DS 4400

Machine Learning and Data Mining I
Spring 2024

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February 13 2022

Outline

- Evaluation of classifiers
  - Accuracy, error, precision, recall
  - ROC curves and the AUC metric
  - Why multiple metrics

- Midterm exam review
- Final project announcements

Classifier Evaluation

- Classification is a supervised learning problem
  - Prediction is binary or multi-class
- Classification techniques
  - Linear classifiers
    - Logistic regression (probabilistic interpretation)
  - Instance learners
    - kNN: need to store entire training data
- Cross-validation should be used for parameter selection and estimation of model error

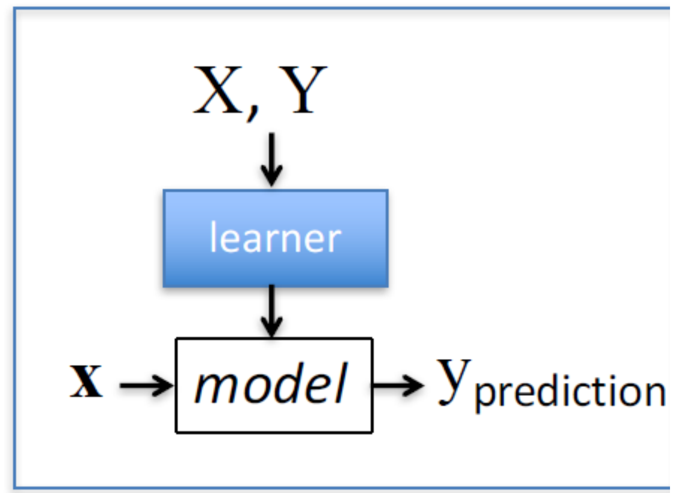
Evaluation of classifiers

Given: labeled training data $X, Y = \{\langle \boldsymbol{x}_i, y_i \rangle\}_{i=1}^{n}$

- Assumes each $\boldsymbol{x}_i \sim \mathcal{D}(\mathcal{X})$

Train the model:

model ← *classifier*.train(X, Y)



Apply the model to new data:

- Given: new unlabeled instance $\boldsymbol{x} \sim \mathcal{D}(\mathcal{X})$

$\mathrm{y}_{\text{prediction}}$ ← *model*.predict($\mathbf{x}$)

Classification Metrics

$$\text{accuracy} = \frac{\#\ \text{correct predictions}}{\#\ \quad\quad\ \text{instances}}$$

$$\text{error} = 1 - \text{accuracy} = \frac{\#\ \text{incorrect predictions}}{\#\ \quad\quad\ \text{instances}}$$

- Can evaluate on both training or testing
- Training set accuracy and error
- Testing set accuracy and error

Confusion Matrix

Given a dataset of P positive instances and N negative instances:

		Predicted Class	
		Yes	No
Actual Class	Yes	TP	FN
	No	FP	TN

Accuracy and Error

Given a dataset of P positive instances and N negative instances:

Actual Class \ Predicted Class	Yes	No
Yes	TP	FN
No	FP	TN

Actual Class \ Predicted Class	Yes	No
Yes	TP	FN
No	FP	TN

$$\text{accuracy} = \frac{TP + TN}{P + N}$$

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

Confusion Matrix

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$$\text{accuracy} = \frac{TP + TN}{P + N}$$

- Imagine using classifier to identify positive cases (i.e., for information retrieval)

$$\text{precision} = \frac{TP}{TP + FP}$$

$$\text{recall} = \frac{TP}{TP + FN}$$

Probability that classifier predicts positive correctly

Probability that actual class is predicted correctly

Why One Metric is Not Enough

Assume that in your training data, Spam email is 1% of data, and Ham email is 99% of data

- Scenario 1
  - Have classifier always output HAM!
  - What is the accuracy?
- Scenario 2
  - Predict one SPAM email as SPAM, all other emails as legitimate
  - What is the precision?
- Scenario 3
  - Output always SPAM!
  - What is the recall?

Why One Metric is Not Enough

Assume that in your training data, Spam email is 1% of data, and Ham email is 99% of data

- Scenario 1
  - Have classifier always output HAM!
  - What is the accuracy? 99%
- Scenario 2
  - Predict one SPAM email as SPAM, all other emails as legitimate
  - What is the precision? 100%
- Scenario 3
  - Output always SPAM!
  - What is the recall? 100%

Precision & Recall

Precision

- the fraction of positive predictions that are correct
- P(is pos | predicted pos)

$$\text{precision} = \frac{TP}{TP + FP}$$

Recall

- fraction of positive instances that are identified
- P(predicted pos | is pos)

$$\text{recall} = \frac{TP}{TP + FN}$$

- You can get high recall (but low precision) by only predicting positive
- Recall is a non-decreasing function of the # positive predictions
- Typically, precision decreases as either the number of positive predictions or recall increases
- Precision & recall are widely used in information retrieval

F-Score

- Combined measure of precision/recall tradeoff

$$F_1 = 2 \times \frac{\text{precision} \times \text{recall}}{\text{precision} + \text{recall}}$$

  - This is the harmonic mean of precision and recall
  - In the F_1 measure, precision and recall are weighted evenly
  - Can also have biased weightings that emphasize either precision or recall more (F_2 = 2 × recall; $F_{0.5}$ = 2 × precision)

- Limitations:
  - F-measure can exaggerate performance if balance between precision and recall is incorrect for application
    - Don't typically know balance ahead of time

A Word of Caution

- Consider binary classifiers A, B, C:

		A	.	B	.	C	.
		1	0	1	0	1	0
Predictions	1	0.9	0.1	0.8	0	0.78	0
	0	0	0	0.1	0.1	0.12	0.1

A Word of Caution

- Consider binary classifiers A, B, C:

		A	.	B	.	C	.
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Predictions	1	0.9	0.1	0.8	0	0.78	0
	0	0	0	0.1	0.1	0.12	0.1

- Clearly A is useless, since it always predicts 1
- B is slightly better than C
  - less probability mass wasted on the off-diagonals
- But, here are the performance metrics:

Metric	A	B	C
Accuracy	0.9	0.9	0.88
Precision	0.9	1.0	1.0
Recall	1.0	0.888	0.8667
F-score	0.947	0.941	0.9286

Classifiers can be tuned

- Logistic regression sets by default the threshold at 0.5 for classifying positive and negative instances
- Some applications have strict constraints on false positives (or other metrics)
  - Example: very low false positives in security (spam)

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- Logistic regression sets by default the threshold at 0.5 for classifying positive and negative instances
- Some applications have strict constraints on false positives (or other metrics)
  – Example: very low false positives in security (spam)
- Solution: choose different threshold

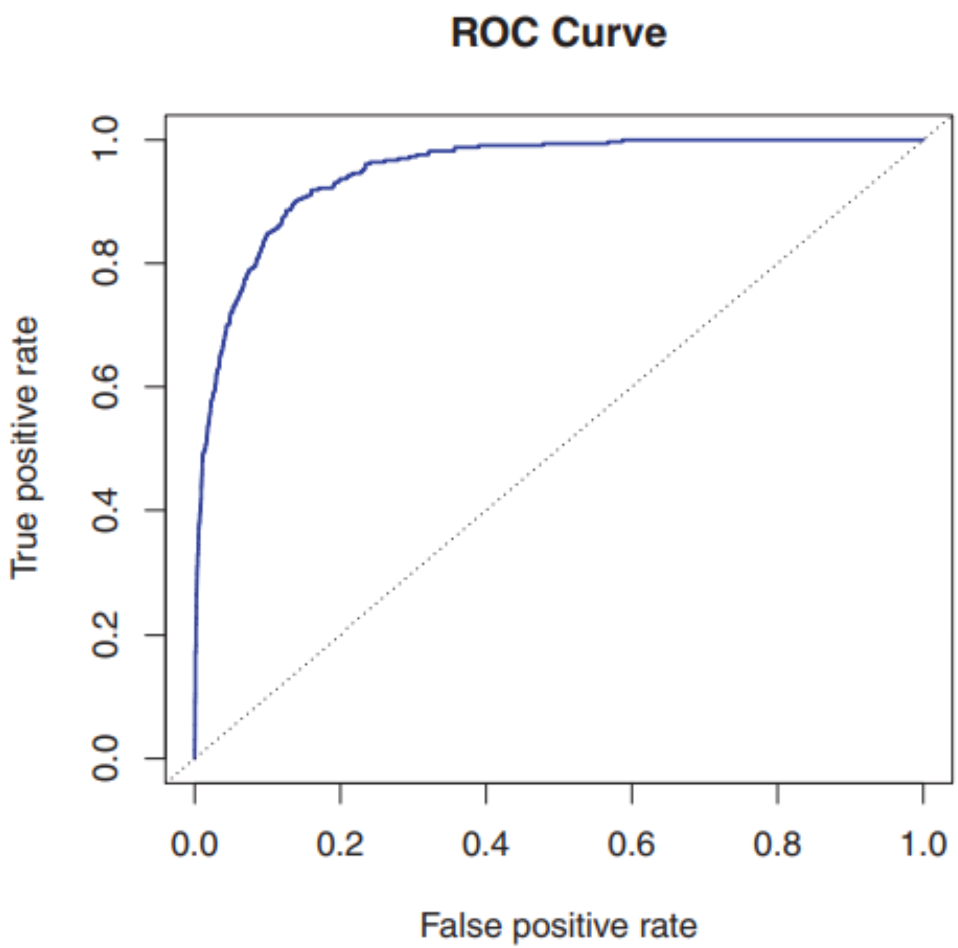
Probabilistic model $h_{\theta(x)} = \mathrm{P}[y = 1 | x; \theta]$

– Predict y = 1 if $h_{\theta}(x) \geq$ T

– Predict y = 0 if $h_{\theta}(x) <$ T

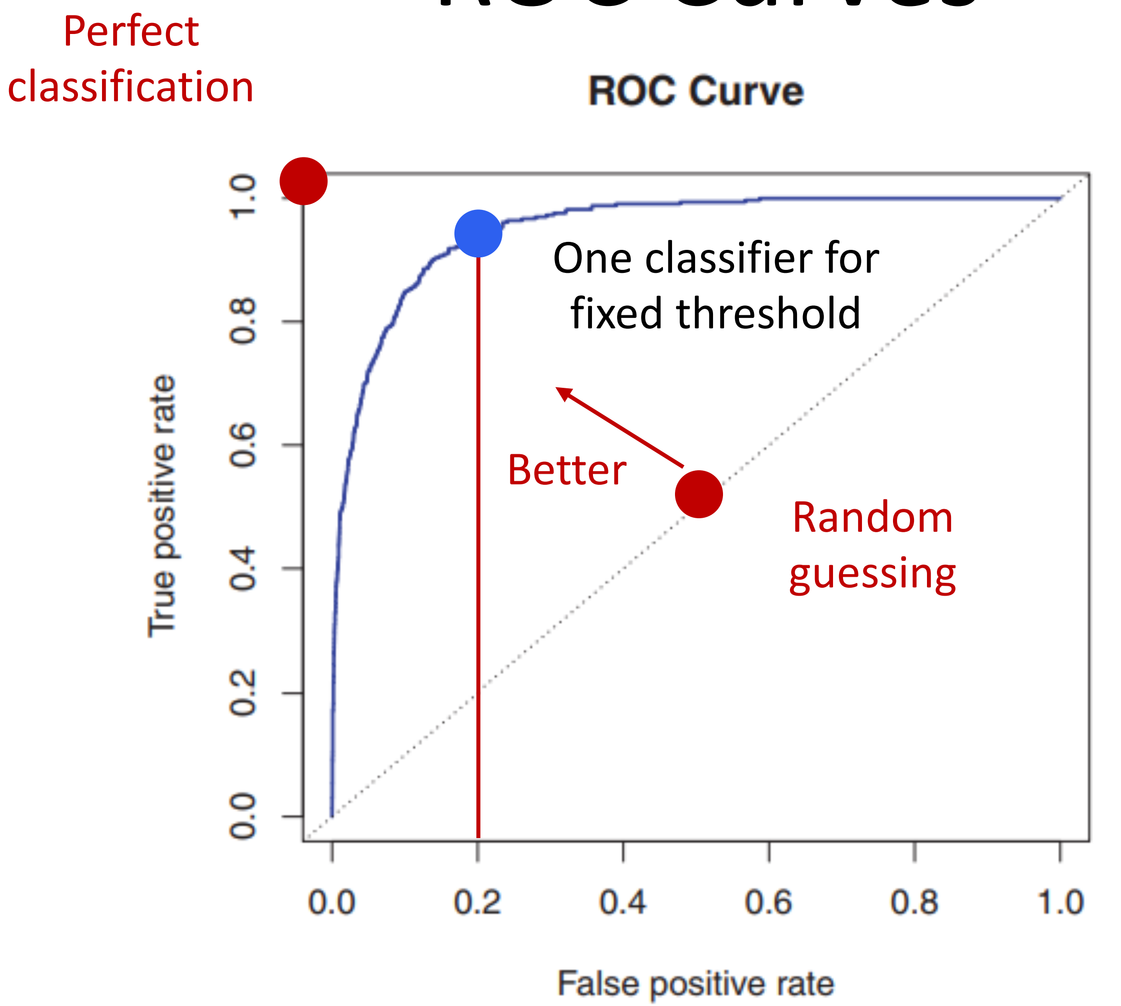
Higher T, lower FP
Lower T, lower FN

ROC Curves



- Receiver Operating Characteristic (ROC)
- Determine operating point (e.g., by fixing false positive rate)

ROC Curves

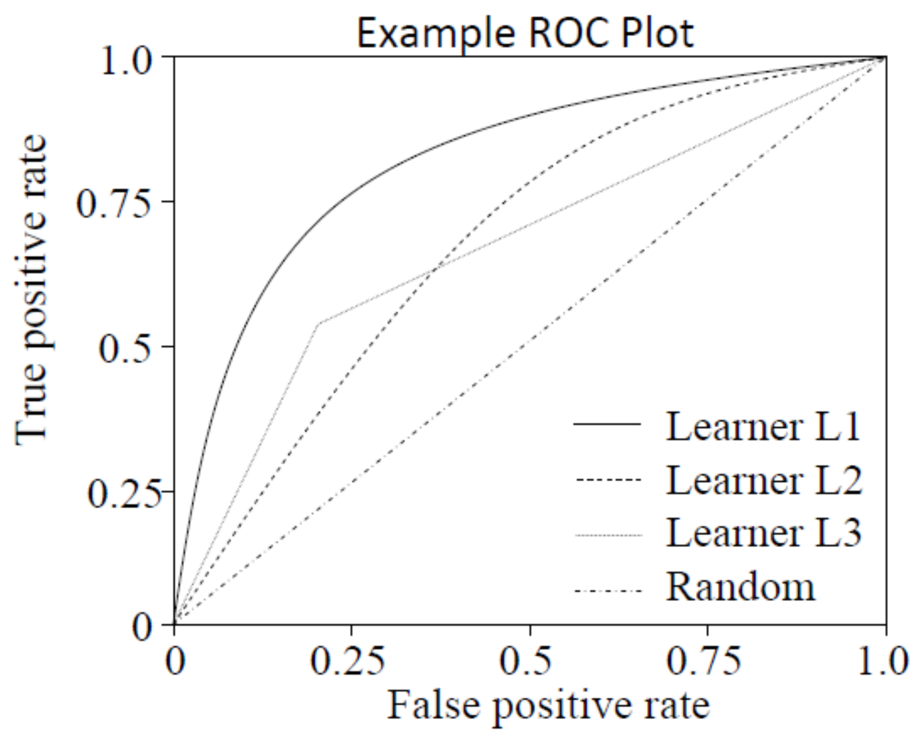


- Receiver Operating Characteristic (ROC)
- Determine operating point (e.g., by fixing false positive rate)

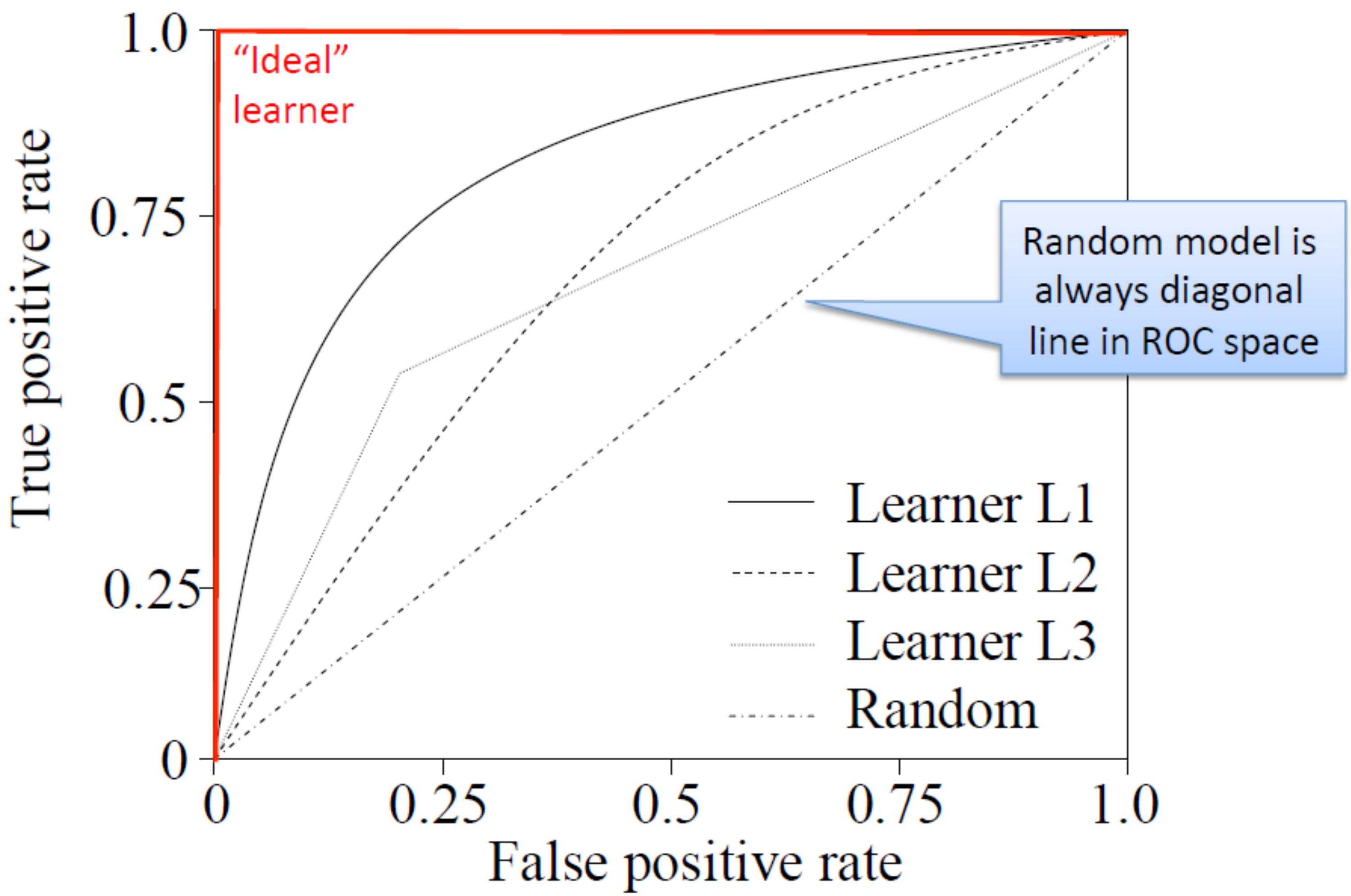
Performance Depends on Threshold

Predict positive if $\mathrm{P}(y = 1 \mid \mathbf{x}) > T$ otherwise negative

- Number of TPs and FPs depend on threshold T
- As we vary T we get different (TPR, FPR) points

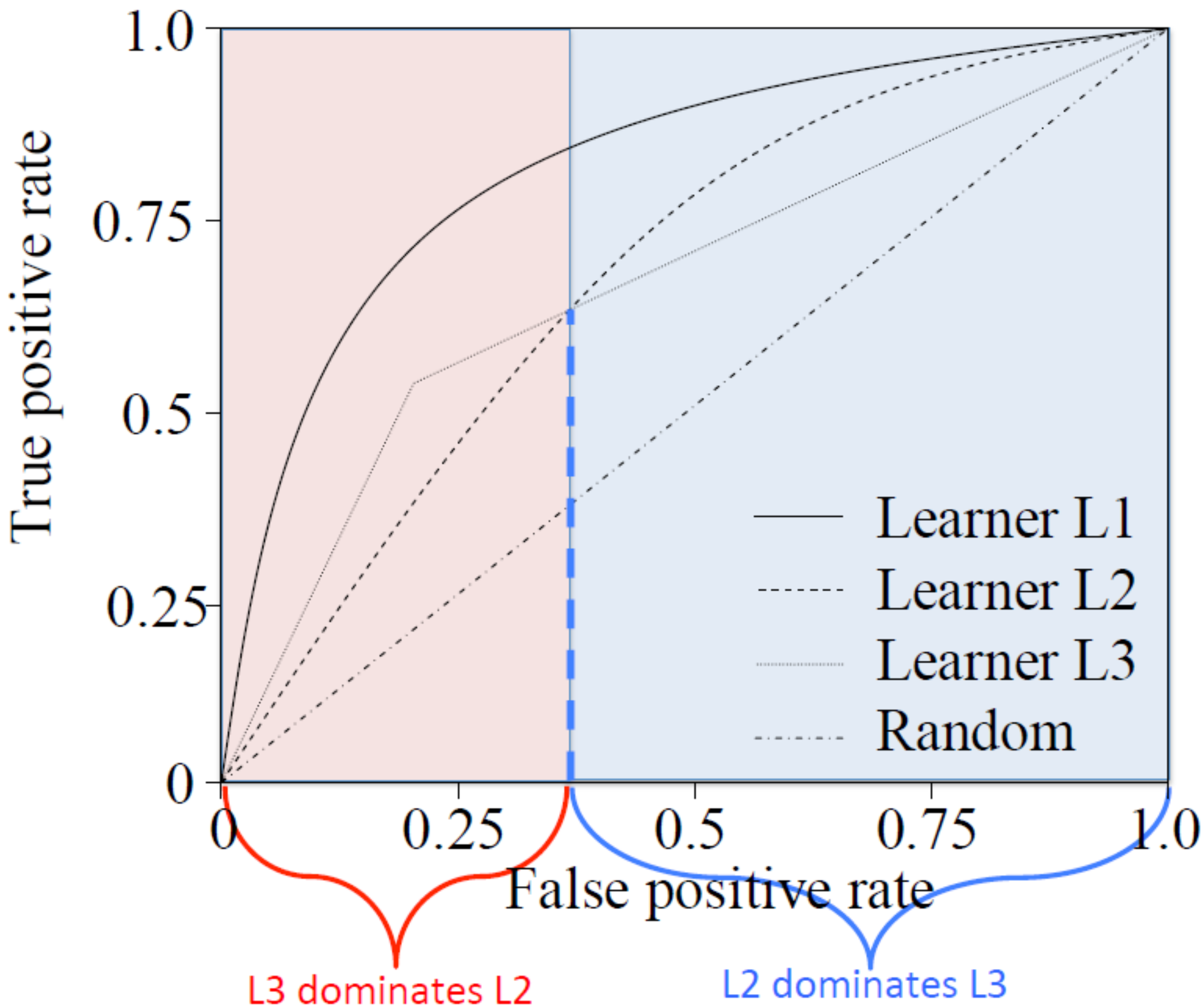


ROC Curve



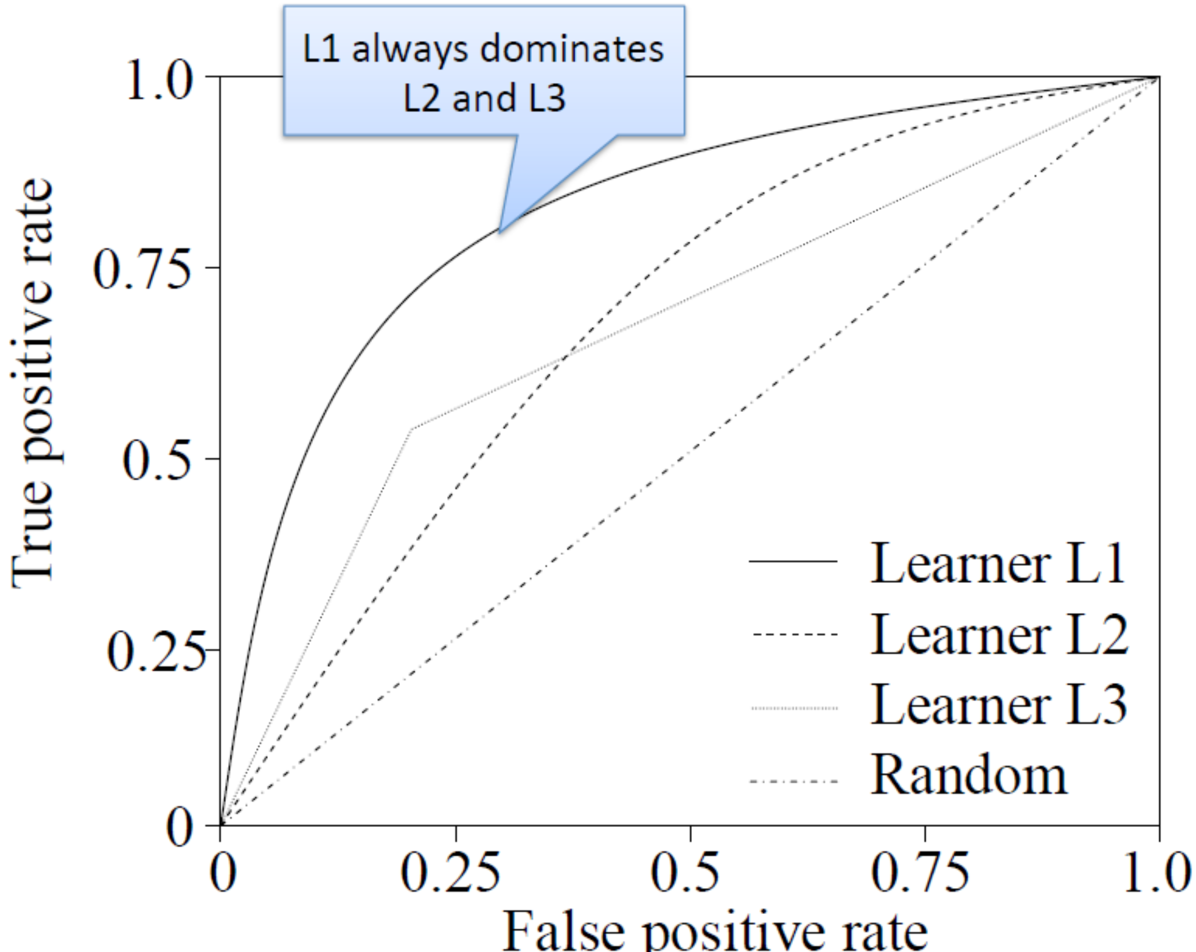
1.0
0.75
0.5
0.25
0
True positive rate
"Ideal" learner
Random model is always diagonal line in ROC space
Learner L1
Learner L2
Learner L3
Random
0
0.25
0.5
0.75
1.0
False positive rate

ROC Curve



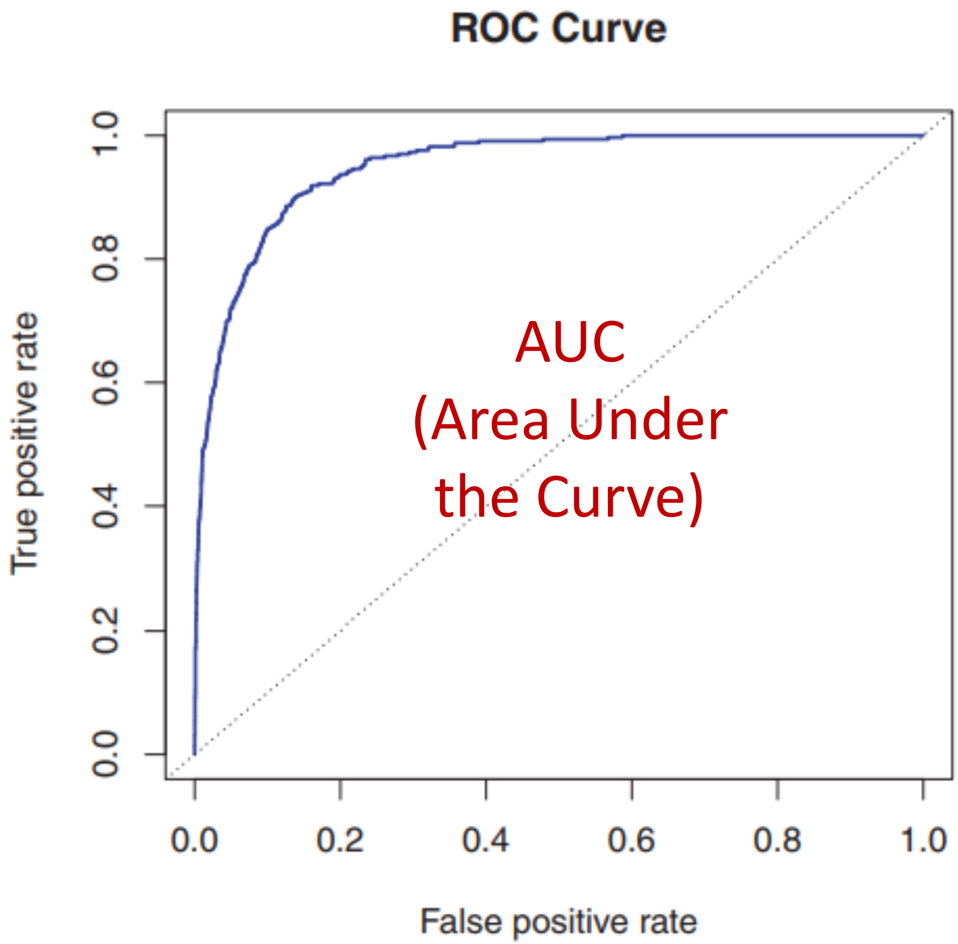
1.0
0.75
0.5
0.25
0
True positive rate
0
0.25
0.5
0.75
1.0
False positive rate
Learner L1
Learner L2
Learner L3
Random
L3 dominates L2
L2 dominates L3

ROC Curve



L1 always dominates L2 and L3
1.0
0.75
0.5
0.25
0
True positive rate
0
0.25
0.5
0.75
1.0
False positive rate
Learner L1
Learner L2
Learner L3
Random

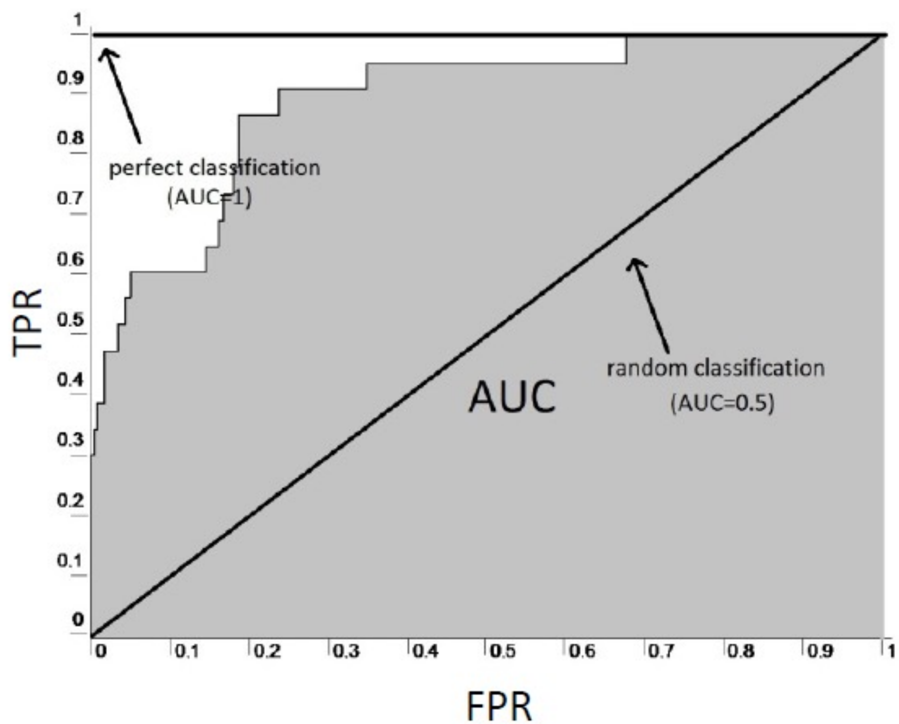
ROC Curves

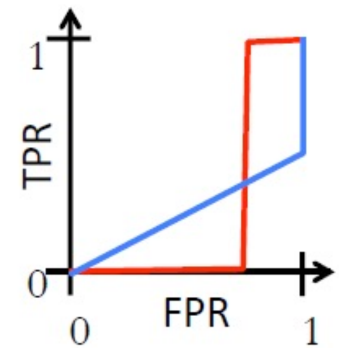


- Another useful metric: Area Under the Curve (AUC)
- The closest to 1, the better!

Area Under the ROC Curve

- Can take area under the ROC curve to summarize performance as a single number
  - Be cautious when you see only AUC reported without a ROC curve; AUC can hide performance issues





Same AUC, very different performance

ROC Example

i	y_i	$p(y_i = 1 \mid \mathbf{x}_i)$	$h(\mathbf{x_i} \mid T = 0)$	$h(\mathbf{x_i} \mid T = 0.5)$	$h(\mathbf{x_i} \mid T = 1)$
1	1	0.9	1	1	0
2	1	0.8	1	1	0
3	1	0.7	1	1	0
4	1	0.6	1	1	0
5	1	0.5	1	1	0
6	0	0.4	1	0	0
7	0	0.3	1	0	0
8	0	0.2	1	0	0
9	0	0.1	1	0	0
			$TPR =$	$TPR =$	$TPR =$
			$FPR =$	$FPR =$	$FPR =$

ROC Example

i	y_i	$p(y_i = 1 \mid \mathbf{x}_i)$	$h(\mathbf{x_i} \mid \theta = 0)$	$h(\mathbf{x_i} \mid \theta = 0.5)$	$h(\mathbf{x_i} \mid \theta = 1)$
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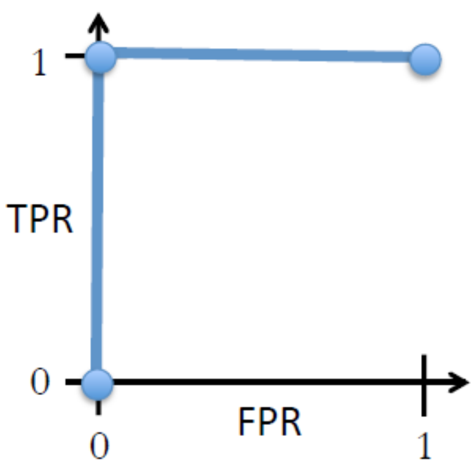
2	1	0.8	1	1	0
3	1	0.7	1	1	0
4	1	0.6	1	1	0
5	1	0.5	1	1	0
6	0	0.4	1	0	0
7	0	0.3	1	0	0
8	0	0.2	1	0	0
9	0	0.1	1	0	0
			$TPR = 5/5 = 1$	$TPR = 5/5 = 1$	$TPR = 0/5 = 0$
			$FPR = 4/4 = 1$	$FPR = 0/4 = 0$	$FPR = 0/4 = 0$



ROC Example

i	y_i	$p(y_i = 1 \mid \mathbf{x}_i)$	$h(\mathbf{x_i} \mid T = 0)$	$h(\mathbf{x_i} \mid T = 0.5)$	$h(\mathbf{x_i} \mid T = 1)$
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2	1	0.8	1	1	0
3	1	0.7	1	1	0
4	1	0.6	1	1	0
5	1	**0.2**	1	**0**	0
6	0	**0.6**	1	**1**	0
7	0	0.3	1	0	0
8	0	0.2	1	0	0
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			$TPR =$	$TPR =$	$TPR =$
			$FPR =$	$FPR =$	$FPR =$

ROC Example

i	y_i	$p(y_i = 1 \mid \mathbf{x}_i)$	$h(\mathbf{x_i} \mid \theta = 0)$	$h(\mathbf{x_i} \mid \theta = 0.5)$	$h(\mathbf{x_i} \mid \theta = 1)$
1	1	0.9	1	1	0
2	1	0.8	1	1	0
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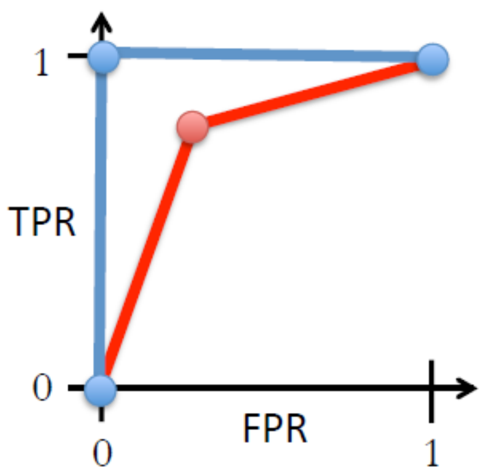
5	1	**0.2**	1	**0**	0
6	0	**0.6**	1	**1**	0
7	0	0.3	1	0	0
8	0	0.2	1	0	0
9	0	0.1	1	0	0
			$TPR = 5/5 = 1$ $FPR = 4/4 = 1$	$TPR = 4/5 = 0.8$ $FPR = 1/4 = 0.25$	$TPR = 0/5 = 0$ $FPR = 0/4 = 0$



Classifier Evaluation

- Accuracy and error are not sufficient for classifier evaluation
- Always include multiple metrics
  - Precision and recall for imbalance cases (plot precision-recall curve by varying the thresholds)
  - F1 score is a single metric averaging precision and recall
- Classifiers can be tuned by changing the threshold for prediction
  - Respect application constraints (e.g., low false positives, high recall)
  - Plot ROC curve and report AUC
- Confusion matrix and metrics can be extended to multi-class classification

MIDTERM PREPARATION

Topics

- Bias-variance trade off
- Probability and linear algebra review
- Simple linear regression
- Correlation
- Multiple linear regression
- Gradient descent
- Regularization. Ridge and lasso regression
- K-Nearest Neighbors
- Cross Validation
- Logistic Regression
- Precision, Recall, ROC curves

Content through **today's** lecture.

Question Format

Majority of the exam is conceptual questions. i.e. short answer verbal response.

Allowed one cheat sheet. Double sided handwritten or printed. That said, focus of exam is not on memorizing formulas.

*stay tuned on logistics for those who have been approved for extra time.

Example Questions

- Give an example of an algorithm that does not have a closed-form solution and explain why one does not exist.
- Explain the difference between the validation dataset and the test dataset
- In K-Nearest Neighbors, if we increase K, how does bias change? How does variance change?
- Given a dataset, describe the steps needed to determine the optimal value of λ
- If I multiply X and y by 2, how does that affect the optimal linear regression coefficients?

Example Questions

- Let A be a matrix with n rows and m columns. If the system of equations $Ax = 0$ has no solutions besides $x = 0$, what does that tell us about the rank of A? If the system has infinite solutions?

- If a matrix is n x m where m < n, then what is the maximum possible rank of the matrix?

- Given a fixed θ when does a logistic regression predict "class 1" and when does it predict "class 0"?

- What are the list one pro and one con of increasing the validation set from 20% of the original data to 30%?