# Machine Learning: Chenhao Tan

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LECTURE 4

Slides adapted from Chris Ketelsen, Noah Smith

## Logistics

- HW1 available on Github, due in 10 days

## Learning objectives

- Understand supervised learning and induction bias
- Understand hyperparameters, underfitting, and overfitting
- Understand bias-variance tradeoff

## Outline

Supervised learning and induction bias

Hyperparameters, underfitting, and overfitting

Bias-variance tradeoff

## Outline

## Supervised Learning

**Hutzler #571 Banana Slicer**

The only banana slicer you will ever need.

Gourmac's easy-to-use Banana Slicer provides a quick solution to slice a banana uniformly each and every time. Simply press the slicer on a peeled banana and the work is done. Safe, fun and easy for children to use. Kids just love eating bananas with this as their favorite kitchen tool. The Banana Slicer may also be used as a quick way to add healthy bananas to breakfast cereal or to make uniform slices for a fruit salad or ice cream dessert.

Data

$X$

Labels

$Y$

- **Supervised methods** find patterns in **fully observed** data and then try to predict something from **partially observed** data.

## Formal Definitions

- Labels $Y$, e.g., binary labels $y \in \{+1, -1\}$
- Instance space $X$, all the possible instances (based on data representation)
- Target function $f$: $X \to Y$ ($f$ is unknown)

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- Instance space $X$, all the possible instances (based on data representation)
- Target function $f$: $X \to Y$ ($f$ is unknown)
- Example/instance $(\boldsymbol{x}, y)$
- Training data $S_{\text{train}}$: collection of examples observed by the algorithm

## Formal Definitions

- Goal of a learning algorithm:

  Find a function $h : X \to Y$ from training data $S_{\text{train}}$ so that $h$ approximates $f$

## Supervised learning in a nutshell

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Given a loss function $l$ and $(\boldsymbol{x}, y) \sim D$, expected loss is defined as:

$$\epsilon \triangleq \mathbb{E}_{(\boldsymbol{x},y)\sim D}\left[l(h(\boldsymbol{x}), y)\right] = \sum_{\boldsymbol{x}\in X, y\in Y} D(X = \boldsymbol{x}, Y = y) l(h(\boldsymbol{x}), y),$$

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but we only have access to training error for a training sample $S_{\text{train}} = \{(\boldsymbol{x}_i, y_i), i = 1, \ldots, N\}$:

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Minimizing training error is not ideal.

## No Free Lunch Theorems

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  Corollary I: there is no single ML algorithm that works for everything.
  Corollary II: every successful ML algorithm makes assumptions.
- No free lunch for search/optimization [Wolpert and Macready, 1997]: All algorithms that search for an extremum of a cost function perform exactly the same when averaged over all possible cost functions.

## So how does machine learning work at all?

## An Exercise, Daume [2017], chapter 2.

Class A

Class B

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Test

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We will see an example in decision tree and change our algorithm slightly.

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- training sample $S_{\text{train}}$
- test sample $S_{\text{test}}$

## Sample Error vs. Generalization Error

- Generalization error of a hypothesis $h$ for a learning task:

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- Use test sample to estimate $\epsilon$:

$$\hat{\epsilon}_{\text{test}} \triangleq \frac{1}{|S_{\text{test}}|} \sum_{(\boldsymbol{x}_i,y_i)\in S_{\text{test}}} l(h(\boldsymbol{x}_i),y_i).$$

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## A concrete hypothetical example

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- What is the problem of generalization error estimation?

[Lazer et al., 2014]

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- What is the problem of generalization error estimation?

[Lazer et al., 2014]
Predicting future is hard!

## Outline

## Greedily Building a Decision Tree (Binary Features)

**Algorithm:** DTREETRAIN
**Data:** data $D$, feature set $\Phi$
**Result:** decision tree
**if** *all examples in* $D$ *have the same label* $y$*, or* $\Phi$ *is empty and* $y$ *is the best guess* **then**
  return LEAF($y$);
**else**
  **for** *each feature* $\phi$ *in* $\Phi$ **do**
    partition $D$ into $D_0$ and $D_1$ based on $\phi$-values;
    let mistakes($\phi$) = (non-majority answers in $D_0$) + (non-majority answers in $D_1$);
  **end**
  let $\phi^*$ be the feature with the smallest number of mistakes;
  return NODE($\phi^*$, {0 $\rightarrow$ DTREETRAIN($D_0, \Phi \setminus \{\phi^*\}$), 1 $\rightarrow$ DTREETRAIN($D_1, \Phi \setminus \{\phi^*\}$)});
**end**

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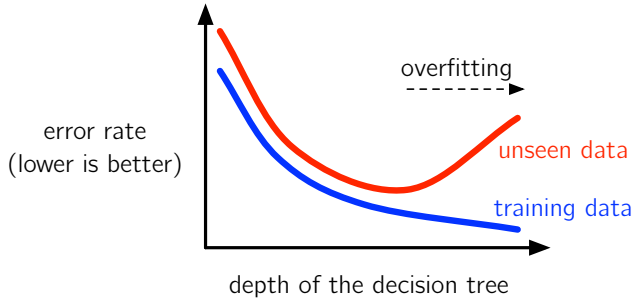
  let $\phi^*$ be the feature with the smallest number of mistakes;
  return Node($\phi^*$, {0 $\rightarrow$ DTreeTrain($D_0, \Phi \setminus \{\phi^*\}$), 1 $\rightarrow$ DTreeTrain($D_1, \Phi \setminus \{\phi^*\}$)});
**end**

Is this algorithm ideal for optimizing generalization error?

## Danger: Overfitting



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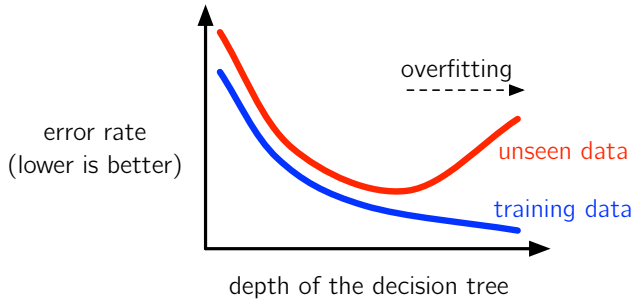


*Underfitting* refers to when your model is not fitting the training data well enough.

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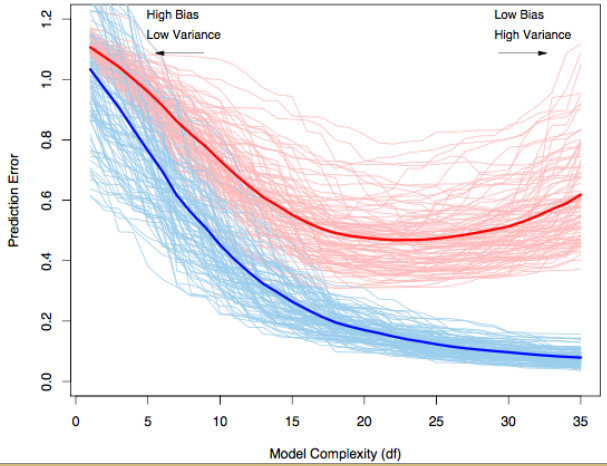
Splitting your data into training/development/test requires careful thinking.
One common starting point is to randomly shuffle examples with an 80%/10%/10% split.

## Outline

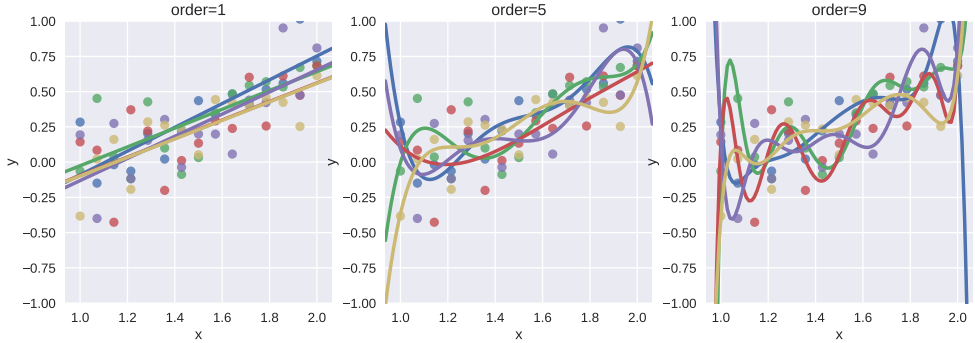
## A more general view of overfitting




[Friedman et al., 2001]

## Example

$$f(x) = 0.5x^2 - 0.8x + 0.3 + \epsilon, \epsilon \sim \mathcal{N}(0, 1)$$



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$$
\begin{aligned}
\mathrm{Err}(x_0) &= \mathrm{E}[(y - h(x_0))^2] \\
&= \sigma_\epsilon^2 + [\mathrm{E}h(x_0) - f(x_0)]^2 + \mathrm{E}[h(x_0) - \mathrm{E}h(x_0)]^2 \\
&= \sigma_\epsilon^2 + \mathrm{Bias}^2(h(x_0)) + \mathrm{Var}(h(x_0)) \\
&= \text{Irreducible Error} + \text{Bias}^2 + \text{Variance}
\end{aligned}
$$

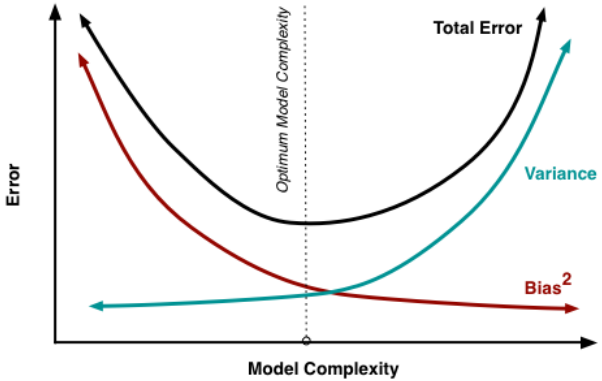
## Bias-Variance Tradeoff

$$\text{Generailization error} \quad = \quad \text{Irreducible Error} + \text{Bias}^2 + \text{Variance}$$

- $[\mathrm{E}h(x_0) - f(x_0)]^2$, high bias means that even with all training data, the error is still high. Model is not flexible enough to model the true function.
- $\mathrm{E}[h(x_0) - \mathrm{E}h(x_0)]^2$, high variance means that a small variation of training data leads to a great change in the learned model. Model is very sensitive to training data.

## Revisit Overfitting

$$\text{Generailization error} = \text{Irreducible Error} + \text{Bias}^2 + \text{Variance}$$




http://scott.fortmann-roe.com/docs/BiasVariance.html

## References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