CSC 411: Introduction to Machine Learning

Lecture 4: Ensemble I

Mengye Ren and Matthew MacKay

University of Toronto

Overview

- We've seen two particular classification algorithms: KNN and decision trees
- Next two lectures: **combine multiple classifiers into an ensemble** which performs better than the individual members
    - Generic class of techniques that can be applied to almost any learning algorithm...
    - ... 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 classify new examples
    - E.g., (possibly weighted) majority vote
- For this to be nontrivial, the classifiers 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 the algorithm predicts y, but the target is actually t.
- Example: **0-1 loss** for classification

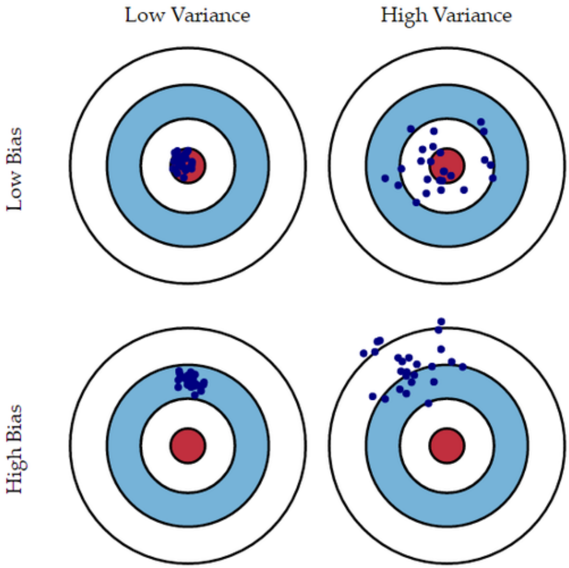
$$L_{0-1}(y, t) = \begin{cases} 0 & \text{if } y = t \\ 1 & \text{if } y \neq t \end{cases}$$

  - 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

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

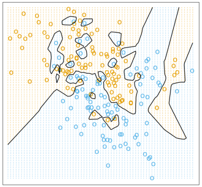
  - The average squared error loss is called **mean squared error (MSE)**.

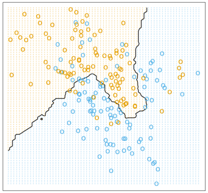
Bias and Variance

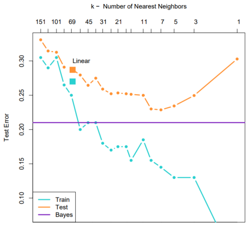


Bias-Variance Decomposition

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



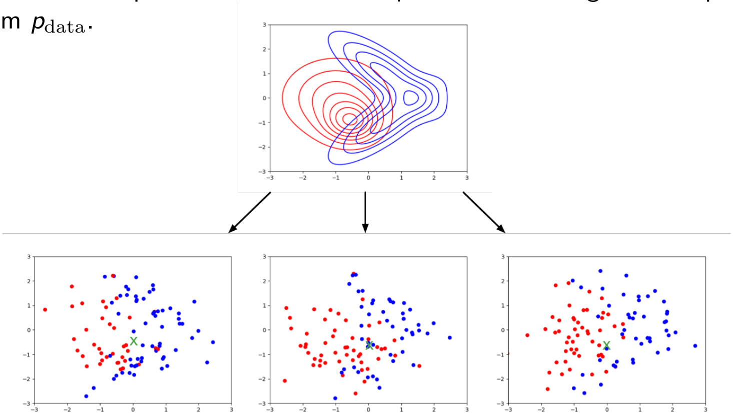




- We can quantify this effect in terms of the **bias/variance decomposition**.
  - Bias and variance of what?

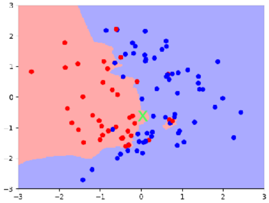
Bias-Variance Decomposition: Basic Setup

- Suppose the training set $\mathcal{D}$ consists of pairs $(\mathbf{x}_i, t_i)$ sampled **independent and identically distributed (i.i.d.)** from a single **data generating distribution** p_{data}.
- 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_{data}.

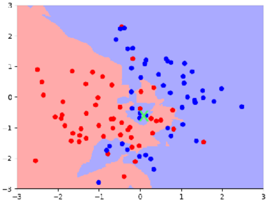


Bias-Variance Decomposition: Basic Setup

- Let's run our learning algorithm on each training set, and compute its prediction y at the query point $\mathbf{x}$.
- We can view y as a random variable, where the randomness comes from the choice of training set.
- The classification accuracy is determined by the distribution of y.



y = 🔴



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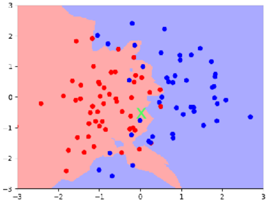

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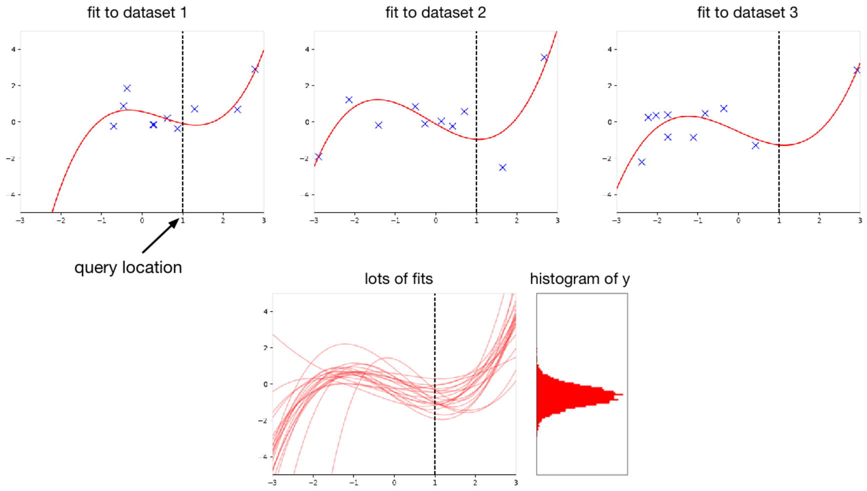
Bias-Variance Decomposition: Basic Setup

Here is the analogous setup for regression:



Since y is a random variable, we can talk about its expectation, variance, etc.

Bias-Variance Decomposition: Basic Setup

- Recap of basic setup:
  - Fix a query point $\mathbf{x}$.
  - Repeat:
    - Sample a random training dataset $\mathcal{D}$ i.i.d. from the data generating distribution p_{data}.
    - Run the learning algorithm on $\mathcal{D}$ to get a prediction y at $\mathbf{x}$.
    - Sample the (true) target from the conditional distribution $p(t|\mathbf{x})$.
    - Compute the loss $L(y, t)$.
- Notice: y is independent of t. (Why?)
- This gives a distribution over the loss at $\mathbf{x}$, with expectation $\mathbb{E}[L(y, t) \,|\, \mathbf{x}]$.
- For each query point $\mathbf{x}$, the expected loss is different. We are interested in minimizing the expectation of this with respect to $\mathbf{x} \sim p_{\text{data}}$.

Bayes Optimality

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

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

Bayes Optimality

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

- The first term is nonnegative, and can be made 0 by setting $y = y_*$.
- 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_* based on $p(t \mid \mathbf{x})$ is an example of **decision theory**.

Bayes Optimality

- Now return to treating y as a random variable (where the randomness comes from the choice of dataset).
- We can decompose out the expected loss (suppressing the conditioning on $\mathbf{x}$ for clarity):

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

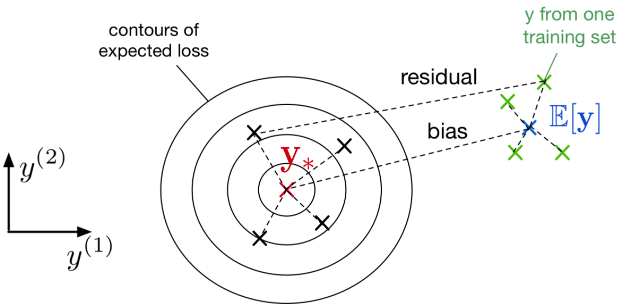
Bayes Optimality

$$\mathbb{E}[(y-t)^2] = \underbrace{(y_* - \mathbb{E}[y])^2}_{\text{bias}} + \underbrace{\mathrm{Var}(y)}_{\text{variance}} + \underbrace{\mathrm{Var}(t)}_{\text{Bayes error}}$$

- We just split the expected loss into three terms:
  - **bias**: how wrong the expected prediction is (corresponds to underfitting)
  - **variance**: the amount of variability in the predictions (corresponds to overfitting)
  - Bayes error: the inherent unpredictability of the targets
- Even though this analysis only applies to squared error, we often loosely use "bias" and "variance" as synonyms for "underfitting" and "overfitting".

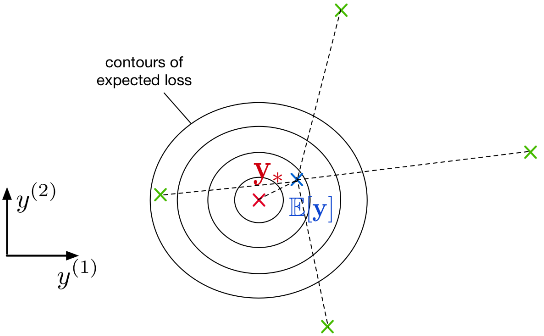
Bias/Variance Decomposition: Another Visualization

- 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. KNN 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. KNN 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)



Bagging

Now, back to bagging!

Bagging: Motivation

- Suppose we could somehow sample m independent training sets from p_{data}.
- We could then compute the prediction y_i based on each one, and take the average $y = \frac{1}{m}\sum_{i=1}^{m} y_i$.
- How does this affect the three terms of the expected loss?
  - **Bayes error: unchanged**, since we have no control over it
  - **Bias: unchanged**, since the averaged prediction has the same expectation

$$\mathbb{E}[y] = \mathbb{E}\left[\frac{1}{m}\sum_{i=1}^{m} y_i\right] = \mathbb{E}[y_i]$$

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

$$\mathrm{Var}[y] = \mathrm{Var}\left[\frac{1}{m}\sum_{i=1}^{m} y_i\right] = \frac{1}{m^2}\sum_{i=1}^{m}\mathrm{Var}[y_i] = \frac{1}{m}\mathrm{Var}[y_i].$$

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

$$\mathrm{Var}\left(\frac{1}{m}\sum_{i=1}^{m} y_i\right) = \frac{1}{m}(1-\rho)\sigma^2 + \rho\sigma^2.$$

- 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

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.