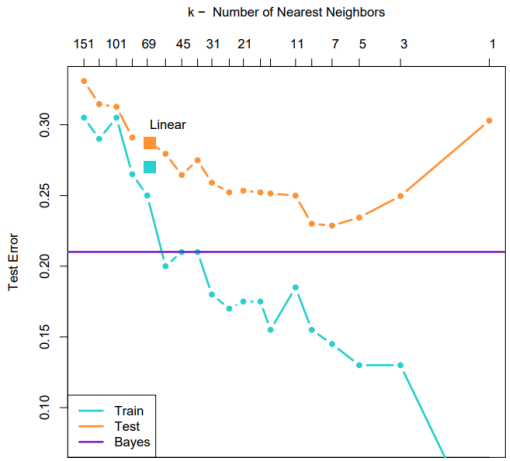
  - The average squared error loss is called **mean squared error (MSE)**.

Bias-Variance Decomposition

- Recall that overly simple models underfit the data, and overly complex models overfit.



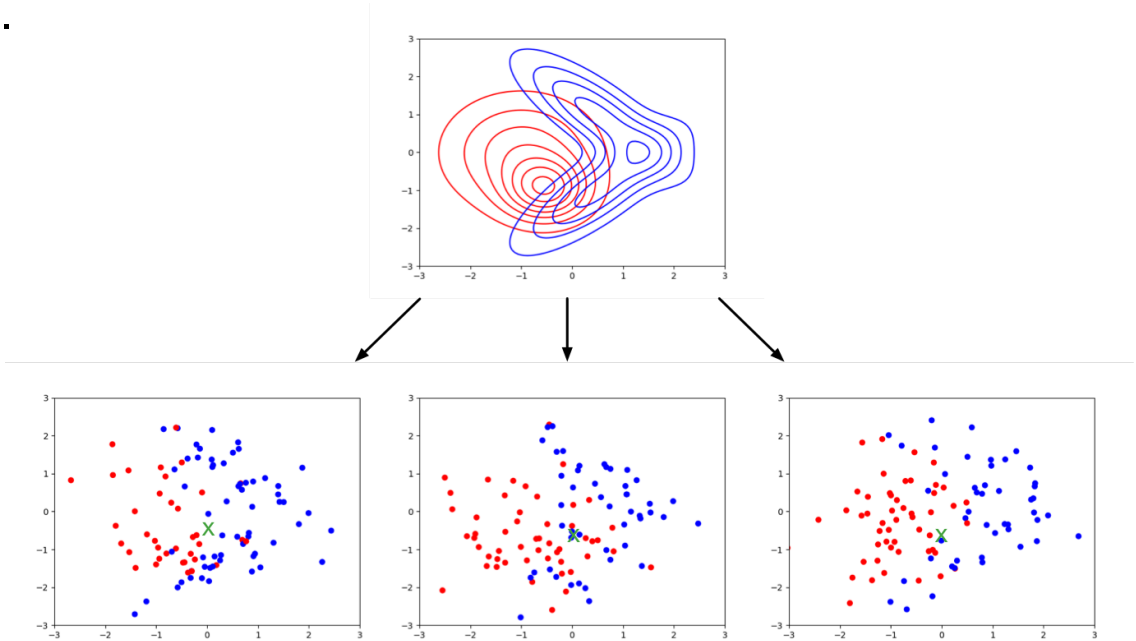




- We can quantify this effect in terms of the **bias/variance decomposition**.
- Bias and variance of what?

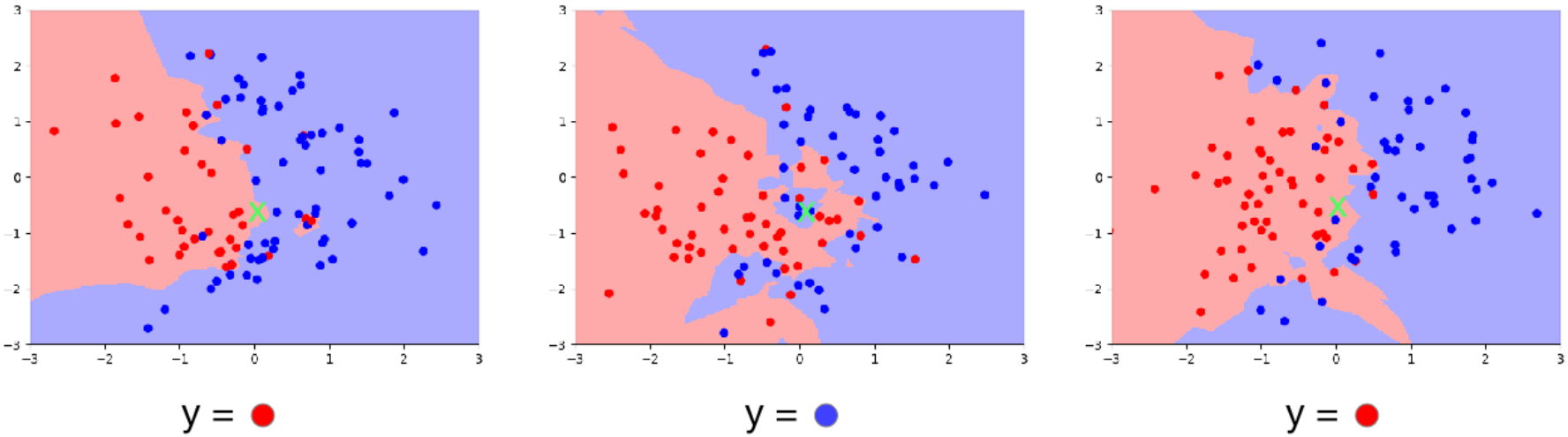
Bias-Variance Decomposition: Basic Setup

- Suppose the training set $\mathcal{D}$ consists of N pairs $(\mathbf{x}_i, t_i)$ sampled **independent and identically distributed (i.i.d.)** from a single **data generating distribution** p_{data}.
  - Let p_{train} denote the induced distribution over training sets
- Pick a fixed query point $\mathbf{x}$ (denoted with a green x).
- Consider an experiment where we sample lots of training sets independently from p_{train}.



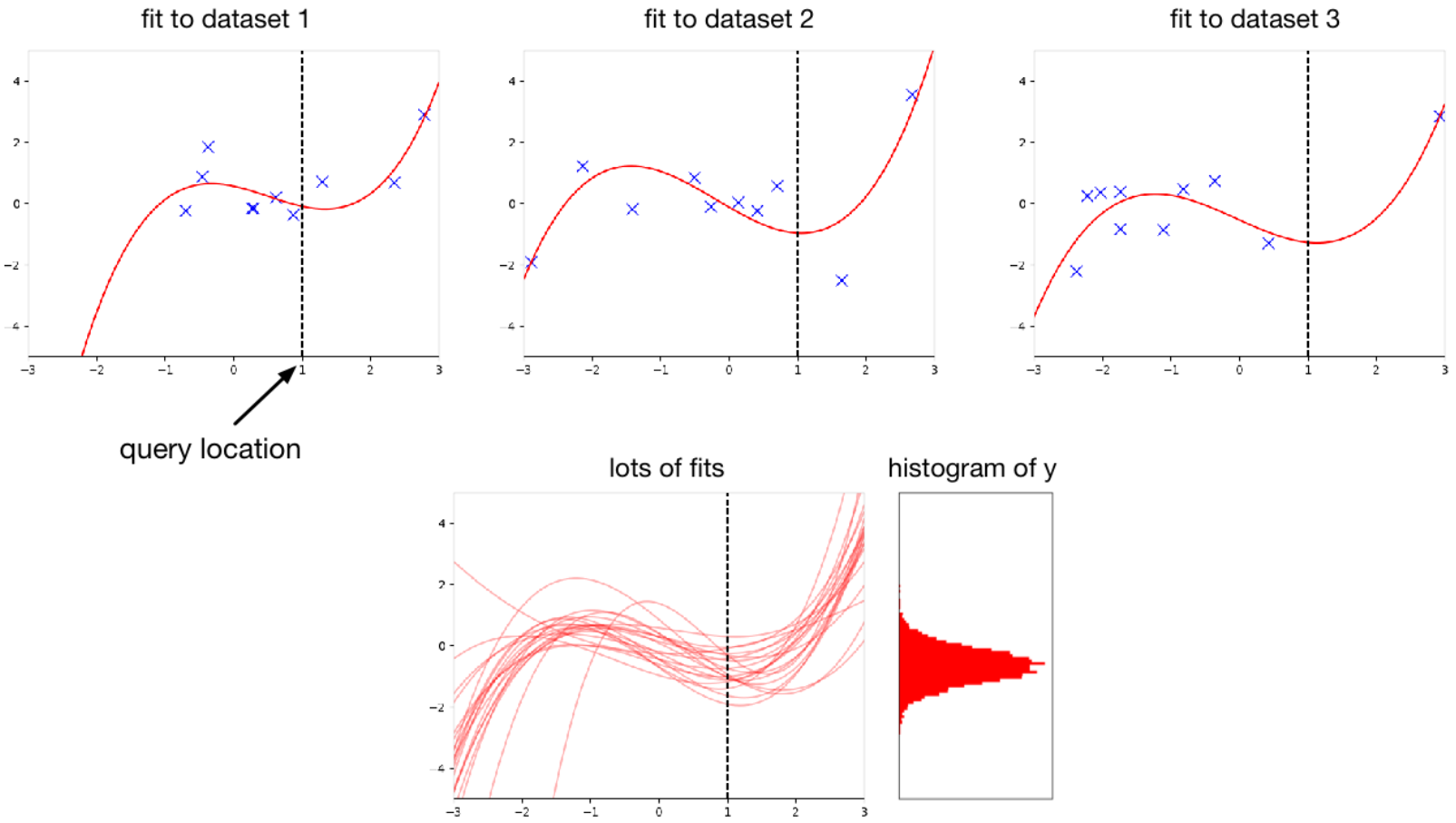
Bias-Variance Decomposition: Basic Setup

- Let's run our learning algorithm on each training set $\mathcal{D}$, producing a classifier $h_{\mathcal{D}}$
- We can compute each classifier's prediction $h_{\mathcal{D}}(\mathbf{x}) = y$ at the query point $\mathbf{x}$.
- y is a random variable, where the **randomness comes from the choice of training set**
  - $\mathcal{D}$ is random $\implies$ $h_{\mathcal{D}}$ is random $\implies$ $h_{\mathcal{D}}(\mathbf{x})$ is random



Bias-Variance Decomposition: Basic Setup

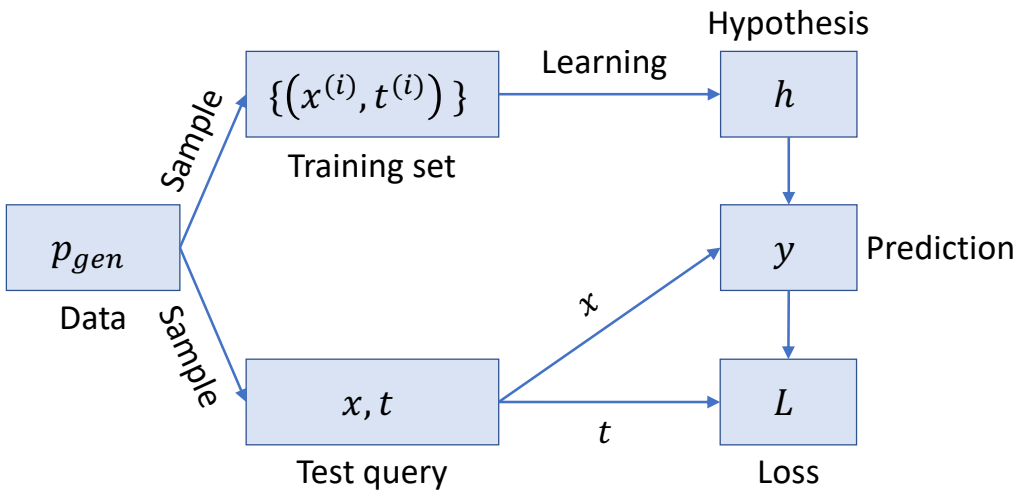
Here is the analogous setup for regression:



Since $y = h_{\mathcal{D}}(\mathbf{x})$ is a random variable, we can talk about its expectation, variance, etc. over the distribution of training sets p_{train}

Bias-Variance Decomposition: Basic Setup

- Recap of basic setup:



- Assume (for the moment) that t is deterministic given x
- There is a distribution over the loss at $\mathbf{x}$, with expectation $\mathbb{E}_{\mathcal{D} \sim p_{\text{train}}}[L(h_{\mathcal{D}}(\mathbf{x}), t)]$.
- For each query point $\mathbf{x}$, the expected loss is different. We are interested in quantifying how well our classifier does over the distribution p_{data}, averaging over training sets: $\mathbb{E}_{\mathbf{x} \sim p_{\text{data}}, \mathcal{D} \sim p_{\text{train}}}[L(h_{\mathcal{D}}(\mathbf{x}), t)]$.

Bias-Variance Decomposition

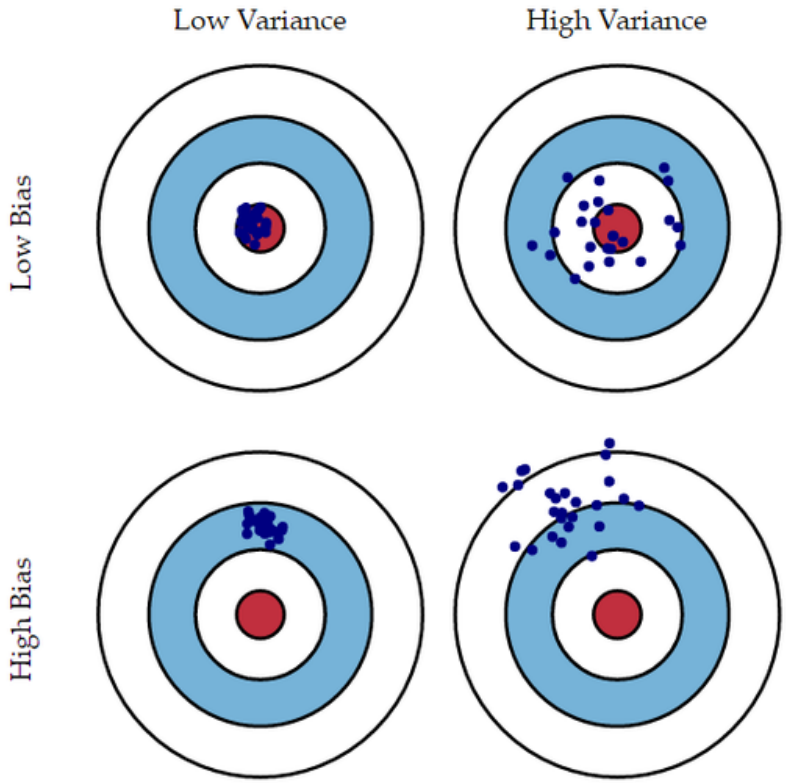
- For now, focus on squared error loss, $L(y, t) = \frac{1}{2}(y - t)^2$.
- We can decompose the expected loss (suppressing distributions $\mathbf{x}$, $\mathcal{D}$ drawn from for compactness):

$$\begin{aligned}
\mathbb{E}_{\mathbf{x},\mathcal{D}}[(h_{\mathcal{D}}(\mathbf{x}) - t)^2] &= \mathbb{E}_{\mathbf{x},\mathcal{D}}[(h_{\mathcal{D}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})] + \mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})] - t)^2] \\
&= \mathbb{E}_{\mathbf{x},\mathcal{D}}[(h_{\mathcal{D}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})])^2 + (\mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})] - t)^2 + \\
&\qquad 2(h_{\mathcal{D}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})])(\mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})] - t)] \\
&= \underbrace{\mathbb{E}_{\mathbf{x},\mathcal{D}}[(h_{\mathcal{D}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})])^2]}_{\text{variance}} + \underbrace{\mathbb{E}_{\mathbf{x}}[(\mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})] - t)^2]}_{\text{bias}}
\end{aligned}$$

- Bias: On average, how close is our classifier to true target? (corresponds to underfitting)
- Variance: How widely dispersed are our predictions as we generate new datasets? (corresponds to overfitting)

Bias and Variance

- Throwing darts = predictions for each draw of a dataset



- What doesn't this capture?
- We average over points **x** from the data distribution

Bagging

Now, back to bagging!

Bagging: Motivation

- Suppose we could somehow sample m independent training sets $\{\mathcal{D}_i\}_{i=1}^m$ from p_{train}.
- We could then learn a predictor $h_i := h_{\mathcal{D}_i}$ based on each one, and take the average $h = \frac{1}{m}\sum_{i=1}^m h_i$.
- How does this affect the terms of the expected loss?
  - **Bias: unchanged**, since the averaged prediction has the same expectation

$$\mathbb{E}_{\mathcal{D}_1,\ldots,\mathcal{D}_m \overset{iid}{\sim} p_{\text{train}}}[h(\mathbf{x})] = \frac{1}{m}\sum_{i=1}^m \mathbb{E}_{\mathcal{D}_i \sim p_{\text{train}}}[h_i(\mathbf{x})] = \mathbb{E}_{\mathcal{D}\sim p_{\text{train}}}[h_{\mathcal{D}}(\mathbf{x})]$$

  - **Variance: reduced**, since we're averaging over independent samples

$$\operatorname*{Var}_{\mathcal{D}_1,\ldots,\mathcal{D}_m}[h(\mathbf{x})] = \frac{1}{m^2}\sum_{i=1}^m \operatorname*{Var}_{\mathcal{D}_i}[h_i(\mathbf{x})] = \frac{1}{m}\operatorname*{Var}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})].$$

Bagging: The Idea

- In practice, we don't have access to the underlying data generating distribution p_{data}.
- It is expensive to independently collect many datasets.
- Solution: **bootstrap aggregation**, or **bagging**.
  - Take a single dataset $\mathcal{D}$ with n examples.
  - Generate m new datasets, each by sampling n training examples from $\mathcal{D}$, with replacement.
  - Average the predictions of models trained on each of these datasets.

Bagging: The Idea

- Problem: the datasets are not independent, so we don't get the $1/m$ variance reduction.
  - Possible to show that if the sampled predictions have variance σ^2 and correlation ρ, then

$$\text{Var}\left(\frac{1}{m}\sum_{i=1}^{m} h_i(\mathbf{x})\right) = \frac{1}{m}(1-\rho)\sigma^2 + \rho\sigma^2.$$

- Ironically, it can be advantageous to introduce *additional* variability into your algorithm, as long as it reduces the correlation between samples.
  - Intuition: you want to invest in a diversified portfolio, not just one stock.
  - Can help to use average over multiple algorithms, or multiple configurations of the same algorithm.

Random Forests

- **Random forests** = bagged decision trees, with one extra trick to decorrelate the predictions
- When choosing each node of the decision tree, choose a random set of d input features, and only consider splits on those features
- Random forests are probably the best black-box machine learning algorithm — they often work well with no tuning whatsoever.
  - one of the most widely used algorithms in Kaggle competitions

Bayes Optimality

- Let's return to quantifying expected loss and make the situation slightly more complicated (and realistic): what if t is not deterministic given $\mathbf{x}$? i.e. have $p(t|\mathbf{x})$
- Can no longer measure bias as expected distance from true target, since there's a distribution over targets!
- Instead, we'll measure distance from $y_*(\mathbf{x}) = \mathbb{E}[t \mid \mathbf{x}]$
  - This is the best possible prediction, in the sense that it minimizes the expected loss

Bayes Optimality

- **Proof:** Start by fixing $\mathbf{x}$. Want to show: $\text{argmin}_y \mathbb{E}_t[(y-t)^2] = y_* = \mathbb{E}_t[t]$ (Distribution of t is $p(t|\mathbf{x})$)

$$\begin{aligned}
\mathbb{E}_t[(y-t)^2] &= \mathbb{E}_t[y^2 - 2yt + t^2] \\
&= y^2 - 2y\mathbb{E}_t[t] + \mathbb{E}_t[t^2] \\
&= y^2 - 2y\mathbb{E}_t[t] + \mathbb{E}_t[t]^2 + \text{Var}[t \,|\, \mathbf{x}] \\
&= y^2 - 2yy_* + y_*^2 + \text{Var}[t \,|\, \mathbf{x}] \\
&= (y-y_*)^2 + \text{Var}[t \,|\, \mathbf{x}]
\end{aligned}$$

- The first term is nonnegative, and can be made 0 by setting $y = y_*$.
- The second term doesn't depend on y! 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**.

Bayes Optimality

- We can again decompose the expected loss, this time including t in our expectation (check this!):

$$\mathbb{E}_{\mathbf{x},\mathcal{D},t}[(h_{\mathcal{D}}(\mathbf{x}) - t)^2] = \underbrace{\mathbb{E}_{\mathbf{x}}[(\mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})] - y_*(\mathbf{x}))^2]}_{\text{bias}} + \underbrace{\mathbb{E}_{\mathbf{x},\mathcal{D}}[(h_{\mathcal{D}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})])^2]}_{\text{variance}} + \underbrace{\mathsf{Var}[t \mid \mathbf{x}]}_{\text{Bayes}}$$

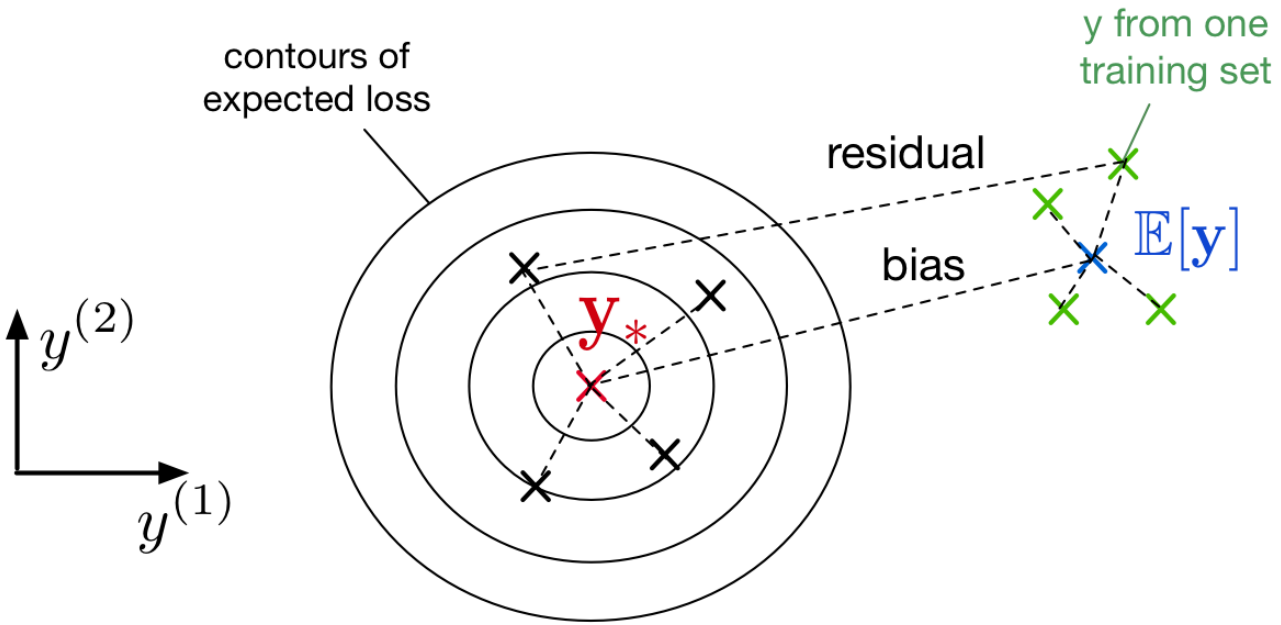
- Contrast if t is not random:

$$\underbrace{\mathbb{E}_{\mathbf{x}}[(\mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})] - t)^2]}_{\text{bias}} + \underbrace{\mathbb{E}_{\mathbf{x},\mathcal{D}}[(h_{\mathcal{D}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})])^2]}_{\text{variance}}$$

- We have no control over the Bayes error! In particular, bagging/boosting do not help

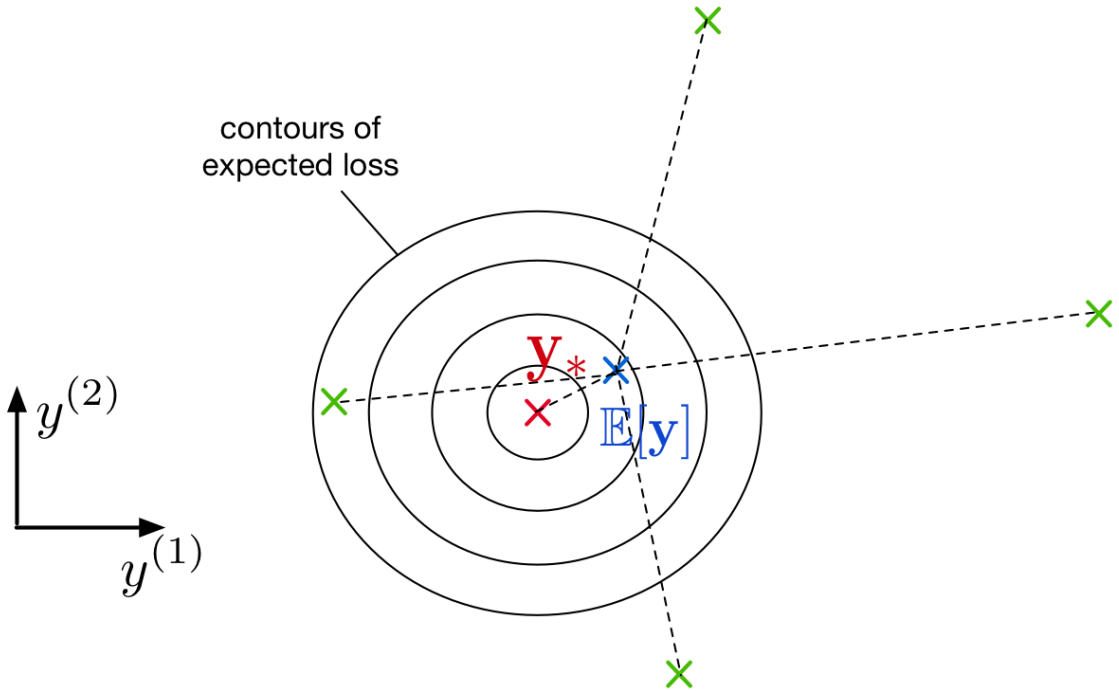
Bias/Variance Decomposition: Another Visualization

- We can visualize this decomposition in **output space**, where the axes correspond to predictions on the test examples.
- If we have an overly simple model (e.g. k-NN with large k), it might have
  - high bias (because it's too simplistic to capture the structure in the data)
  - low variance (because there's enough data to get a stable estimate of the decision boundary)



Bias/Variance Decomposition: Another Visualization

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



Summary

- Bagging reduces overfitting by averaging predictions.
- Used in most competition winners
  - Even if a single model is great, a small ensemble usually helps.
- Limitations:
  - Does not reduce bias.
  - There is still correlation between classifiers.
- Random forest solution: Add more randomness.