DS 4400

Machine Learning and Data Mining I
Spring 2024

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Outline

- Review of Cross Validation
- Logistic regression
  - Objective for logistic regression
  - Gradient descent training
  - Regularization
- Logistic regression lab
- Evaluation of classifiers
  - Accuracy, error, precision, recall
  - ROC curves and the AUC metric
  - Why multiple metrics

Announcements

Based on class feedback there will be frequent code demos / examples to complement lecture slides.

Many of these will be the textbook's labs. However, in coming weeks I will likely create my own code demos as well.

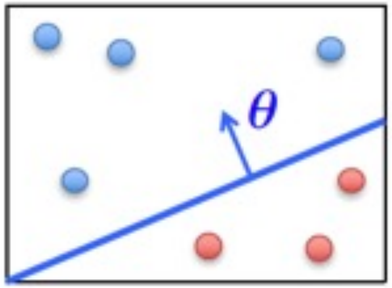
Lab Demo for Cross Validation and Regularization

LOGISTIC REGRESSION

Linear Classifiers

- **Linear classifiers**: represent decision boundary by hyperplane

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix} \quad \boldsymbol{x}^\intercal = \begin{bmatrix} 1 & x_1 & \dots & x_d \end{bmatrix}$$



$h_\theta(x) = f(\theta^T x)$ linear classifier

- If $\theta^T x > 0$ classify "Class 1"
- If $\theta^T x < 0$ classify "Class 0"

All the points x on the hyperplane satisfy: $\theta^T x = 0$

Logistic Regression

- Setup
  - Training data: $\{x_i, y_i\}$, for $i = 1, \dots, N$
  - Labels: $y_i \in \{0,1\}$
- Goals
  - Learn $h_\theta(x) = P(Y = 1|X = x)$
- Highlights
  - Probabilistic output
  - At the basis of more complex models (e.g., neural networks)
  - Supports regularization (Ridge, Lasso)
  - Can be trained with Gradient Descent

Logistic Regression

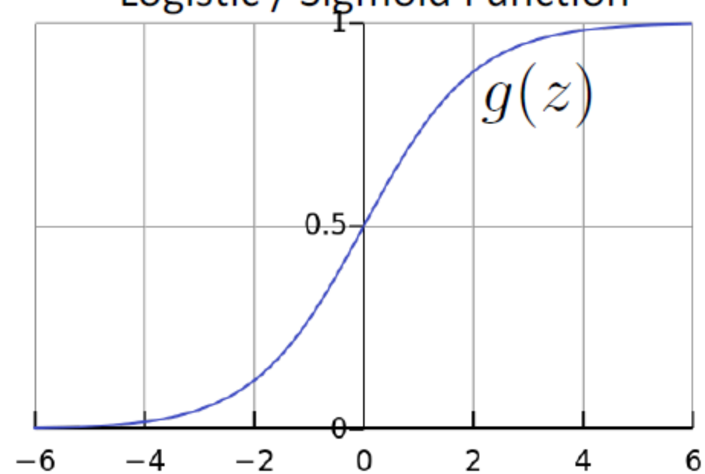
- Takes a probabilistic approach to learning discriminative functions (i.e., a classifier)
- $h_{\boldsymbol{\theta}}(\boldsymbol{x})$ should give $P(Y = 1|X; \theta)$
  - Want $0 \leq h_{\boldsymbol{\theta}}(\boldsymbol{x}) \leq 1$
- Logistic regression model:

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = g\left(\boldsymbol{\theta}^\top \boldsymbol{x}\right)$$

$$g(z) = \frac{1}{1 + e^{-z}}$$

$$\boxed{h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^\top \boldsymbol{x}}}}$$

Logistic / Sigmoid Function



Maximum Likelihood Estimation (MLE)

Training data $X = \{x_1, \dots, x_N\}$, labels $Y = \{y_1, \dots, y_N\}$

What is the likelihood of training data for parameter θ?

Define likelihood function $\quad Max_\theta \, L(\theta) = P[Y|X;\theta]$

Assumption: *training labels are conditionally independent*

$$L(\theta) = \prod_{i=1}^{N} P[Y = y_i | X = x_i; \theta]$$

Log likelihood has the same maximum

$$\log L(\theta) = \sum_{i=1}^{N} \log P[Y = y_i | X = x_i; \theta]$$

MLE for Logistic Regression

$$\mathrm{P}(Y = y_i | X = x_i; \theta) = h_\theta(x_i)^{y_i}\left(1 - h_\theta(x_i)\right)^{1-y_i}$$

$$\theta_{MLE} = \mathrm{argmax}_\theta \textstyle\sum_{i=1}^{N} \log P[Y = y_i | X = x_i; \theta]$$

$$= \mathrm{argmax}_\theta \sum_{i=1}^{N} \mathrm{y_i} \log h_\theta(x_i) + (1 - y_i) \log\left(1 - h_\theta(x_i)\right)$$

Logistic Regression Cross-Entropy Loss Objective

$$\min_\theta J(\theta)$$

$$J(\theta) = -\sum_{i=1}^{N} [\mathrm{y_i} \log h_\theta(x_i) + (1 - y_i) \log\left(1 - h_\theta(x_i)\right)]$$

Cross-Entropy Objective

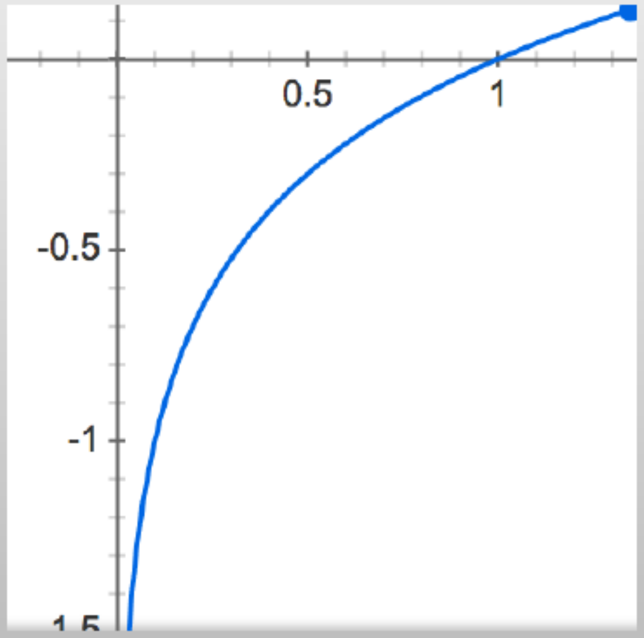
$$J(\theta) = -\sum_{i=1}^{N}[y_{\mathrm{i}}\log h_\theta(x_i) + (1-y_i)\log\left(1-h_\theta(x_i)\right)]$$

- Loss of a single instance:

Intuition

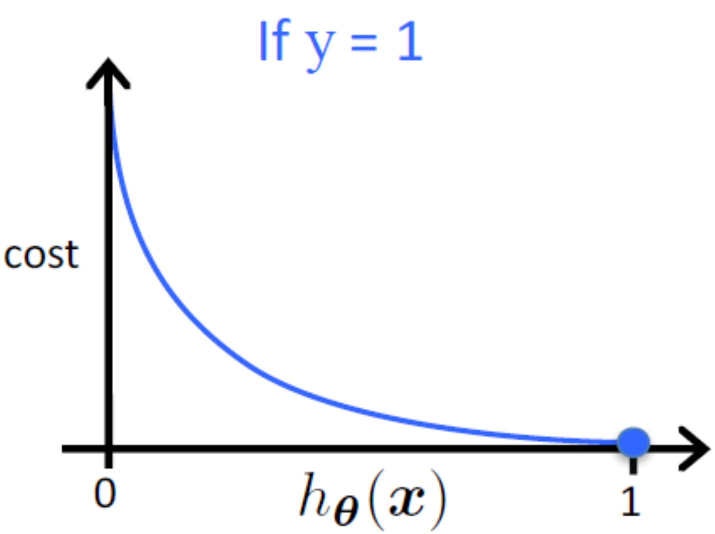
$$\text{loss } (h_{\boldsymbol{\theta}}(\boldsymbol{x}), y) = \begin{cases} -\log(h_{\boldsymbol{\theta}}(\boldsymbol{x})) & \text{if } y = 1 \\ -\log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x})) & \text{if } y = 0 \end{cases}$$

Aside: Recall the plot of log(z)



Intuition

$$\text{loss}\ \ (h_{\boldsymbol{\theta}}(\boldsymbol{x}), y) = \begin{cases} \boxed{\quad -\log(h_{\boldsymbol{\theta}}(\boldsymbol{x})) \quad \text{if } y = 1} \\ -\log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x})) \quad \text{if } y = 0 \end{cases}$$

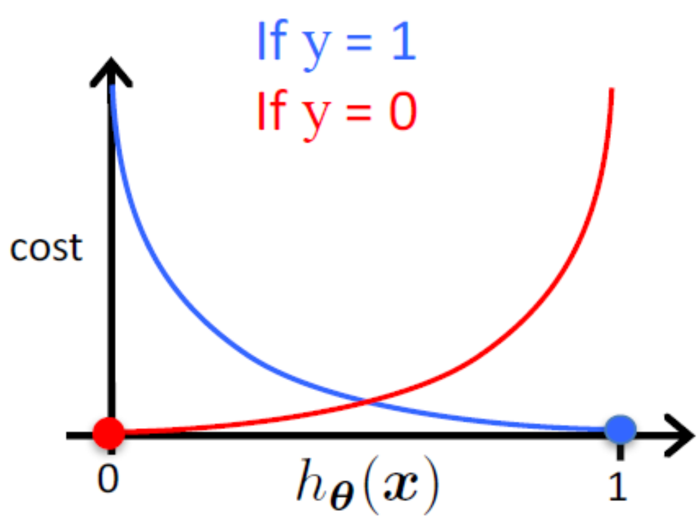


If y = 1

- loss = 0 if prediction is correct
- As $h_{\boldsymbol{\theta}}(\boldsymbol{x}) \to 0$, loss $\to \infty$
- Captures intuition that larger mistakes should get larger penalties
  - e.g., predict $h_{\boldsymbol{\theta}}(\boldsymbol{x}) = 0$, but y = 1

Intuition

$$\text{loss}\ (h_{\boldsymbol{\theta}}(\boldsymbol{x}), y) = \begin{cases} \boxed{-\log(h_{\boldsymbol{\theta}}(\boldsymbol{x})) \quad \text{if } y = 1} \\ \boxed{-\log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x})) \quad \text{if } y = 0} \end{cases}$$



If y = 0

- loss = 0 if prediction is correct
- As $(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x})) \rightarrow 0$, loss $\rightarrow \infty$
- Captures intuition that larger mistakes should get larger penalties

Gradient Descent for Logistic Regression

$$J(\theta) = -\sum_{i=1}^{N}[y_{\mathrm{i}}\log h_\theta(x_i) + (1-y_i)\log\big(1-h_\theta(x_i)\big)]$$

Want $\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta})$$

simultaneous update
for j = 0 ... d

Gradient Computation

$$J(\theta) = -\sum_{i=1}^{N}[y_{\mathrm{i}}\log h_\theta(x_i) + (1-y_i)\log\left(1-h_\theta(x_i)\right)]$$

Derivative Facts to Know:

$$\frac{d}{dx}\log x = \frac{1}{x}$$

If $\mathrm{f}(x) = \frac{1}{1+e^{-x}}$, then

$$\frac{df}{dx} = f(x)(1-f(x))$$

Computing Gradients

- Derivative of sigmoid
  - $g(z) = \frac{1}{1+e^{-z}}$; $g'(z) = \frac{e^{-z}}{(1+e^{-z})^2} = g(z)(1-g(z))$
- Derivative of hypothesis
  - $h_\theta(x) = g(\theta^T x) = g(\theta_j x_j + \sum_{k \neq j} \theta_k x_k)$
  - $\frac{\partial h_\theta(x)}{\partial \theta_j} = \frac{\partial g\left(\theta^T x\right)}{\partial \theta_j} x_j = g(\theta^T x)\left(1 - g(\theta^T x)\right) x_j$
- Derivation of C_i
  - $\frac{\partial C_i}{\partial \theta_j} = y_i \frac{1}{h_\theta(x_i)} \mathrm{g}(\theta^T x_i)\left(1 - \mathrm{g}(\theta^T x_i)\right) x_{ij}$ -

    $(1 - y_i) \frac{1}{1-h_\theta(x_i)} \mathrm{g}(\theta^T x_i)\left(1 - \mathrm{g}(\theta^T x_i)\right) x_{ij}$

    $= \left(y_i - h_\theta(x_i)\right) x_{ij}$

Gradient Descent for Logistic Regression

$$J(\theta) = -\sum_{i=1}^{N} [y_{\mathrm{i}} \log h_\theta(x_i) + (1 - y_i) \log \left(1 - h_\theta(x_i)\right)]$$

Want $\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence (simultaneous update for j = 0 ... d)

$$\theta_0 \leftarrow \theta_0 - \alpha \textstyle\sum_{i=1}^{N} (h_\theta(x_i) - y_i)$$

$$\theta_j \leftarrow \theta_j - \alpha \sum_{i=1}^{N} (h_\theta(x_i) - y_i) x_{ij}$$

Gradient Descent for Logistic Regression

Want $\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence (simultaneous update for j = 0 ... d)

$$\theta_0 \leftarrow \theta_0 - \alpha \sum_{i=1}^{N} (h_\theta(x_i) - y_i)$$

$$\theta_j \leftarrow \theta_j - \alpha \sum_{i=1}^{N} (h_\theta(x_i) - y_i) x_{ij}$$

This looks IDENTICAL to Linear Regression!

- However, the form of the model is very different:

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^\top \boldsymbol{x}}}$$

Regularized Logistic Regression

$$J(\theta) = -\sum_{i=1}^{N}[y_{\mathrm{i}}\log h_\theta(x_i) + (1-y_i)\log\left(1-h_\theta(x_i)\right)]$$

- We can regularize logistic regression exactly as before:

$$\begin{aligned} J_{\text{regularized}}(\boldsymbol{\theta}) &= J(\boldsymbol{\theta}) + \lambda\sum_{j=1}^{d}\theta_j^2 \\ &= J(\boldsymbol{\theta}) + \lambda\|\boldsymbol{\theta}_{[1:d]}\|_2^2 \end{aligned}$$

L2 regularization

Logistic Regression
Lab Example

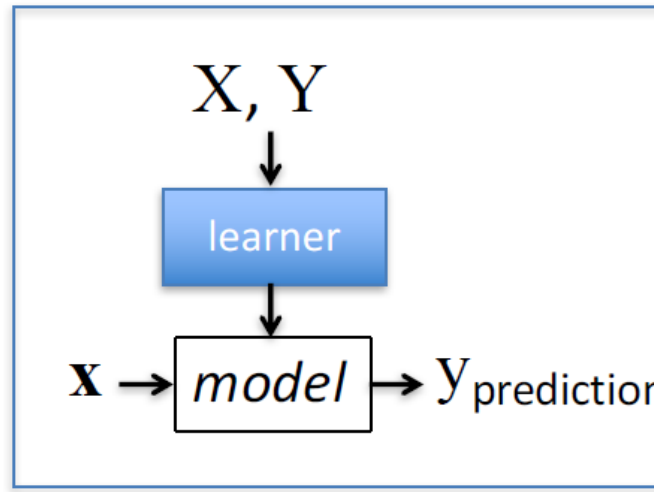
Classifier Evaluation

- 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

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

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

- 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

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

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

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?

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	.
		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

- 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:

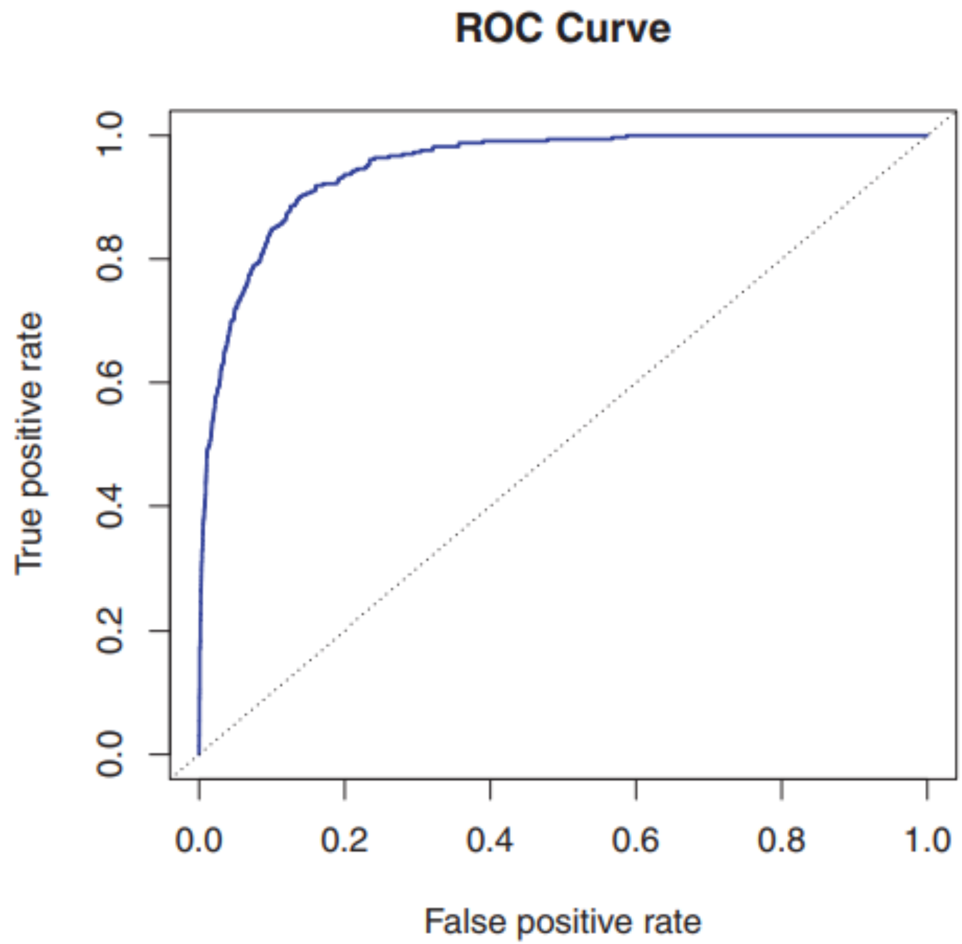
Metric	A	B	C
Accuracy	0.9	0.9	0.88
Precision	0.9	1.0	1.0
Recall	1.0	0.888	0.8667
F-score	0.947	0.941	0.9286

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)

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

ROC Curves

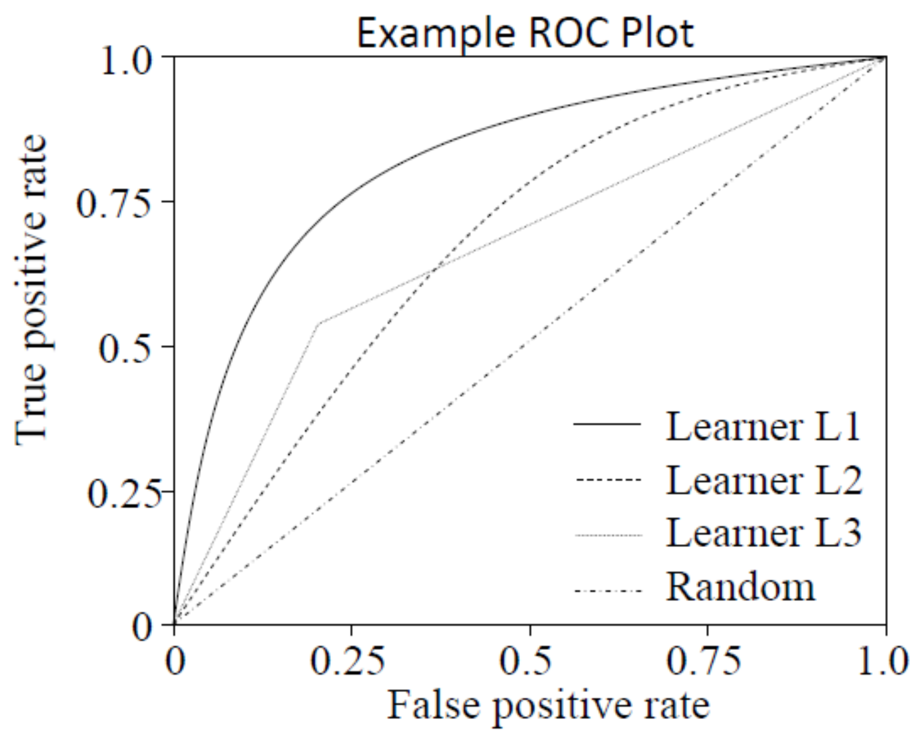


- Receiver Operating Characteristic (ROC)
- Determine operating point (e.g., by fixing false positive rate)

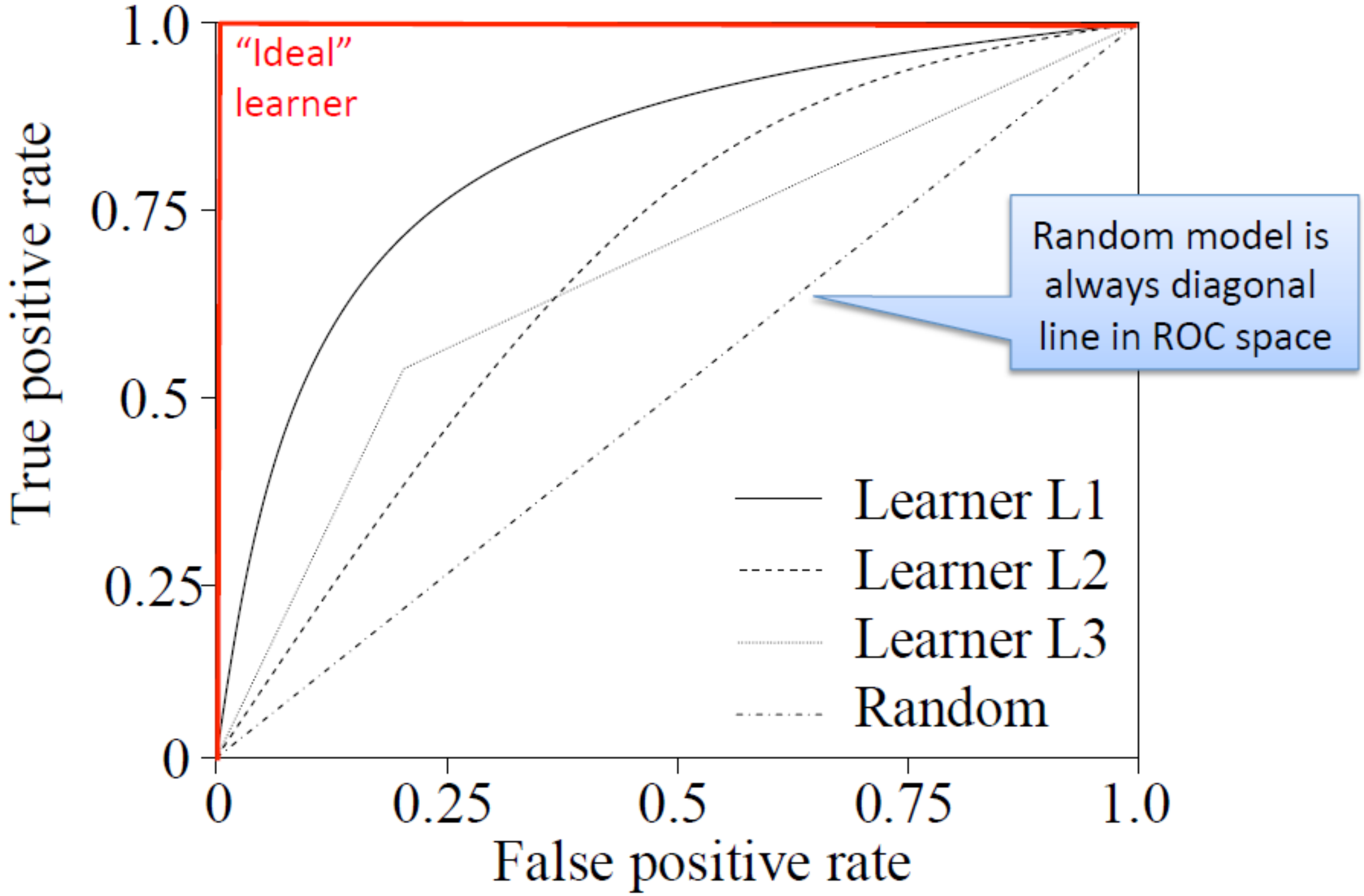
Performance Depends on Threshold

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

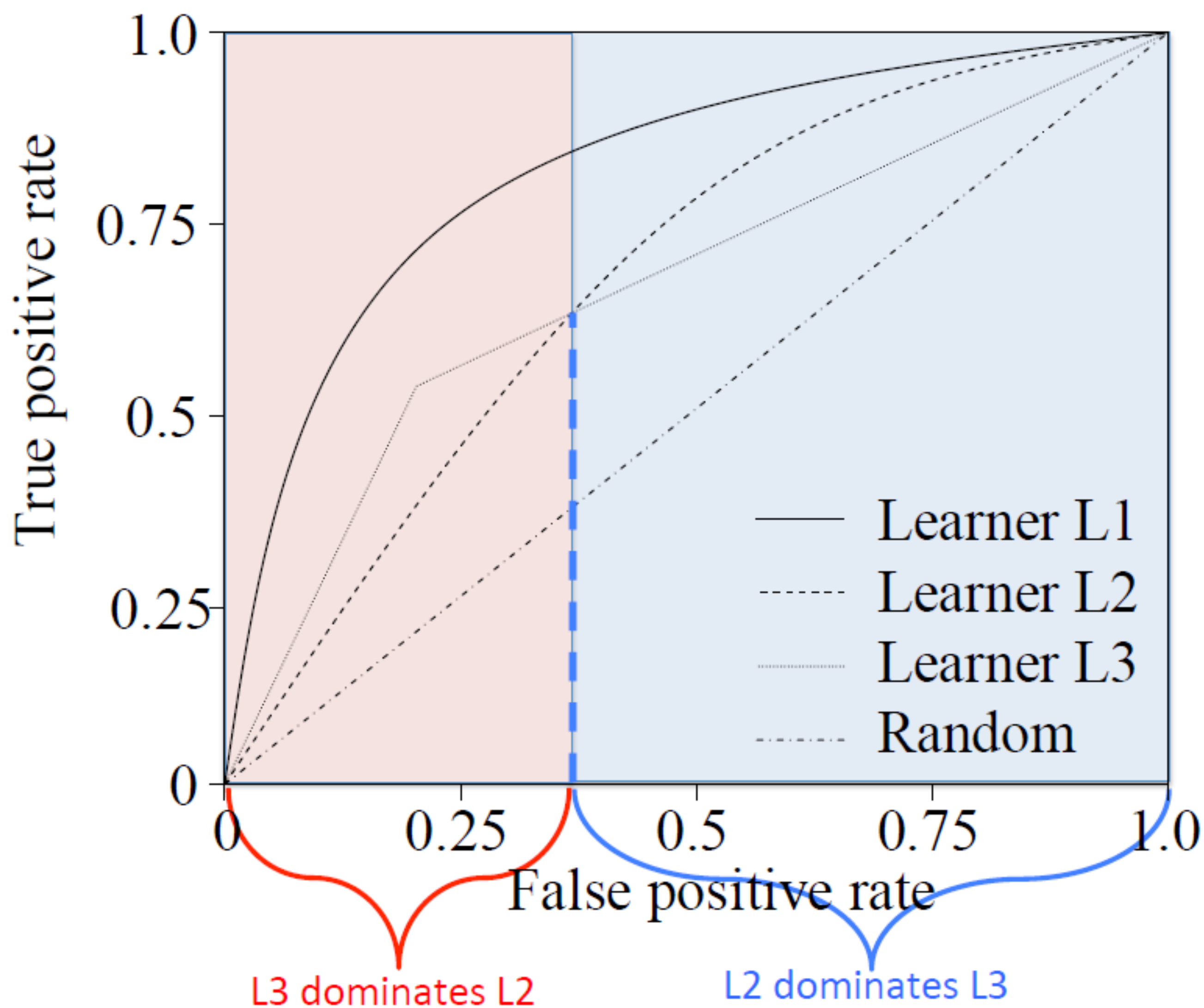


ROC Curve



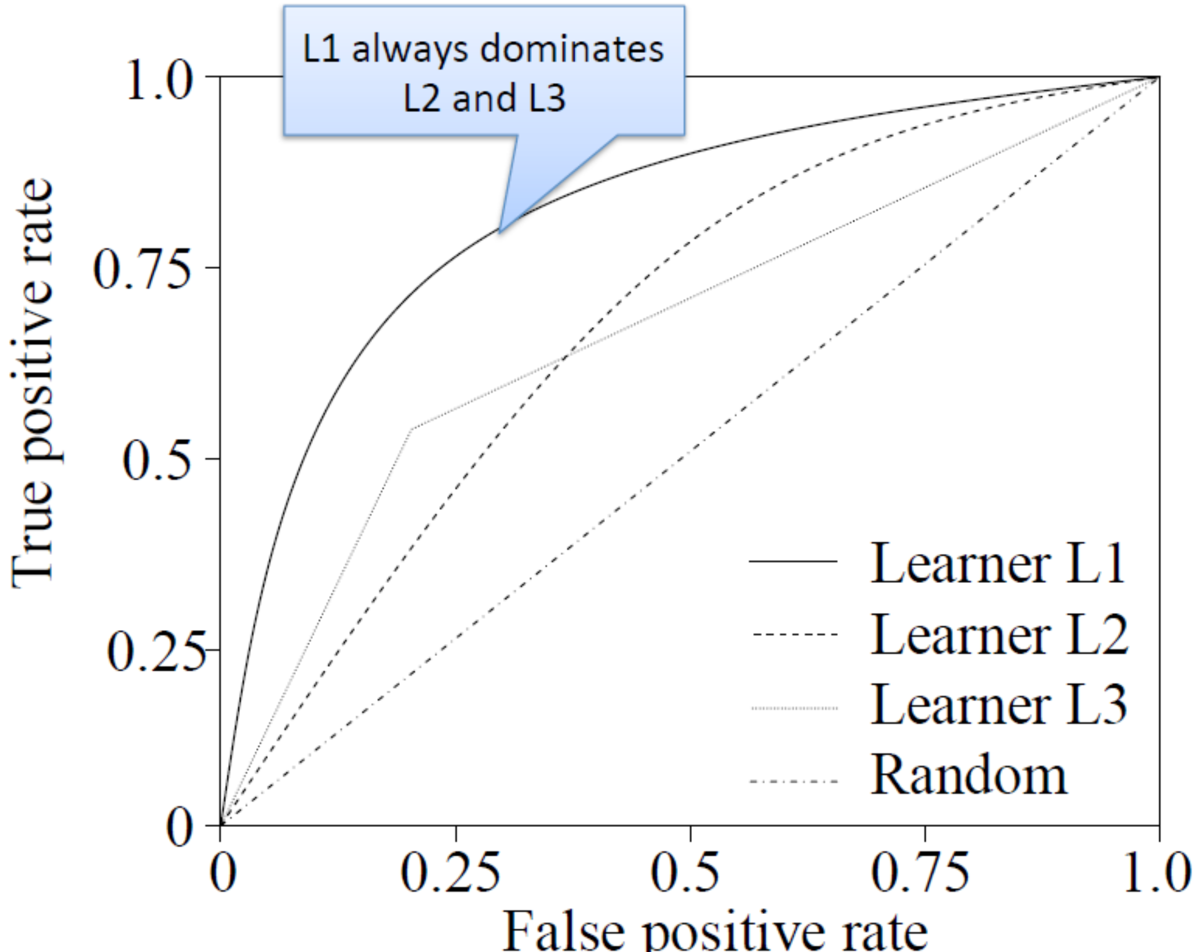
1.0
0.75
0.5
0.25
0
True positive rate
"Ideal"
learner
Random model is always diagonal line in ROC space
Learner L1
Learner L2
Learner L3
Random
0
0.25
0.5
0.75
1.0
False positive rate

ROC Curve



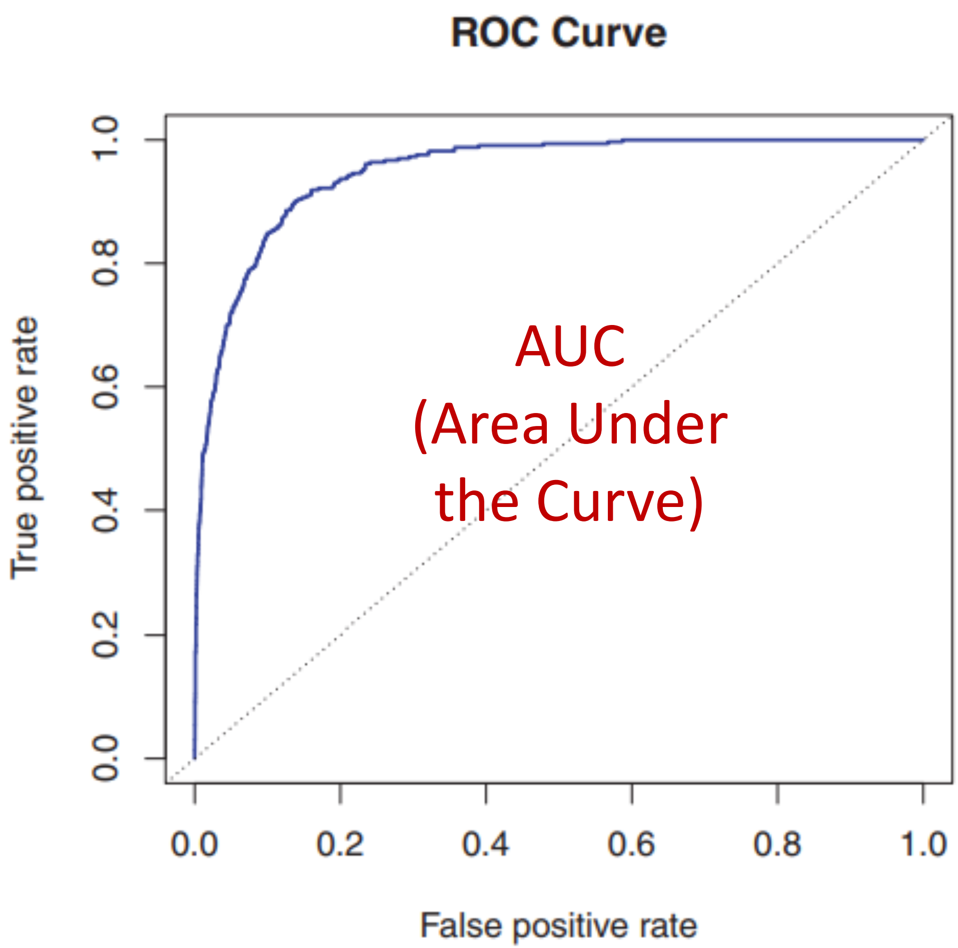
1.0
0.75
0.5
0.25
0
True positive rate
Learner L1
Learner L2
Learner L3
Random
0
0.25
0.5
0.75
1.0
False positive rate
L3 dominates L2
L2 dominates L3

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

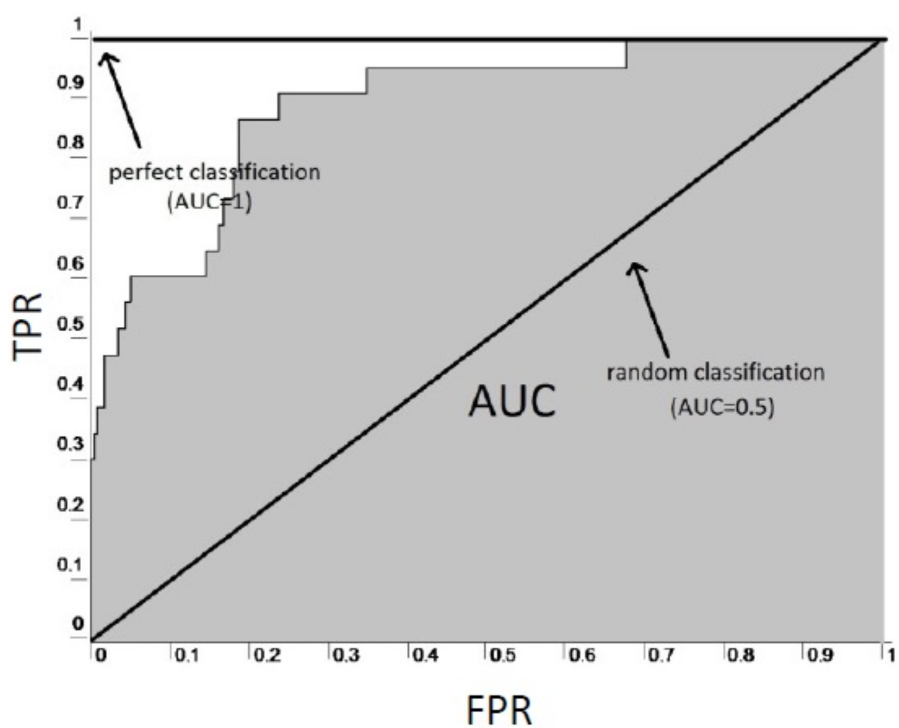
ROC Curves

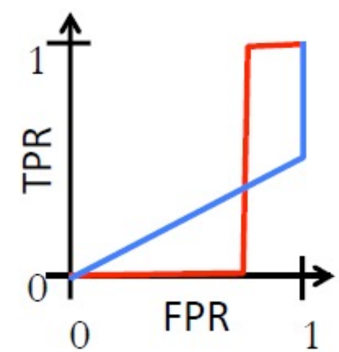


- Another useful metric: Area Under the Curve (AUC)
- The closest to 1, the better!

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	$p(y_i = 1 \mid \mathbf{x}_i)$	$h(\mathbf{x_i} \mid T = 0)$	$h(\mathbf{x_i} \mid T = 0.5)$	$h(\mathbf{x_i} \mid T = 1)$
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	**0.2**	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
			$TPR =$	$TPR =$	$TPR =$
			$FPR =$	$FPR =$	$FPR =$

Review

- Maximum Likelihood Estimation (MLE) is a general statistical method for parameter estimation
- Logistic regression is a linear classifier that predicts class probability
  - Cross-entropy objective derived with MLE
- Can be trained with Gradient Descent
- Multiple metrics for classifier evaluation
  - Accuracy, error, precision, recall, F1 score
  - RIC curves and AUC