Tying up some loose ends

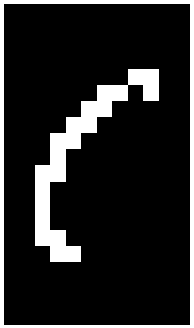
Multi-class classification, Model Selection, and Evaluation

CS534

MULTICLASS CLASSIFICATION

Adapted from slides by Ben Taskar and Simon Lacoste-Julien

Basic Classification in ML

	Input $\mathbf{x} \in \mathcal{X}$	Output $y \in \mathcal{Y}$
Spam filtering		**Binary** 
Character recognition		**Multi-Class** **C**

[thanks to Ben Taskar for slide!]

Multi-Class Classification

- Multi-class classification : direct approaches

Perceptron	Logistic regression	SVM	Naïve Bayes	Decision Tree	Neural Network
?	Softmax $P(y=i\|x) = \frac{\exp w_i^T x}{\sum_j \exp w_j^T x}$	?	No change $P(y=i)$ & $P(x\|y=i)$ $i=1,\dots,K$	No change	K output nodes with softmax activation

- Multi-class classification through binary classification
  - One-vs-All
  - All-vs-all
  - …

Linear classification

- Each class has a parameter vector (w_k,b_k)
- x is assigned to class k iff $w_k^\top x + b_k \geq \max_j w_j^\top x + b_j$

- For simplicity set $b_k = 0$ (add the bias dimension in x and add b_k to w_k)
- So learning goal given separable data: choose w_k s.t.

$$\forall (x^i, y^i), \quad {w_{y^i}}^\top x^i \geq \max_j w_j^\top x^i$$

K-class Perceptron and SVM

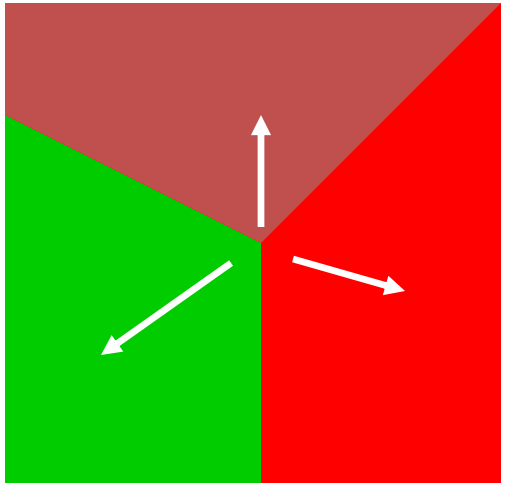
Perceptron: $\max_W \sum_i \left[{w_{y^i}}^\top x^i - \max_k w_k^\top x^i \right]$

K-class SVM: $\max_W \sum_i \left[{w_{y^i}}^\top x^i - \max_k (w_k^\top x^i + \mathbf{1}\{k \neq y^i\}) \right]$

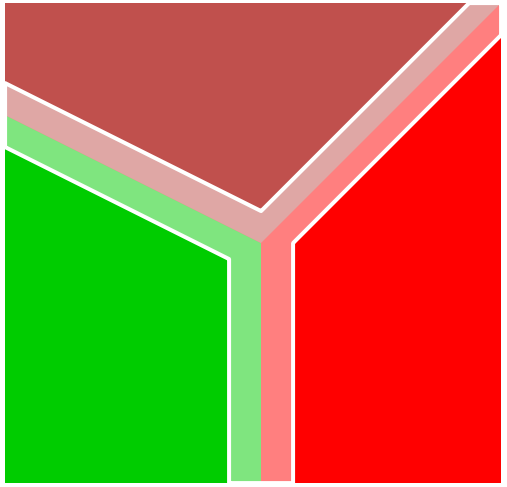
Without regularization

Geometry of Linear classification

Perceptron



K-class SVM



Multiclass Perceptron

Online: for each datapoint

Predict: $\widehat{y}_i = \arg\max_y \ w_y^\top x^i$

Update: if $\widehat{y}_i \neq y^i$ then

$$\begin{cases} w_{y^i,t+1} = w_{y^i,t} + \alpha x^i \\ w_{\widehat{y}_i,t+1} = w_{\widehat{y}_i,t} - \alpha x^i \end{cases}$$

Multi-class SVM

Primal problem: QP

$$\min_{w_1,\ldots,w_K} \quad \frac{1}{2}\|(w_1,\ldots,w_K)\|^2 + C\sum_{ik}\xi_{ik}$$

$$\text{s.t.} \quad \forall(i,k), \quad {w_{y^i}}^\top x^i - w_k^\top x^i \geq 1\{k \neq y^i\} - \xi_{ik}$$

Again can be solved in the dual formulation, also Quadratic Program

Combining binary classifiers

One-vs-all For each class build a classifier for that class vs the rest

- Often very imbalanced classifiers --- often challenging to learn a good classifier

All-vs-all build a classifier for each pair of classes

- A priori a large number of classifiers $\binom{n}{2}$ to build ***but…***
  - The pairwise classification are way much faster
  - The classifications are balanced

… so that in many cases it is faster than one-vs-all

MODEL SELECTION

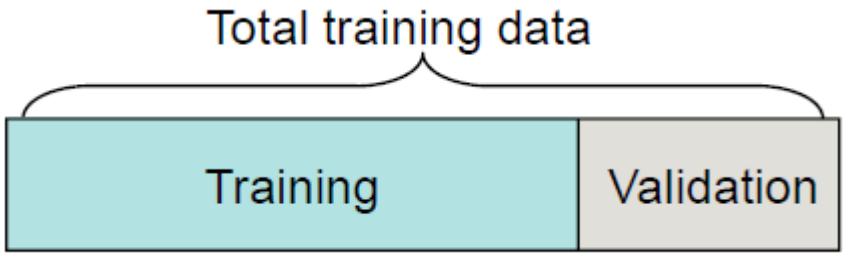
General Model Selection Problem

- Assume that we have a set of models M=$\{M_1, M_2, \cdots, M_d\}$ that we are trying to select from. Some examples include:
  - **Feature Selection:** each M_i corresponds to using a different feature subset from a large set of potential features
  - **Algorithm Selection:** each M_i corresponds to an algorithm, e.g., Naïve Bayes, Logistic Regression, DT …
  - **Parameter selection/tuning:** each M_i corresponds to a particular parameter choice, e.g., the choice of kernel and C for SVM

Approaches to Model Selection

- **Holdout and Cross-validation methods**
  - Experimentally determine when overfitting occurs and which model works well on the specific data in hand
- Penalty methods - regularization based, introducing penalty on complex models
  - MAP Penalty
  - Minimum Description Length – an alternative approach to MAP
- You can also avoid model selection and use ensembles
  - Instead of choosing, consider many possibilities and let them vote, or learn to combine their decisions

Simple Holdout Method

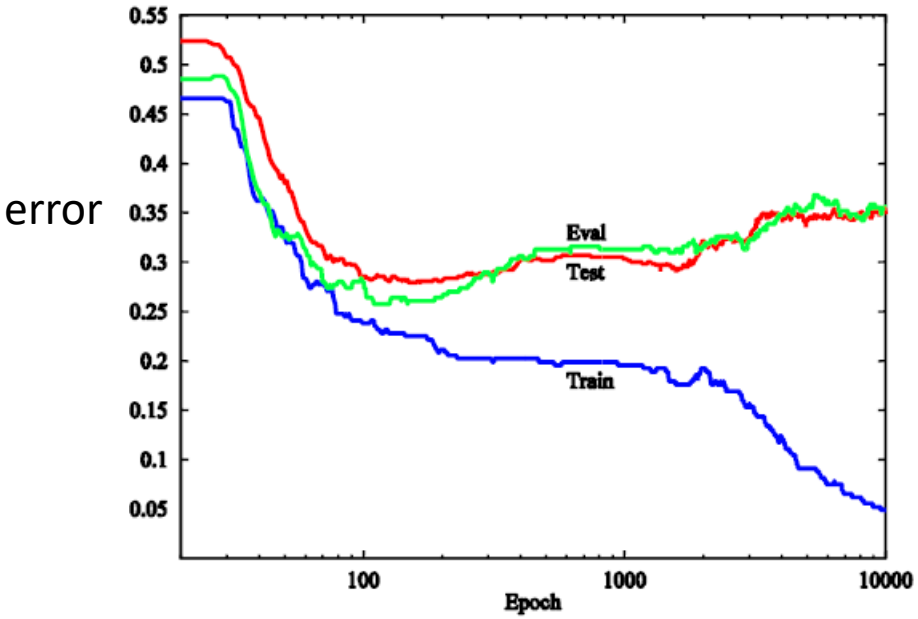


1. Divide training set S into S_{train} and S_{valid}
2. Train each model M_i on S_{train} to get a hypothesis h_i
3. Choose and output h_i with the smallest error rate on S_{valid}

Could retrain the selected model on the whole dataset to get the final hypothesis *h* - this will improve the original h_i because of more training data

Notes on hold-out methods

- Hold-out method often used for choosing among nested hypotheses:
  - Deciding # of training epochs for Neural net
  - Deciding when to stop growing or pruning a decision tree
  - Deciding when to stop growing an ensemble



Example:

Selecting # of epochs for neural net

Issues

- It wastes part of the data
  - The model selection choice is still made using only part of the data
  - Still possible to overfit the validation data since it is a relatively small set of data

- To address these problems, we can use **Cross-Validation**

k-fold Cross-validation

- Partition (randomly) S into k disjoint subsets $S_1, \cdots, S_k$ (preferably in a class-balanced way)
- To evaluate model M_j:

for i=1:K

1. *Train* M_j *on* $S \backslash S_i$ *(*S *removing* S_i*)* $\rightarrow h_{ji}$
2. *Test* h_{ji} *on* $S_i \rightarrow \epsilon_j(i)$

End for

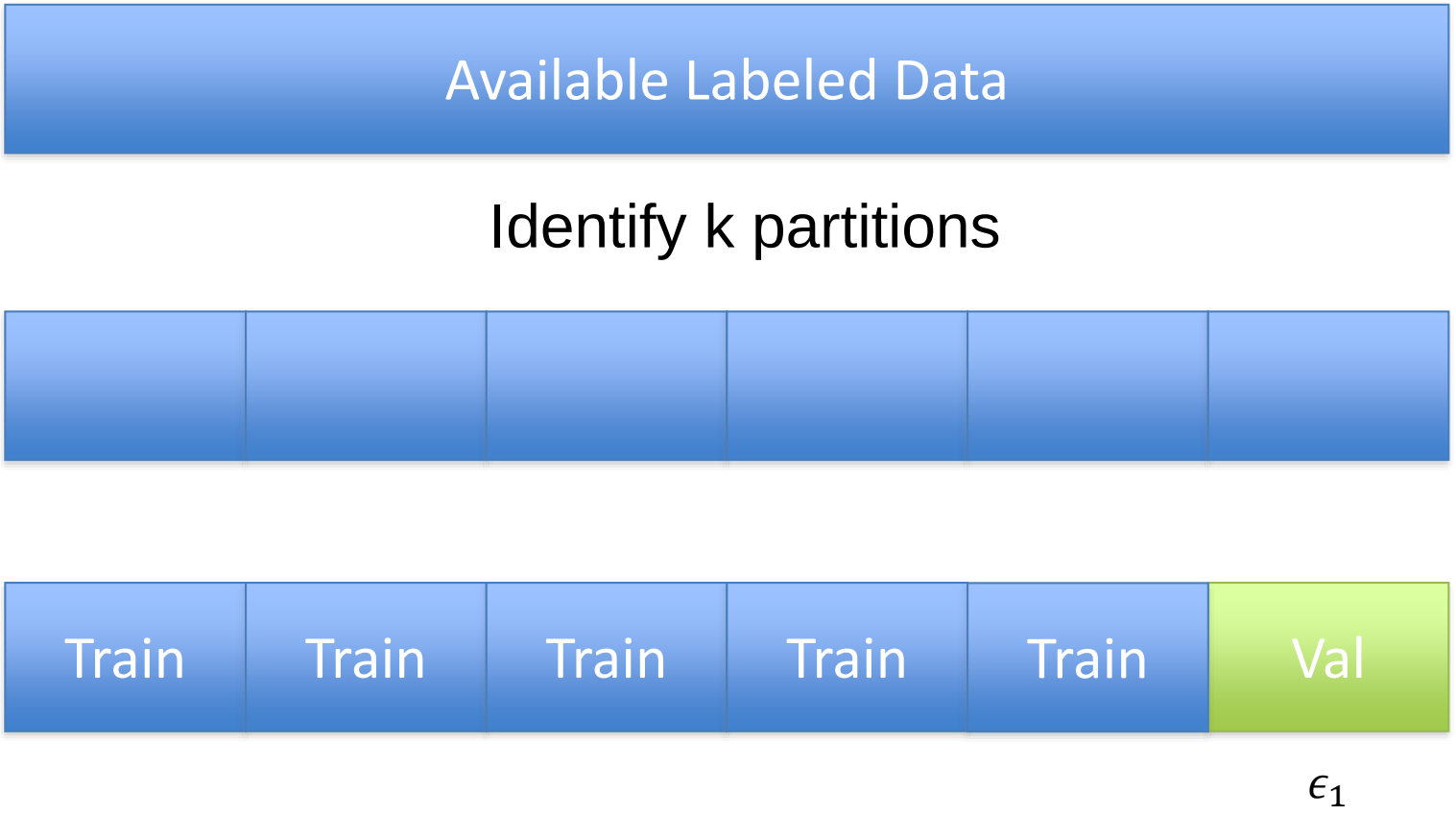
$$\epsilon_j = \frac{1}{K} \sum_i \epsilon_j(i)$$

- Select model that minimizes the error:

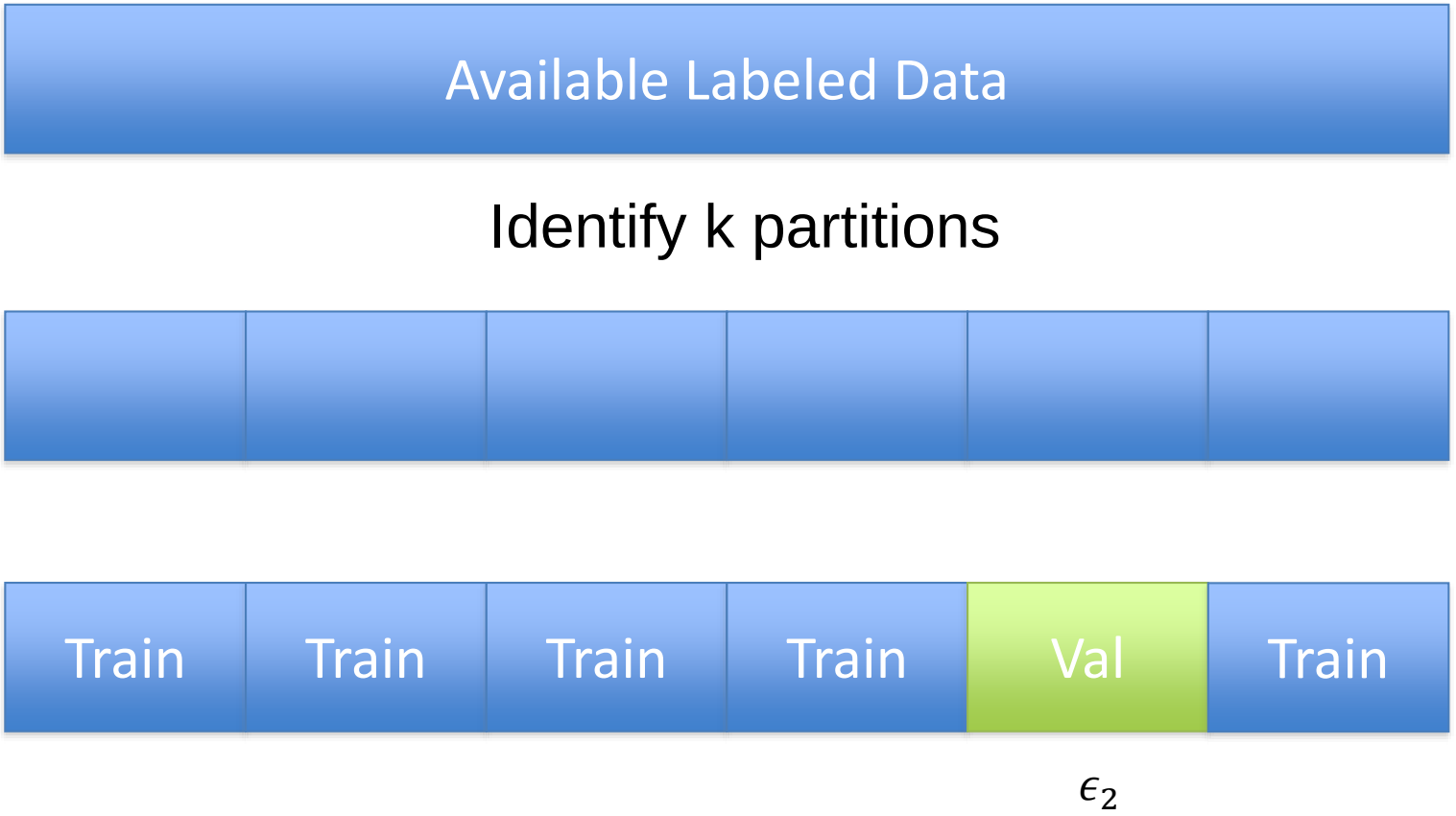
$$M^* = \underset{M_j}{\operatorname{argmin}}\, \epsilon_j$$

- Train M^* on S and output resulting hypothesis

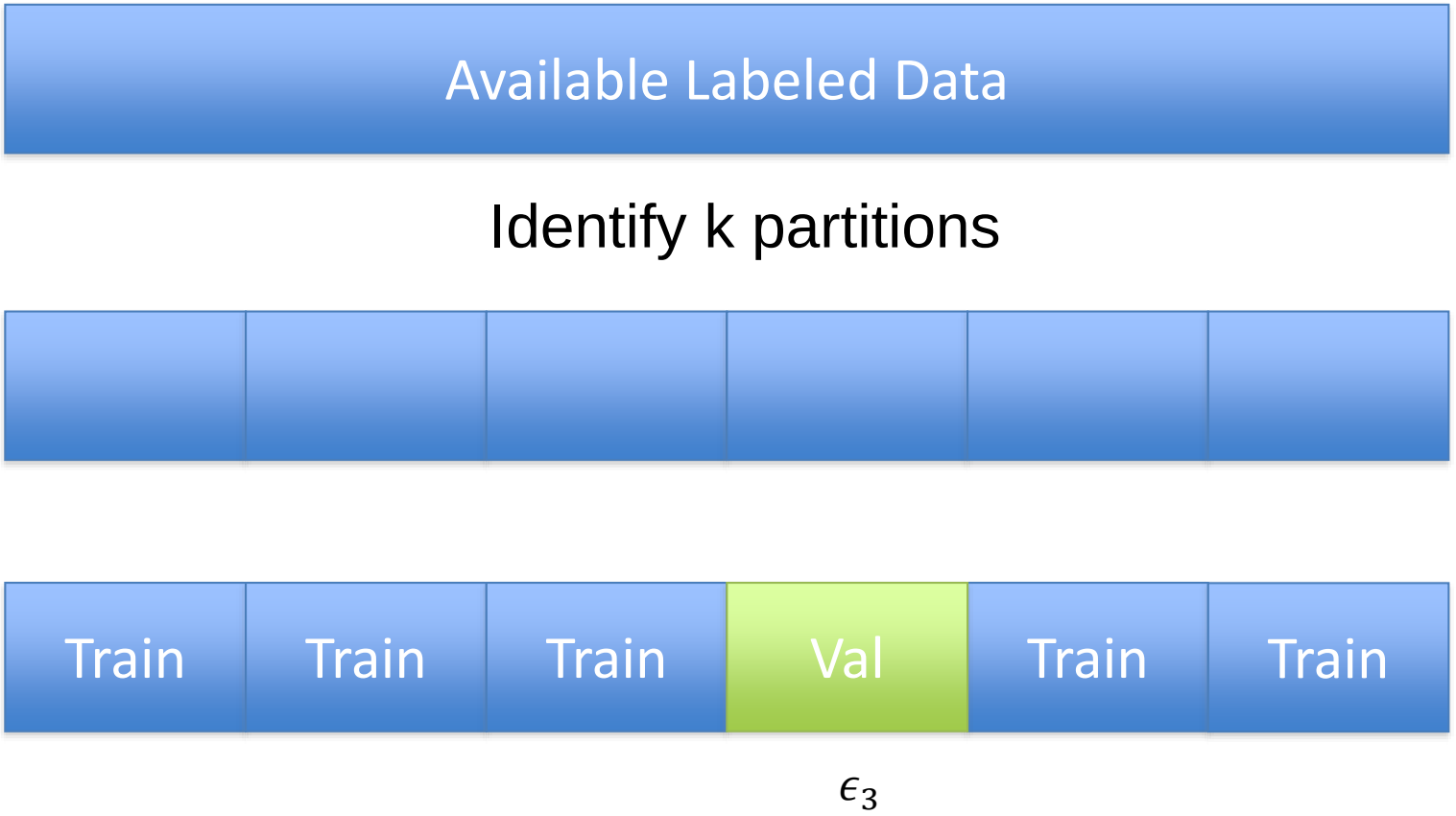
Cross-validation visualized



Cross-validation visualized



Cross-validation visualized



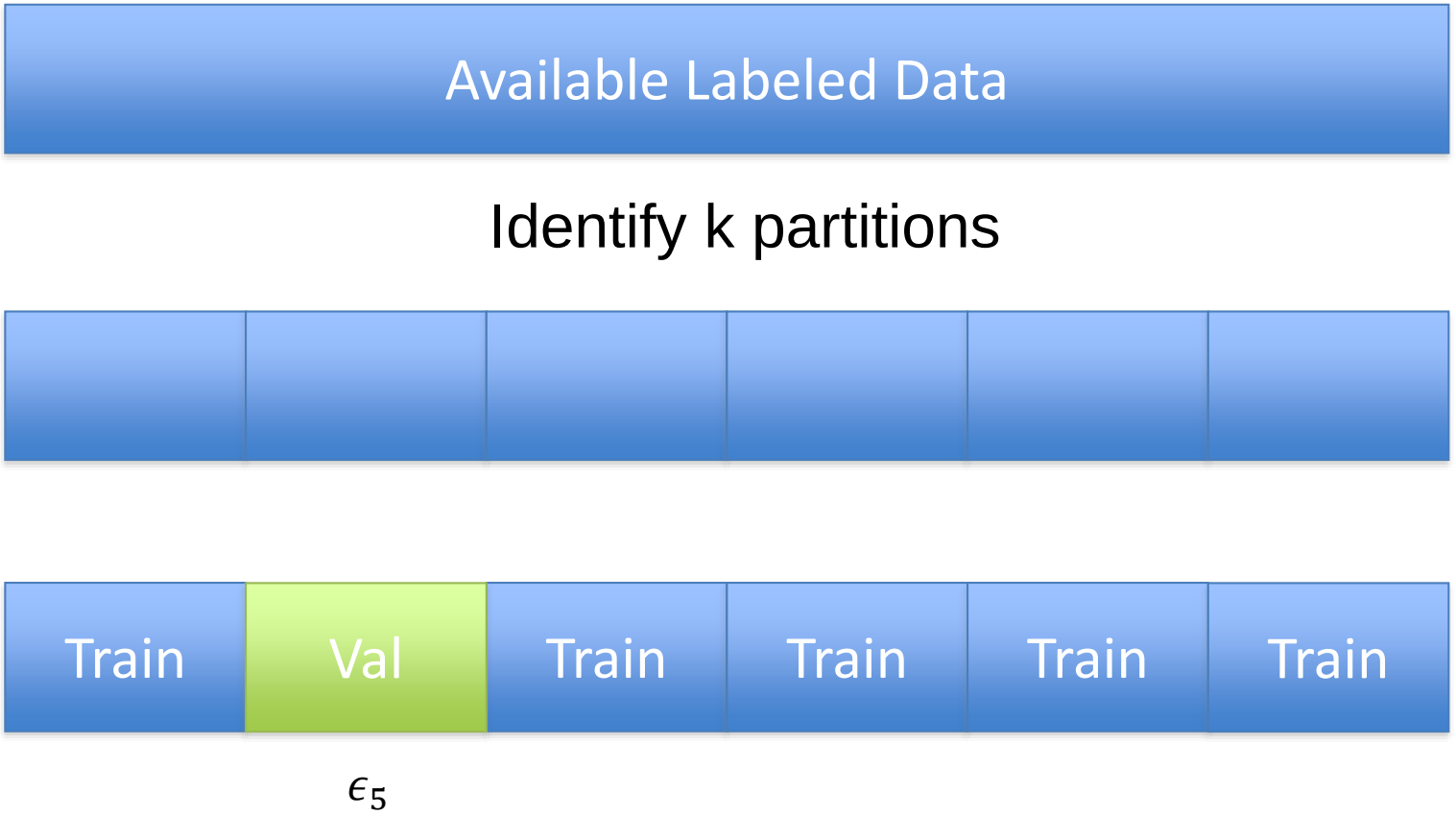
Cross-validation visualized

Identify k partitions

Fold 4

ϵ_4

Cross-validation visualized



Cross-validation visualized

Identify k partitions

Fold 6

ϵ_6

Comments on k-fold Cross-Validation

- Computationally more expensive than simple hold-out method but better use of data
  - Every data point in the training set is used in validating the model selection choices
- If the data is really scarce, we can use the extreme choice of $k = |S|$
  - Each validation set contains only one data point
  - Often referred to as Leave-one-out (LOO) cross-validation

EVALUATION OF CLASSIFIERS

How do we valuate a classifier?

- What measure to use?
  - Accuracy
  - Precision, recall, F-Measure
  - ROC Curves
- What sampling method to use?
  - Train/test split
  - Cross-validation
  - Leave-one-out
- How to tell if the difference is significant?

Performance Measure: Accuracy

- Easily the most common and intuitive measure of classification performance.

$$Accuracy = \frac{\#correct}{N}$$

Confusion matrix

		True Values	
		Positive	**Negative**
Pred. Values	**Positive**	True Positive	False Positive
	Negative	False Negative	True Negative

Definition: Accuracy

		True Values	
		Positive	Negative
Pred. Values	Positive	TP	FP
	Negative	FN	TN

$$Accuracy = \frac{TP + TN}{TP + FP + TN + FN}$$

Precision, Recall, F-measure

		True Values	
		Positive	Negative
Pred. Values	Positive	TP	FP
	Negative	FN	TN

- Precision: how many predicted positives were true positives

$$P = \frac{TP}{TP + FP}$$

- Recall: how many of the true positives were identified $R = \frac{TP}{TP + FN}$

- F-Measure: Harmonic mean of precision and recall $F = \frac{2PR}{P + R}$

What's wrong with Accuracy?

True class →	Pos	Neg
Pos	0	0
Neg	100	900
	P=100	N=900

True class →	Pos	Neg
Pos	90	90
Neg	10	810
	P=100	N=900

- Both classifiers obtain 90% accuracy
- They exhibit very different behaviors:
  - On the left: classifier completely give up on the positive class
  - On the right: classifier is able to catch some positive examples

What's wrong with Precision/Recall?

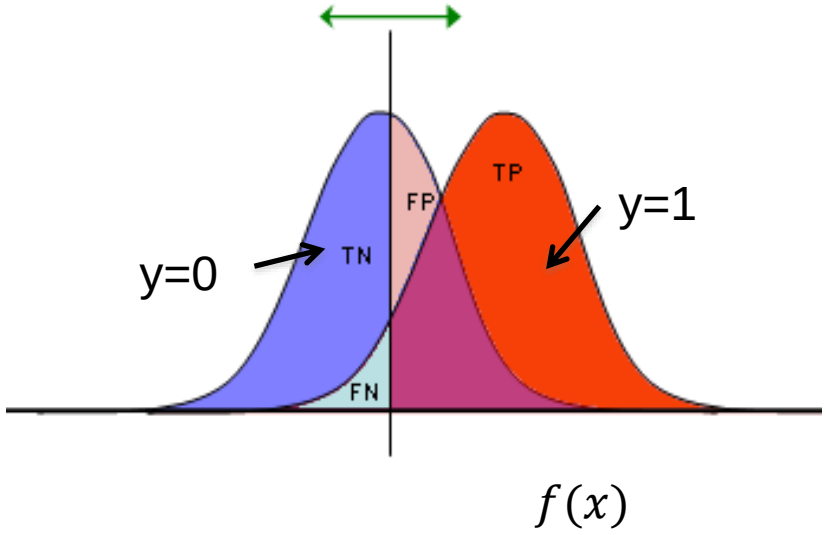
True class →	Pos	Neg
Pos	200	100
Neg	300	400
	P=500	N=500

True class →	Pos	Neg
Pos	200	100
Neg	300	0
	P=500	N=100

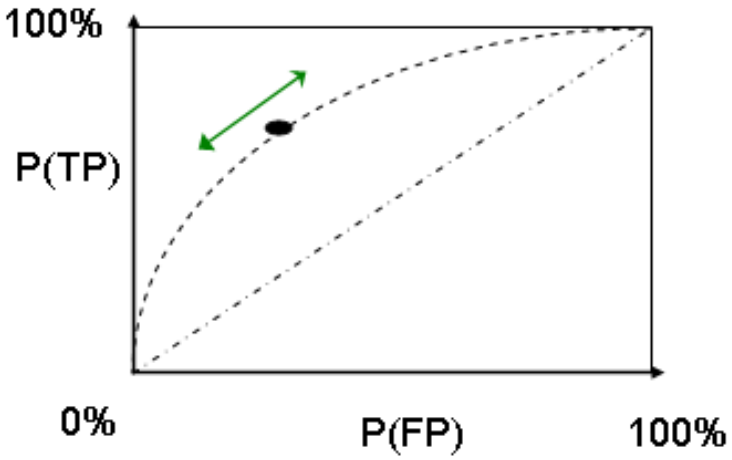
- Both classifiers obtain the same precision and recall values of 66.7% and 40%
- They exhibit very different behaviors:
  - Same positive recognition rate
  - Extremely different negative recognition rate: strong on the left / nil on the right
- Note: Accuracy has no problem catching this!

ROC Curve

- Assume your binary classifier outputs a score f(x)
- If we can plot the class conditional density of the score, it might look like this

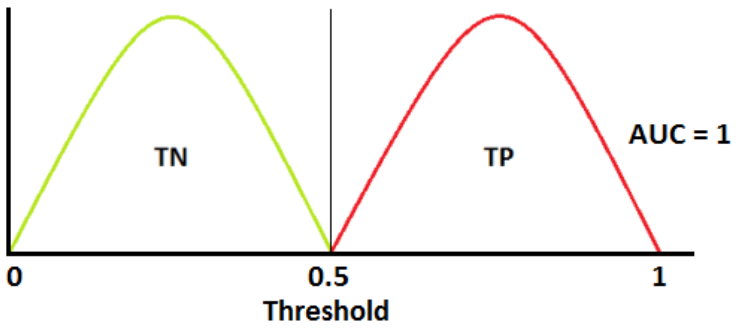


- We apply a threshold to the score $f(x)$ for prediction: $y = I(f(x) > \theta)$
- As you change the value θ the true positive rate (TP) and the false positive rate (FP) will change.
-
- By plotting the entire curve you can see the tradeoffs.

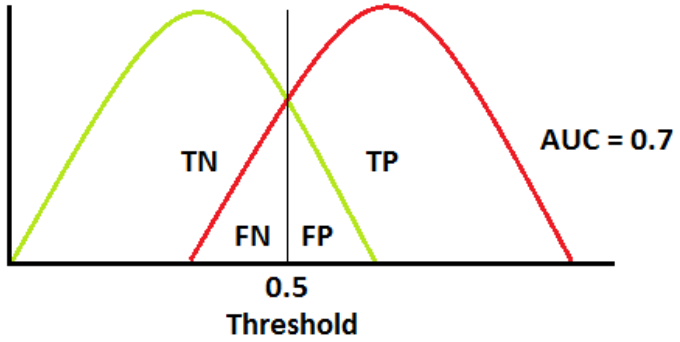


ROC measures how the learned score $f(x)$ separates positive from negative

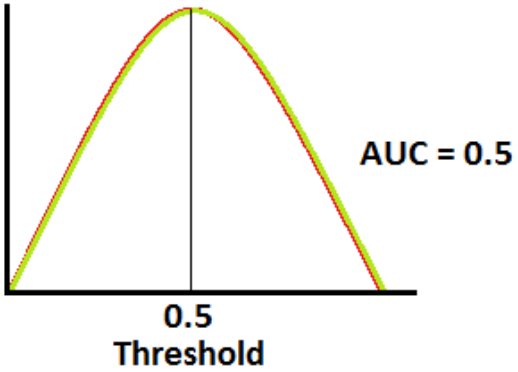
A. Complete separation



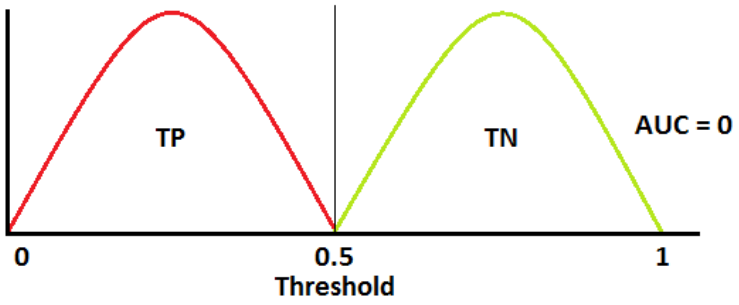
B. Some overlap



C. Complete overlap

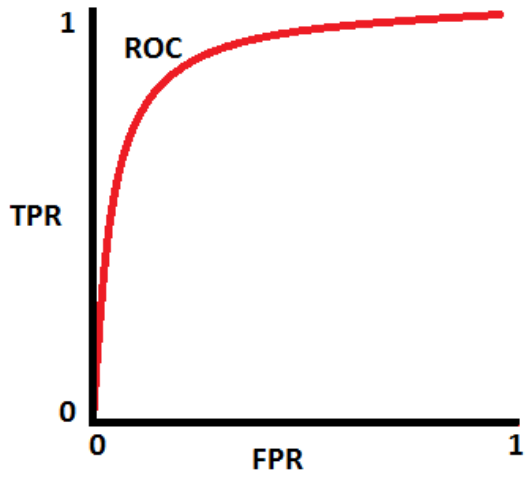


D. Separate but reversed

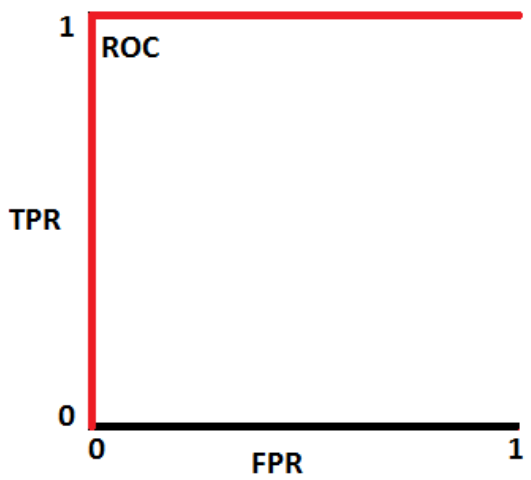


What do their corresponding ROC curves look like?

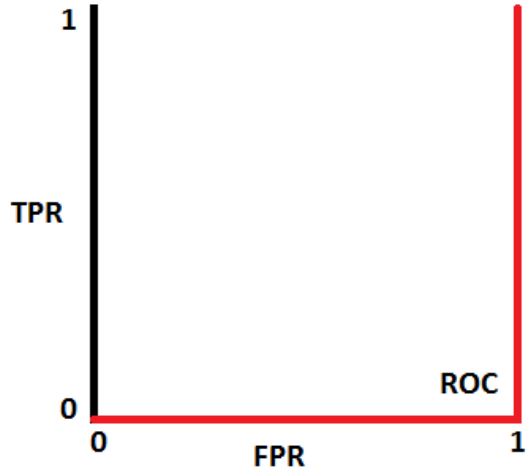
(i)


1
ROC
TPR
0
0
FPR
1

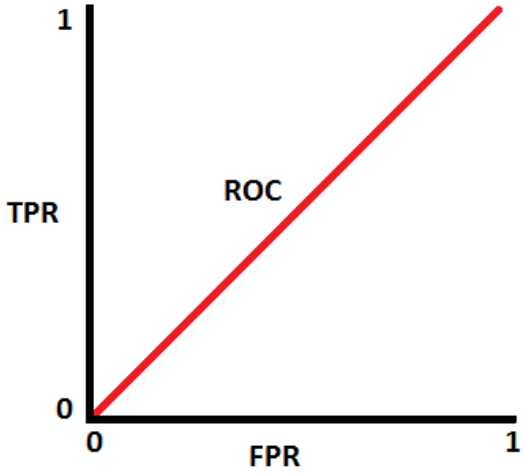
(ii)


1
ROC
TPR
0
0
FPR
1

(iii)


1
TPR
0
ROC
0
FPR
1

(iv)


1
TPR
ROC
0
0
FPR
1

Area under the ROC curves

- Area Under the Curve (AUC) measures the area under the ROC curve
- AUC = the probability that a randomly selected positive example will score higher than a randomly selected negative example
- AUC = 1 model achieves perfect separation
- AUC = 0.5 complete overlap, equivalent to random guessing
- AUC = 0 completely reversed

Comparing classifiers statistically

- Say I have two classifiers.

- A = 50% accuracy
- B = 75% accuracy

- B is better, right?

Comparing classifiers statistically

- Say I have another two classifiers

- A = 50% accuracy
- B = 50.5% accuracy

- Is B better?

Basic Evaluation

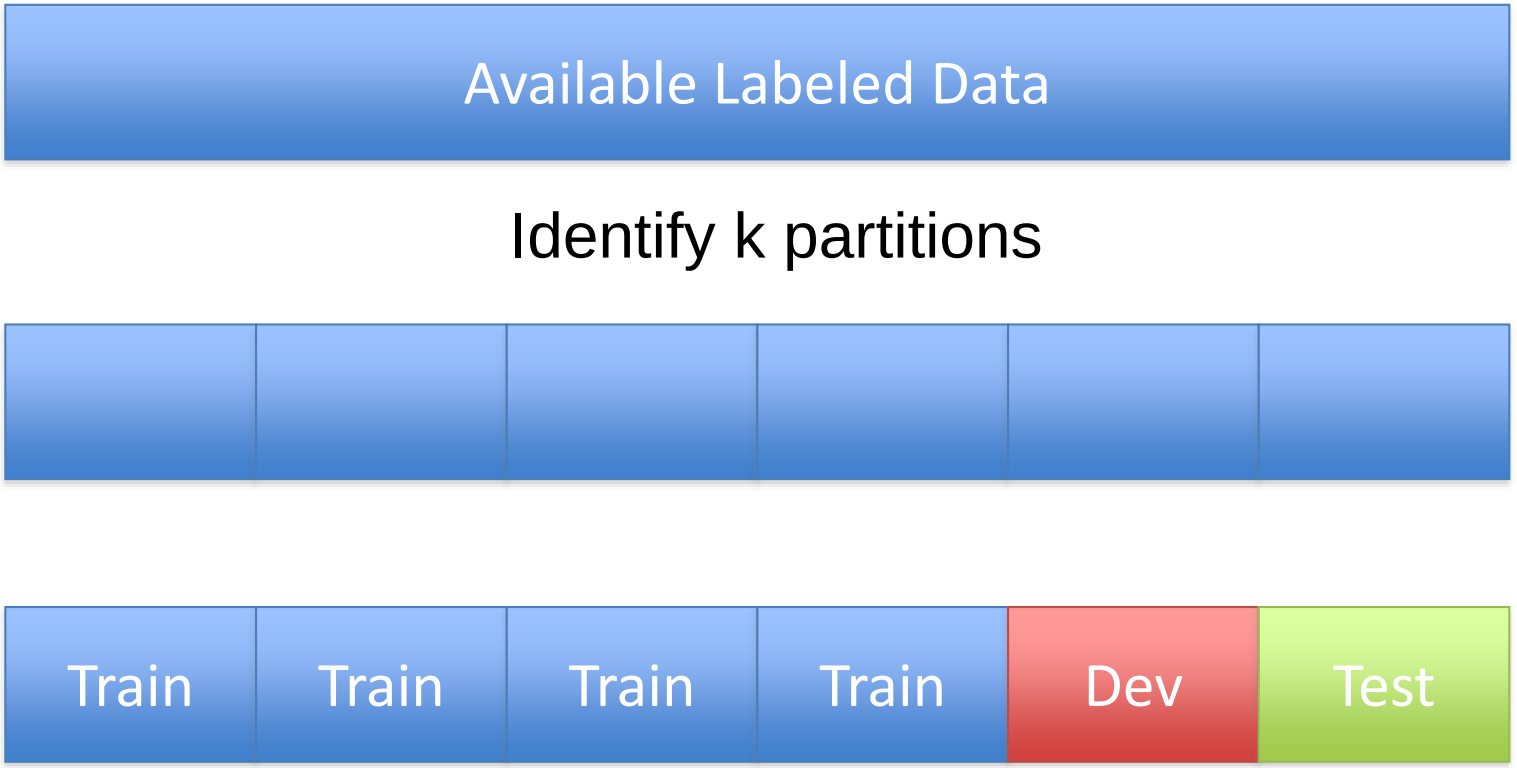
- Training data – used to identify model parameters
- Testing data – used for evaluation
- Optionally: Development / tuning data – used to identify model hyperparameters.

- Difficult to get significance or confidence values

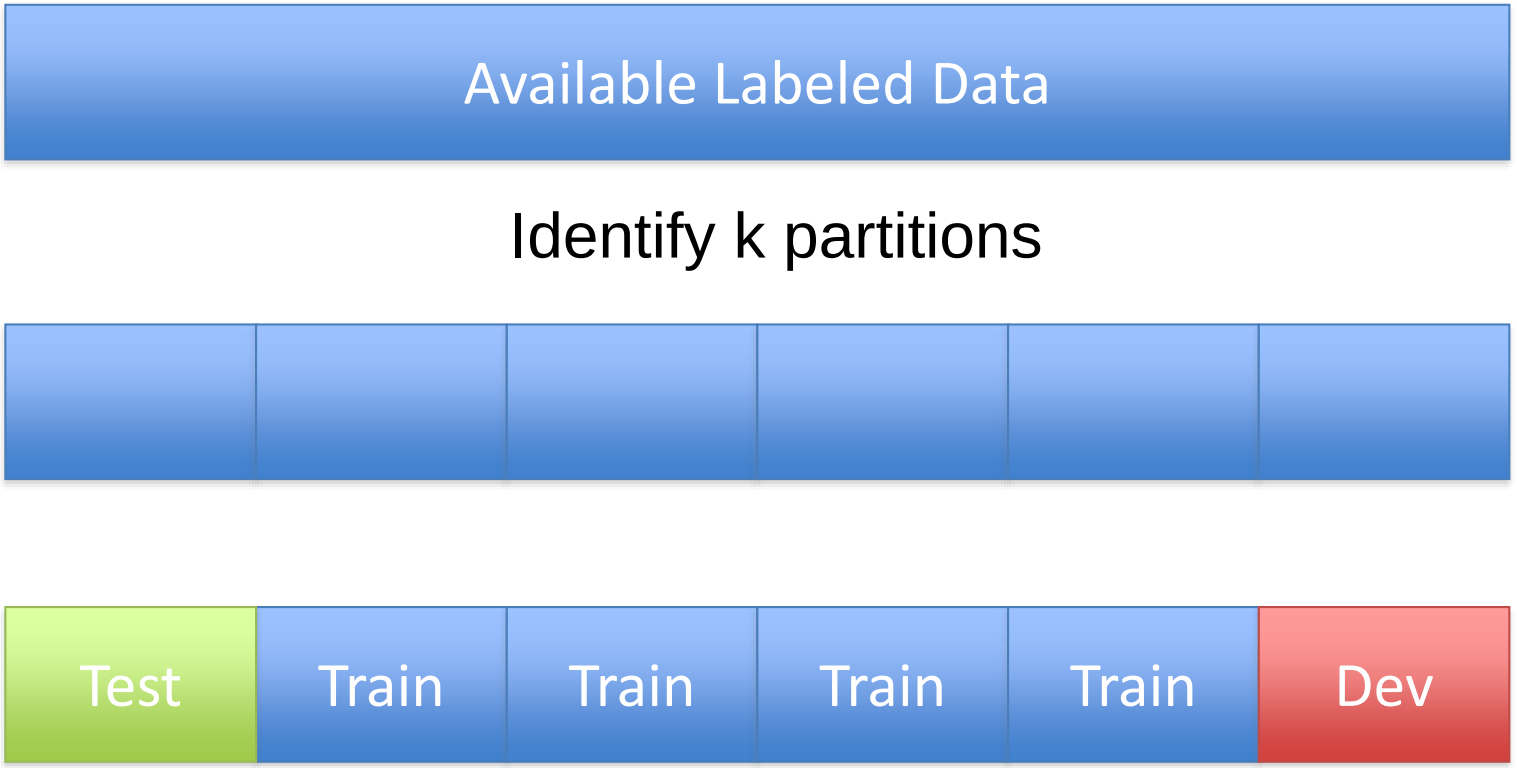
k-fold Cross validation

- Partition the available data into k folds
- Train on $k-1$ folds
- Test on the remaining fold.
- In the extreme $k = N,$ this is known as "**leave-one-out**" (LOO) cross validation
- k-fold cross validation gives k samples of the performance of the classifier.

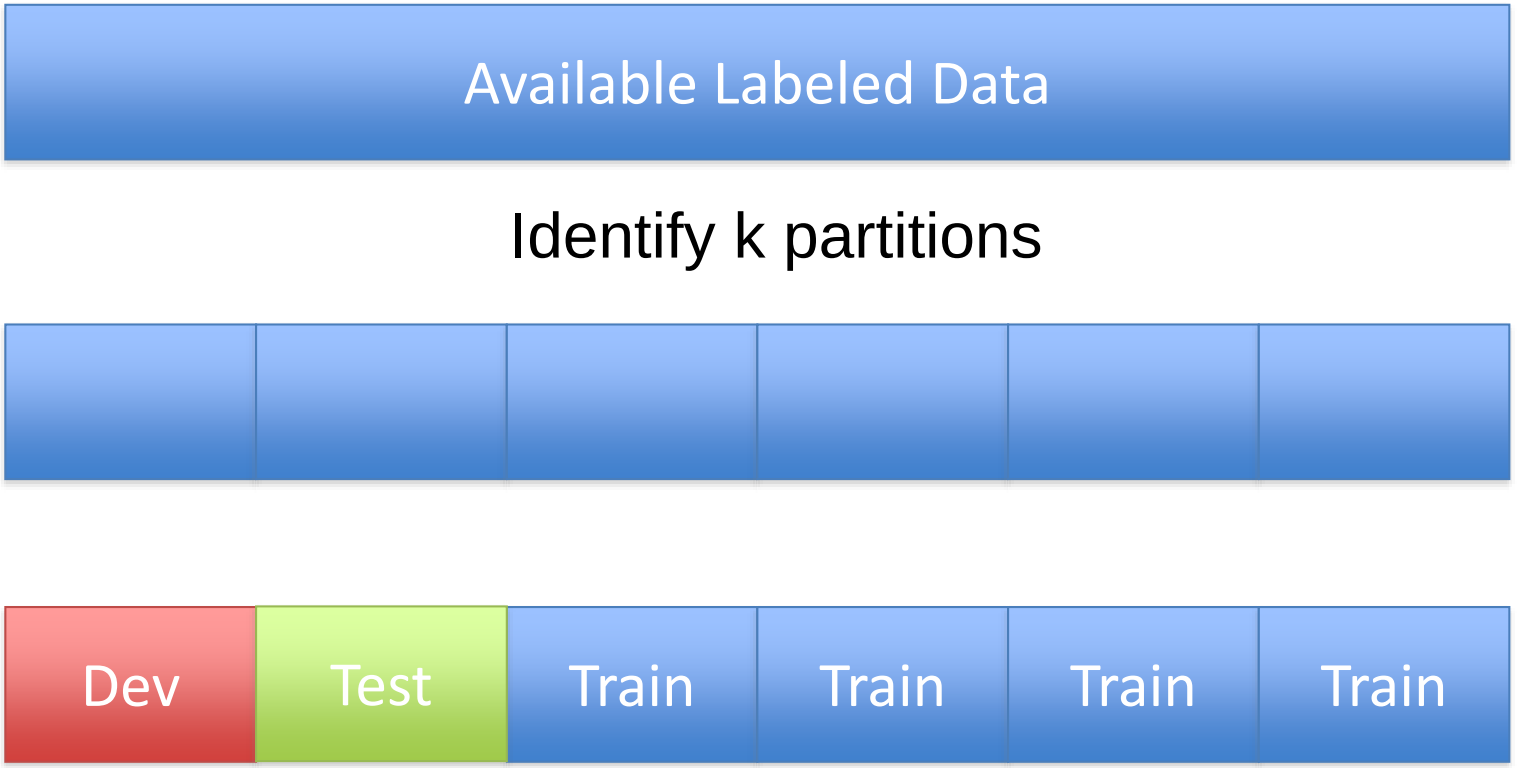
Cross-validation visualized



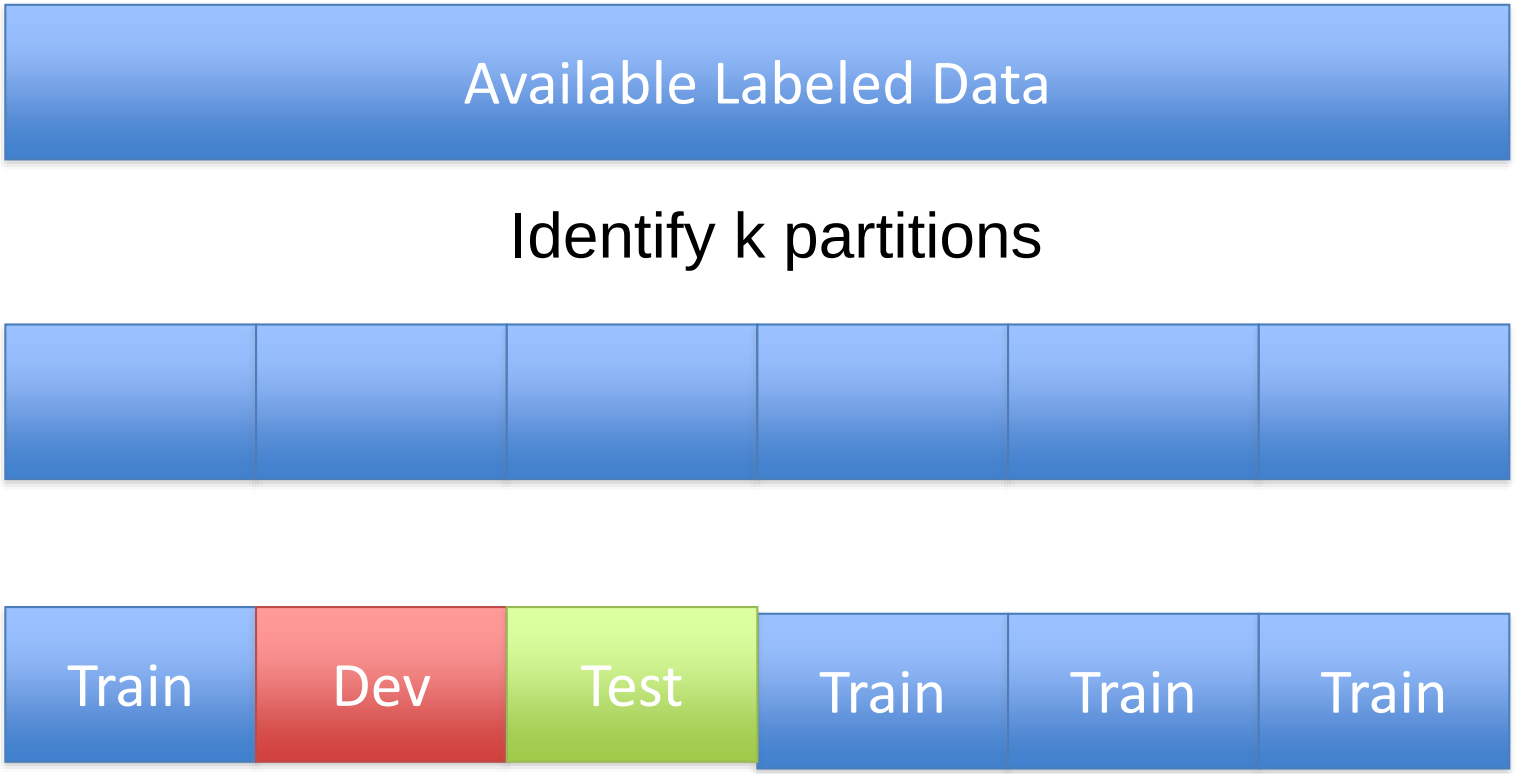
Cross-validation visualized



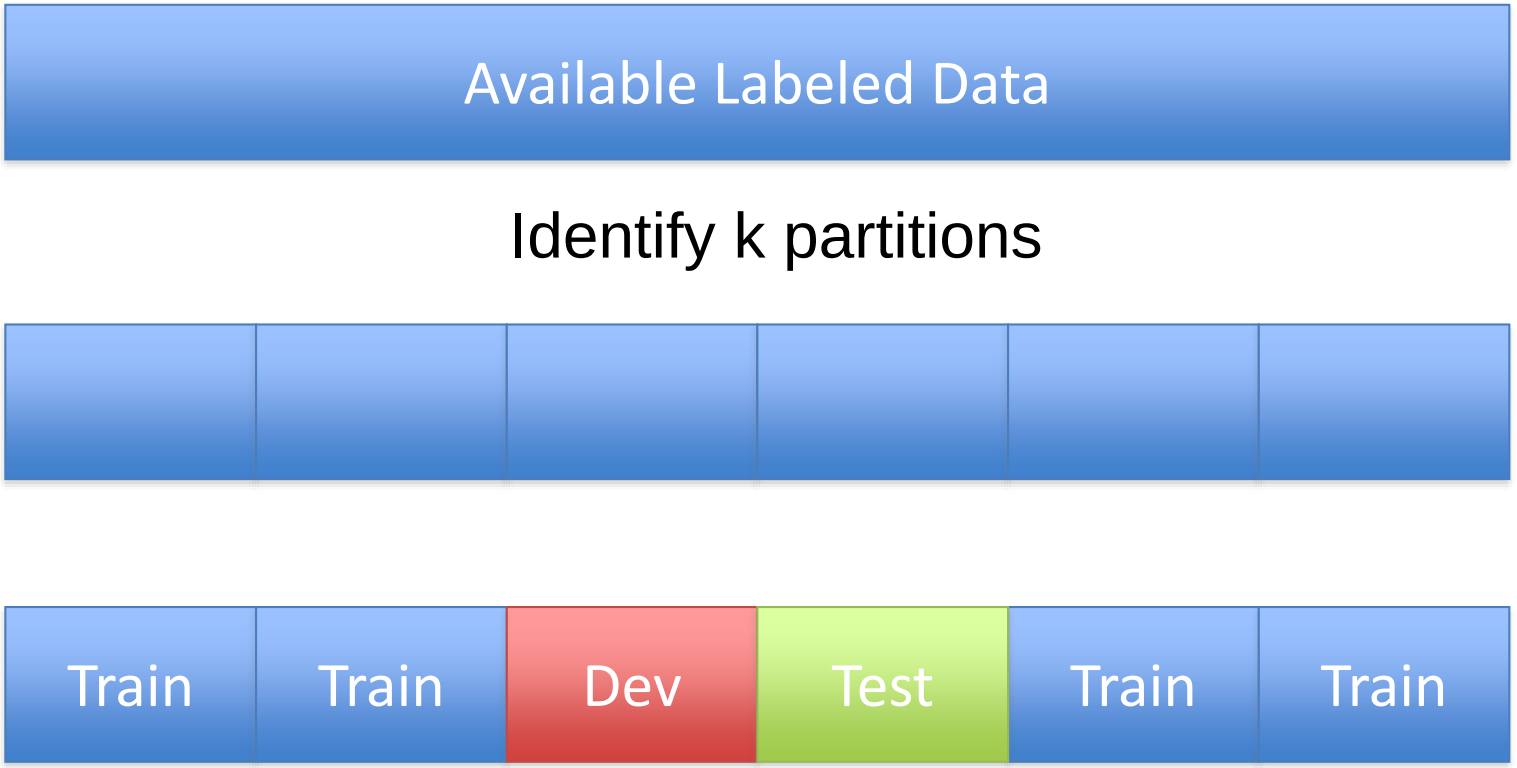
Cross-validation visualized



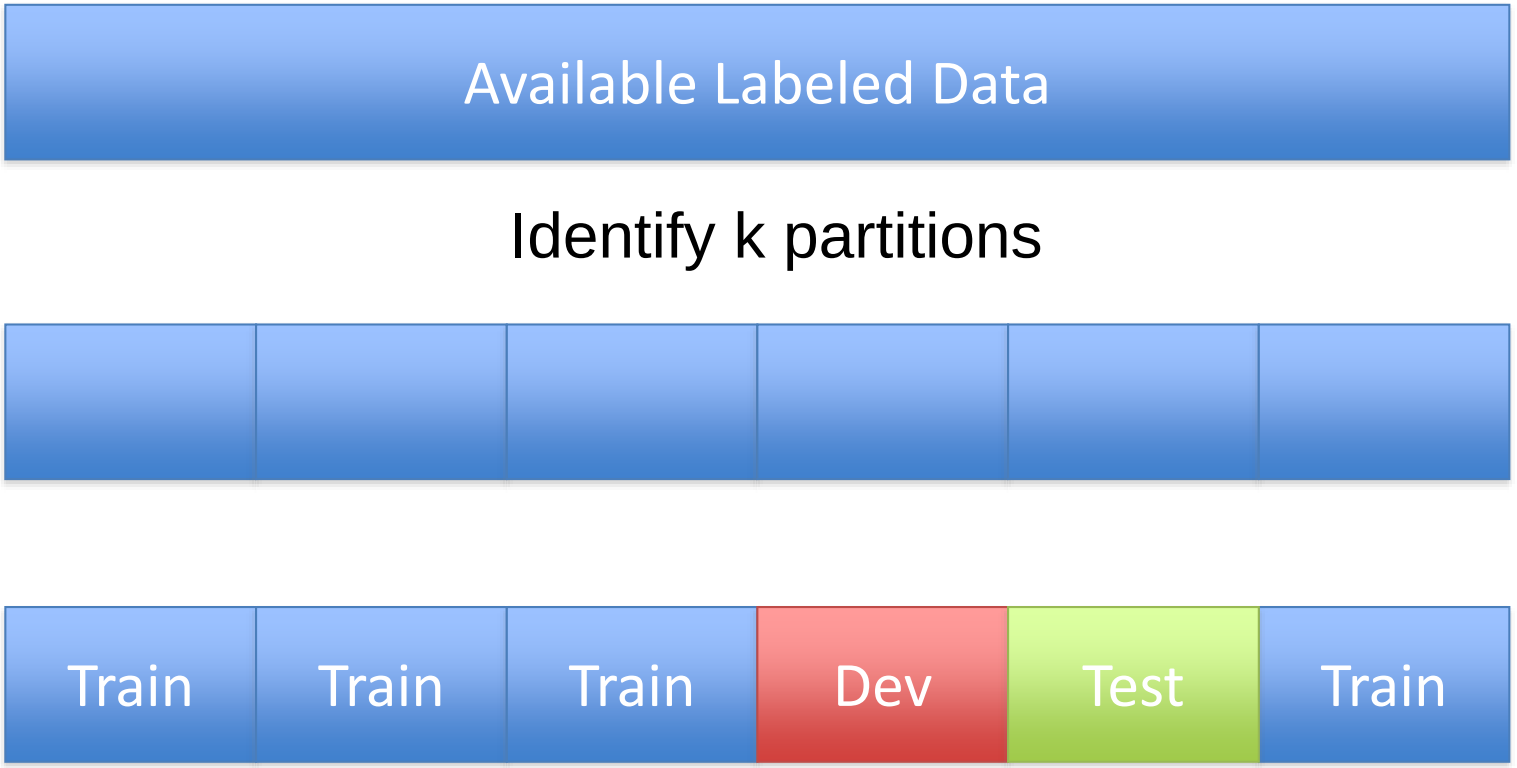
Cross-validation visualized



Cross-validation visualized



Cross-validation visualized



Calculate Average Performance

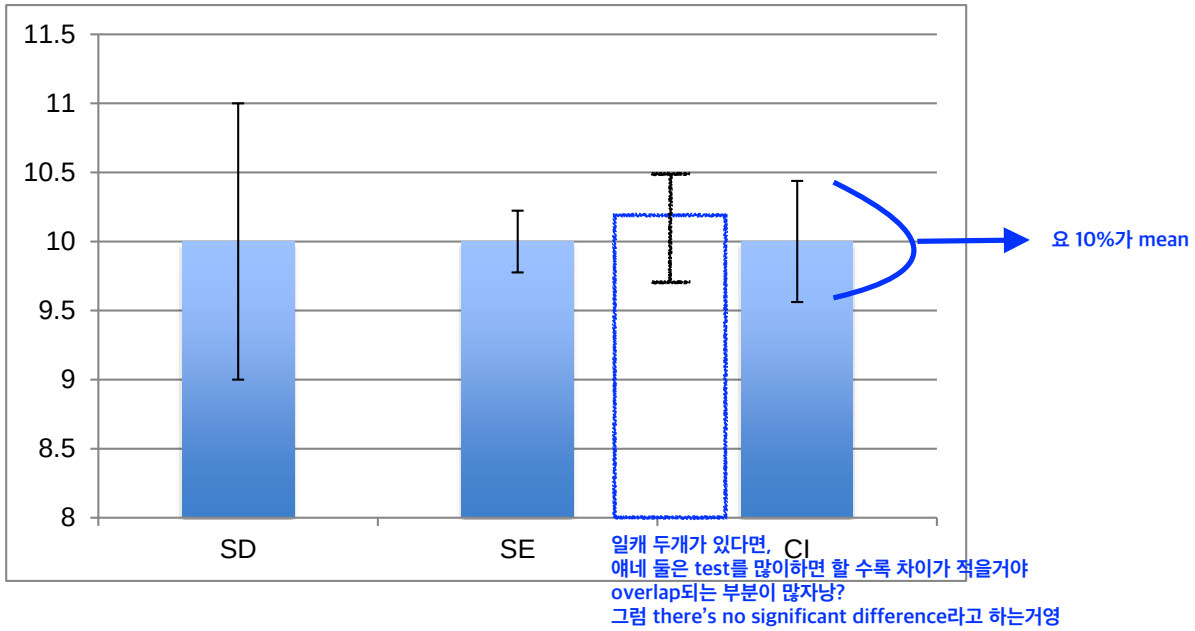
Confidence interval

- Given k samples of performance measures, we can compute the mean of the performance, μ
- While mean is important, the variance information should also be included
  - Standard deviation (SD): σ
  - Standard error (SE):$\frac{\sigma}{\sqrt{k}}$
  - Confidence interval ($CI_{\alpha\%}$)

$$CI_{95\%} = \mu \pm 1.96 * \frac{\sigma}{\sqrt{k}}$$

Confidence Bars

- Variance information is often represented as an error bar or confidence bar around the mean performance
- 95% confidence interval has the clearest interpretation.



Criticisms of cross-validation

- While the test data is independently sampled, there is a lot of overlap in training data.
  - The model performance may be correlated.
  - **Underestimation** of variance.
  - **Overestimation** of significant differences.
- One proposed solution* is to repeat **2-fold** cross-validation 5 times rather than **10-fold** cross validation
  - It more directly measures variation due to the choice of training set

*Dietterich, Thomas G. "Approximate statistical tests for comparing supervised classification learning algorithms." *Neural computation* 10.7 (1998): 1895-1923.

Significance Testing

- Is the performance of two classifiers different with statistical significance?
- Testing the means
  - If we have two samples of classifier performance (accuracy), we want to determine if they are drawn from the same distribution (Null hypothesis: no difference) or two different distributions.
- Statistical testing is extensively studied in the stat 561, 562, 563 sequence

Baseline Classifiers

- Majority Class baseline
  - Every data point is classified as the class that is most frequently represented in the training data
- Random baseline
  - Randomly assign one of the classes to each data point.
    - with an even distribution
    - with the training class distribution

Proper Evaluation: summary

- How do you measure performance?
  - Accuracy, precision/recall/F1, ROC/AUC --- often it is good to look at multiple measures and carefully think about which measure makes sense for your application
- How certain are you about the performance you claim?
  - Include variance information using SD, SE or Confidence interval
- How do you compare two algorithms and decide if one performs better than another?
  - Consider multiple runs of the algorithm on different samples, e.g., Cross-validation, or bootstrapping, and consider statistical testing when appropriate
- What algorithm you should compare to?
  - In addition to state-of-the-art, it is also important to compare against some dummy baselines