

Lec09: Decision Trees and Ensembles

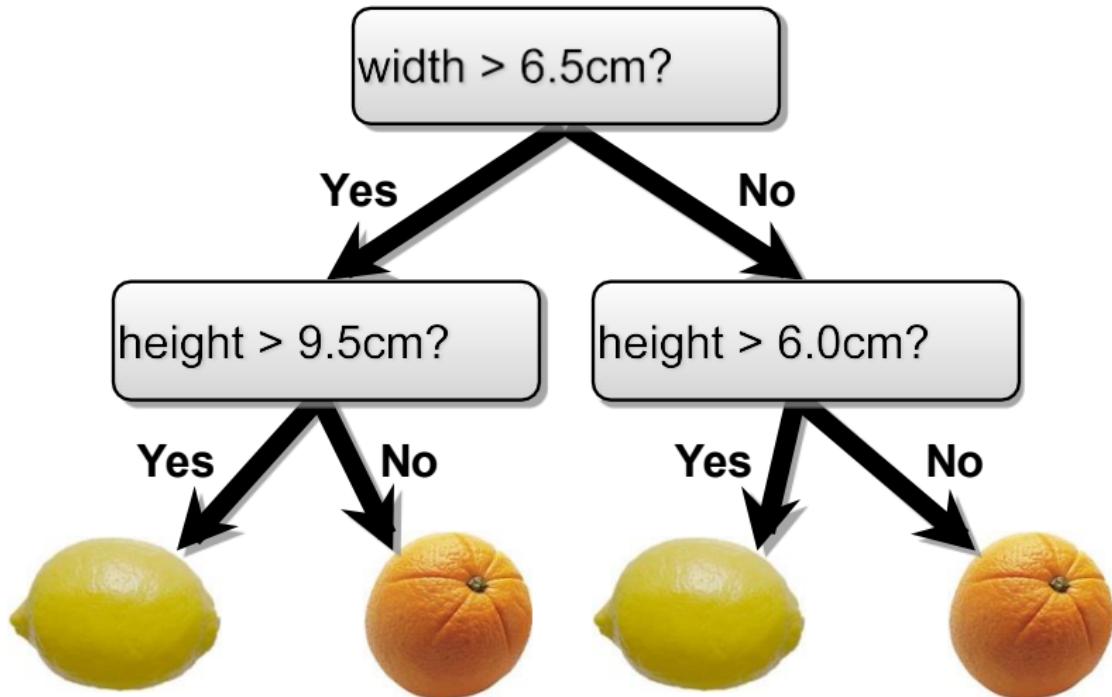
Xiaojun Chang

University of Science and Technology of China

Overview

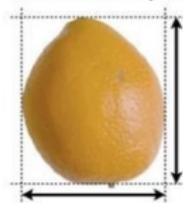
- Decision Trees
 - ▶ Simple but powerful learning algorithm
 - ▶ One of the most widely used learning algorithms in Kaggle competitions
- Lets us introduce ensembles, a key idea in ML more broadly
- Useful information theoretic concepts (entropy, mutual information, etc.)

Decision Trees



Decision Trees

Test example



width > 6.5cm?

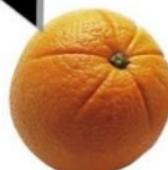
Yes

height > 9.5cm?

Yes



No



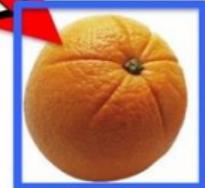
No

height > 6.0cm?

Yes

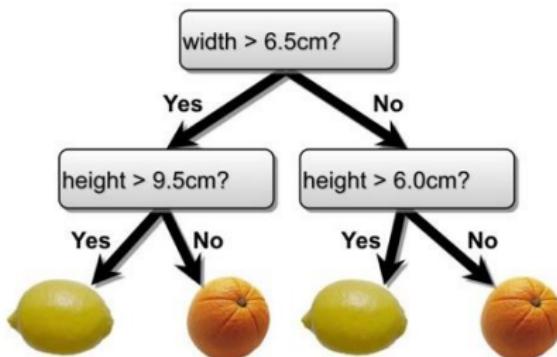
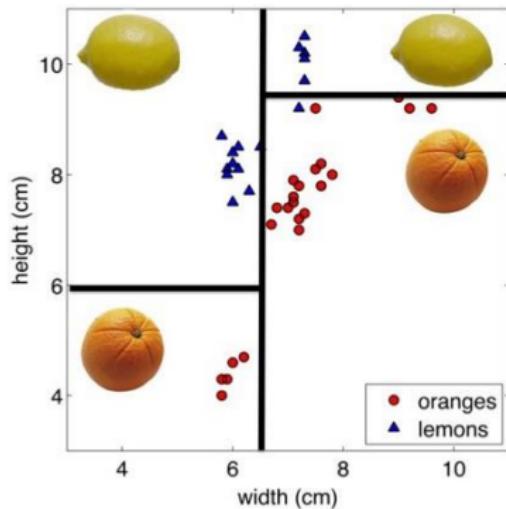


No



Decision Trees

- Decision trees make predictions by recursively splitting on different attributes according to a tree structure.



Example with Discrete Inputs

- What if the attributes are discrete?

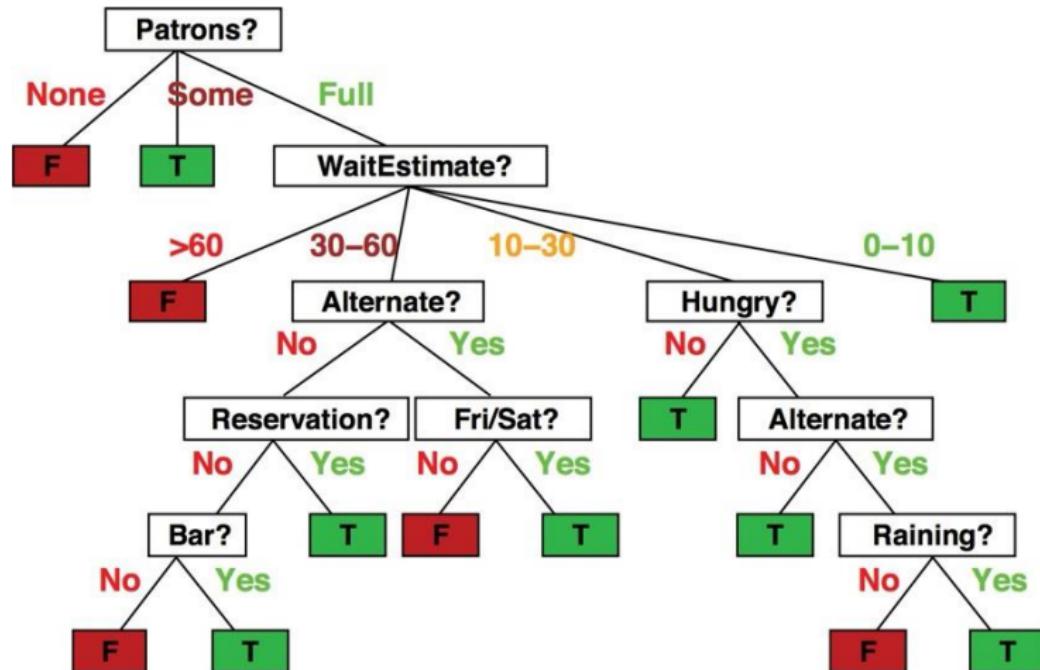
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x ₁₂	Yes	Yes	Yes	Yes	Full	\$	No	No	Burger	30-60	y ₁₂ = Yes

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8.	Reservation: whether we made a reservation.
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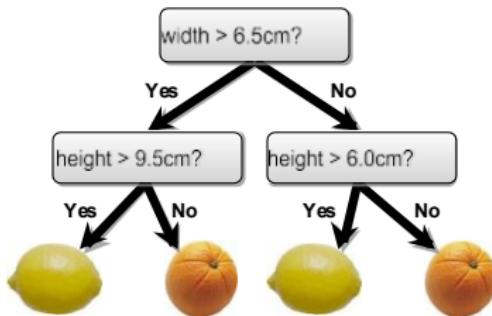
Attributes:

Decision Tree: Example with Discrete Inputs

- The tree to decide whether to wait (T) or not (F)



Decision Trees



- Internal nodes test attributes
- Branching is determined by attribute value
- Leaf nodes are outputs (predictions)

Decision Tree: Classification and Regression

- Each path from root to a leaf defines a region R_m of input space
- Let $\{(x^{(m_1)}, t^{(m_1)}), \dots, (x^{(m_k)}, t^{(m_k)})\}$ be the training examples that fall into R_m

- **Classification tree:**

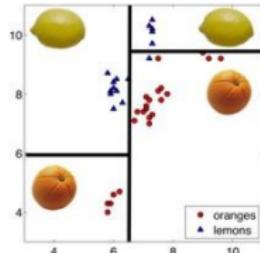
- ▶ discrete output
- ▶ leaf value y^m typically set to the most common value in $\{t^{(m_1)}, \dots, t^{(m_k)}\}$

- **Regression tree:**

- ▶ continuous output
- ▶ leaf value y^m typically set to the mean value in $\{t^{(m_1)}, \dots, t^{(m_k)}\}$

Note: We will focus on classification

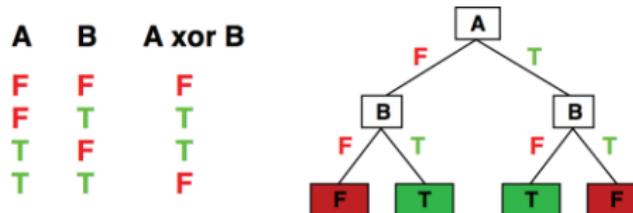
[Slide credit: S. Russell]



Expressiveness

- Discrete-input, discrete-output case:

- ▶ Decision trees can express any function of the input attributes
- ▶ E.g., for Boolean functions, truth table row → path to leaf:



- Continuous-input, continuous-output case:

- ▶ Can approximate any function arbitrarily closely
- Trivially, there is a consistent decision tree for any training set w/ one path to leaf for each example (unless f nondeterministic in x) but it probably won't generalize to new examples

[Slide credit: S. Russell]

How do we Learn a Decision Tree?

- How do we construct a useful decision tree?

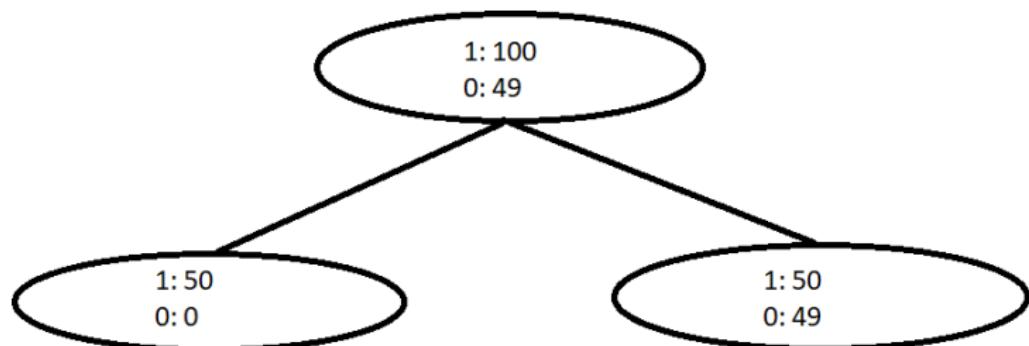
Learning Decision Trees

Learning the simplest (smallest) decision tree is an NP complete problem [if you are interested, check: Hyafil & Rivest'76]

- Resort to a **greedy heuristic**:
 - ▶ Start from an empty decision tree
 - ▶ Split on the “best” attribute
 - ▶ Recurse
- Which attribute is the “best”?
 - ▶ Choose based on accuracy?

Choosing a Good Split

- Why isn't accuracy a good measure?



- Is this split good? Zero accuracy gain.
- Instead, we will use techniques from **information theory**

Idea: Use counts at leaves to define probability distributions, so we can measure uncertainty

Choosing a Good Split

- Which attribute is better to split on, X_1 or X_2 ?
 - ▶ Deterministic: good (all are true or false; just one class in the leaf)
 - ▶ Uniform distribution: bad (all classes in leaf equally probable)
 - ▶ What about distributions in between?

Note: Let's take a slight detour and remember concepts from information theory

[Slide credit: D. Sontag]

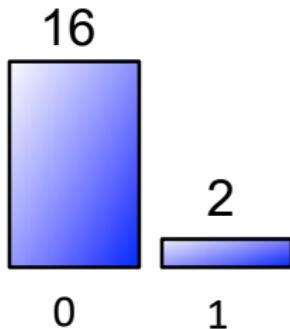
We Flip Two Different Coins

Sequence 1:

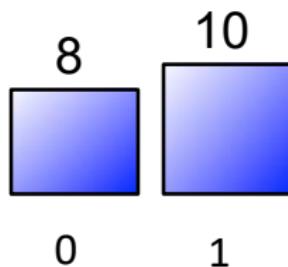
0 0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 ... ?

Sequence 2:

0 1 0 1 0 1 1 0 1 0 0 1 1 0 1 0 1 ... ?



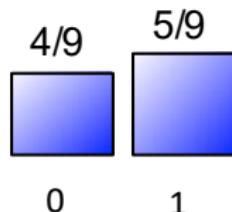
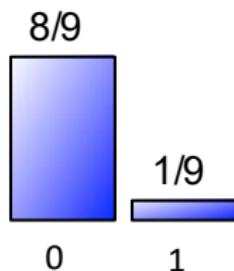
versus



Quantifying Uncertainty

Entropy is a measure of expected “surprise”:

$$H(X) = - \sum_{x \in X} p(x) \log_2 p(x)$$



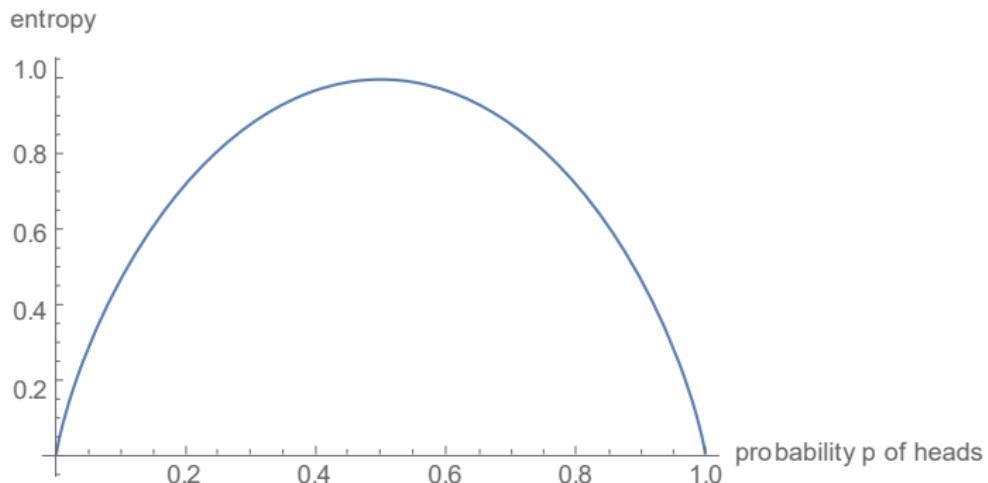
$$-\frac{8}{9} \log_2 \frac{8}{9} - \frac{1}{9} \log_2 \frac{1}{9} \approx \frac{1}{2}$$

$$-\frac{4}{9} \log_2 \frac{4}{9} - \frac{5}{9} \log_2 \frac{5}{9} \approx 0.99$$

- Measures the information content of each observation
- Unit = bits
- A fair coin flip has 1 bit of entropy

Quantifying Uncertainty

$$H(X) = - \sum_{x \in X} p(x) \log_2 p(x)$$



Entropy

- “High Entropy”:
 - ▶ Variable has a uniform like distribution
 - ▶ Flat histogram
 - ▶ Values sampled from it are less predictable
- “Low Entropy”
 - ▶ Distribution of variable has many peaks and valleys
 - ▶ Histogram has many lows and highs
 - ▶ Values sampled from it are more predictable

[Slide credit: Vibhav Gogate]

Entropy of a Joint Distribution

- Example: $X = \{\text{Raining, Not raining}\}$, $Y = \{\text{Cloudy, Not cloudy}\}$

		Cloudy	Not Cloudy
Raining	24/100	1/100	
Not Raining	25/100	50/100	

$$\begin{aligned}H(X, Y) &= - \sum_{x \in X} \sum_{y \in Y} p(x, y) \log_2 p(x, y) \\&= -\frac{24}{100} \log_2 \frac{24}{100} - \frac{1}{100} \log_2 \frac{1}{100} - \frac{25}{100} \log_2 \frac{25}{100} - \frac{50}{100} \log_2 \frac{50}{100} \\&\approx 1.56 \text{ bits}\end{aligned}$$

Specific Conditional Entropy

- Example: $X = \{\text{Raining, Not raining}\}$, $Y = \{\text{Cloudy, Not cloudy}\}$

		Cloudy	Not Cloudy
Raining	24/100	1/100	
Not Raining	25/100	50/100	

- What is the entropy of cloudiness Y , **given that it is raining?**

$$\begin{aligned}H(Y|X=x) &= -\sum_{y \in Y} p(y|x) \log_2 p(y|x) \\&= -\frac{24}{25} \log_2 \frac{24}{25} - \frac{1}{25} \log_2 \frac{1}{25} \\&\approx 0.24 \text{ bits}\end{aligned}$$

- We used: $p(y|x) = \frac{p(x,y)}{p(x)}$, and $p(x) = \sum_y p(x,y)$ (sum in a row)

Conditional Entropy

		Cloudy	Not Cloudy
Raining	24/100	1/100	
Not Raining	25/100	50/100	

- The expected conditional entropy:

$$\begin{aligned} H(Y|X) &= \sum_{x \in X} p(x) H(Y|X = x) \\ &= - \sum_{x \in X} \sum_{y \in Y} p(x, y) \log_2 p(y|x) \end{aligned}$$

Conditional Entropy

- Example: $X = \{\text{Raining, Not raining}\}$, $Y = \{\text{Cloudy, Not cloudy}\}$

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- What is the entropy of cloudiness, given the knowledge of whether or not it is raining?

$$\begin{aligned}H(Y|X) &= \sum_{x \in X} p(x) H(Y|X=x) \\&= \frac{1}{4} H(\text{cloudy}|\text{is raining}) + \frac{3}{4} H(\text{cloudy}|\text{not raining}) \\&\approx 0.75 \text{ bits}\end{aligned}$$

Conditional Entropy

- Some useful properties:
 - H is always non-negative
 - Chain rule: $H(X, Y) = H(X|Y) + H(Y) = H(Y|X) + H(X)$
 - If X and Y independent, then X doesn't tell us anything about Y :
 $H(Y|X) = H(Y)$
 - But Y tells us everything about Y : $H(Y|Y) = 0$
 - By knowing X , we can only decrease uncertainty about Y :
 $H(Y|X) \leq H(Y)$

Information Gain

	Cloudy	Not Cloudy
Raining	24/100	1/100
Not Raining	25/100	50/100

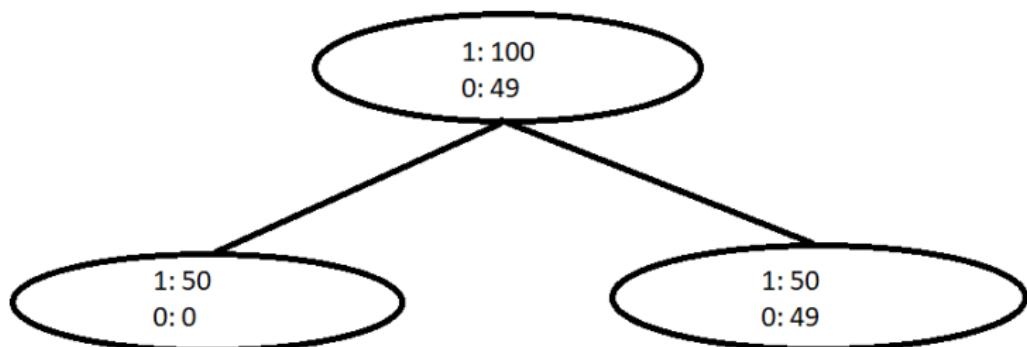
- How much information about cloudiness do we get by discovering whether it is raining?

$$\begin{aligned}IG(Y|X) &= H(Y) - H(Y|X) \\&\approx 0.25 \text{ bits}\end{aligned}$$

- This is called the **information gain** in Y due to X , or the **mutual information** of Y and X
- If X is completely uninformative about Y : $IG(Y|X) = 0$
- If X is completely informative about Y : $IG(Y|X) = H(Y)$

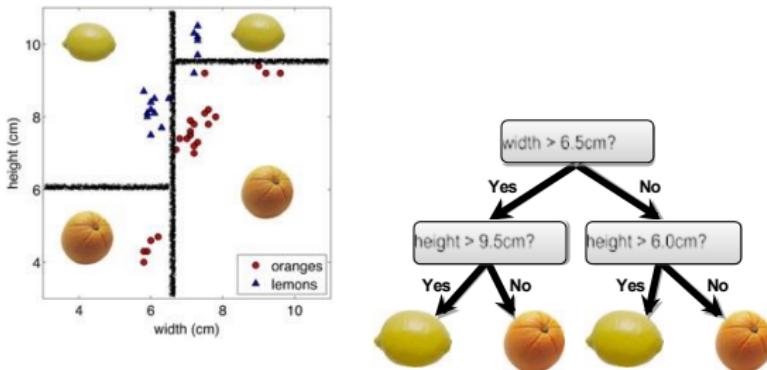
Revisiting Our Original Example

- Information gain measures the informativeness of a variable, which is exactly what we desire in a decision tree attribute!
- What is the information gain of this split?



- Root entropy: $H(Y) = - \frac{49}{149} \log_2\left(\frac{49}{149}\right) - \frac{100}{149} \log_2\left(\frac{100}{149}\right) \approx 0.91$
- Leafs entropy: $H(Y/left) = 0$, $H(Y/right) \approx 1$.
- $IG(split) \approx 0.91 - \left(\frac{1}{3} \cdot 0 + \frac{2}{3} \cdot 1\right) \approx 0.24 > 0$

Constructing Decision Trees



- At each level, one must choose:
 - Which variable to split.
 - Possibly where to split it.
- Choose them based on how much information we would gain from the decision! (choose attribute that gives the highest gain)

Decision Tree Construction Algorithm

- Simple, greedy, recursive approach, builds up tree node-by-node
 - 1. pick an attribute to split at a non-terminal node
 - 2. split examples into groups based on attribute value
 - 3. for each group:
 - ▶ if no examples – return majority from parent
 - ▶ else if all examples in same class – return class
 - ▶ else loop to step 1

Back to Our Example

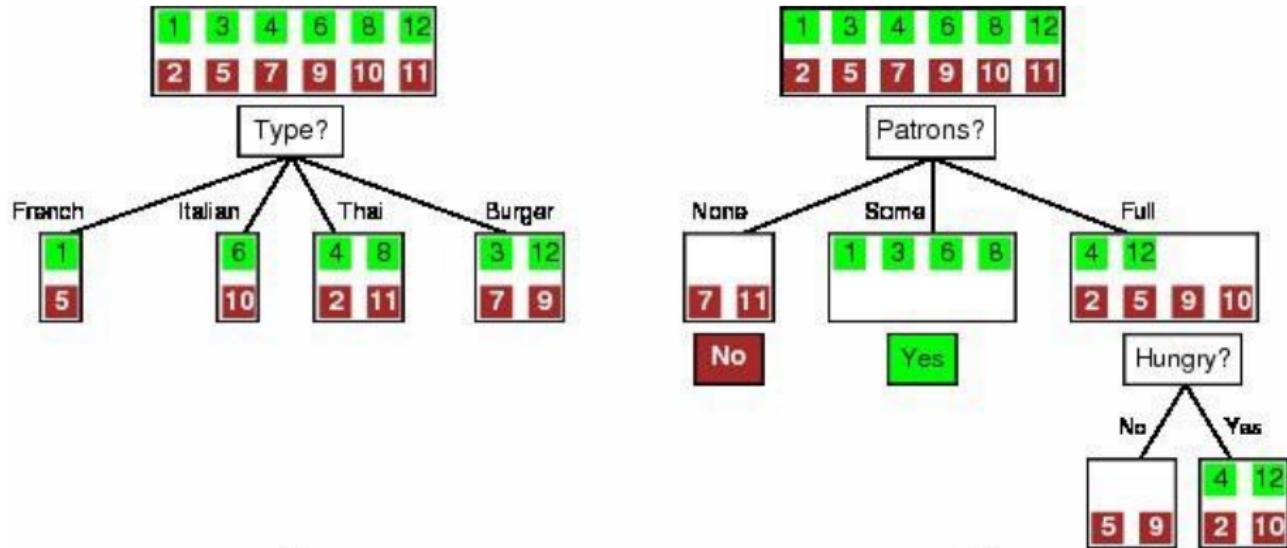
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Attributes:

[from: Russell & Norvig]

Attribute Selection

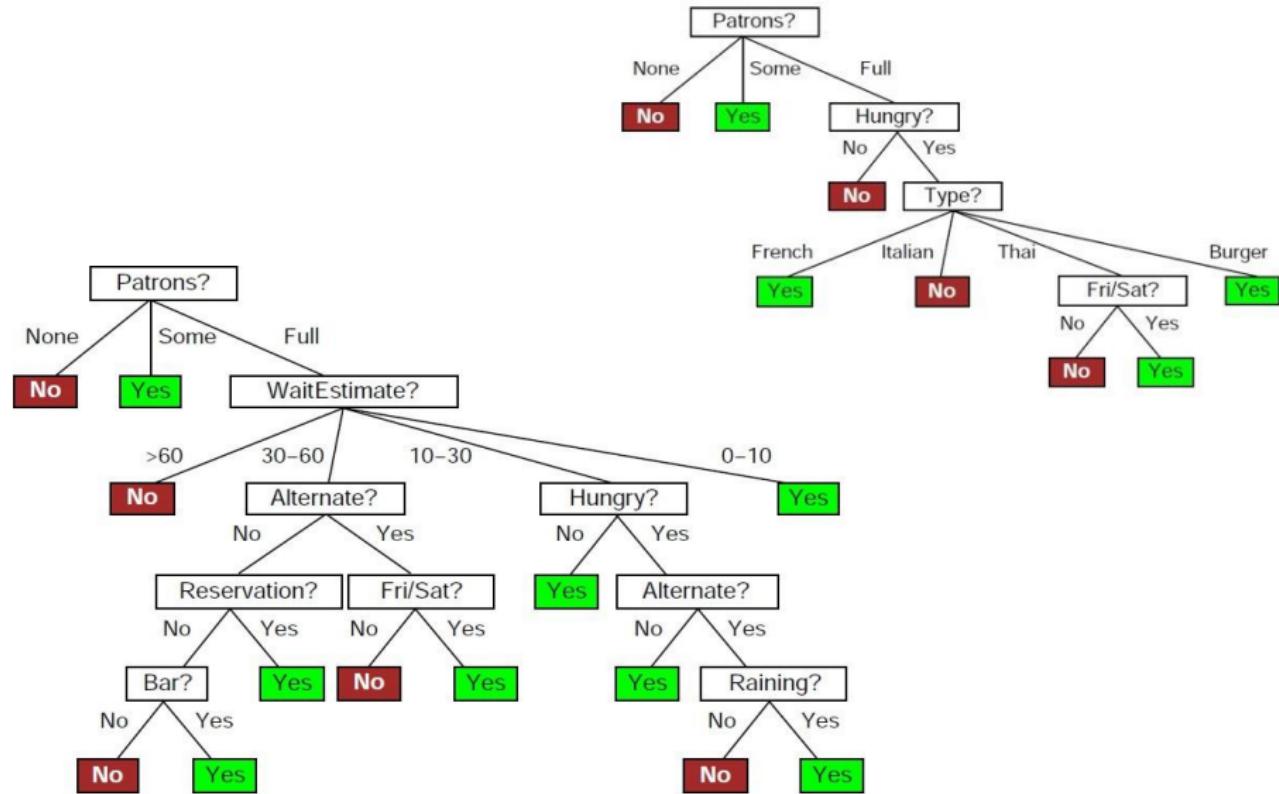


$$IG(Y) = H(Y) - H(Y|X)$$

$$IG(\text{type}) = 1 - \left[\frac{2}{12}H(Y|\text{Fr.}) + \frac{2}{12}H(Y|\text{It.}) + \frac{4}{12}H(Y|\text{Thai}) + \frac{4}{12}H(Y|\text{Bur.}) \right] = 0$$

$$IG(\text{Patrons}) = 1 - \left[\frac{2}{12}H(0, 1) + \frac{4}{12}H(1, 0) + \frac{6}{12}H\left(\frac{2}{6}, \frac{4}{6}\right) \right] \approx 0.541$$

Which Tree is Better?



What Makes a Good Tree?

- Not too small: need to handle important but possibly subtle distinctions in data
- Not too big:
 - ▶ Computational efficiency (avoid redundant, spurious attributes)
 - ▶ Avoid over-fitting training examples
 - ▶ Human interpretability
- “Occam’s Razor”: find the simplest hypothesis that fits the observations
 - ▶ Useful principle, but hard to formalize (how to define simplicity?)
 - ▶ See Domingos, 1999, “The role of Occam’s razor in knowledge discovery”
- We desire small trees with informative nodes near the root

Decision Tree Miscellany

- Problems:
 - ▶ You have exponentially less data at lower levels
 - ▶ Too big of a tree can overfit the data
 - ▶ Greedy algorithms don't necessarily yield the global optimum
- Handling continuous attributes
 - ▶ Split based on a threshold, chosen to maximize information gain
- Decision trees can also be used for regression on real-valued outputs. Choose splits to minimize squared error, rather than maximize information gain.

Comparison to k-NN

Advantages of decision trees over KNN

- Good when there are lots of attributes, but only a few are important
- Good with discrete attributes
- Easily deals with missing values (just treat as another value)
- Robust to scale of inputs
- Fast at test time
- More interpretable

Advantages of KNN over decision trees

- Few hyperparameters
- Able to handle attributes/features that interact in complex ways (e.g. pixels)
- Can incorporate interesting distance measures (e.g. shape contexts)
- Typically make better predictions in practice
 - ▶ As we'll see next lecture, ensembles of decision trees are much stronger. But they lose many of the advantages listed above.

Ensembles and Bagging

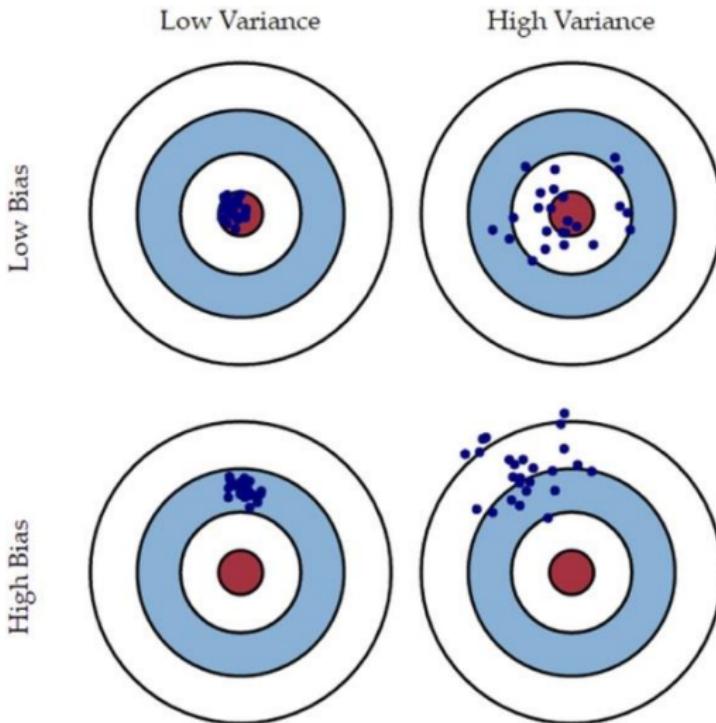
Ensemble methods: Overview

- 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 trivial to implement. The hard part is deciding what kind of ensemble you want, based on your goals.

Ensemble methods: Overview

- This lecture: **bagging**
 - ▶ Train classifiers independently on random subsets of the training data.
- Later 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.

Bias and Variance



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

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

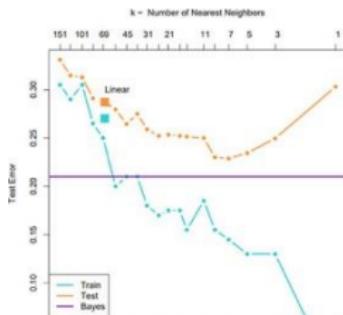
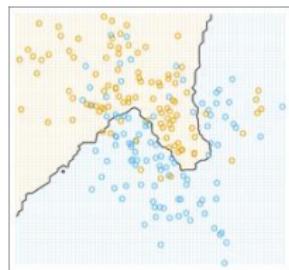
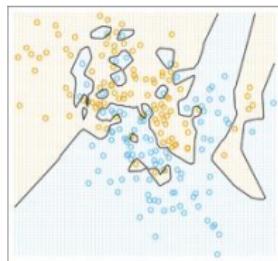
- ▶ Averaging the 0-1 loss over the training set gives the training error rate, and averaging over the test set gives the test error rate.
- Example: squared error loss for regression

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

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

Bias-Variance Decomposition

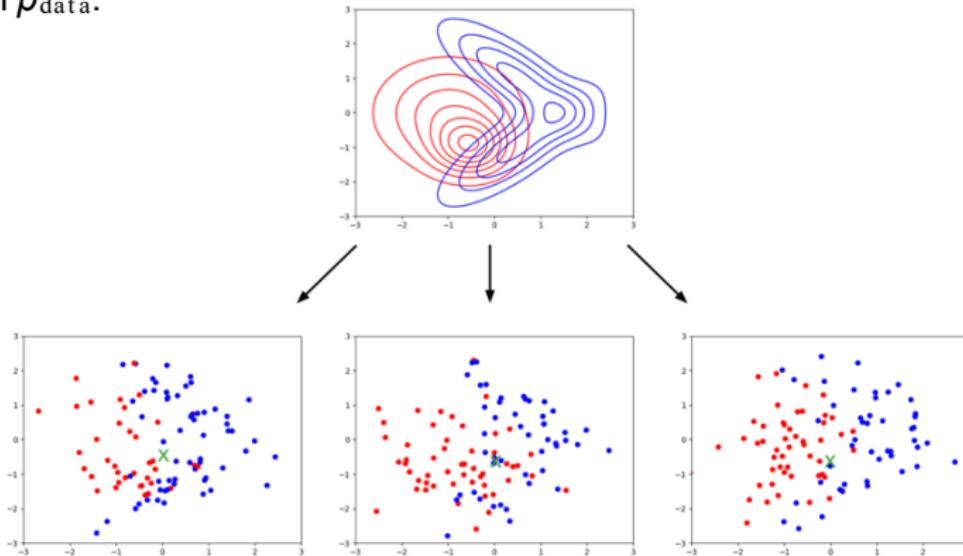
- Recall that overly simple models underfit the data, and overly complex models overfit.



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

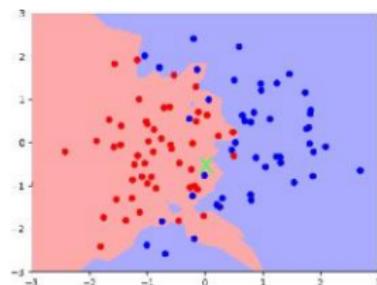
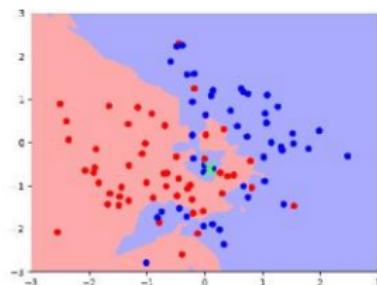
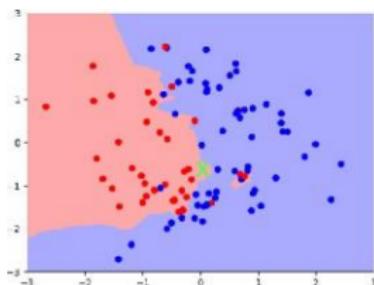
Bias-Variance Decomposition: Basic Setup

- Suppose the training set 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 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 .



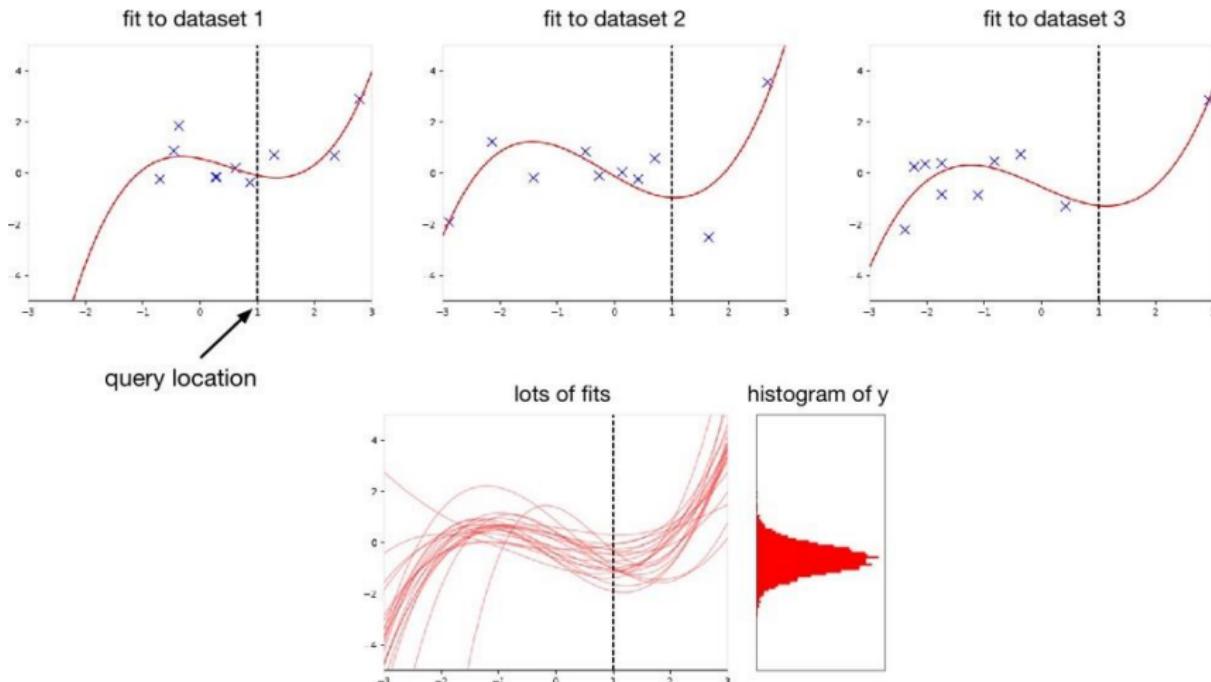
$y = \bullet$

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Bias-Variance Decomposition: Basic Setup

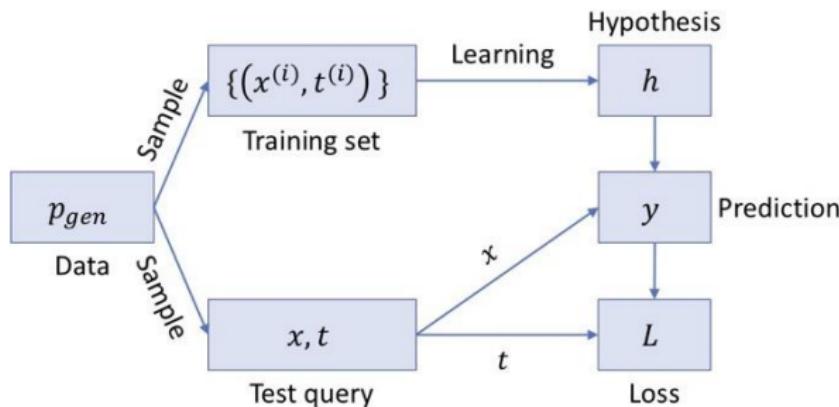
Here is the analogous setup for regression:



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

Bias-Variance Decomposition: Basic Setup

- Recap of basic setup:



- Notice: y is independent of t . (Why?)
- This gives a distribution over the loss at \mathbf{x} , with expectation $E[L(y, t) | \mathbf{x}]$.
- 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 $p(t | \mathbf{x})$. What value y should we predict?
 - Here, we are treating t as a random variable and choosing y .
- Claim:** $y_* = E[t | \mathbf{x}]$ is the best possible prediction.
- Proof:**

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

Bayes Optimality

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

- 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 $p(t | \mathbf{x})$ 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):

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

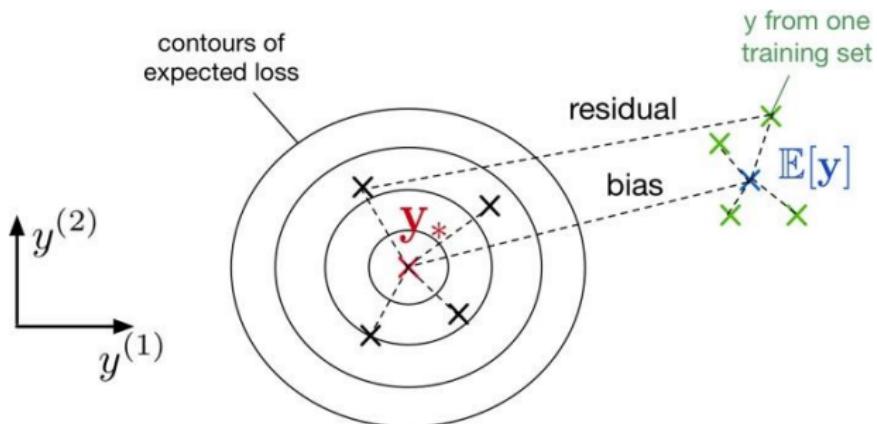
Bayes Optimality

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

- 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”.

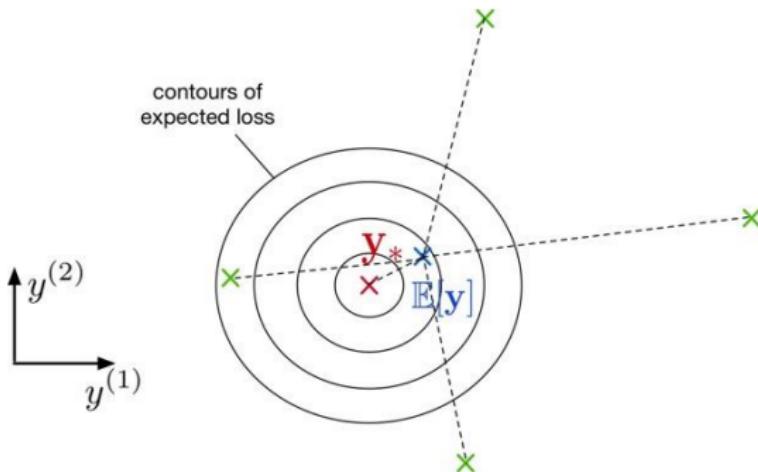
Bias/Variance Decomposition: Another Visualization

- 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

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

Bagging: The Idea

- In practice, running an algorithm separately on independently sampled datasets is very wasteful!
- Solution: **bootstrap aggregation**, or **bagging**.
 - ▶ Take a single dataset D with n examples.
 - ▶ Generate m new datasets, each by sampling n training examples from D , with replacement.
 - ▶ Average the predictions of models trained on each of these datasets.
- The bootstrap is one of the most important ideas in all of statistics!

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

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

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.