

10-701: Introduction to Machine Learning

Lecture 21 – Bagging & Boosting

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* Slides adopted from F24 offering of 10701 by Henry Chai.

Bias-Variance Decomposition

- Suppose $y=f(x)+\varepsilon$, where ε is noise with $\mathbb{E}[\varepsilon] = 0, \text{Var}(\varepsilon) = \sigma^2$.
- The expected squared prediction error at a point x :

$$\mathbb{E}_{D,\varepsilon}[(y - \hat{f}(x))^2] =$$

Bias-Variance Decomposition

- $\mathbb{E}[(f(x) - \hat{f}(x))^2] =$

- $\mathbb{E}[(f(x) - \hat{f}(x))^2] = \underbrace{(f(x) - \mathbb{E}[\hat{f}(x)])^2}_{\text{Bias}^2} + \underbrace{\mathbb{E}[(\hat{f}(x) - \mathbb{E}[\hat{f}(x)])^2]}_{\text{Variance}}$ or

$$\boxed{\mathbb{E}[(y - \hat{f}(x))^2] = \text{Bias}^2[\hat{f}(x)] + \text{Var}[\hat{f}(x)] + \sigma^2}$$

The Wisdom of Crowds

- In 1906, Francis Galton asked ~800 people at a farmer's fair to guess the weight of a cow, including “experts”
 - Actual weight: 1198 lbs
 - Mean guess: 1197 lbs
 - Mean guess was more accurate than any single guess, even the experts

Ensemble Learning

- **Key idea:** Different models make different errors. By aggregating their predictions, ensembles can reduce variance, bias, or both—leading to better accuracy and robustness than any single model alone.
- **Common ensemble methods**
 - **Bagging (Bootstrap Aggregating):**
Trains many models independently on different random subsets of the data to reduce variance and overfitting.
 - **Boosting:**
Trains models sequentially, with each new model focusing on the errors of the previous to reduce bias.
 - **Stacking:**
Combines predictions from multiple models using another model (a *meta-learner*) that learns how best to blend them.

The Netflix Prize



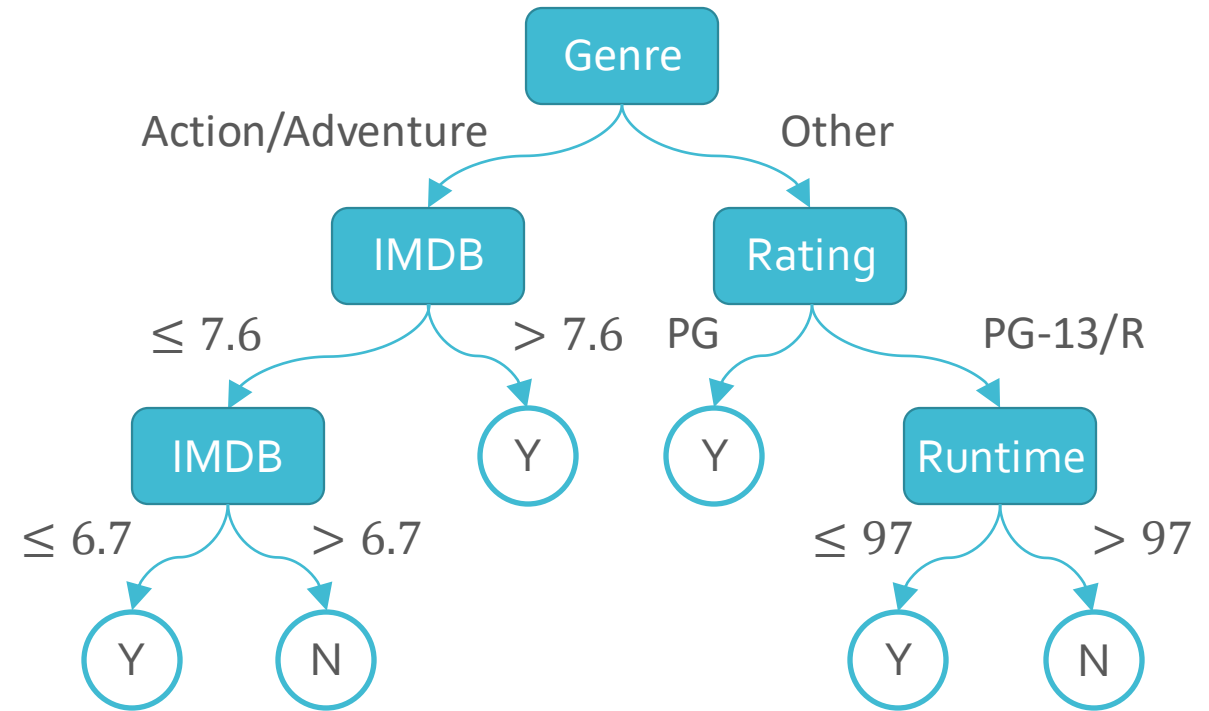
The Netflix Prize

Netflix Prize				
COMPLETED				
Home Rules Leaderboard Update Download				
Leaderboard				
Showing Test Score. Click here to show quiz score				
Display top 20 leaders.				
Rank	Team Name	Best Test Score	% Improvement	Best Submit Time
Grand Prize - RMSE = 0.8567 - Winning Team: BellKor's Pragmatic Chaos				
1	BellKor's Pragmatic Chaos	0.8567	10.06	2009-07-26 18:18:28
2	The Ensemble	0.8567	10.06	2009-07-26 18:38:22
3	Grand Prize Team	0.8582	9.90	2009-07-10 21:24:40
4	Opera Solutions and Vandelay United	0.8588	9.84	2009-07-10 01:12:31
5	Vandelay Industries !	0.8591	9.81	2009-07-10 00:32:20
6	PragmaticTheory	0.8594	9.77	2009-06-24 12:06:56
7	BellKor in BigChaos	0.8601	9.70	2009-05-13 08:14:09
8	Dace	0.8612	9.59	2009-07-24 17:18:43
9	Feeds2	0.8622	9.48	2009-07-12 13:11:51
10	BigChaos	0.8623	9.47	2009-04-07 12:33:59
11	Opera Solutions	0.8623	9.47	2009-07-24 00:34:07
12	BellKor	0.8624	9.46	2009-07-26 17:19:11

MovieID	Runtime	Genre	Budget	Year	IMDB	Rating	Liked?
1	124	Action	18M	1980	8.7	PG	Y
2	105	Action	30M	1984	7.8	PG	Y
3	103	Comedy	6M	1986	7.8	PG-13	N
4	98	Adventure	16M	1987	8.1	PG	Y
5	128	Comedy	16.4M	1989	8.1	PG	Y
6	120	Comedy	11M	1992	7.6	R	N
7	120	Drama	14.5M	1996	6.7	PG-13	N
8	136	Action	115M	1999	6.5	PG	Y
9	90	Action	90M	2001	6.6	PG-13	Y
10	161	Adventure	100M	2002	7.4	PG	N
11	201	Action	94M	2003	8.9	PG-13	Y
12	94	Comedy	26M	2004	7.2	PG-13	Y
13	157	Biography	100M	2007	7.8	R	N
14	128	Action	110M	2007	7.1	PG-13	N
15	107	Drama	39M	2009	7.1	PG-13	N
16	158	Drama	61M	2012	7.6	PG-13	N
17	169	Adventure	165M	2014	8.6	PG-13	Y
18	100	Biography	9M	2016	6.7	R	N
19	130	Action	180M	2017	7.9	PG-13	Y
20	141	Action	275M	2019	6.5	PG-13	Y

Movie Recommendations

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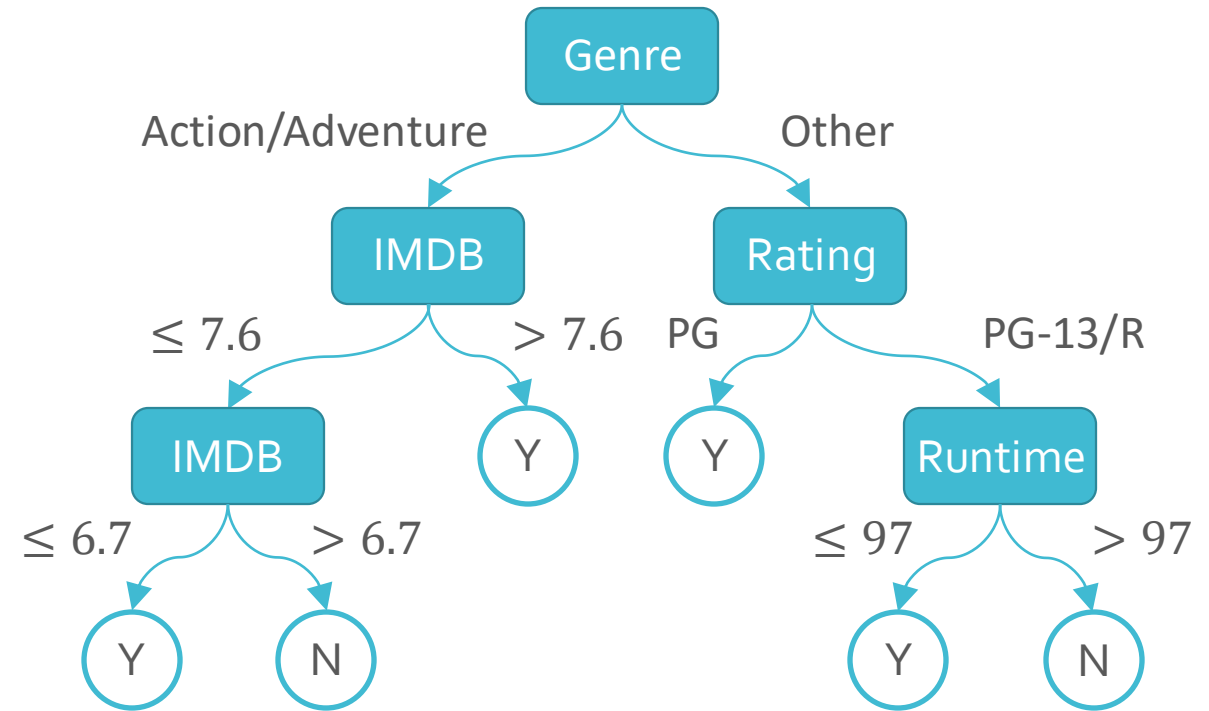


Decision Trees

Recall: Decision Tree Pros & Cons

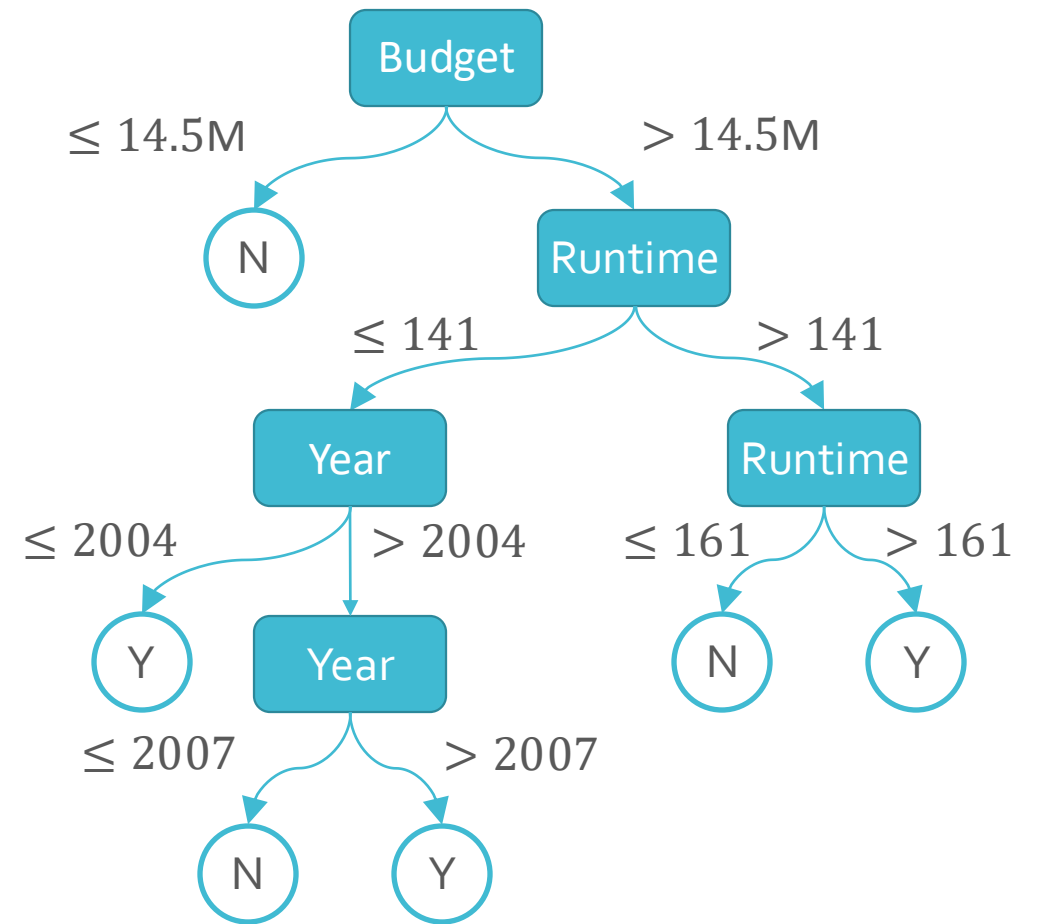
- Pros
 - Interpretable
 - Efficient (computational cost and storage)
 - Can be used for classification and regression tasks
 - Compatible with categorical and real-valued features
- Cons
 - Learned greedily: each split only considers the immediate impact on the splitting criterion
 - Not guaranteed to find the smallest (fewest number of splits) tree that achieves a training error rate of 0.
 - Prone to overfit
 - High variance

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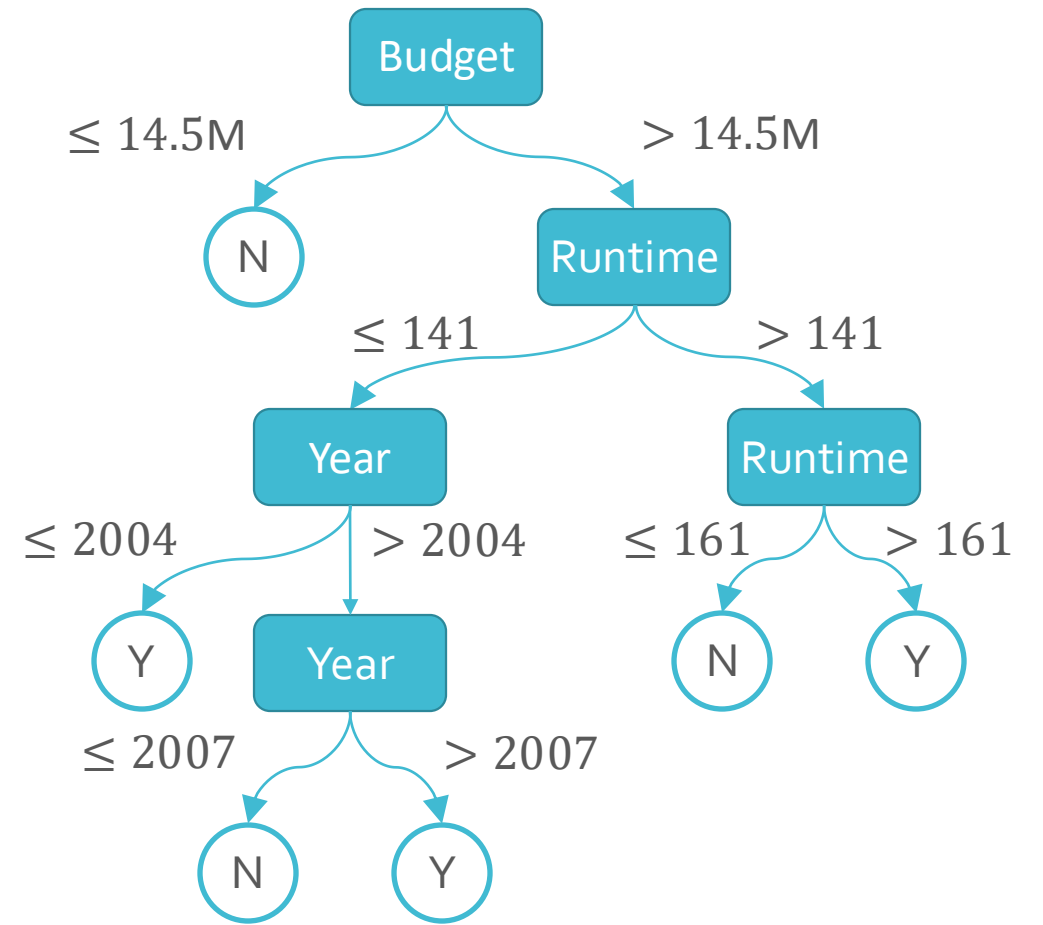
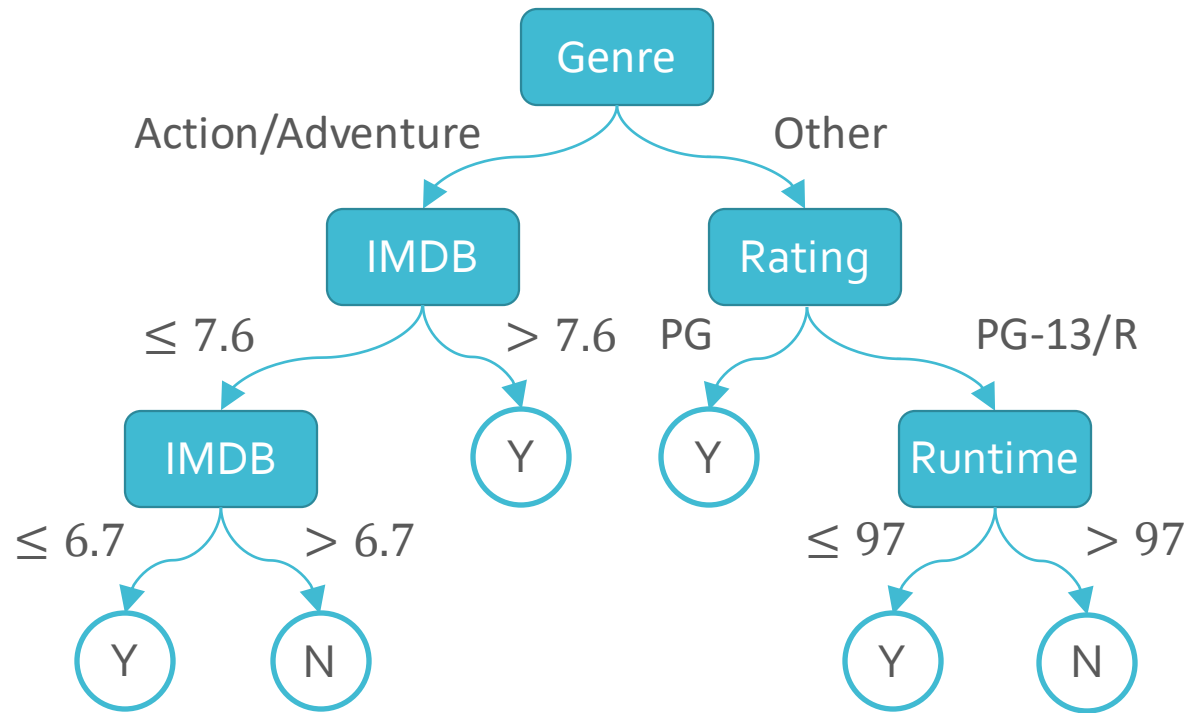


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Decision Trees

Decision Trees: Pros & Cons

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 - Not guaranteed to find the smallest (fewest number of splits) tree that achieves a training error rate of 0.
 - Prone to overfit
 - High variance
 - **Can be addressed via ensembles → random forests**

Random Forests

- Combines the prediction of many diverse decision trees to reduce their variability
- If B independent random variables $x^{(1)}, x^{(2)}, \dots, x^{(B)}$ all have variance σ^2 , then the variance of $\frac{1}{B} \sum_{b=1}^B x^{(b)}$ is $\frac{\sigma^2}{B}$
- Random forests = bagging + split-feature randomization
= bootstrap aggregating + split-feature randomization

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Aggregating

- How can we combine multiple decision trees, $\{t_1, t_2, \dots, t_B\}$, to arrive at a single prediction?
- Regression - average the predictions:

$$\bar{t}(\mathbf{x}) = \frac{1}{B} \sum_{b=1}^B t_b(\mathbf{x})$$

- Classification - plurality (or majority) vote; for binary labels encoded as $\{-1, +1\}$:

$$\bar{t}(\mathbf{x}) = \text{sign} \left(\frac{1}{B} \sum_{b=1}^B t_b(\mathbf{x}) \right)$$

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Random Forests

- Combines the prediction of many **diverse** decision trees to reduce their variability
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Bootstrapping

- Insight: one way of generating different decision trees is by changing the training data set
- Issue: often, we only have one fixed set of training data
- Idea: resample the data multiple times ***with replacement***

MovieID	...
1	...
2	...
3	...
⋮	⋮
19	...
20	...

Training data

MovieID	...
1	...
1	...
1	...
⋮	⋮
14	...
19	...

Bootstrapped
Sample 1

MovieID	...
4	...
4	...
5	...
⋮	⋮
16	...
16	...

Bootstrapped
Sample 2

...

...

Bootstrapping

- Idea: resample the data multiple times *with replacement*
 - Each bootstrapped sample has the same number of data points as the original data set
 - Duplicated points cause different decision trees to focus on different parts of the input space

MovieID	...
1	...
2	...
3	...
⋮	⋮
19	...
20	...

Training data

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1	...
1	...
1	...
⋮	⋮
14	...
19	...

Bootstrapped
Sample 1

MovieID	...
4	...
4	...
5	...
⋮	⋮
16	...
16	...

Bootstrapped
Sample 2

...

...

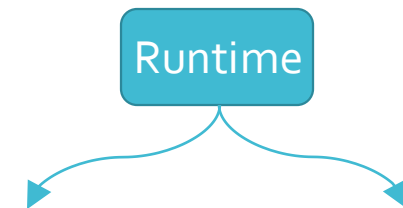
Split-feature Randomization

- Issue: decision trees trained on bootstrapped samples still tend to behave similarly...
- Idea: in addition to sampling the data points (i.e., the rows), also sample the features (i.e., the columns)
- Each time a split is being considered, limit the possible features to a randomly sampled subset

Runtime	Genre	Budget	Year	IMDB	Rating
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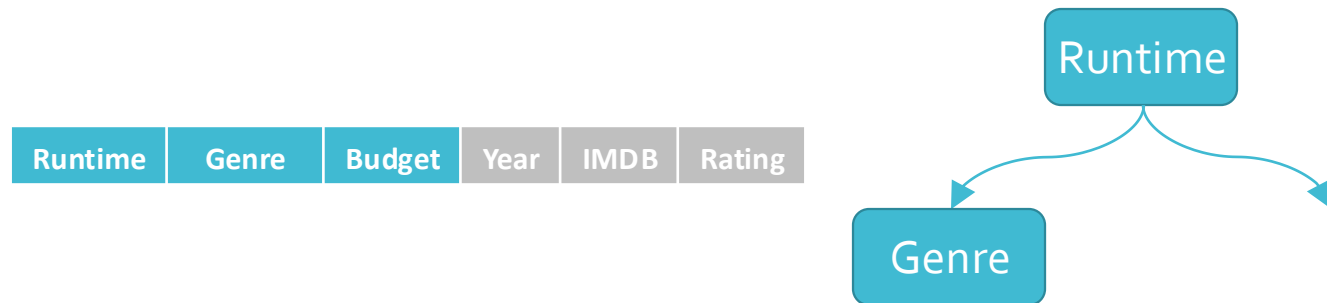
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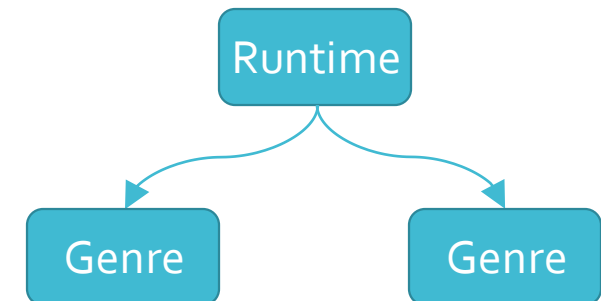
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- Each time a split is being considered, limit the possible features to a randomly sampled subset



Random Forests

- Input: $\mathcal{D} = \{(\mathbf{x}^{(n)}, y^{(n)})\}_{n=1}^N, B, \rho$
- For $b = 1, 2, \dots, B$
 - Create a dataset, \mathcal{D}_b , by sampling N points from the original training data \mathcal{D} **with replacement**
 - Learn a decision tree, t_b , using \mathcal{D}_b and the ID3 algorithm **with split-feature randomization**, sampling ρ features for each split
- Output: $\bar{t} = f(t_1, \dots, t_B)$, the aggregated hypothesis

How can we set B and ρ ?

- Input: $\mathcal{D} = \{(\mathbf{x}^{(n)}, y^{(n)})\}_{n=1}^N, B, \rho$
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Recall: Validation Sets



- Suppose we want to compare multiple hyperparameter settings $\theta_1, \dots, \theta_K$
- For $k = 1, 2, \dots, K$
 - Train a model on D_{train} using θ_k
 - Evaluate each model on D_{val} and find the best hyperparameter setting, θ_{k^*}
 - Compute the error of a model trained with θ_{k^*} on D_{test}

Out-of-bag Error

- For each training point, $\mathbf{x}^{(n)}$, there are some decision trees which $\mathbf{x}^{(n)}$ was not used to train (roughly B/e trees or 37%)
 - Let these be $\mathbf{t}^{(-n)} = \{t_1^{(-n)}, t_2^{(-n)}, \dots, t_{N-n}^{(-n)}\}$
- Compute an aggregated prediction for each $\mathbf{x}^{(n)}$ using the trees in $\mathbf{t}^{(-n)}$, $\bar{t}^{(-n)}(\mathbf{x}^{(n)})$
- Compute the out-of-bag (OOB) error, e.g., for regression

$$E_{OOB} = \frac{1}{N} \sum_{n=1}^N (\bar{t}^{(-n)}(\mathbf{x}^{(n)}) - y^{(n)})^2$$

Out-of-bag Error

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- Compute an aggregated prediction for each $\mathbf{x}^{(n)}$ using the trees in $\mathbf{t}^{(-n)}$, $\bar{\mathbf{t}}^{(-n)}(\mathbf{x}^{(n)})$

- Compute the out-of-bag (OOB) error, e.g., for classification

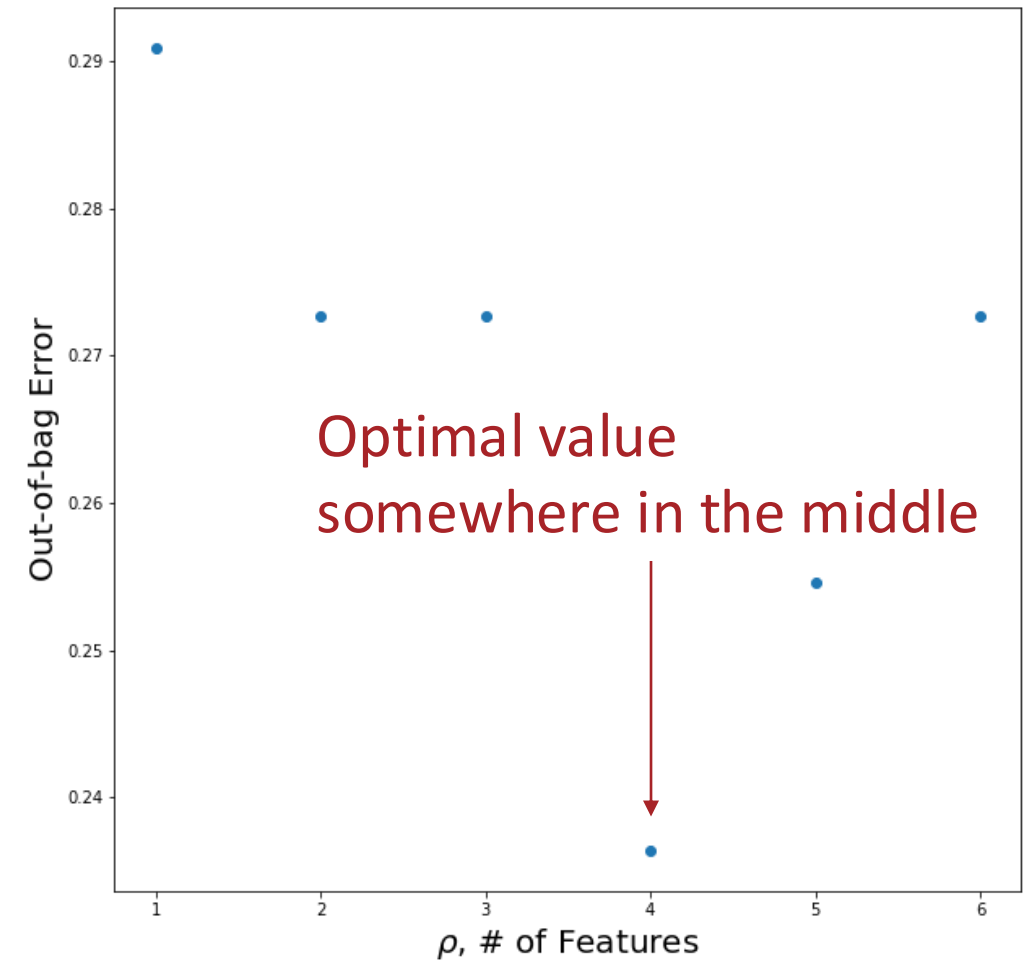
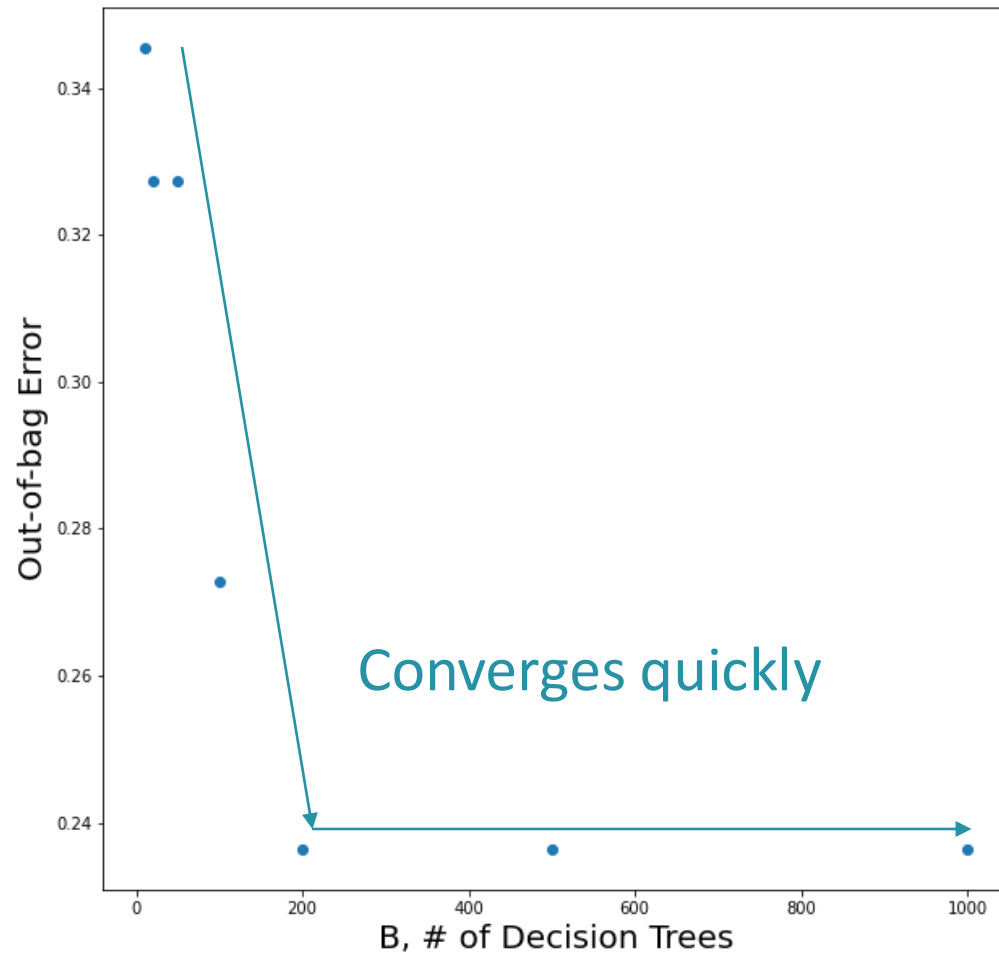
$$E_{OOB} = \frac{1}{N} \sum_{n=1}^N \mathbb{1}(\bar{\mathbf{t}}^{(-n)}(\mathbf{x}^{(n)}) \neq y^{(n)})$$

- E_{OOB} can be used for hyperparameter optimization!

Out-of-bag Error



- Suppose we want to compare different numbers of trees in our random forest B_1, \dots, B_K
- For $k = 1, 2, \dots, K$
 - Train a random forest on D_{train} with B_k trees
- Compute E_{OOB} for each random forest and find the best number of trees, B_{k^*}
- Evaluate the random forest with B_{k^*} trees on D_{test}

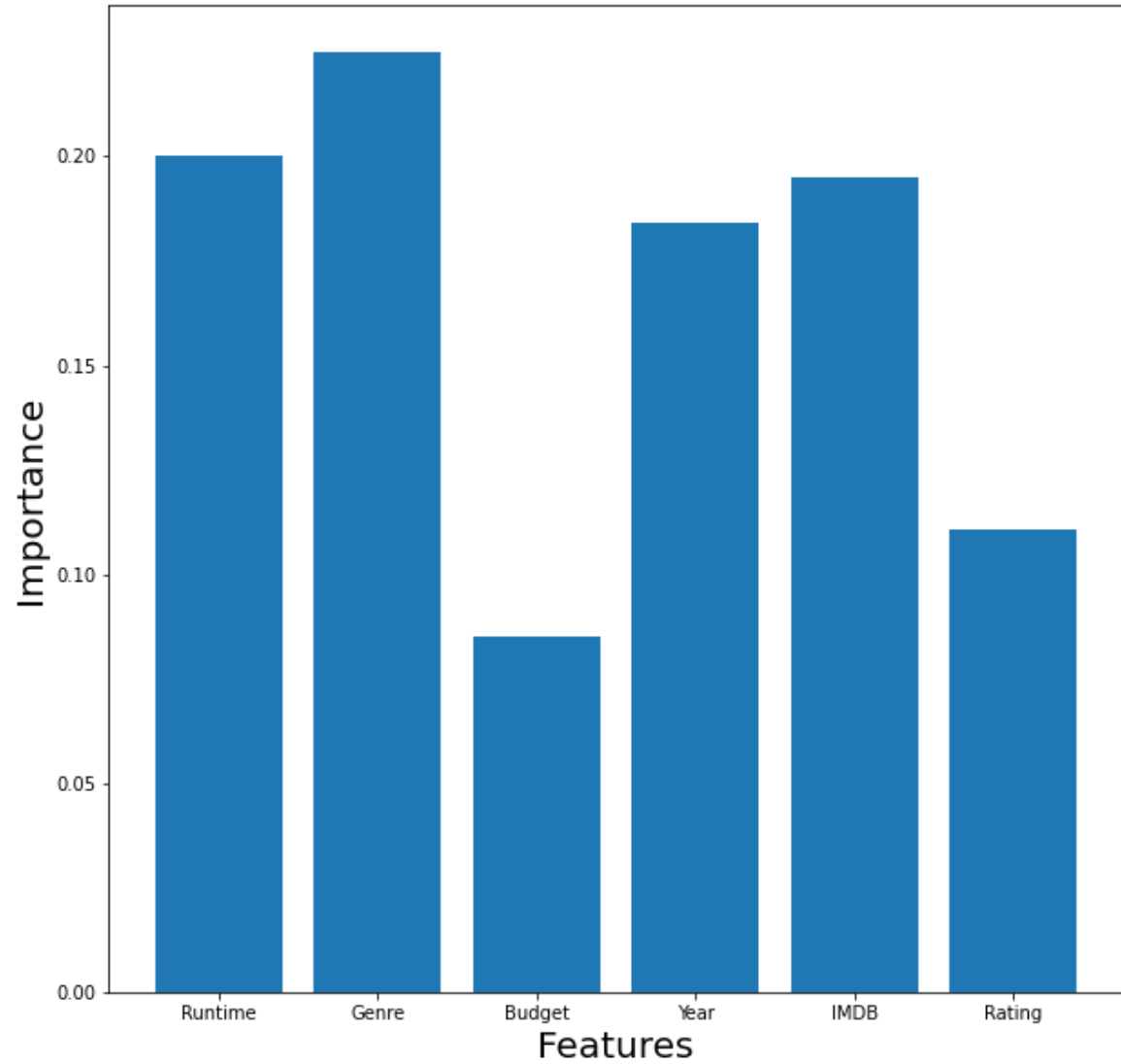


Setting Hyperparameters

Feature Importance

- Some of the interpretability of decision trees gets lost when switching to random forests
- Random forests allow for the computation of “feature importance”, a way of ranking features based on how useful they are at predicting the target
- Initialize each feature’s importance to zero
- Each time a feature is chosen to be split on, add the reduction in IG (weighted by the number of data points in the split) to its importance

Feature Importance



Key Takeaways

- Ensemble methods employ a “wisdom of crowds” philosophy
 - Can reduce the variance of high variance methods
- Random forests = bagging + split-feature randomization
 - Aggregate multiple decision trees together
 - Bootstrapping and split-feature randomization increase diversity in the decision trees
 - Use out-of-bag errors for hyperparameter optimization

Decision Trees: Pros & Cons

- Pros
 - ...
- Cons
 - Learned greedily: each split only considers the immediate impact on the splitting criterion
 - Not guaranteed to find the smallest (fewest number of splits) tree that achieves a training error rate of 0.
 - Prone to overfit
 - High variance
 - Can be addressed via **bagging** → random forests
 - Limited expressivity/high bias (especially short trees)
 - Can be addressed via **boosting**

AdaBoost

- Intuition: iteratively reweight inputs, giving more weight to inputs that are difficult-to-predict correctly
- Analogy:
 - You all have to take a test (😱) ...
 - ... but you're going to be taking it one at a time.
 - After you finish, you get to tell the next person the questions you struggled with.
 - Hopefully, they can cover for you because...
 - ... if “enough” of you get a question right, you'll all receive full credit for that problem

- Input: $\mathcal{D} \left(y^{(n)} \in \{-1, +1\} \right), T$
- Initialize data point weights: $\omega_0^{(1)}, \dots, \omega_0^{(N)} = \frac{1}{N}$
- For $t = 1, \dots, T$
 1. Train a weak learner, h_t , by minimizing the *weighted* training error
 2. Compute the *weighted* training error of h_t :

$$\epsilon_t = \sum_{n=1}^N \omega_{t-1}^{(n)} \mathbb{1} \left(y^{(n)} \neq h_t(\mathbf{x}^{(n)}) \right)$$

3. Compute the **importance** of h_t :

$$\alpha_t = \frac{1}{2} \log \left(\frac{1 - \epsilon_t}{\epsilon_t} \right)$$

4. Update the data point weights:

$$\omega_t^{(n)} = \frac{\omega_{t-1}^{(n)}}{Z_t} \times \begin{cases} e^{-\alpha_t} & \text{if } h_t(\mathbf{x}^{(n)}) = y^{(n)} \\ e^{\alpha_t} & \text{if } h_t(\mathbf{x}^{(n)}) \neq y^{(n)} \end{cases} = \frac{\omega_{t-1}^{(n)} e^{-\alpha_t y^{(n)} h_t(\mathbf{x}^{(n)})}}{Z_t}$$

- Output: an aggregated hypothesis

$$g_T(\mathbf{x}) = \text{sign}(H_T(\mathbf{x})) \\ = \text{sign} \left(\sum_{t=1}^T \alpha_t h_t(\mathbf{x}) \right)$$

Setting α_t

α_t determines the contribution of h_t to the final, aggregated hypothesis:

$$g(x) = \text{sign} \left(\sum_{t=1}^T \alpha_t h_t(x) \right)$$

Intuition: we want good weak learners to have high importances

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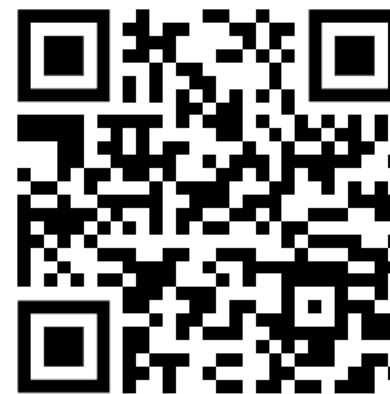
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$$\alpha_t = \frac{1}{2} \log \left(\frac{1 - \epsilon_t}{\epsilon_t} \right)$$

In-class Poll:

How does the importance of a very bad/mostly incorrect classifier compare to that of a very good/mostly correct classifier?

- Same sign and similar magnitude
- Same sign, different magnitude
- Different sign, similar magnitude
- Different sign, different magnitude



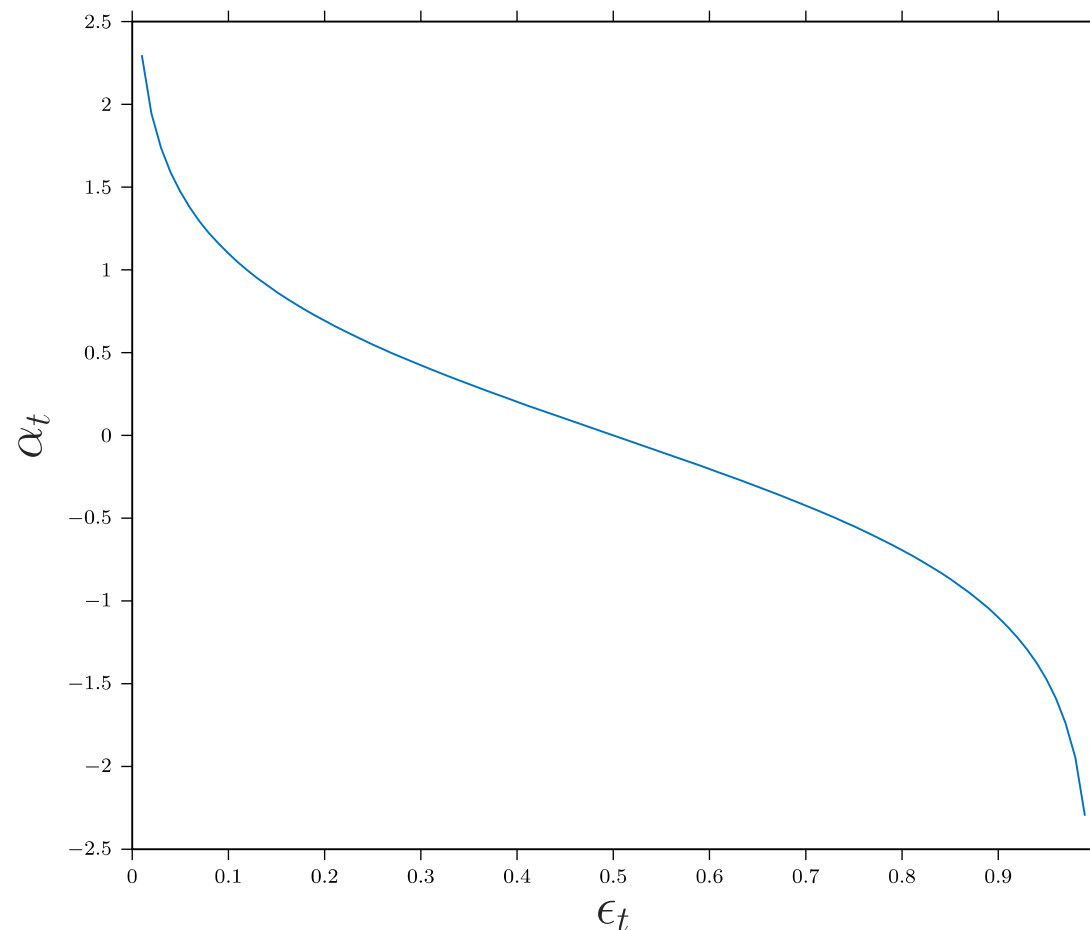
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Updating $\omega^{(n)}$

- Intuition: we want incorrectly classified inputs to receive a higher weight in the next round

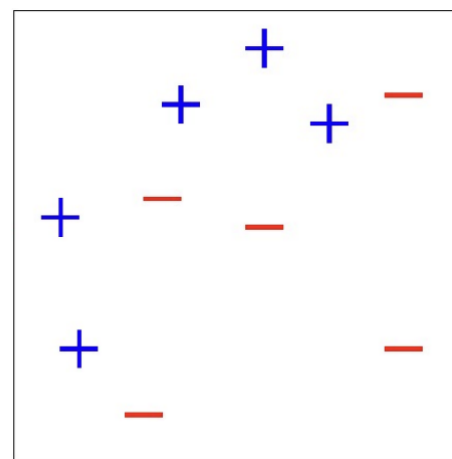
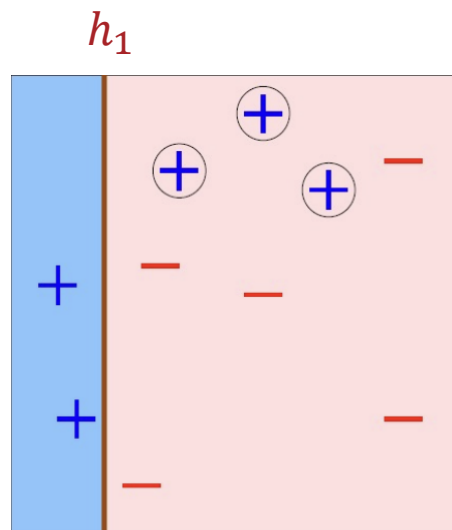
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- If $\epsilon_t < \frac{1}{2}$, then $\frac{1-\epsilon_t}{\epsilon_t} > 1$
- If $\frac{1-\epsilon_t}{\epsilon_t} > 1$, then $\alpha_t = \frac{1}{2} \log \left(\frac{1-\epsilon_t}{\epsilon_t} \right) > 0$
- If $\alpha_t > 0$, then $e^{-\alpha_t} < 1$ and $e^{\alpha_t} > 1$

AdaBoost: Example

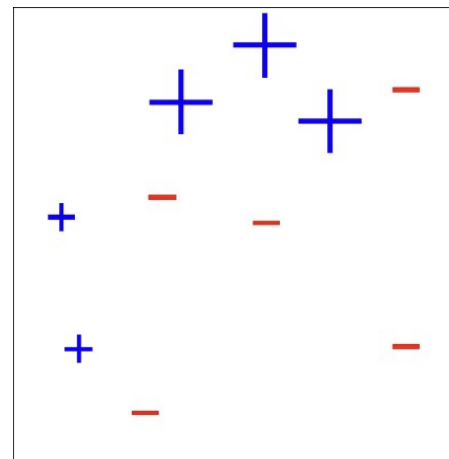
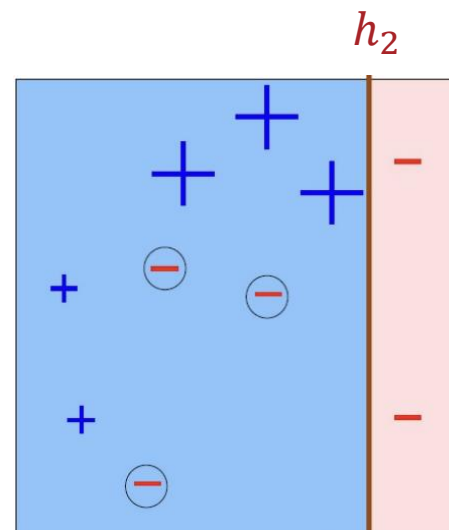
$$\epsilon_1 = 0.3$$

$$\alpha_1 = 0.42$$



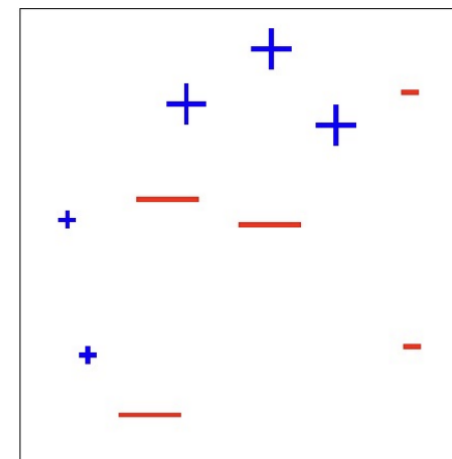
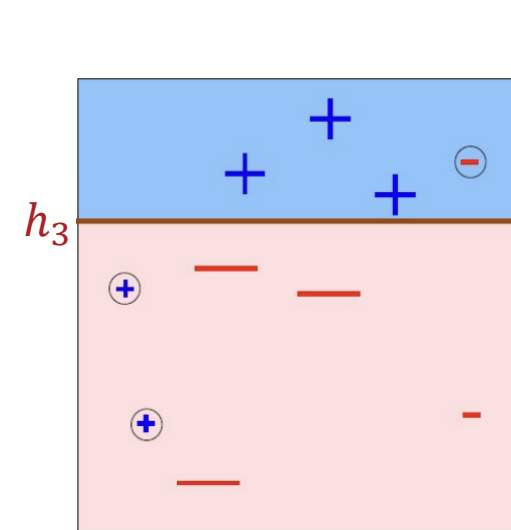
$$\epsilon_2 = 0.21$$

$$\alpha_2 = 0.65$$



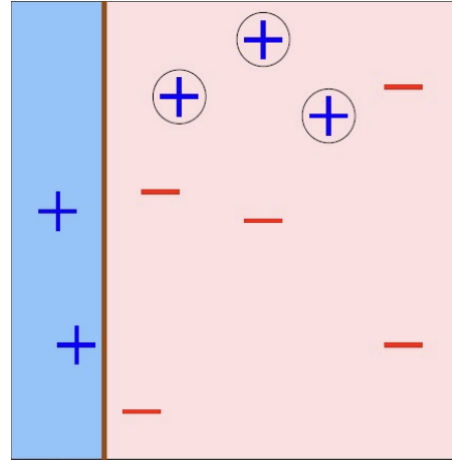
$$\epsilon_3 = 0.14$$

$$\alpha_3 = 0.92$$



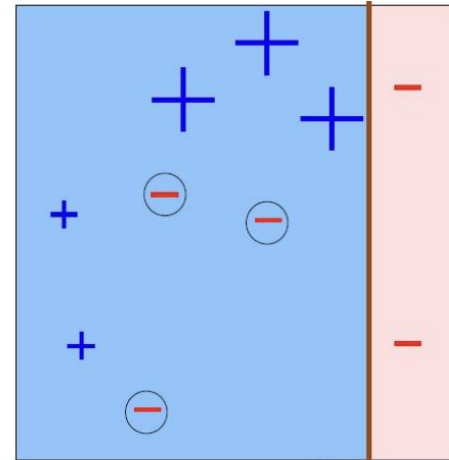
AdaBoost: Example

$0.42 h_1$

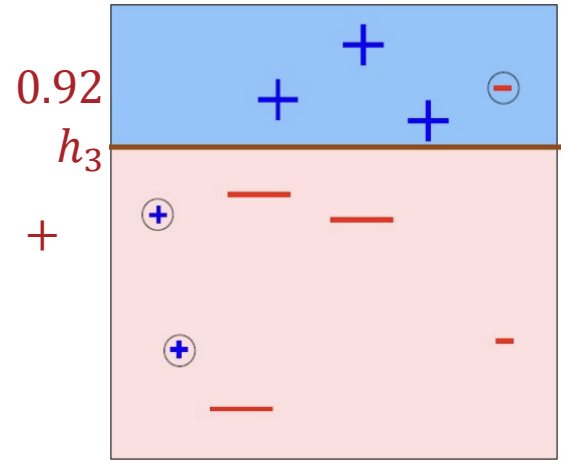


+

$0.65 h_2$

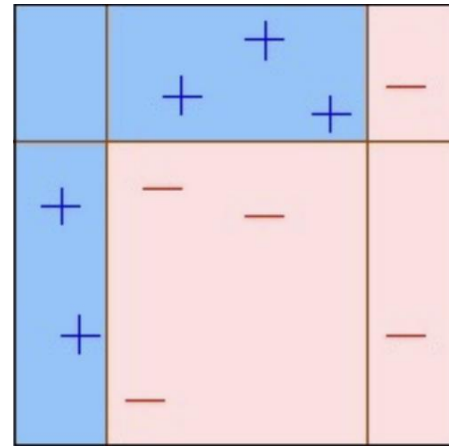


$0.92 h_3$



+

=



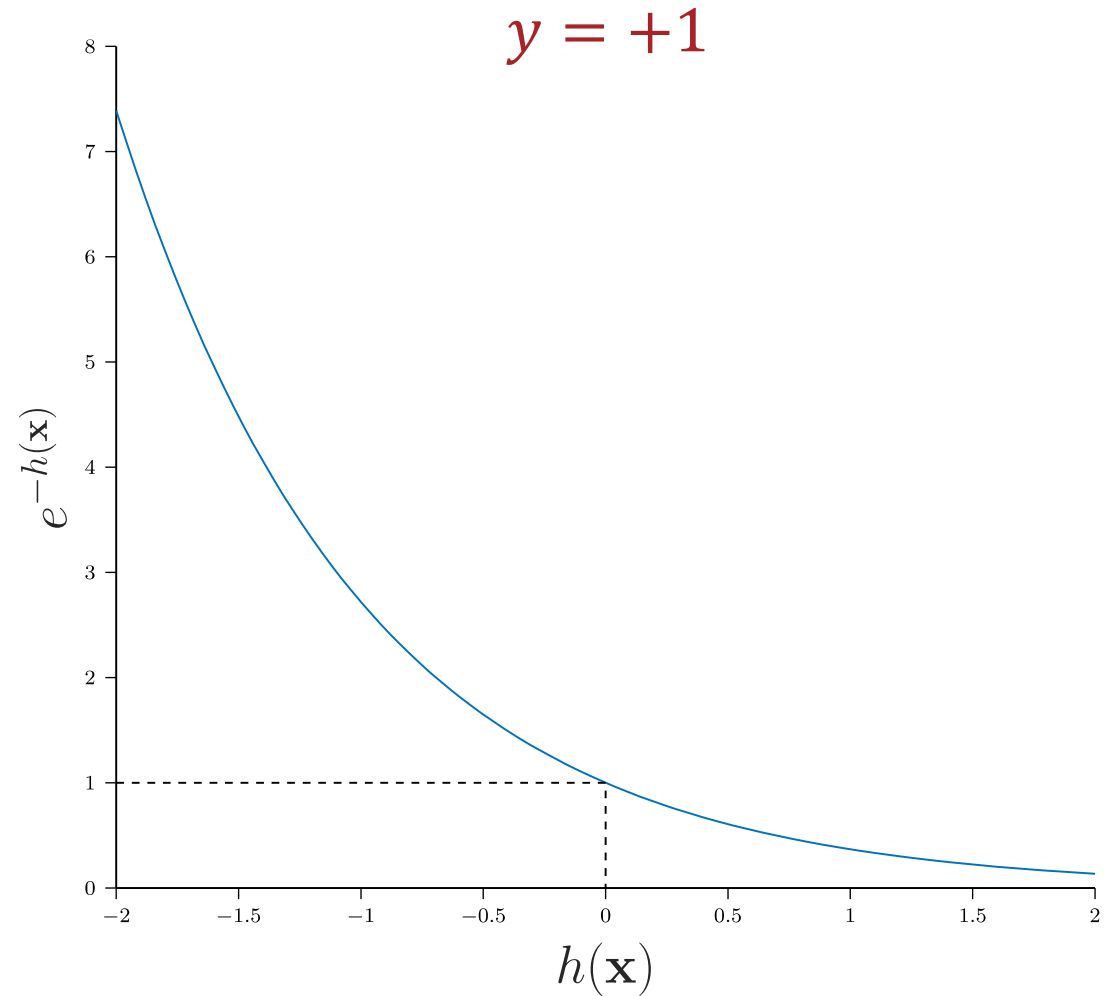
Why AdaBoost?

1. If you want to use weak learners ...
 2. ... and want your final hypothesis to be a weighted combination of weak learners, ...
 3. ... then Adaboost greedily minimizes the exponential loss:
$$e(h(\mathbf{x}), y) = e^{-yh(\mathbf{x})}$$
1. Because they're low variance / computational constraints
 2. Because weak learners are not great on their own
 3. Because the exponential loss upper bounds binary error!

Exponential Loss

$$e(h(\mathbf{x}), y) = e^{-yh(\mathbf{x})}$$

The more $h(\mathbf{x})$ “agrees with” y , the smaller the loss and the more $h(\mathbf{x})$ “disagrees with” y , the greater the loss



Exponential Loss

- Claim:

$$\frac{1}{N} \sum_{n=1}^N e^{(-y^{(n)} h(\mathbf{x}^{(n)}))} \geq \frac{1}{N} \sum_{n=1}^N \mathbb{1} \left(\text{sign} \left(h(\mathbf{x}^{(n)}) \right) \neq y^{(n)} \right)$$

- Consequence:

$$\frac{1}{N} \sum_{n=1}^N e^{(-y^{(n)} h(\mathbf{x}^{(n)}))} \rightarrow 0$$

$$\Rightarrow \frac{1}{N} \sum_{n=1}^N \mathbb{1} \left(\text{sign} \left(h(\mathbf{x}^{(n)}) \right) \neq y^{(n)} \right) \rightarrow 0$$

Key Takeaways

- Boosting targets simple models, i.e., weak learners
- Greedily minimizes the exponential loss, an upper bound of the classification error
- Theoretical (and empirical) results show resilience to overfitting by targeting training margin