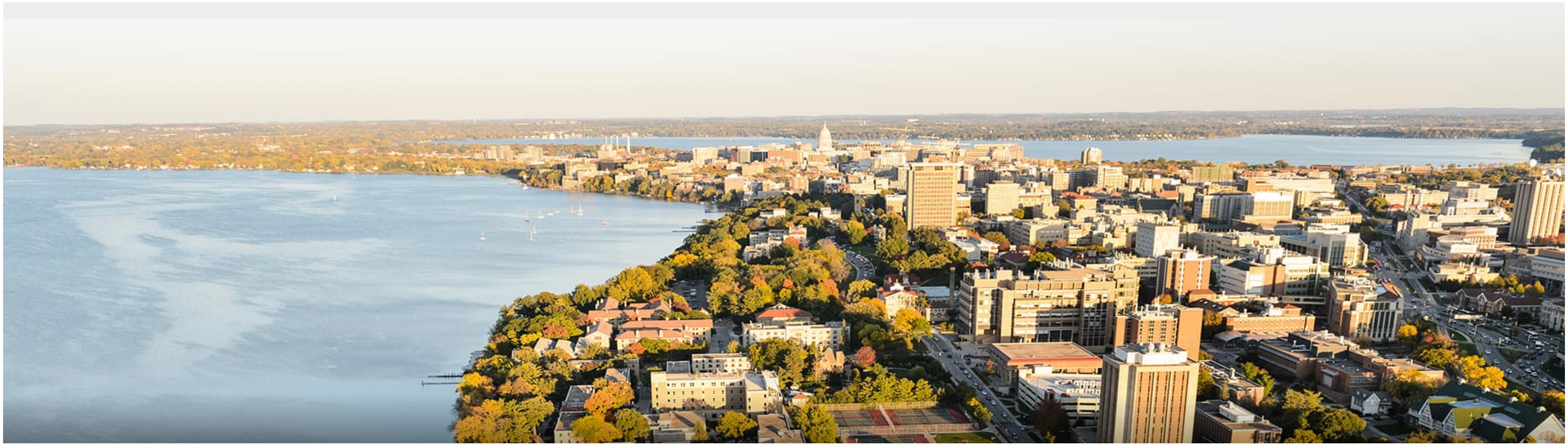

CS 760: Machine Learning
Decision Trees & Evaluation

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Sept. 22, 2022

Announcements

- **Announcements**:
  - HW 2 released Tuesday
- **Class roadmap:**

Thursday Sept. 22	Evaluation
Tuesday Sept. 27	Regression I
Thursday Sept. 29	Regression II
Tuesday, Oct. 4	Naive Bayes
Thursday, Oct. 6	Neural Networks I

Supervised Learning

Outline

- **Continuing from last time: Decision trees**
  - Information gain, stopping criteria, overfitting, pruning, variations
- **Evaluation: Generalization**
  - Train/test split, random sampling, cross validation
- **Evaluation: Metrics**
  - Confusion matrices, ROC curves, precision/recall

Outline

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DT Learning: InfoGain Limitations

- InfoGain is biased towards tests with many outcomes
  - A feature that uniquely identifies each instance
  - Splitting on it results in many branches, each of which is “pure” (has instances of only one class)
  - **Maximal** information gain!

- Use **GainRatio**: normalize information gain by entropy

$$\mathrm{GainRatio}(D, S) = \frac{\mathrm{InfoGain}(D,S)}{H_D(S)} = \frac{H_D(Y) - H_D(Y|S)}{H_D(S)}$$

DT Learning: GainRatio

- Why?
  - Suppose S is a *binary split*. InfoGain limited to 1 bit, no matter what.

$$\mathrm{InfoGain}(D,S) = H_D(Y) - H_D(Y|S)$$

Intuition: at most, S tells us Y is in one half of its classes or the other

  - Now suppose S is different for each instance (i.e., student number).
    - Uniquely determines Y for each point, but useless for generalization.
    - But, then $H_D(Y|S) = 0$, so maximal information gain!
  - Control this by normalizing by $H_D(S)$.
    - Above: for *n* instances, $H_D(S) = \log_2(n)$

$$\mathrm{GainRatio}(D,S) = \frac{\mathrm{InfoGain}(D,S)}{H_D(S)} = \frac{H_D(Y)-H_D(Y|S)}{H_D(S)}$$

DT Learning: Stopping Criteria

Form a leaf when

- All of the given subset of instances are same class
- We've exhausted all of the candidate splits

- Stop earlier?

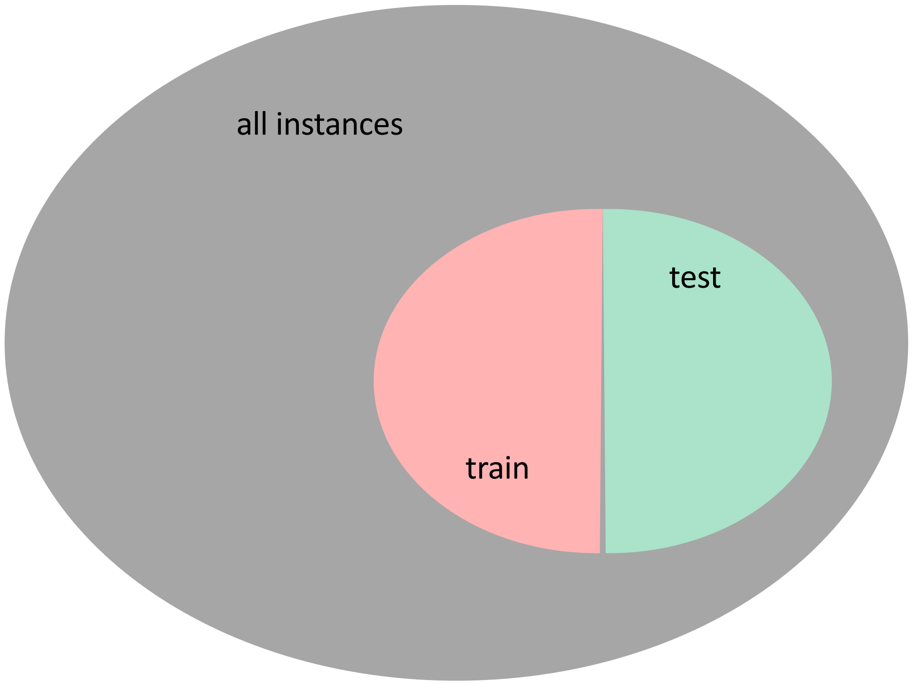
Evaluation: Accuracy

- Can we just calculate the fraction of training instances that are correctly classified?
- Consider a problem domain in which instances are assigned labels at random with $P(Y = 1) = 0.5$
  - How accurate would a learned decision tree be on previously unseen instances?
  - How accurate would it be on its training set?

Evaluation: Accuracy

To get unbiased estimate of model accuracy, we must use a set of instances that are **held-aside** during learning

- This is called a **test set**



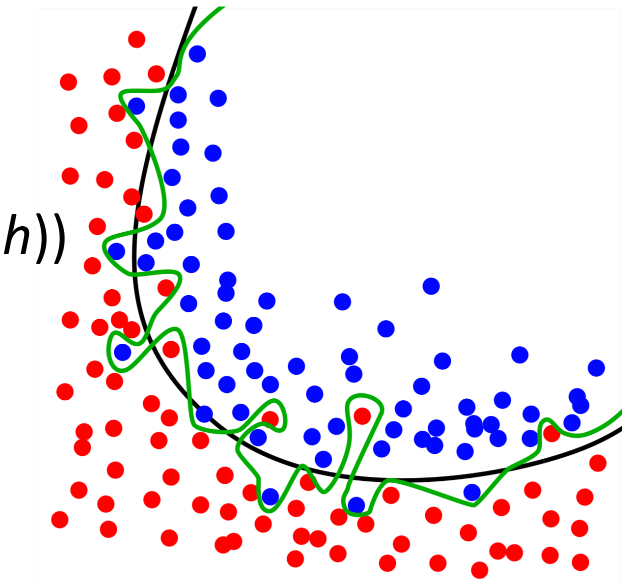
Overfitting

Notation: error of model *h* over

- training data: $\mathrm{error}_{\mathrm{D}}(h)$
- entire distribution of data: $\mathrm{error}_{D}(h)$

Model *h* **overfits** training data if it has

- a low error on the training data (low $\mathrm{error}_{\mathrm{D}}(h)$)
- high error on the entire distribution (high $\mathrm{error}_{D}(h)$)



Wikipedia

Overfitting Example: Noisy Data

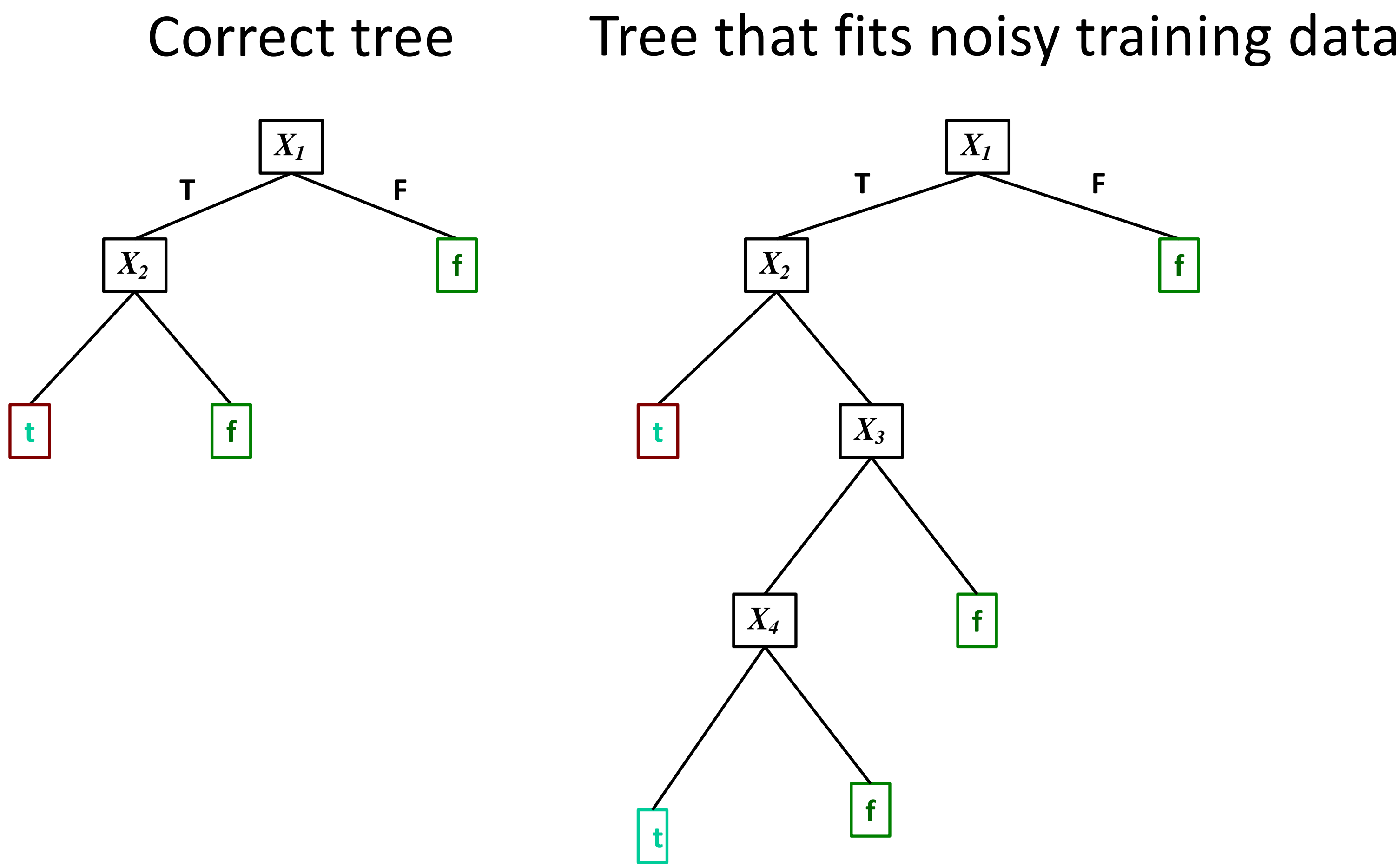
Target function is $Y = X_1 \wedge X_2$

- There is **noise** in some feature values
- Training set:

X_1	X_2	X_3	X_4	X_5	…	Y
t	t	t	t	t	…	t
t	t	f	f	t	…	t
t	f	t	t	f	…	t
t	f	f	t	f	…	f
t	f	t	f	f	…	f
f	t	t	f	t	…	f

noisy value

Overfitting Example: Noisy Data



Overfitting Example: Noise-Free Data

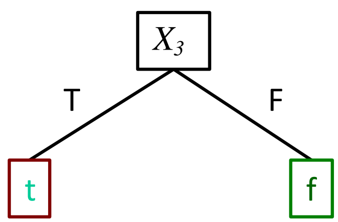
Target function is $Y = X_1 \wedge X_2$

- P(X_3 = t) = 0.5 for both classes
- P(Y = t) = 0.67
- Training set:

X_1	X_2	X_3	X_4	X_5	…	Y
t	t	t	t	t	…	t
t	t	t	f	t	…	t
t	t	t	t	f	…	t
t	f	f	t	f	…	f
f	t	f	f	t	…	f

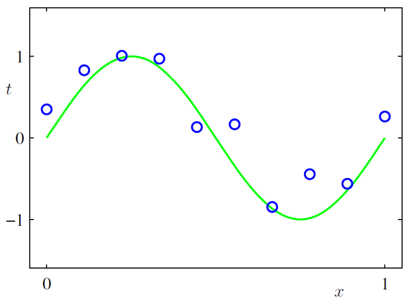
Overfitting Example: Noise-Free Data

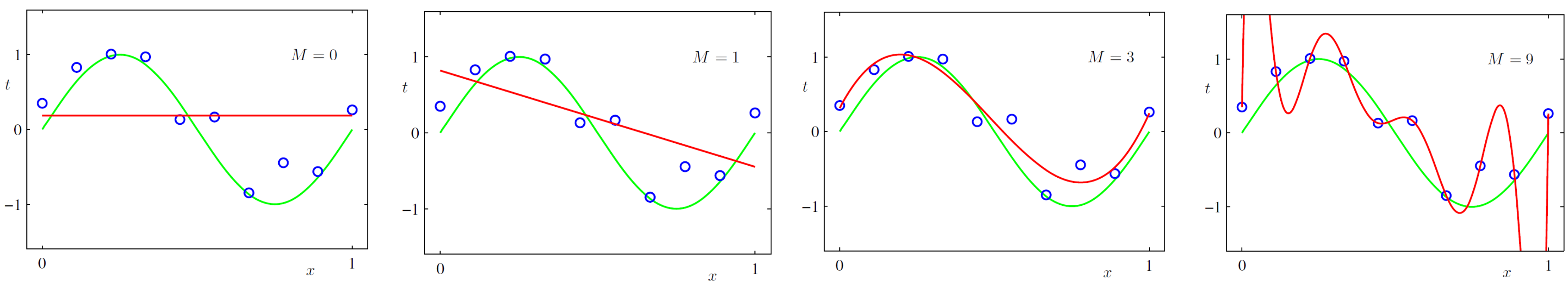
- Training set is a **limited sample.** There might be (combinations of) features that are correlated with the target concept by chance

	Training set accuracy	**Test set accuracy**
	100%	50%
	66%	66%

Overfitting Example: Polynomial Regression

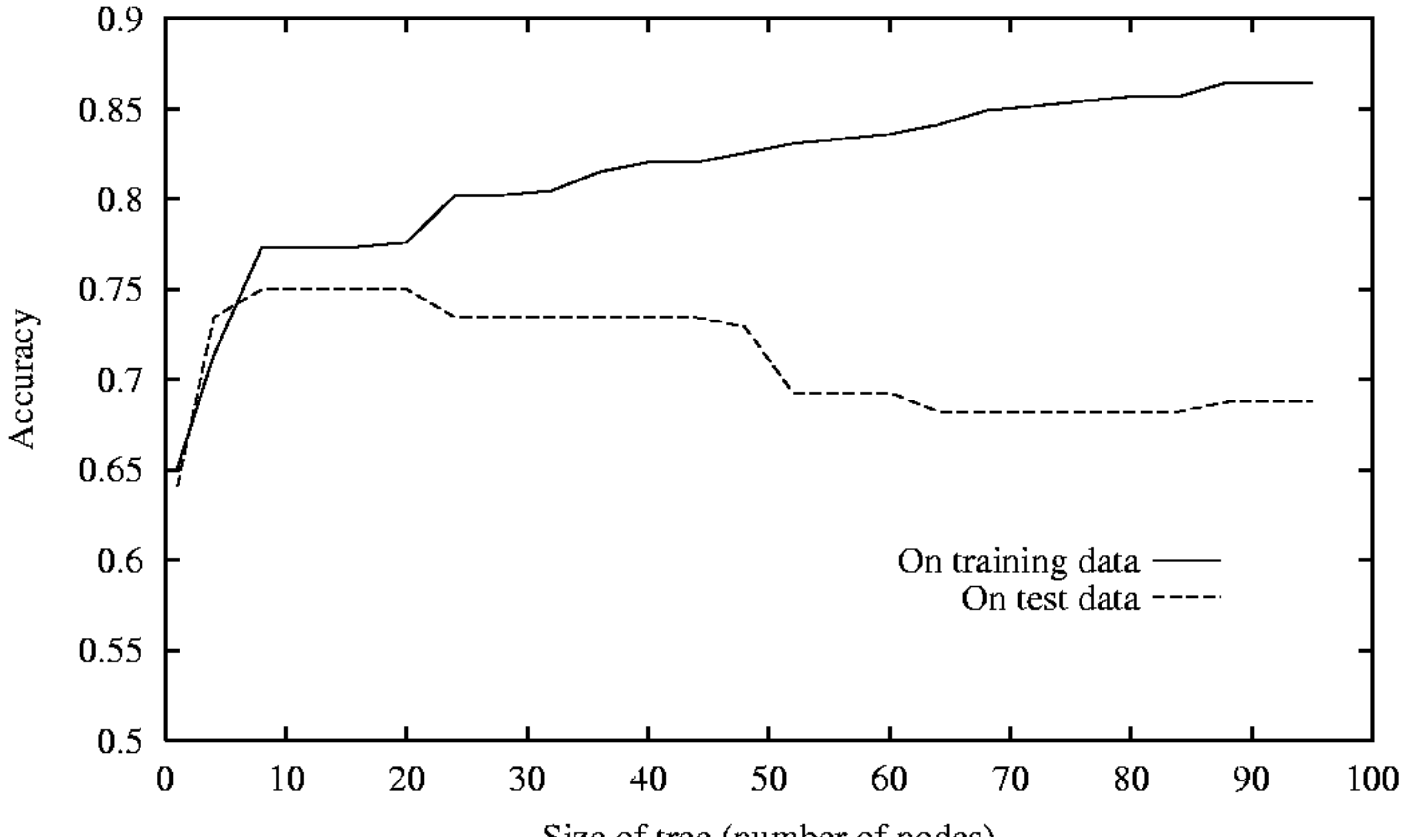
- Training set is a **limited sample.** There might be (combinations of) features that are correlated with the target concept by chance





Overfitting: Tree Size vs. Accuracy

- Tree size vs accuracy



General Phenomenon

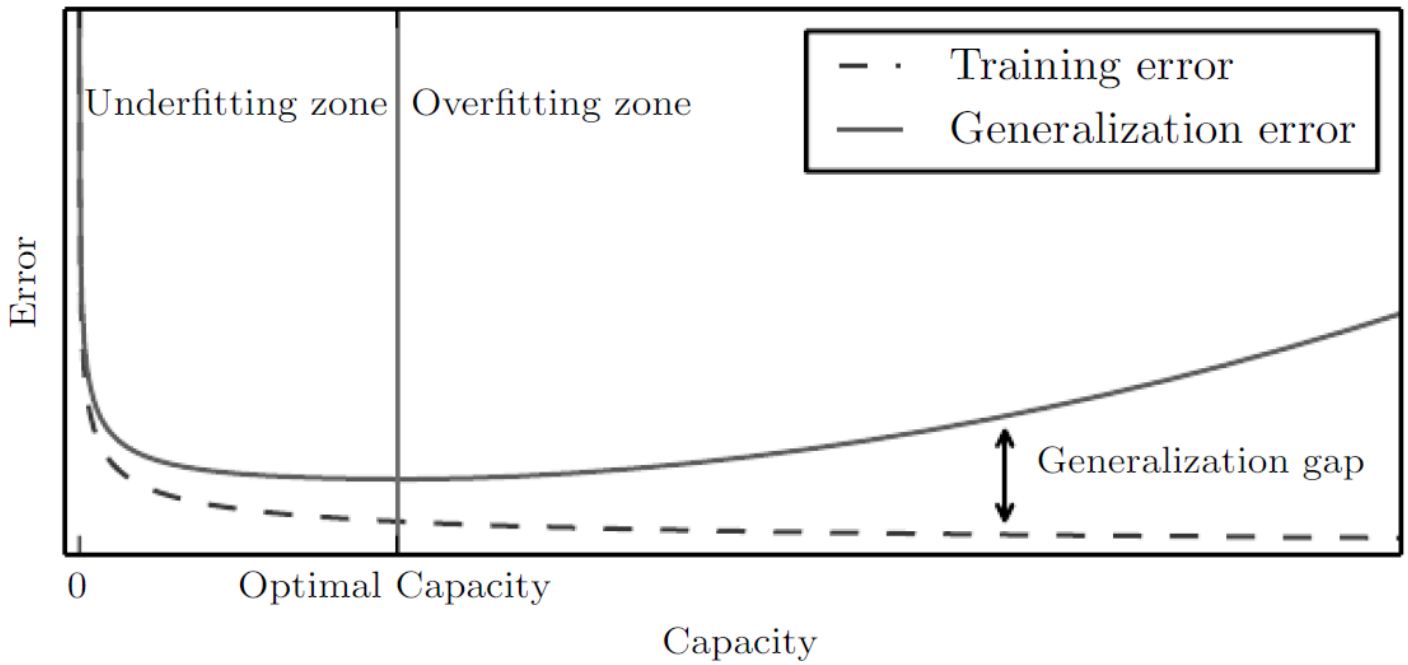


Figure from *Deep Learning*, Goodfellow, Bengio and Courville

DT Learning: Avoiding Overfitting

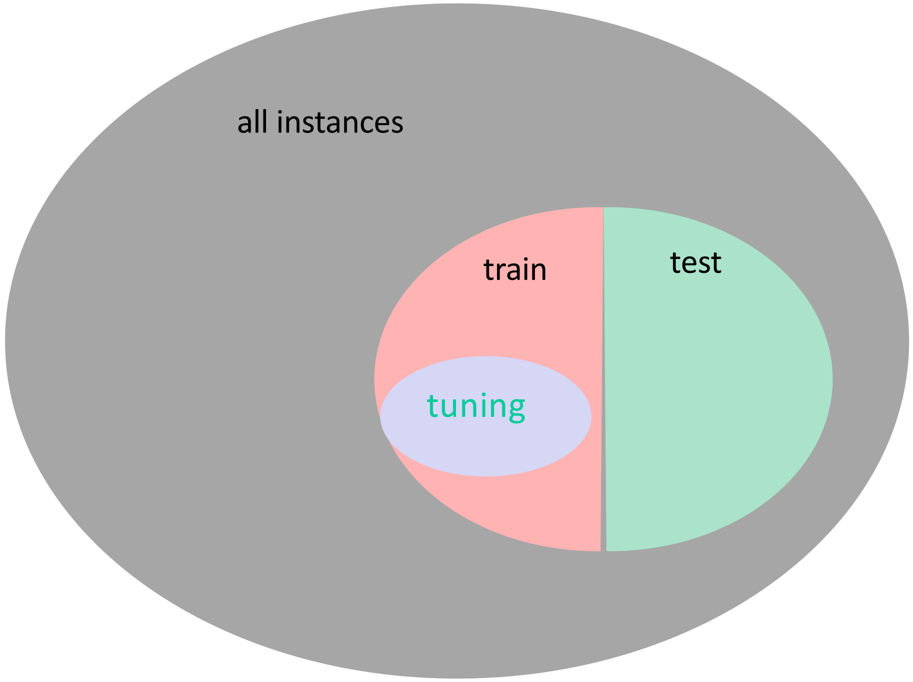
Two **general strategies** to avoid overfitting

1. ***early stopping***: stop if further splitting not justified by a statistical test

2. ***post-pruning***: grow a large tree, then prune back some nodes
   - Ex: evaluate impact on tuning-set accuracy of pruning each node
   - Greedily remove the one that most improves tuning-set accuracy

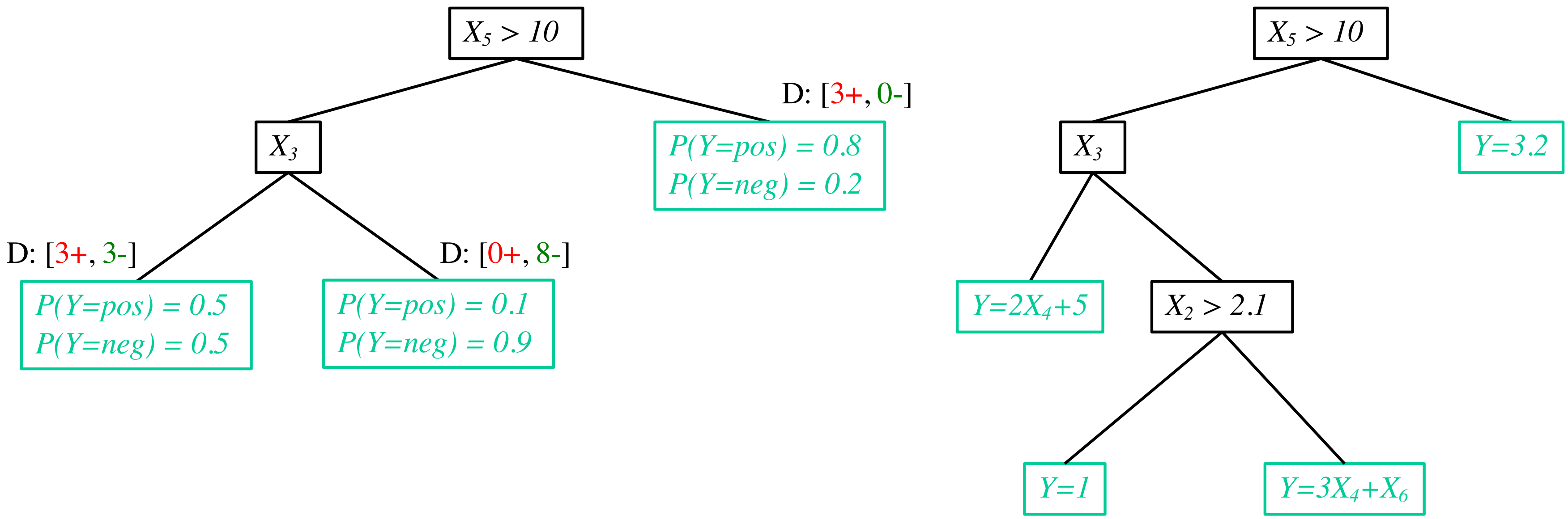
Validation Sets

- A *validation set* (a.k.a. *tuning set*) is
  - not used for primary training process (e.g. tree growing)
  - but used to select among models (e.g. trees pruned to varying degrees)



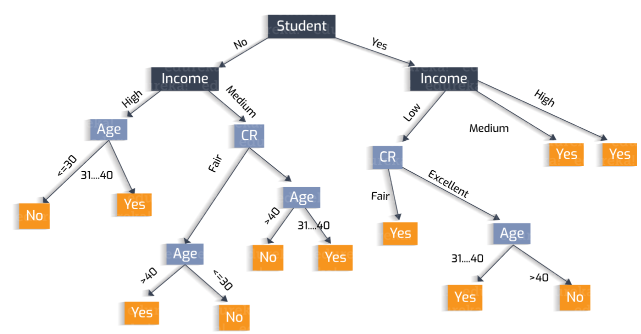
Variations

- Probability estimation trees
  - Leaves: estimate the probability of each class
- Regression trees
  - Either numeric values on leaves, or functions (e.g., linear functions)



Decision Trees: Comments

- Widely used approach
  - Many variations
- Provides humanly comprehensible models
  - When trees not too big
- Insensitive to monotone transformations of numeric features
- Standard methods not suited to on-line setting
- **Usually** not among most accurate learning methods



Break & Quiz

Q2-1: How many distinct (binary classification) decision trees are possible with *4* Boolean attributes? Here distinct means representing different functions.

1. 2^4
2. 2^8
3. 2^{16}
4. 2^{32}

Q2-1: How many distinct (binary classification) decision trees are possible with *4* Boolean attributes? Here distinct means representing different functions.

1. 2^4
2. 2^8
3. 2^{16}
4. 2^{32}

#distinct decision trees
= #distinct Boolean functions
= #functions of 2^4 = 16 inputs, binary label for each input
= $\mathbf{2^{16}}$

Q2-2: Which of the following statements is TRUE?

1. If there is no noise, then there is no overfitting.
2. Overfitting may improve the generalization ability of a model.
3. Generalization error is monotone with respect to the capacity/complexity of a model.
4. More training data may help preventing overfitting.

Q2-2: Which of the following statements is TRUE?

1. If there is no noise, then there is no overfitting.
2. Overfitting may improve the generalization ability of a model.
3. Generalization error is monotone with respect to the capacity/complexity of a model.
4. More training data may help preventing overfitting.

1. We can still have false correlation that leads to overfitting.
2. Overfitting would undermine the generalization ability.
3. Generalization error would first decrease and then increase as the model capacity increases.
4. Increasing training data size would help better approximate the true distribution.

Outline

- **Continuing from last time: Decision trees**
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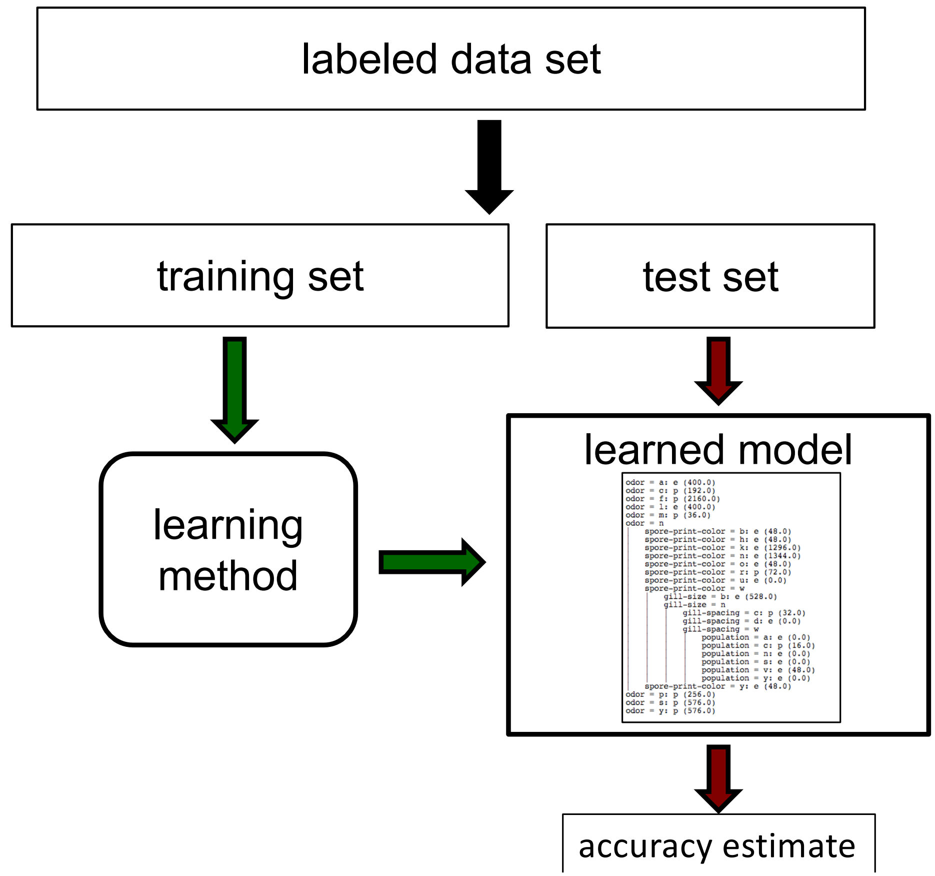
Bias: Accuracy of a Model

- How can we get an **unbiased** estimate of the accuracy of a learned model?



- Unbiased estimate of θ

$$\mathbb{E}[\hat{\theta}] = \theta$$

Bias: Using a Test Set

- How can we get an unbiased estimate of the accuracy of a learned model?
  - When learning a model, you should pretend that you don’t have the test data yet (it is “in the mail”)
  - If the test-set labels influence the learned model in any way, accuracy estimates will be **biased**

- **Don’t train on the test set!**

Bias: Learning Curves

- Accuracy of a method as a function of the train set size?
  - Plot ***learning curves***

Training/test set partition

- for each sample size s on learning curve
  - (optionally) repeat n times
    - randomly select s instances from training set
    - learn model
    - evaluate model on test set to determine accuracy a
    - plot (s, a) or (s, avg. accuracy and error bars)

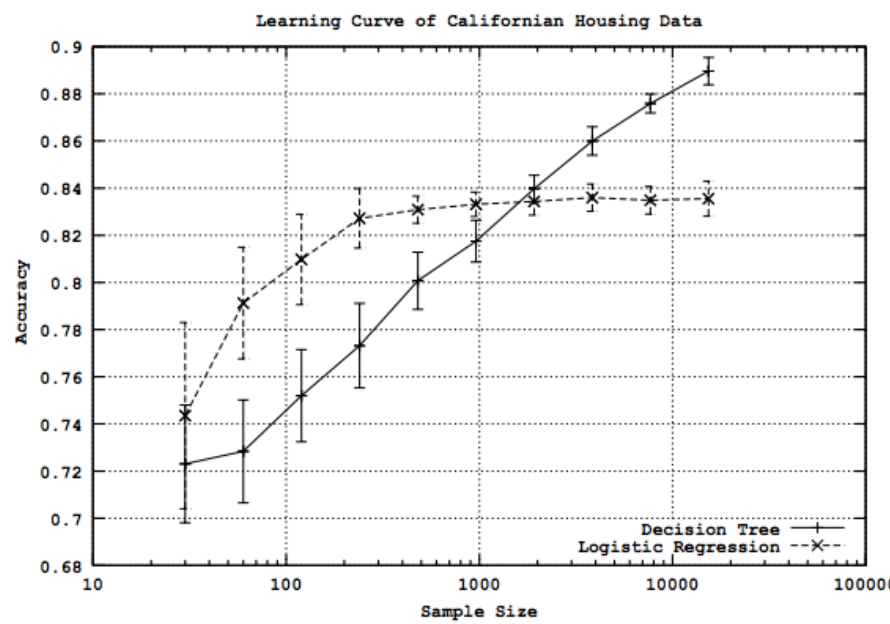
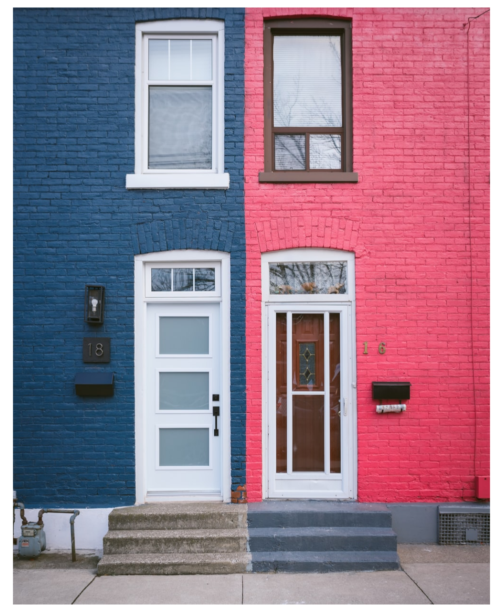


Figure from Perlich et al. *Journal of Machine Learning Research*, 2003

Single Train/Test Split: Limitations

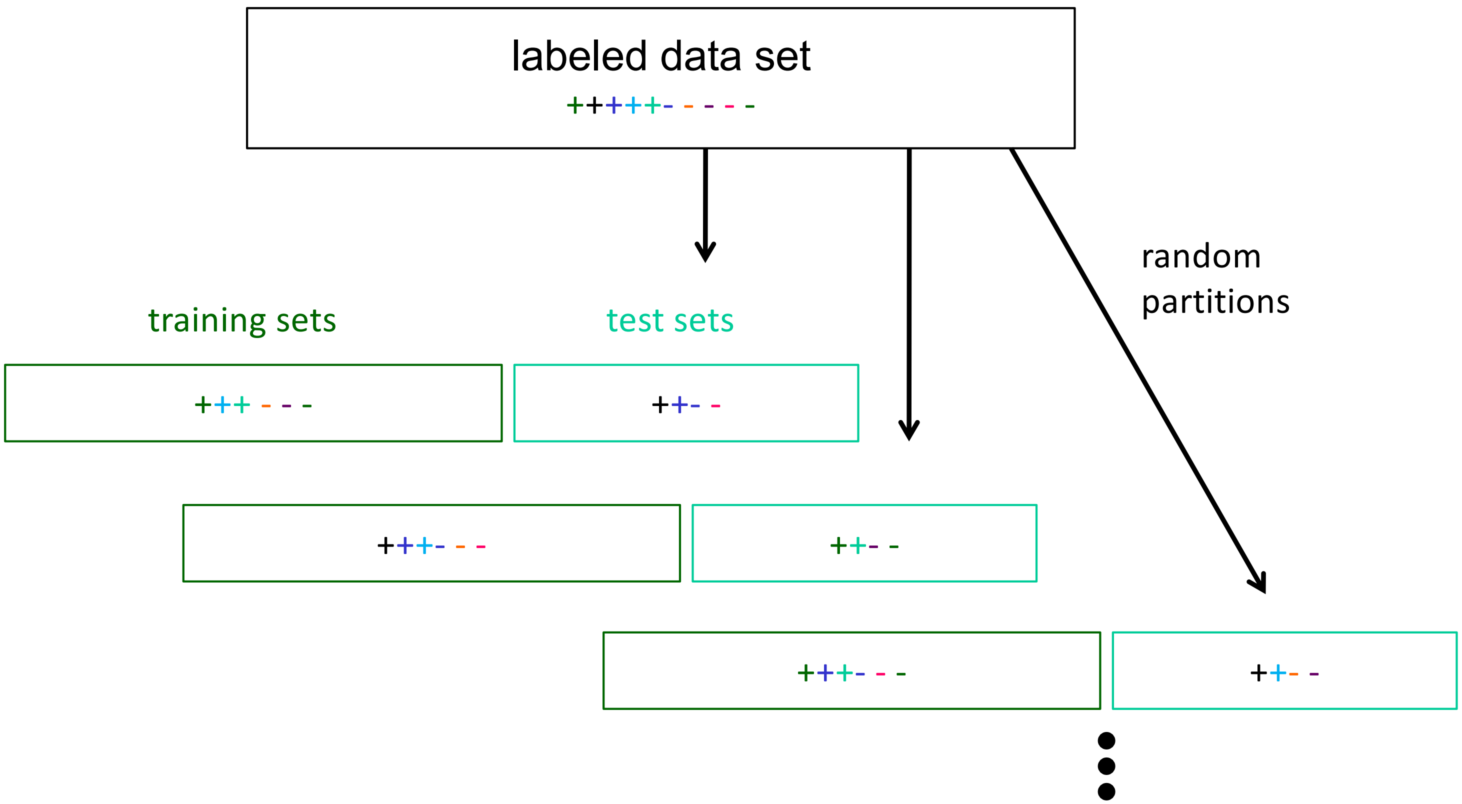
- May not have enough data for sufficiently large training/test sets
  - A **larger test set** gives us more reliable estimate of accuracy (i.e. a lower variance estimate)
  - But… a **larger training set** will be more representative of how much data we actually have for learning process



- A single training set does not tell us how sensitive accuracy is to a particular training sample

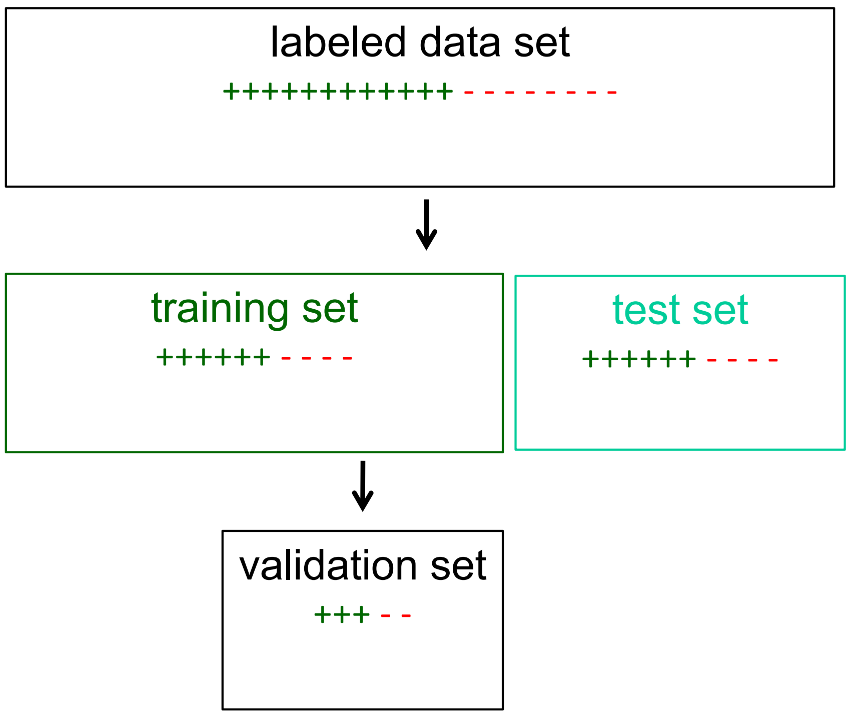
Strategy I: Random Resampling

- Address the second issue by repeatedly randomly partitioning the available data into training and test sets.



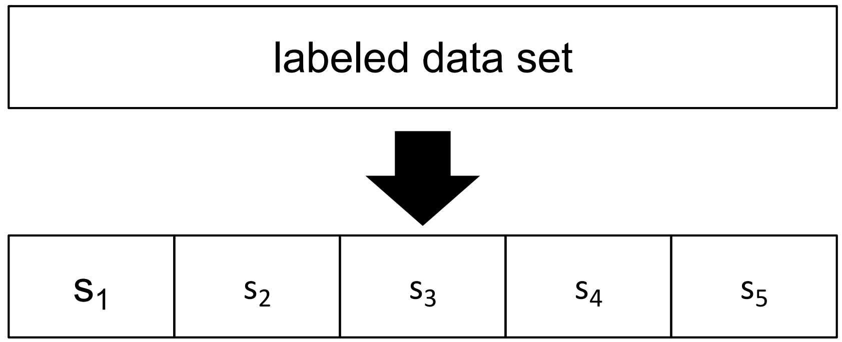
Strategy I: Stratified Sampling

- When randomly selecting training or validation sets, we may want to ensure that **class proportions** are maintained in each selected set



This can be done via stratified sampling: first stratify instances by class, then randomly select instances from each class proportionally.

Strategy II: Cross Validation



Partition data
into *n* subsamples

Iteratively leave one subsample out for the test set, train on the rest

iteration	train on	test on
1	s_2 s_3 s_4 s_5	s_1
2	s_1 s_3 s_4 s_5	s_2
3	s_1 s_2 s_4 s_5	s_3
4	s_1 s_2 s_3 s_5	s_4
5	s_1 s_2 s_3 s_4	s_5

Strategy II: Cross Validation Example

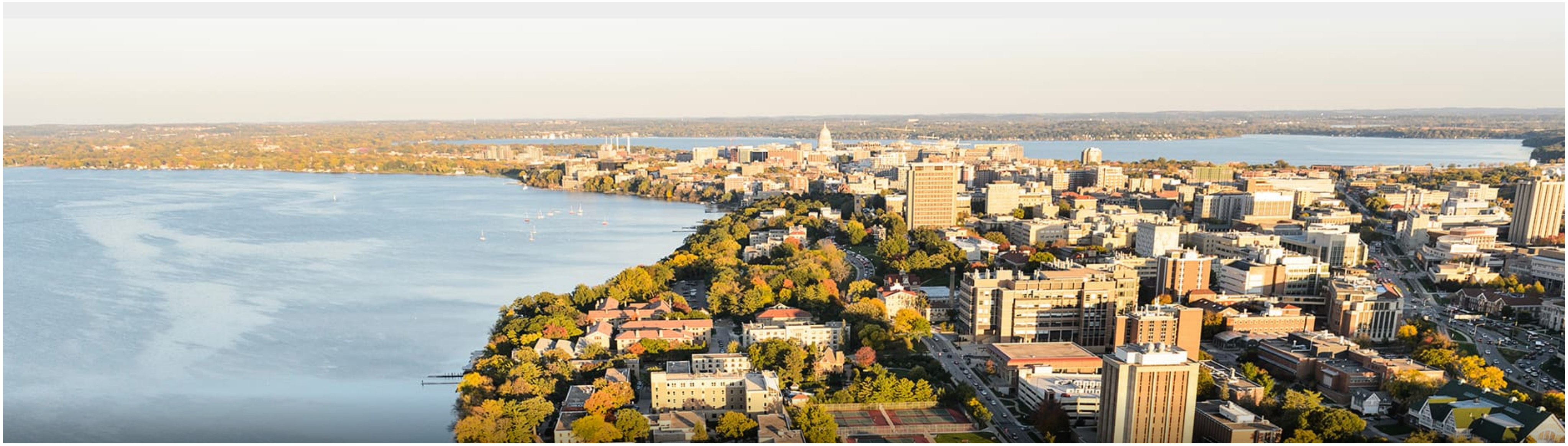
- Suppose we have 100 instances, and we want to estimate accuracy with cross validation

iteration	**train on**	**test on**	**correct**
1	s_2 s_3 s_4 s_5	s_1	11 / 20
2	s_1 s_3 s_4 s_5	s_2	17 / 20
3	s_1 s_2 s_4 s_5	s_3	16 / 20
4	s_1 s_2 s_3 s_5	s_4	13 / 20
5	s_1 s_2 s_3 s_4	s_5	16 / 20

accuracy = 73/100 = 73%

Strategy II: Cross Validation Tips

- 10-fold cross validation is common, but smaller values of *n* are often used when learning takes a lot of time
- in *leave-one-out* cross validation, *n* = # instances
- in *stratified* cross validation, stratified sampling is used when partitioning the data
- CV makes efficient use of the available data for testing
- note that whenever we use multiple training sets, as in CV and random resampling, we are evaluating a <u>learning method</u> as opposed to an <u>individual learned hypothesis</u>



Break & Quiz

Q2-1: Are these statements true or not?
(A) The accuracy of a model is the training set accuracy, and its estimator is the test set accuracy.
(B) An unbiased estimator $\hat{\theta}$ always equals to its corresponding true parameter θ.

1. True, True
2. True, False
3. False, True
4. False, False

Q2-1: Are these statements true or not?
(A) The accuracy of a model is the training set accuracy, and its estimator is the test set accuracy.
(B) An unbiased estimator $\hat{\theta}$ always equals to its corresponding true parameter θ.

1. True, True
2. True, False
3. False, True
4. False, False

(A) The accuracy of a model should be based on the true distribution. The training set and test set only approximate the true distribution.
(B) An unbiased estimator equals to the true parameter in expectation, which means that they won't always be the same for single estimate but the average of a large number of estimates would well approximate the true parameter. An unbiased estimator just makes sure that there's no systematic error.

Q2-2: Are these statements true or not?
(A) The sample size on the learning curve is the size of test set.
(B) A larger training set would provide a lower variance estimate of the accuracy of a learned model.

1. True, True
2. True, False
3. False, True
4. False, False

Q2-2: Are these statements true or not?
(A) The sample size on the learning curve is the size of test set.
(B) A larger training set would provide a lower variance estimate of the accuracy of a learned model.

1. True, True
2. True, False
3. False, True
4. False, False

(A) The sample size on the learning curve is for training set.
(B) A larger test set rather than a larger training set does so.

Q2-3: Which of the following is NOT true?

1. Random resampling can tell us how sensitive accuracy of a learning method is.
2. Class proportions are maintained same in the stratified sampling.
3. In leave-one-out cross validation, the number of partition equals to the number of instances.
4. In cross validation, we are evaluating the performance of an individual learned hypothesis.

Q2-3: Which of the following is NOT true?

1. Random resampling can tell us how sensitive accuracy of a learning method is.
2. Class proportions are maintained same in the stratified sampling.
3. In leave-one-out cross validation, the number of partition equals to the number of instances.
4. In cross validation, we are evaluating the performance of an individual learned hypothesis.

In cross validation, we are evaluating a learning method as opposed to a specific individual learned hypothesis.

Outline

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Beyond Accuracy: Confusion Matrices

- How can we understand what types of mistakes a learned model makes?

task: activity recognition from video

actual class

	bend	jack	jump	pjump	run	side	skip	walk	wave1	wave2
bend	100	0	0	0	0	0	0	0	0	0
jack	0	100	0	0	0	0	0	0	0	0
jump	0	0	89	0	0	0	11	0	0	0
pjump	0	0	0	100	0	0	0	0	0	0
run	0	0	0	0	89	0	11	0	0	0
side	0	0	0	0	0	100	0	0	0	0
skip	0	0	0	0	0	0	100	0	0	0
walk	0	0	0	0	0	0	0	100	0	0
wave1	0	0	0	0	0	0	0	0	67	33
wave2	0	0	0	0	0	0	0	0	0	100

predicted class

Confusion Matrices: 2-Class Version

		actual class	
		positive	negative
predicted class	positive	true positives (TP)	false positives (FP)
	negative	false negatives (FN)	true negatives (TN)

$$\text{accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{FP} + \text{FN} + \text{TN}}$$

$$\text{error} = 1 - \text{accuracy} = \frac{\text{FP} + \text{FN}}{\text{TP} + \text{FP} + \text{FN} + \text{TN}}$$

Accuracy: Sufficient?

Accuracy may not be useful measure in cases where

- There is a large class skew
  - Is 98% accuracy good when 97% of the instances are negative?
- There are differential misclassification costs – say, getting a positive wrong costs more than getting a negative wrong
  - Consider a medical domain in which a false positive results in an extraneous test but a false negative results in a failure to treat a disease
- We are most interested in a subset of high-confidence predictions

Other Metrics

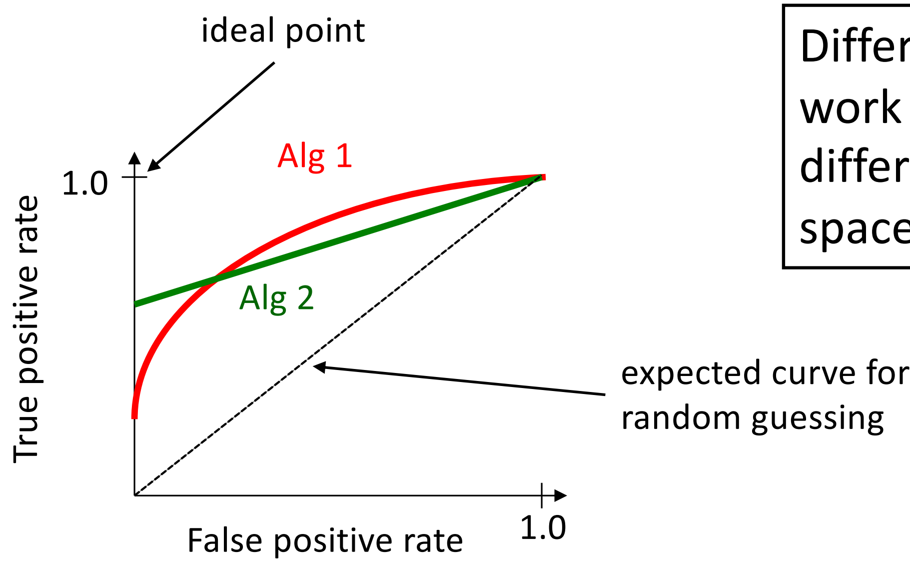
		actual class	
		positive	negative
predicted class	positive	true positives (TP)	false positives (FP)
	negative	false negatives (FN)	true negatives (TN)

$$\text{true positive rate (recall)} = \frac{\text{TP}}{\text{actual pos}} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

$$\text{false positive rate} = \frac{\text{FP}}{\text{actual neg}} = \frac{\text{FP}}{\text{TN} + \text{FP}}$$

Other Metrics: ROC Curves

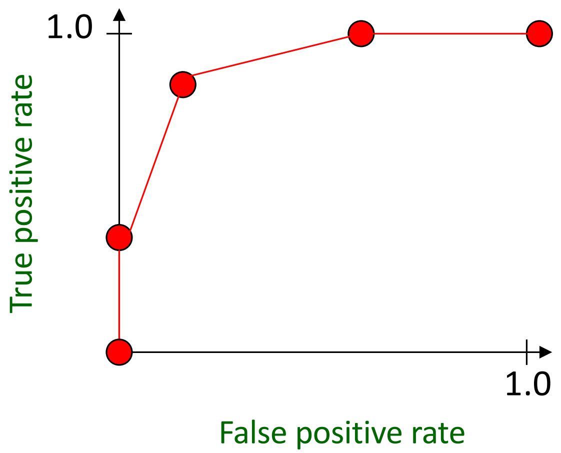
- A *Receiver Operating Characteristic* (*ROC*) curve plots the TP-rate vs. the FP-rate as a threshold on the confidence of an instance being positive is varied



Different methods can work better in different parts of ROC space.

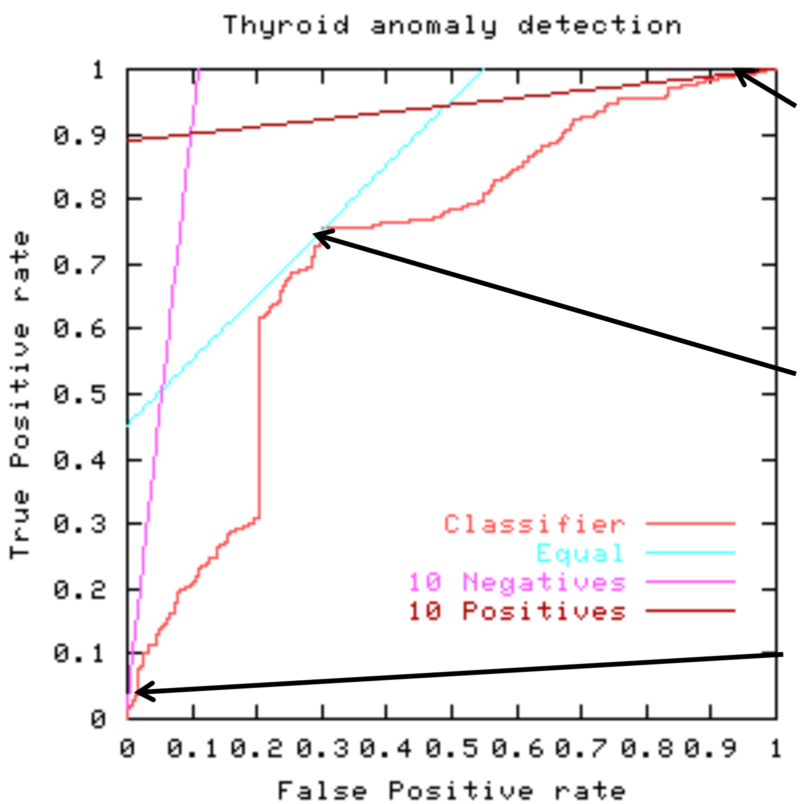
ROC Curves: Plotting

instance	confidence positive		correct class
Ex 9	.99		+
Ex 7	.98	TPR= 2/5, FPR= 0/5	+
Ex 1	.72		-
Ex 2	.70		+
Ex 6	.65	TPR= 4/5, FPR= 1/5	+
Ex 10	.51		-
Ex 3	.39		-
Ex 5	.24	TPR= 5/5, FPR= 3/5	+
Ex 4	.11		-
Ex 8	.01	TPR= 5/5, FPR= 5/5	-



ROC Curves: Misclassification Cost

- The best operating point depends on relative cost of FN and FP misclassifications



best operating point when
FN costs 10× FP

best operating point when
cost of misclassifying positives and
negatives is equal

best operating point when
FP costs 10× FN

Other Metrics: Precision

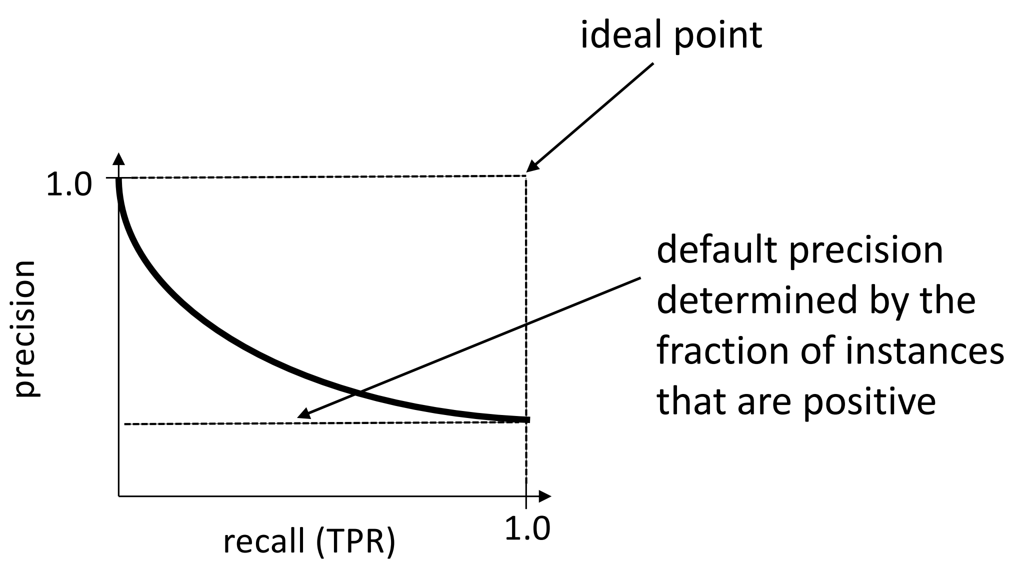
predicted class \ actual class	positive	negative
positive	true positives (TP)	false positives (FP)
negative	false negatives (FN)	true negatives (TN)

$$\text{recall (TP rate)} = \frac{\text{TP}}{\text{actual pos}} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

$$\text{precision (positive predictive value)} = \frac{\text{TP}}{\text{predicted pos}} = \frac{\text{TP}}{\text{TP} + \text{FP}}$$

Other Metrics: Precision/Recall Curve

- A *precision/recall curve* (TP-rate): threshold on the confidence of an instance being positive is varied



predicting patient risk for VTE

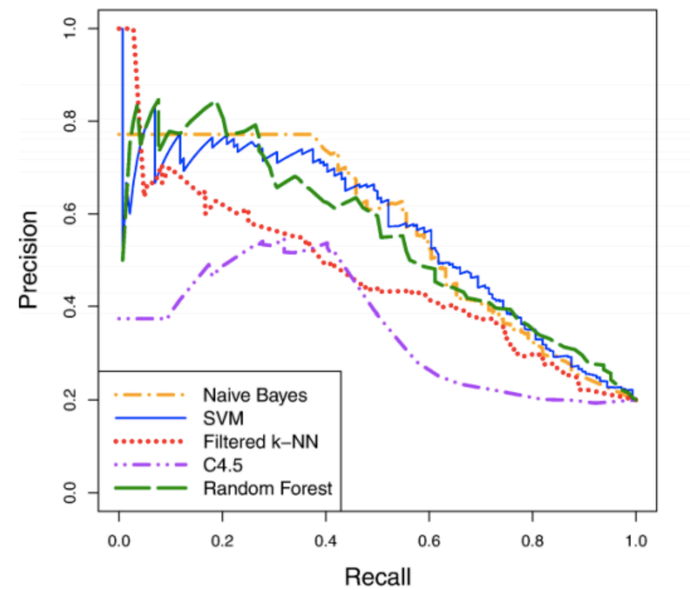


figure from Kawaler et al., *Proc. of AMIA Annual Symposium,* 2012

ROC vs. PR curves

Both

- Allow predictive performance to be assessed at various levels of confidence
- Assume binary classification tasks
- Sometimes summarized by calculating *area under the curve*

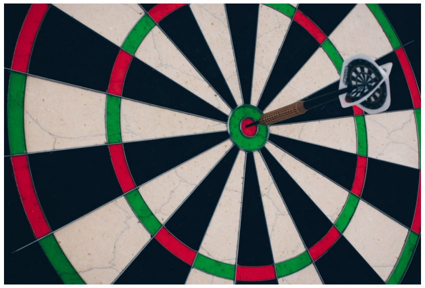
ROC curves

- Insensitive to changes in class distribution (ROC curve does not change if the proportion of positive and negative instances in the test set are varied)
- Can identify optimal classification thresholds for tasks with differential misclassification costs

Precision/recall curves

- Show the fraction of predictions that are false positives
- Well suited for tasks with lots of negative instances

Confidence Intervals

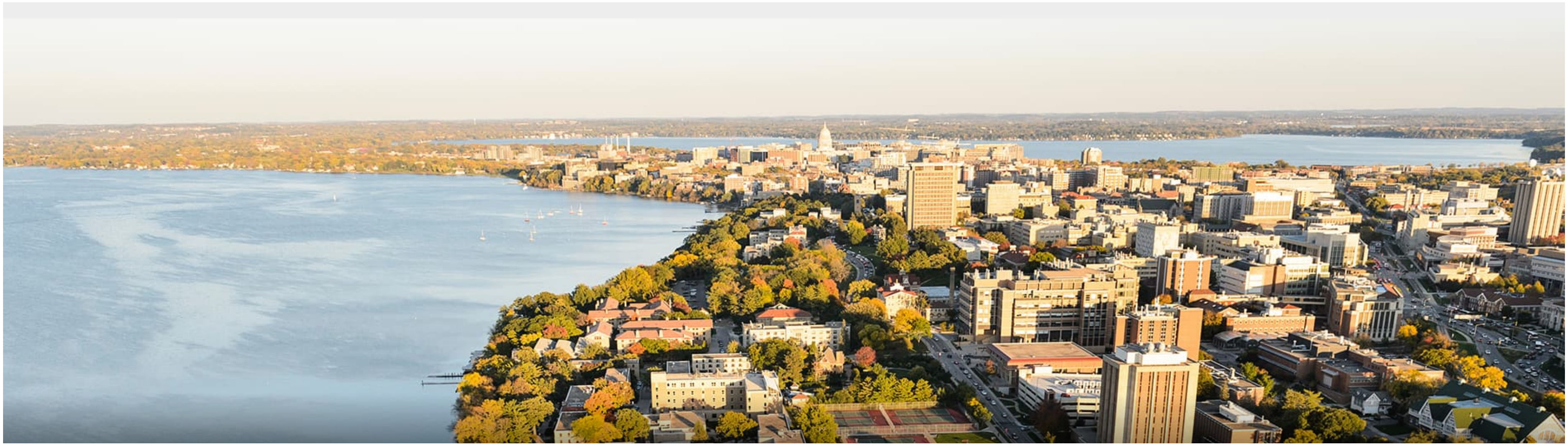


- Back to looking at accuracy on new data.
- **Scenario**:
  - For some model *h*, a test set S with *n* samples
  - We have *h* producing *r* errors out of *n*.
  - Our estimate of the error rate: $\text{error}_S(h) = r/n$

- With C% probability, true error is in interval

$$error_S(h) \pm z_C \sqrt{\frac{error_S(h)(1 - error_S(h))}{n}}$$

  - z_C depends on C. For 95% confidence, it is ~1.96



Thanks Everyone!

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