# 10-301/601: Introduction to Machine Learning Lecture 29 – Random Forests

#### **Front Matter**

- Announcements:
  - HW7 released on 6/10, due 6/13 at 11:59 PM
  - Thursday's lecture will be a guest lecture by Alex Xie on Reinforcement Learning for LLMs
    - Everyone who attends will have their lowest quiz grade down-weighted by 50%
  - Next's weeks lectures (6/16 and 6/17) will start at 11
     AM, not 9:30 AM

#### Final Logistics

- Time and place:
  - Final on 6/20 (next Friday) at **8:30 AM** in BH A36 (here!)
- Closed book/notes
  - 1-page cheatsheet allowed, both back and front; can be typeset or handwritten

#### Final Coverage

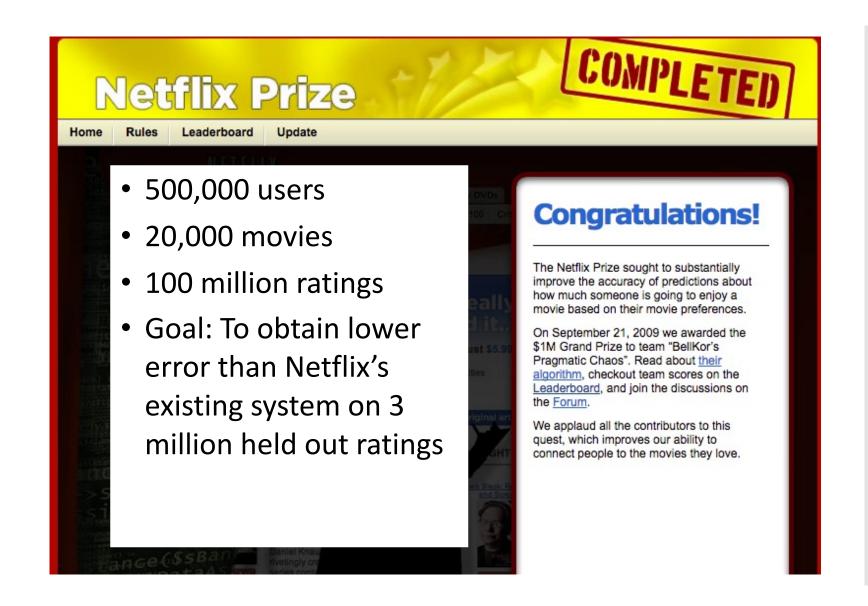
- Lectures: 17 30 (through today's lectures)
  - Learning Theory
  - Deep Learning: CNNs, RNNs, Attention and Transformers
  - Unsupervised Learning: Dimensionality Reduction,
     Clustering
  - Pre-training, Fine-tuning and In-context Learning
  - Reinforcement Learning
  - Ensemble Methods: Boosting, Random Forests
- The final is *not* cumulative: pre-midterm content may be referenced but will not be the *primary* focus of any question

# Final Preparation

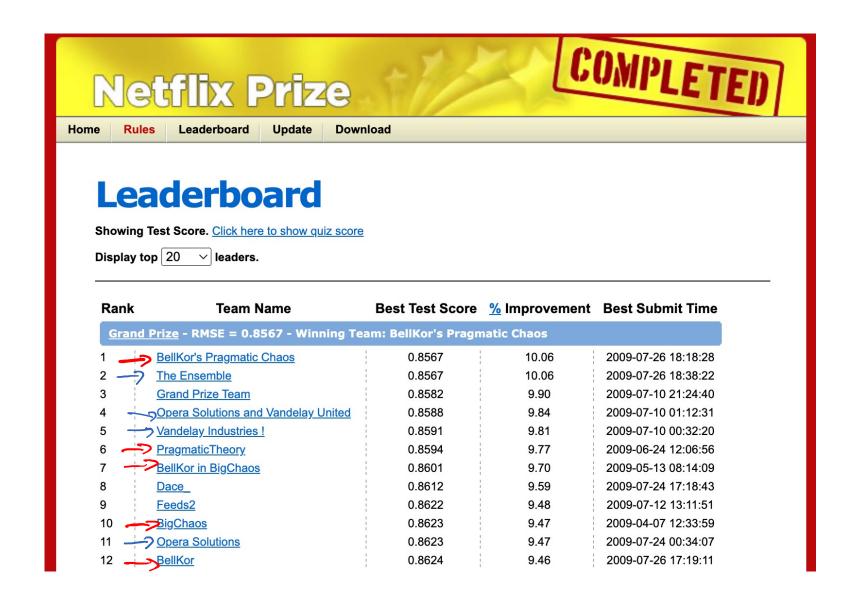


- Review midterm practice problems, to be posted on 6/13 to the course website (under <u>Schedule</u>)
- Attend the exam review recitation on 6/18 at 9:30 AM
- Review the homeworks and study guides
- Consider whether you understand the "Key Takeaways"
   for each lecture / section
- Write your cheat sheet

# The Netflix Prize



# The Netflix Prize



# Ranking Classifiers (Caruana & Niculescu-Mizil, 2006)

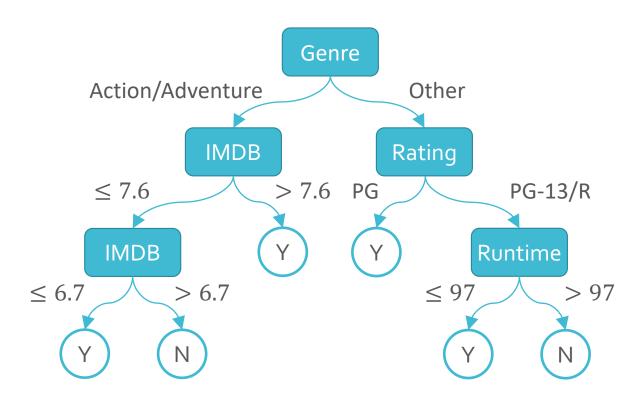
Table 2. Normalized scores for each learning algorithm by metric (average over eleven problems)

MODEL	CAL	ACC	FSC	LFT	ROC	APR	BEP	RMS	MXE	MEAN	OPT-SEL
BST-DT	PLT	.843*	.779	.939	.963	.938	.929*	.880	.896	.896	.917
RF	PLT	.872*	.805	.934*	.957	.931	.930	.851	.858	.892	.898
BAG-DT	_	.846	.781	.938*	.962*	.937*	.918	.845	.872	.887*	.899
BST-DT	ISO	.826*	.860*	.929*	.952	.921	.925*	.854	.815	.885	.917*
RF	_	.872	.790	.934*	.957	.931	.930	.829	.830	.884	.890
BAG-DT	PLT	.841	.774	.938*	.962*	.937*	.918	.836	.852	.882	.895
RF	ISO	.861*	.861	.923	.946	.910	.925	.836	.776	.880	.895
BAG-DT	ISO	.826	.843*	.933*	.954	.921	.915	.832	.791	.877	.894
SVM	PLT	.824	.760	.895	.938	.898	.913	.831	.836	.862	.880
ANN	1 - 1	.803	.762	.910	.936	.892	.899	.811	.821	.854	.885
SVM	ISO	.813	.836 <b>*</b>	.892	.925	.882	.911	.814	.744	.852	.882
ANN	PLT	.815	.748	.910	.936	.892	.899	.783	.785	.846	.875
ANN	ISO	.803	.836	.908	.924	.876	.891	.777	.718	.842	.884
BST-DT	* <u></u>	.834*	.816	.939	.963	.938	.929*	.598	.605	.828	.851
KNN	PLT	.757	.707	.889	.918	.872	.872	.742	.764	.815	.837
KNN	_	.756	.728	.889	.918	.872	.872	.729	.718	.810	.830
KNN	ISO	.755	.758	.882	.907	.854	.869	.738	.706	.809	.844
BST-STMP	PLT	.724	.651	.876	.908	.853	.845	.716	.754	.791	.808
SVM	_	.817	.804	.895	.938	.899	.913	.514	.467	.781	.810
BST-STMP	ISO	.709	.744	.873	.899	.835	.840	.695	.646	.780	.810
BST-STMP	1 - 2	.741	.684	.876	.908	.853	.845	.394	.382	.710	.726
DT	ISO	.648	.654	.818	.838	.756	.778	.590	.589	.709	.774
DT	_	.647	.639	.824	.843	.762	.777	.562	.607	.708	.763
DT	PLT	.651	.618	.824	.843	.762	.777	.575	.594	.706	.761
LR	_	.636	.545	.823	.852	.743	.734	.620	.645	.700	.710
LR	ISO	.627	.567	.818	.847	.735	.742	.608	.589	.692	.703
LR	PLT	.630	.500	.823	.852	.743	.734	.593	.604	.685	.695
NB	ISO	.579	.468	.779	.820	.727	.733	.572	.555	.654	.661
NB	PLT	.576	.448	.780	.824	.738	.735	.537	.559	.650	.654
NB		.496	.562	.781	.825	.738	.735	.347	633	.481	.489

MovieID	Runtime	Genre	Budget	Year	IMDB	Rating	Liked?
1	124	Action	18M	1980	8.7	PG	Υ
2	105	Action	30M	1984	7.8	PG	Υ
3	103	Comedy	6M	1986	7.8	PG-13	N
4	98	Adventure	16M	1987	8.1	PG	Υ
5	128	Comedy	16.4M	1989	8.1	PG	Υ
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	Υ
9	90	Action	90M	2001	6.6	PG-13	Υ
10	161	Adventure	100M	2002	7.4	PG	N
11	201	Action	94M	2003	8.9	PG-13	Υ
12	94	Comedy	26M	2004	7.2	PG-13	Υ
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	Υ
18	100	Biography	9M	2016	6.7	R	N
19	130	Action	180M	2017	7.9	PG-13	Υ
20	141	Action	275M	2019	6.5	PG-13	Υ

### Movie Recommendations

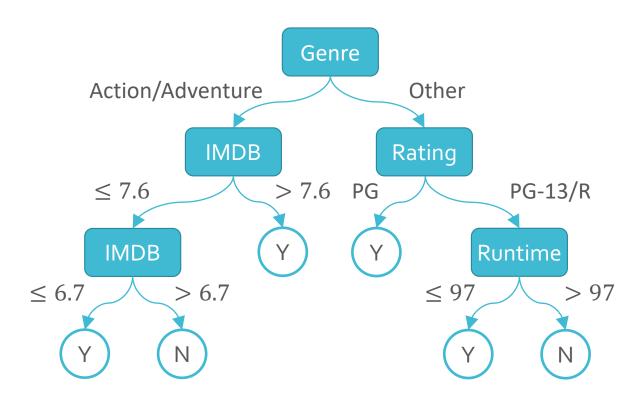
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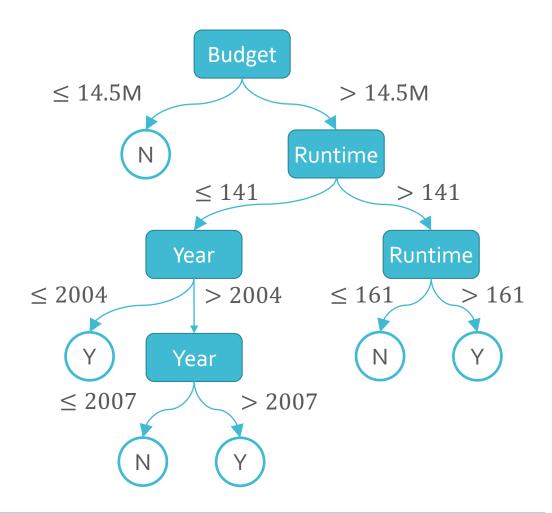
# Decision Trees: Pros & Cons

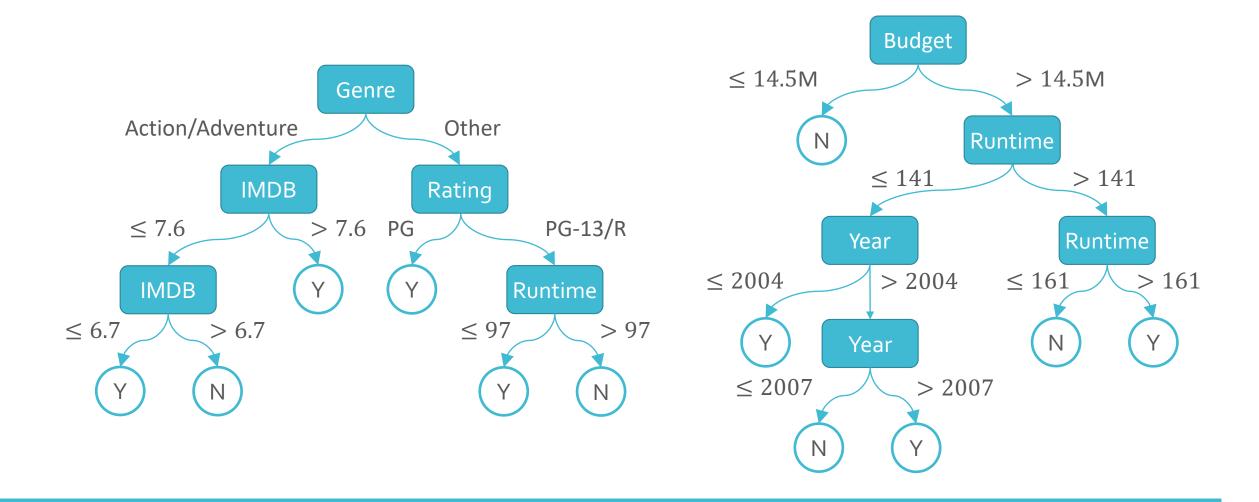
- Pros
  - Interpretable
  - Efficient (computational cost and storage)
  - Can be used for classification and regression tasks
  - Compatible with categorical and real-valued features
- Cons
  - Learned greedily: each split only considers the immediate impact on the splitting criterion
    - Not guaranteed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

MovielD	Runtime	Genre	Budget	Year	IMDB	Rating	Liked?
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#### Random Forests

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

- + split-feature randomization
- = **b**ootstrap **agg**regat**ing** + split-feature randomization

#### Aggregating

- How can we combine multiple decision trees,  $\{t_1, t_2, ..., t_B\}$ , 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  $\{-1, +1\}$ :

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

#### 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

MovielD	•••
1	•••
2	•••
3	•••
:	:
19	•••
20	•••

Train	ing	data
-------	-----	------

MovielD	•••
1	•••
1	•••
1	•••
:	i
14	•••
19	•••

Bootstrapped Sample 1

MovielD	•••	
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

MovielD	•••
1	•••
2	•••
3	•••
:	÷
19	•••
20	•••

MovielD	•••
1	•••
1	•••
1	•••
:	÷
14	•••
19	•••

Bootstrapped Sample 1

MovielD	•••	
4	•••	
4	•••	
5	•••	
:	:	
16	•••	
16	•••	

Bootstrapped Sample 2

- Issue: decision trees trained on bootstrapped samples still 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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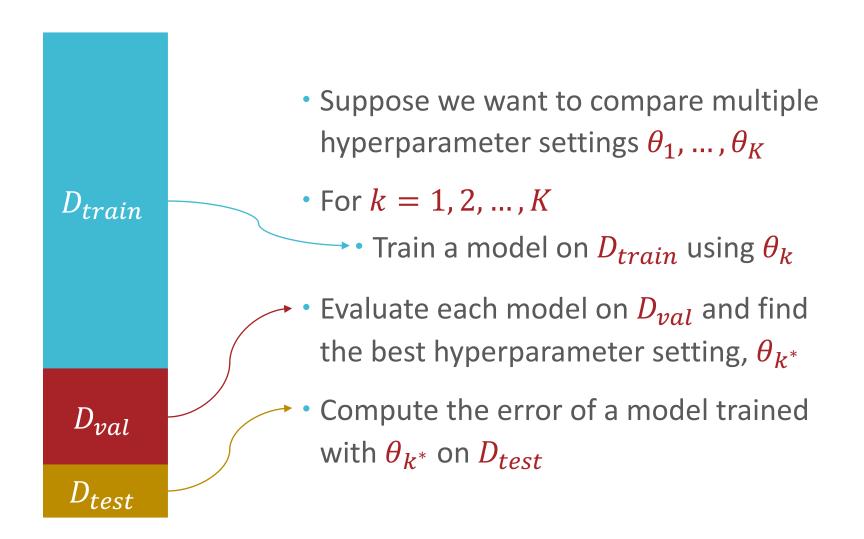


#### Random Forests

• Input: 
$$\mathcal{D} = \{(x^{(n)}, y^{(n)})\}_{n=1}^{N}, B, \rho$$

- For b = 1, 2, ..., 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  $\rho$  features for each split
- Output:  $\bar{t} = f(t_1, ..., t_B)$ , the aggregated hypothesis

# Recall: Validation Sets



• For each training point,  $x^{(n)}$ , there are some decision trees which  $x^{(n)}$  was not used to train (roughly B/e trees or 37%)

• Let these be 
$$t^{(-n)} = \left\{ t_1^{(-n)}, t_2^{(-n)}, \dots, t_{N-n}^{(-n)} \right\}$$

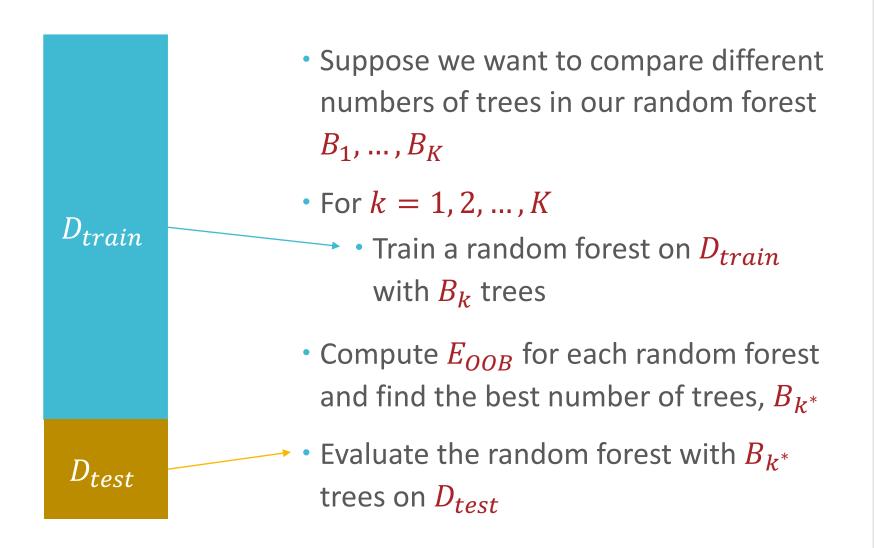
- Compute an aggregated prediction for each  $x^{(n)}$  using the trees in  $t^{(-n)}$ ,  $\bar{t}^{(-n)}(x^{(n)})$
- Compute the out-of-bag (OOB) error, e.g., for regression

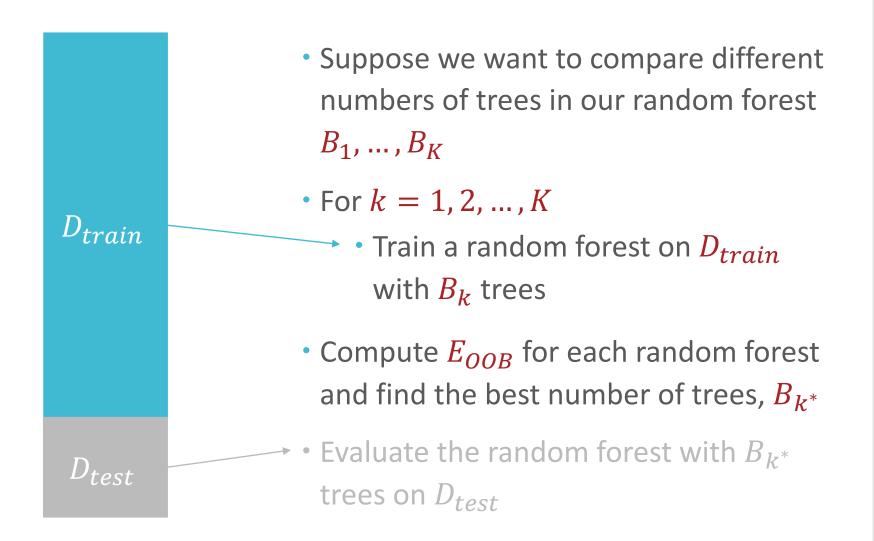
$$E_{OOB} = \frac{1}{N} \sum_{n=1}^{N} (\bar{t}^{(-n)}(x^{(n)}) - y^{(n)})^{2}$$

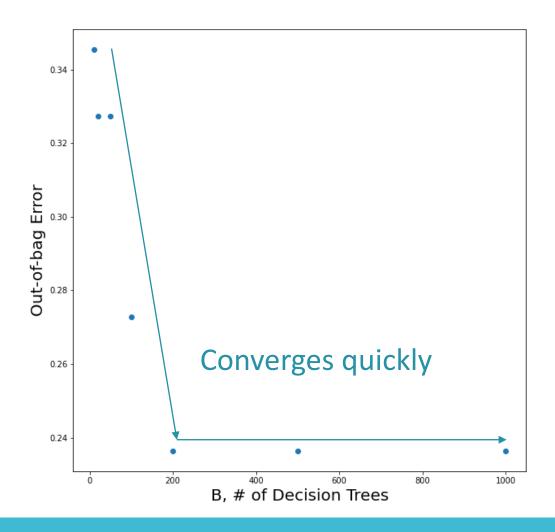
- For each training point,  $\mathbf{x}^{(n)}$ , there are some decision trees which  $\mathbf{x}^{(n)}$  was not used to train (roughly B/e trees or 37%)
  - Let these be  $t^{(-n)} = \left\{ t_1^{(-n)}, t_2^{(-n)}, \dots, t_{N-n}^{(-n)} \right\}$
- Compute an aggregated prediction for each  ${\it x}^{(n)}$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

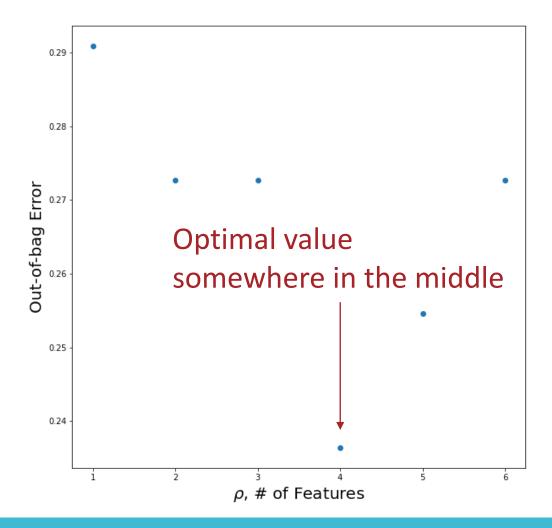
$$E_{OOB} = \frac{1}{N} \sum_{n=1}^{N} \mathbb{1}(\bar{t}^{(-n)}(x^{(n)}) \neq y^{(n)})$$

•  $E_{OOB}$  can be used for hyperparameter optimization!









## Setting Hyperparameters

#### 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