Machine Learning

CS 539

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Department of Computer Science
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Previous Class…

Regularization

Previous Class…

Regularization

Perceptron

Logistic Regression

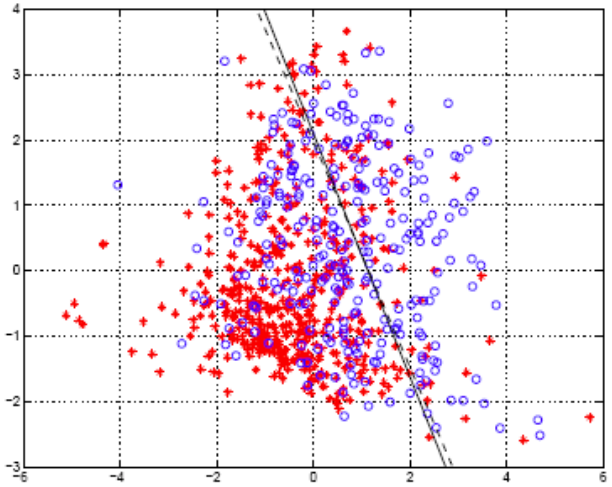
(models probability of output in terms of input)

Classification based on Probability

- Instead of just predicting the class, give the probability of the instance being that class
  - i.e., learn $p(y \mid \boldsymbol{x})$
- Comparison to perceptron:
  - Perceptron doesn't produce probability estimate
  - Perceptron (and other discriminative classifiers) are only interested in producing a discriminative model
- Recall that:

$$0 \leq p(\text{event}) \leq 1$$

$$p(\text{event}) + p(\neg\text{event}) = 1$$



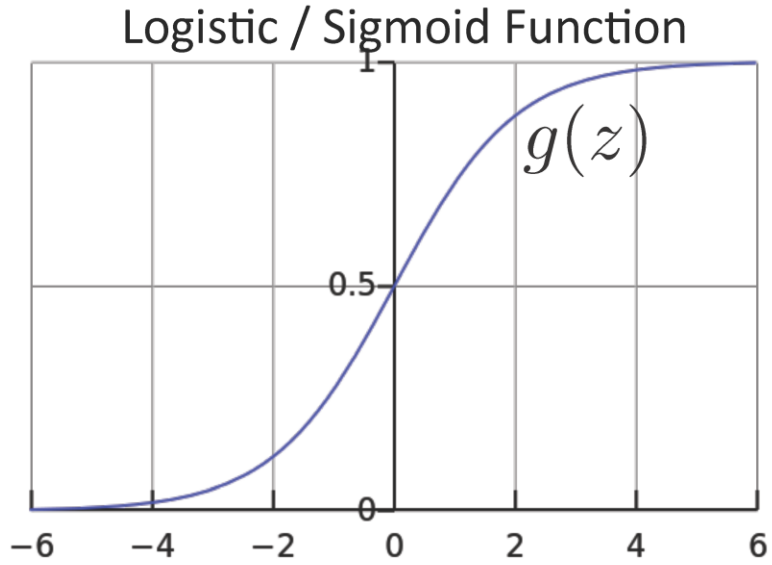
Logistic Regression

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

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

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

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



Interpretation of Hypothesis Output

$h_{\boldsymbol{\theta}}(\boldsymbol{x})$ = estimated $p(y = 1 \mid \boldsymbol{x}; \boldsymbol{\theta})$

Example: Cancer diagnosis from tumor size

$$\boldsymbol{x} = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} 1 \\ \text{tumorSize} \end{bmatrix}$$

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = 0.7$$

→ Tell patient that 70% chance of tumor being malignant

Note that: $p(y = 0 \mid \boldsymbol{x}; \boldsymbol{\theta}) + p(y = 1 \mid \boldsymbol{x}; \boldsymbol{\theta}) = 1$

Therefore, $p(y = 0 \mid \boldsymbol{x}; \boldsymbol{\theta}) = 1 - p(y = 1 \mid \boldsymbol{x}; \boldsymbol{\theta})$

Another Interpretation

- Equivalently, logistic regression assumes that

$$\log \frac{p(y=1 \mid \boldsymbol{x}; \boldsymbol{\theta})}{p(y=0 \mid \boldsymbol{x}; \boldsymbol{\theta})} = \theta_0 + \theta_1 x_1 + \ldots + \theta_d x_d$$

odds of y = 1 (Ratio of y=1 and y=0)

- In other words, logistic regression assumes that the log odds is a linear function of $\boldsymbol{x}$

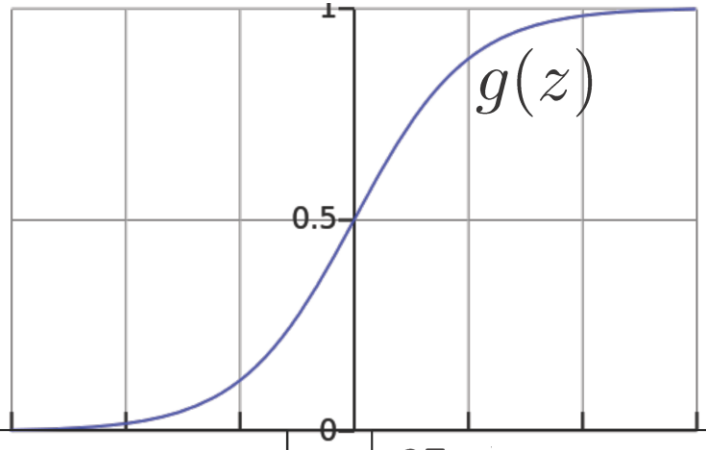
Side Note: the odds in favor of an event is the quantity p / (1 – p), where p is the probability of the event

E.g., If I toss a fair dice, what are the odds that I will have a 6?

Logistic Regression

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

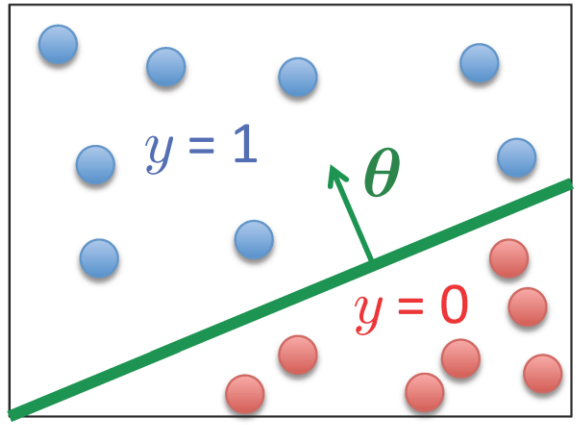
$$g(z) = \frac{1}{1+e^{-z}}$$



$\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}$ should be large negative values for negative instances

$\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}$ should be large positive values for positive instances

- Assume a threshold and...
  - Predict $y = 1$ if $h_{\boldsymbol{\theta}}(\boldsymbol{x}) \geq 0.5$
  - Predict $y = 0$ if $h_{\boldsymbol{\theta}}(\boldsymbol{x}) < 0.5$



Logistic Regression

- Given $\left\{\left(\boldsymbol{x}^{(1)}, y^{(1)}\right), \left(\boldsymbol{x}^{(2)}, y^{(2)}\right), \ldots, \left(\boldsymbol{x}^{(n)}, y^{(n)}\right)\right\}$

  where $\boldsymbol{x}^{(i)} \in \mathbb{R}^d,\ y^{(i)} \in \{0, 1\}$

- Model: $h_{\boldsymbol{\theta}}(\boldsymbol{x}) = g\left(\boldsymbol{\theta}^\intercal \boldsymbol{x}\right)$

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

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

Logistic Regression Objective Function

- Can't just use squared loss as in linear regression:

$$J(\boldsymbol{\theta}) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)^2$$

  - Using the logistic regression model

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

    results in a non-convex optimization

Intuition Behind the Objective (log loss)

$$J(\boldsymbol{\theta}) = -\frac{1}{n}\sum_{i=1}^{n}\left[y^{(i)}\log h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) + \left(1-y^{(i)}\right)\log\left(1-h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})\right)\right]$$

- Cost of a single instance:

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

- Can re-write objective function as

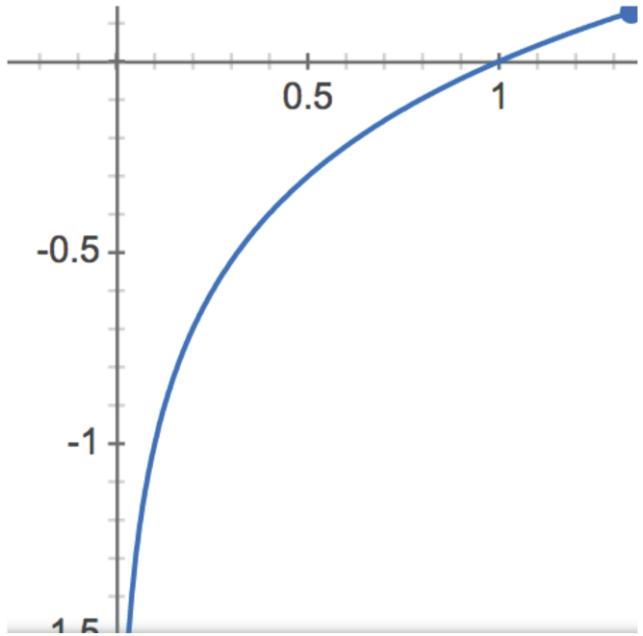
$$J(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\text{cost}\left(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}), y^{(i)}\right)$$

Compare to linear regression: $J(\boldsymbol{\theta}) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)^2$

Intuition Behind the Objective

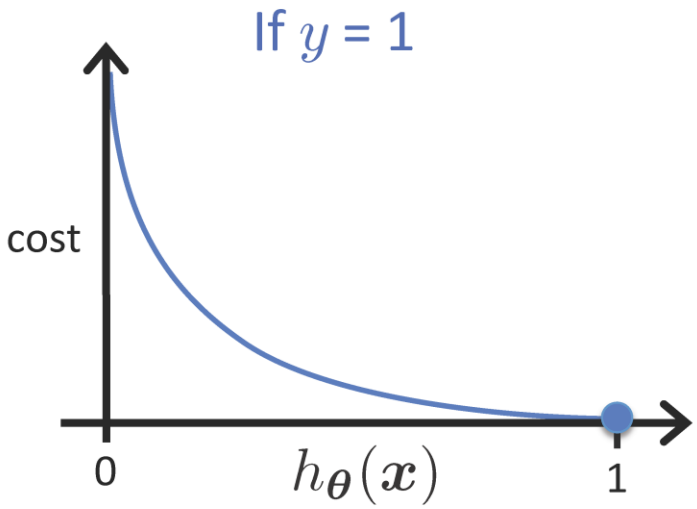
$$\text{cost}\left(h_{\boldsymbol{\theta}}(\boldsymbol{x}), y\right) = \begin{cases} -\log(h_{\boldsymbol{\theta}}(\boldsymbol{x})) & \text{if } y = 1 \\ -\log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x})) & \text{if } y = 0 \end{cases}$$

Aside: Recall the plot of $\log(z)$



Intuition Behind the Objective

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

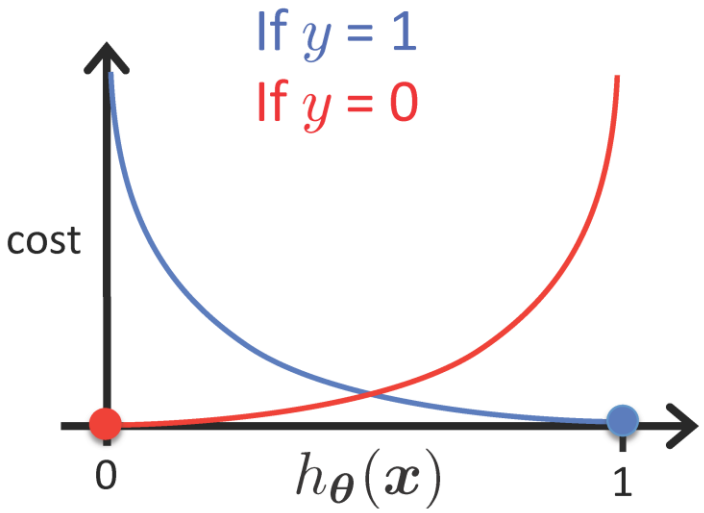


If y = 1

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

Intuition Behind the Objective

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



If y = 0

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

Regularized Logistic Regression

$$J(\boldsymbol{\theta}) = -\frac{1}{n}\sum_{i=1}^{n}\left[y^{(i)}\log h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) + \left(1-y^{(i)}\right)\log\left(1-h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})\right)\right]$$

- We can regularize logistic regression exactly as before:

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

Gradient Descent for Logistic Regression

$$J_{\text{reg}}(\boldsymbol{\theta}) = -\frac{1}{n}\sum_{i=1}^{n}\left[y^{(i)}\log h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) + \left(1-y^{(i)}\right)\log\left(1-h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})\right)\right] + \frac{\lambda}{2}\|\boldsymbol{\theta}_{[1:d]}\|_2^2$$

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

Use the natural logarithm (ln = $\log_e$) to cancel with the exp() in $h_{\boldsymbol{\theta}}(\boldsymbol{x})$

Gradient Descent for Logistic Regression

$$J_{\text{reg}}(\boldsymbol{\theta}) = -\frac{1}{n}\sum_{i=1}^{n}\left[y^{(i)}\log h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) + \left(1-y^{(i)}\right)\log\left(1-h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})\right)\right] + \frac{\lambda}{2}\|\boldsymbol{\theta}_{[1:d]}\|_2^2$$

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

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

$$\theta_0 \leftarrow \theta_0 - \alpha\frac{1}{n}\sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)$$

$$\theta_j \leftarrow \theta_j - \alpha\frac{1}{n}\sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)x_j^{(i)} - \alpha\lambda\theta_j$$

https://stats.stackexchange.com/questions/278771/how-is-the-cost-function-from-logistic-regression-derivated

Gradient Descent for Logistic Regression

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

$$\theta_0 \leftarrow \theta_0 - \alpha \frac{1}{n} \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right)$$

$$\theta_j \leftarrow \theta_j - \alpha \frac{1}{n} \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right) x_j^{(i)} - \alpha \lambda \theta_j$$

This looks IDENTICAL to linear regression!!!

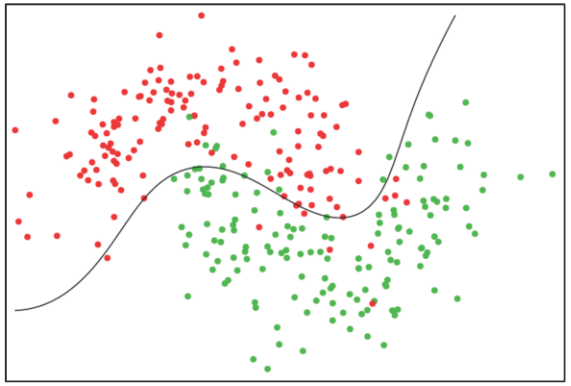
- However, the form of the model is very different:

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

Non-Linear Decision Boundary

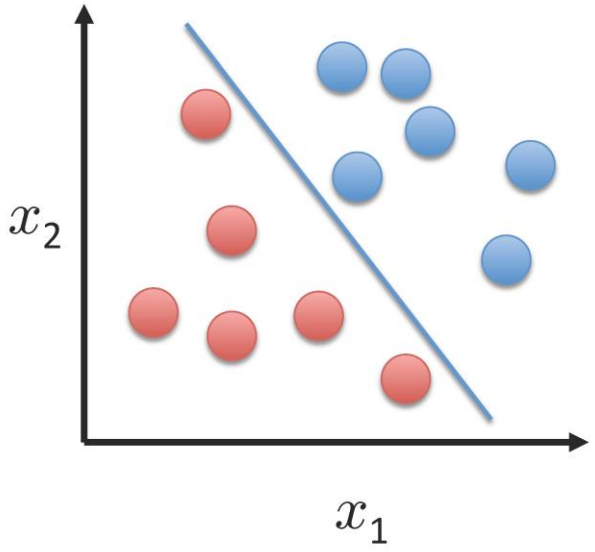
- Can apply basis function expansion to features, same as with linear regression

$$\boldsymbol{x} = \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix} \rightarrow \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ x_1 x_2 \\ x_1^2 \\ x_2^2 \\ x_1^2 x_2 \\ x_1 x_2^2 \\ \vdots \end{bmatrix}$$

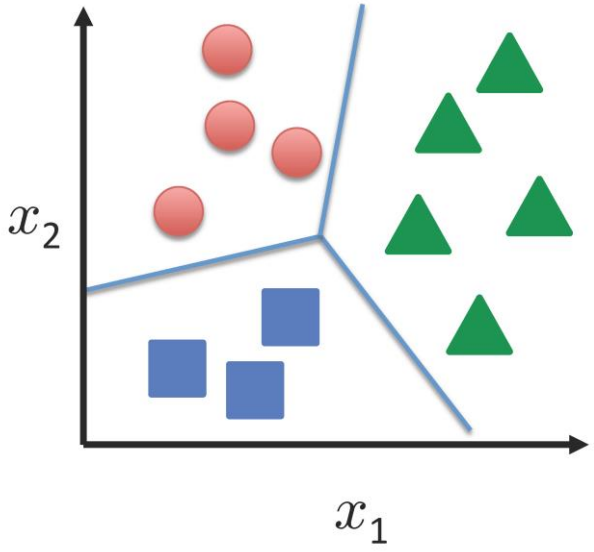


Multi-Class Classification

Binary classification:



Multi-class classification:

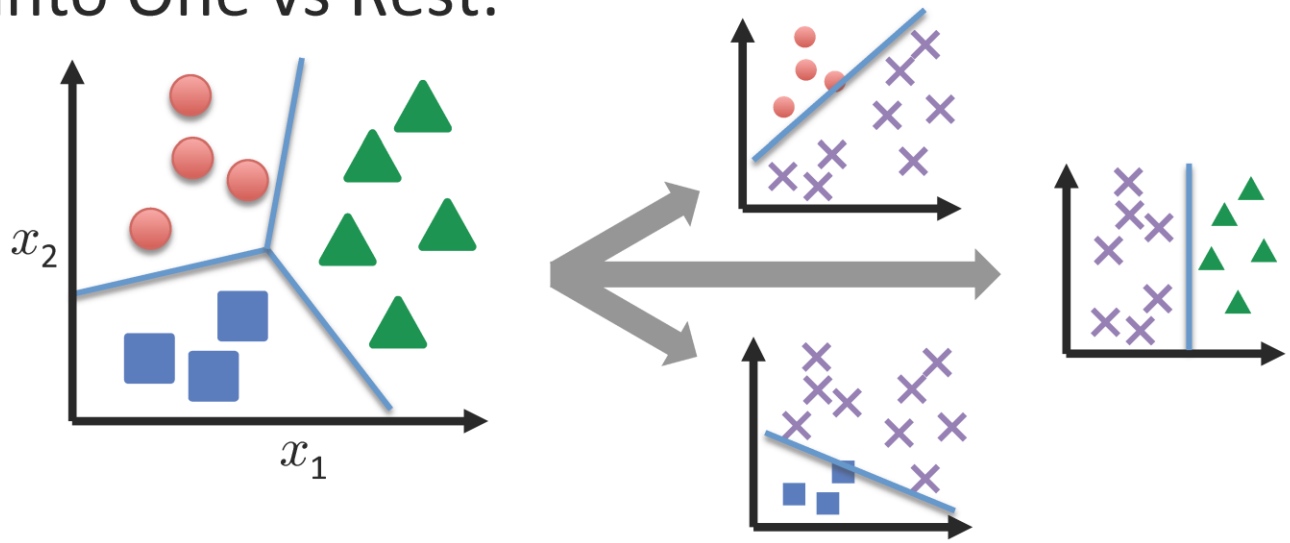


Disease diagnosis: healthy / cold / flu / pneumonia

Object classification: desk / chair / monitor / bookcase

Multi-Class Logistic Regression

Split into One vs Rest:



- Train a logistic regression classifier for each class i to predict the probability that $y = i$ with

$$h_c(\boldsymbol{x}) = \frac{\exp(\boldsymbol{\theta}_c^\mathsf{T}\boldsymbol{x})}{\sum_{c=1}^{C}\exp(\boldsymbol{\theta}_c^\mathsf{T}\boldsymbol{x})}$$

Multi-Class Logistic Regression

- For 2 classes:

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \frac{1}{1+\exp(-\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x})} = \frac{\exp(\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x})}{1+\exp(\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x})}$$

weight assigned to $y = 0$

weight assigned to $y = 1$

- For C classes {1, ..., C}:

$$p(y = c \mid \boldsymbol{x}; \boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_C) = \frac{\exp(\boldsymbol{\theta}_c^{\mathsf{T}}\boldsymbol{x})}{\sum_{c=1}^{C}\exp(\boldsymbol{\theta}_c^{\mathsf{T}}\boldsymbol{x})}$$

  - Called the **softmax** function (normalized exponential)

Implementing Multi-Class Logistic Regression

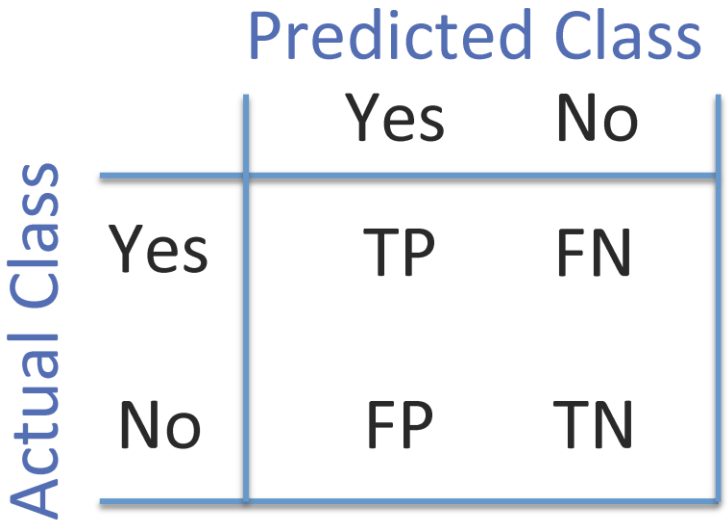
- Use $h_c(\boldsymbol{x}) = \dfrac{\exp(\boldsymbol{\theta}_c^\mathsf{T}\boldsymbol{x})}{\sum_{c=1}^{C}\exp(\boldsymbol{\theta}_c^\mathsf{T}\boldsymbol{x})}$ as the model for class c
- Gradient descent simultaneously updates all parameters for all models
  - Same derivative as before, just with the above $h_c(\boldsymbol{x})$
- Predict class label as the most probable label

$$\max_c h_c(\boldsymbol{x})$$

Advanced Evaluation Metrics

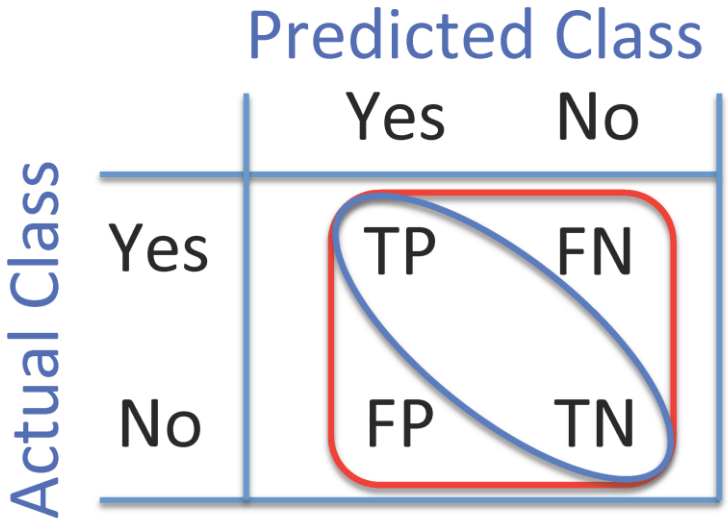
Confusion Matrix

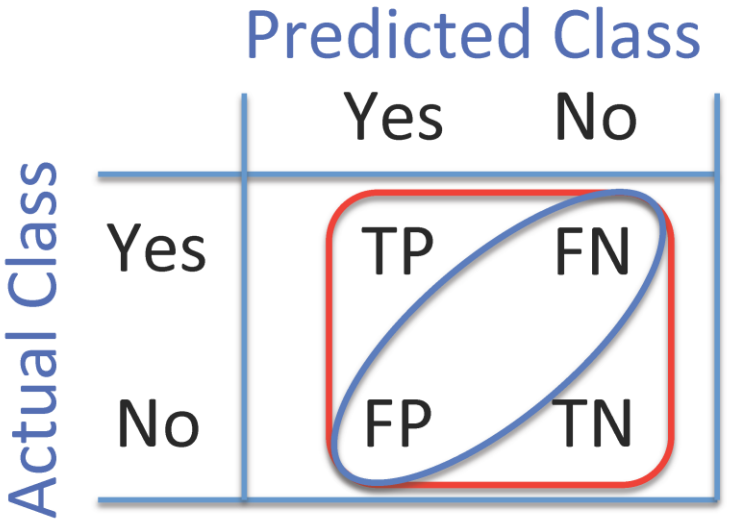
Given a dataset of P positive instances and N negative instances:



Accuracy & Error

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





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

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

$$= \frac{FP + FN}{P + N}$$

Precision & Recall

Precision

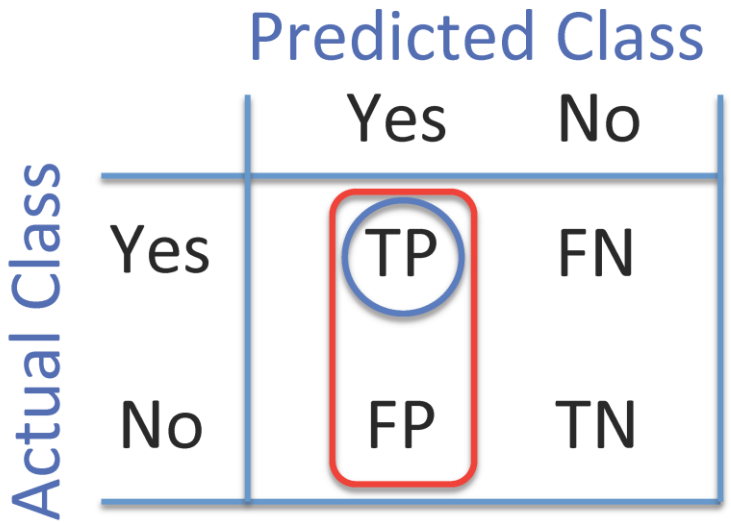
- the fraction of positive predictions that are correct
- P(is pos|predicted pos)

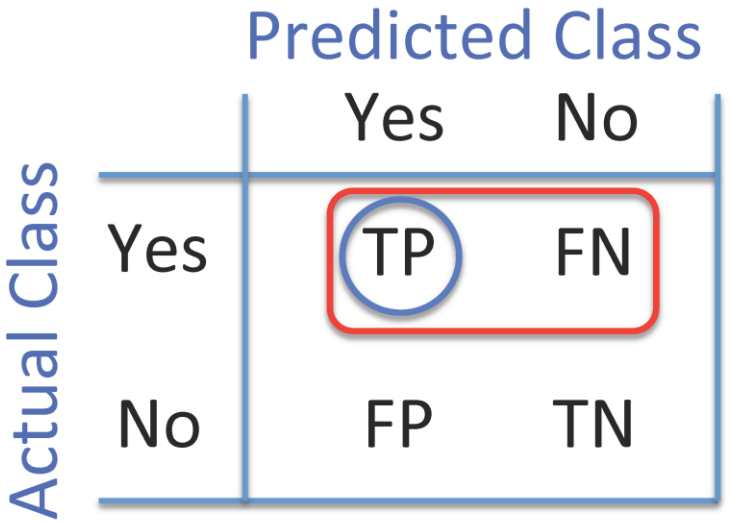
$$\text{precision} = \frac{TP}{TP + FP}$$

Recall

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

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





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-Measure

- 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)

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
Predictions 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
- 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

Receiver Operating Characteristic (ROC)

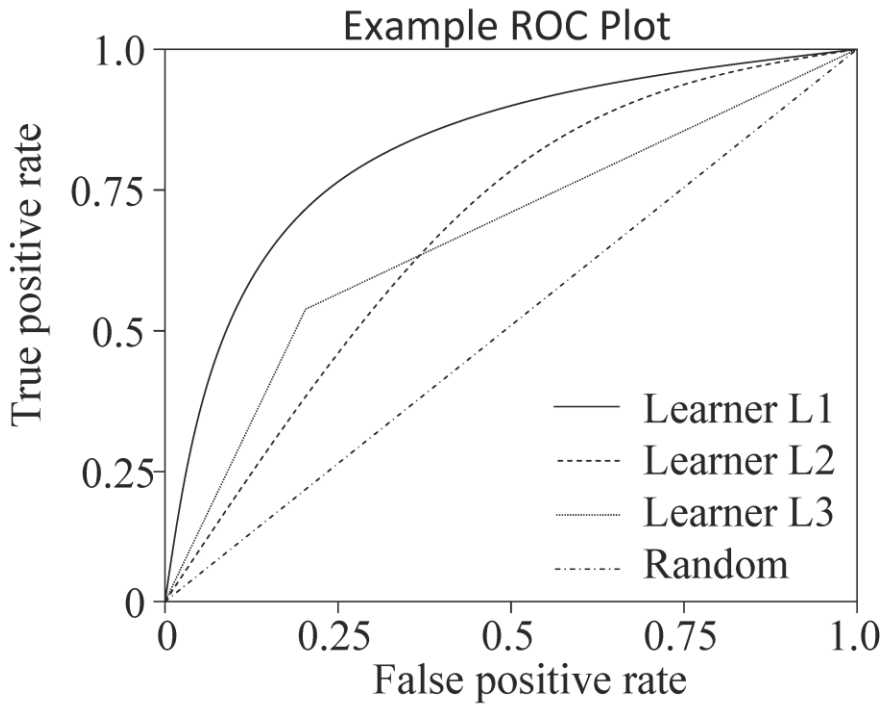
ROC curves assess predictive behavior independent of error costs or class distributions

- Originated from signal detection theory
- Common in medical diagnosis, now used for ML

Plots TP rate vs FP Rate

$$\text{TP rate} = \text{TP}/\text{P}$$
$$\text{FP rate} = \text{FP}/\text{N}$$

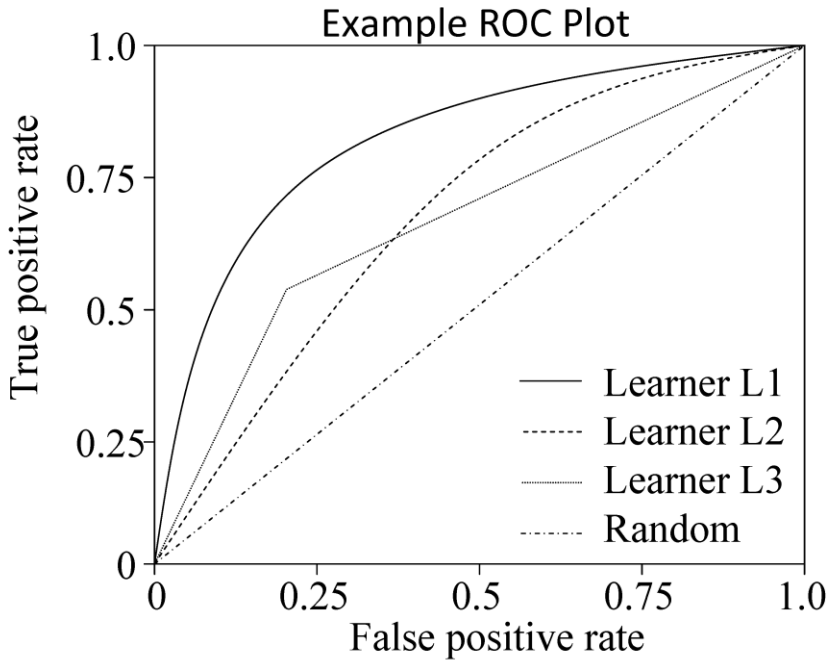
Actual Class \ Predicted Class	Yes	No
Yes	TP	FN
No	FP	TN



Performance Depends on Threshold

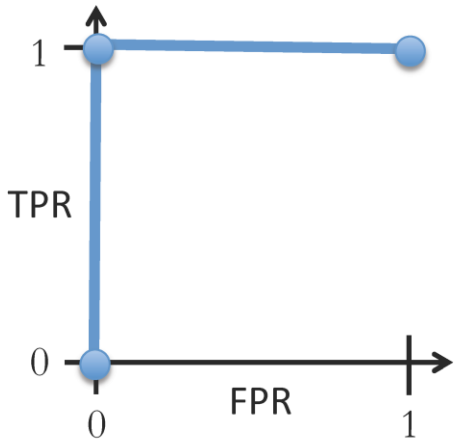
Predict positive if $\mathrm{P}(y = 1 \mid \mathbf{x}) \geq \theta$, otherwise negative

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



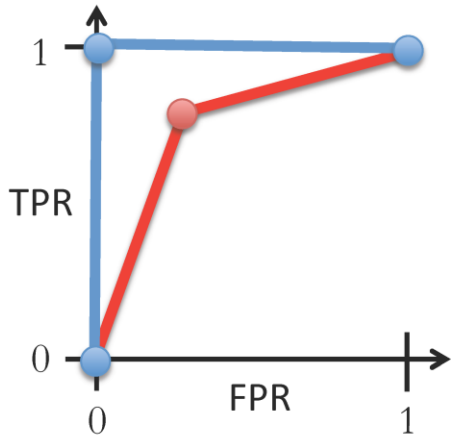
ROC Example

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
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
			$TPR = 5/5 = 1$	$TPR = 5/5 = 1$	$TPR = 0/5 = 0$
			$FPR = 4/4 = 1$	$FPR = 0/4 = 0$	$FPR = 0/4 = 0$

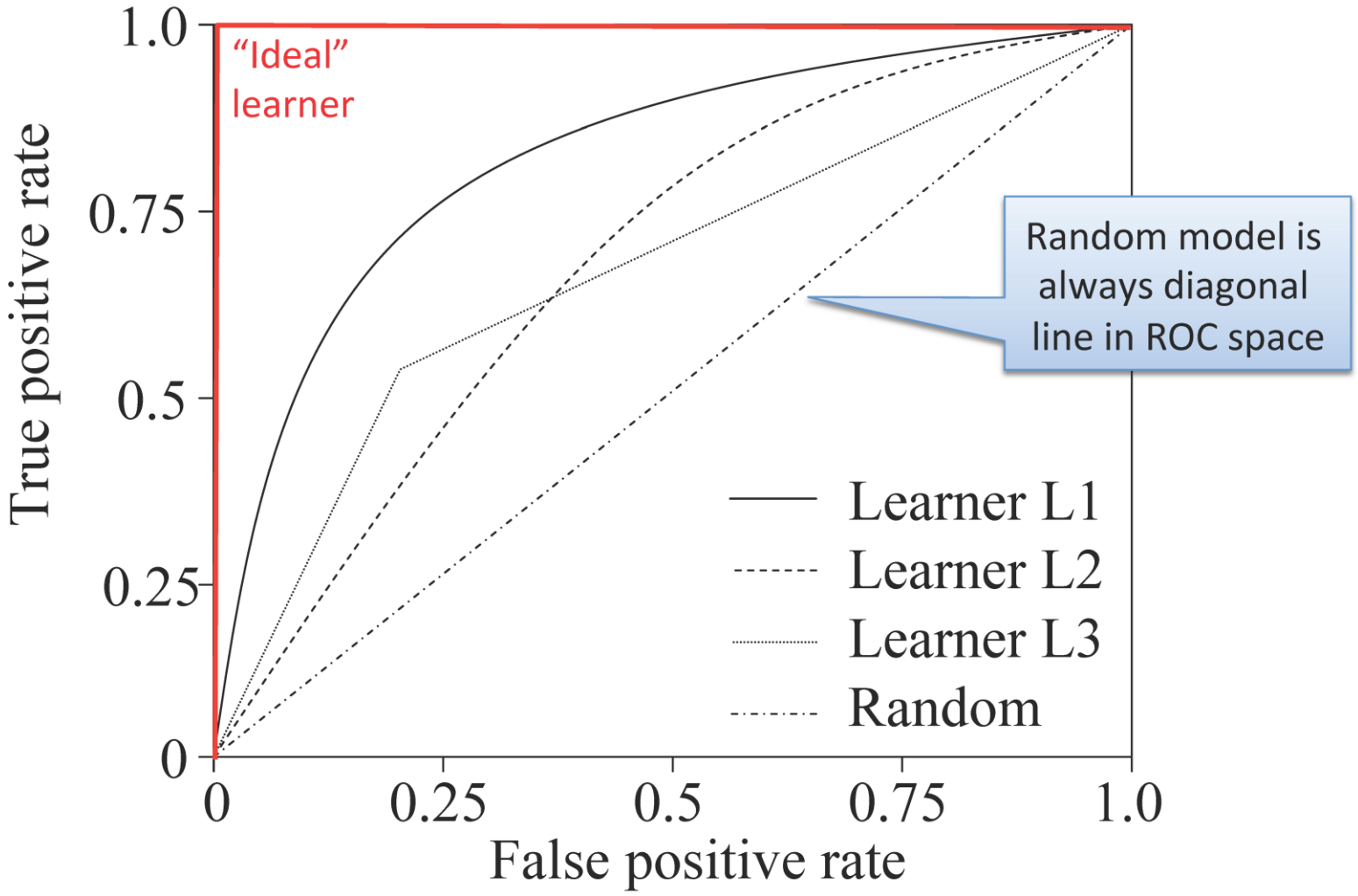


ROC Example

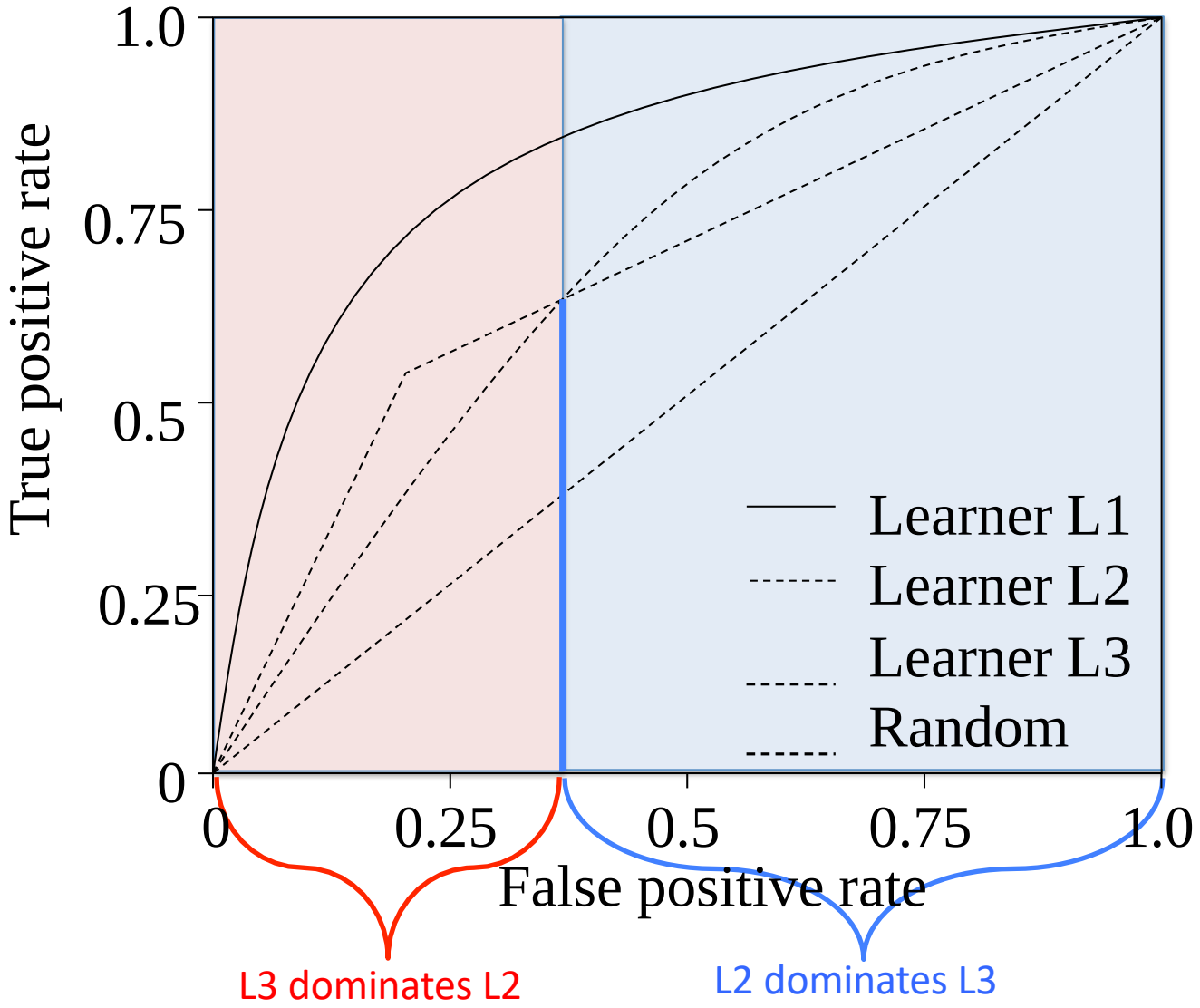
i	y_i	$p(y_i = 1 \mid \mathbf{x}_i)$	$h(\mathbf{x_i} \mid \theta = 0)$	$h(\mathbf{x_i} \mid \theta = 0.5)$	$h(\mathbf{x_i} \mid \theta = 1)$
1	1	0.9	1	1	0
2	1	0.8	1	1	0
3	1	0.7	1	1	0
4	1	0.6	1	1	0
5	1	**0.2**	1	**0**	0
6	0	**0.6**	1	**1**	0
7	0	0.3	1	0	0
8	0	0.2	1	0	0
9	0	0.1	1	0	0
			$TPR = 5/5 = 1$	$TPR = 4/5 = 0.8$	$TPR = 0/5 = 0$
			$FPR = 4/4 = 1$	$FPR = 1/4 = 0.25$	$FPR = 0/4 = 0$



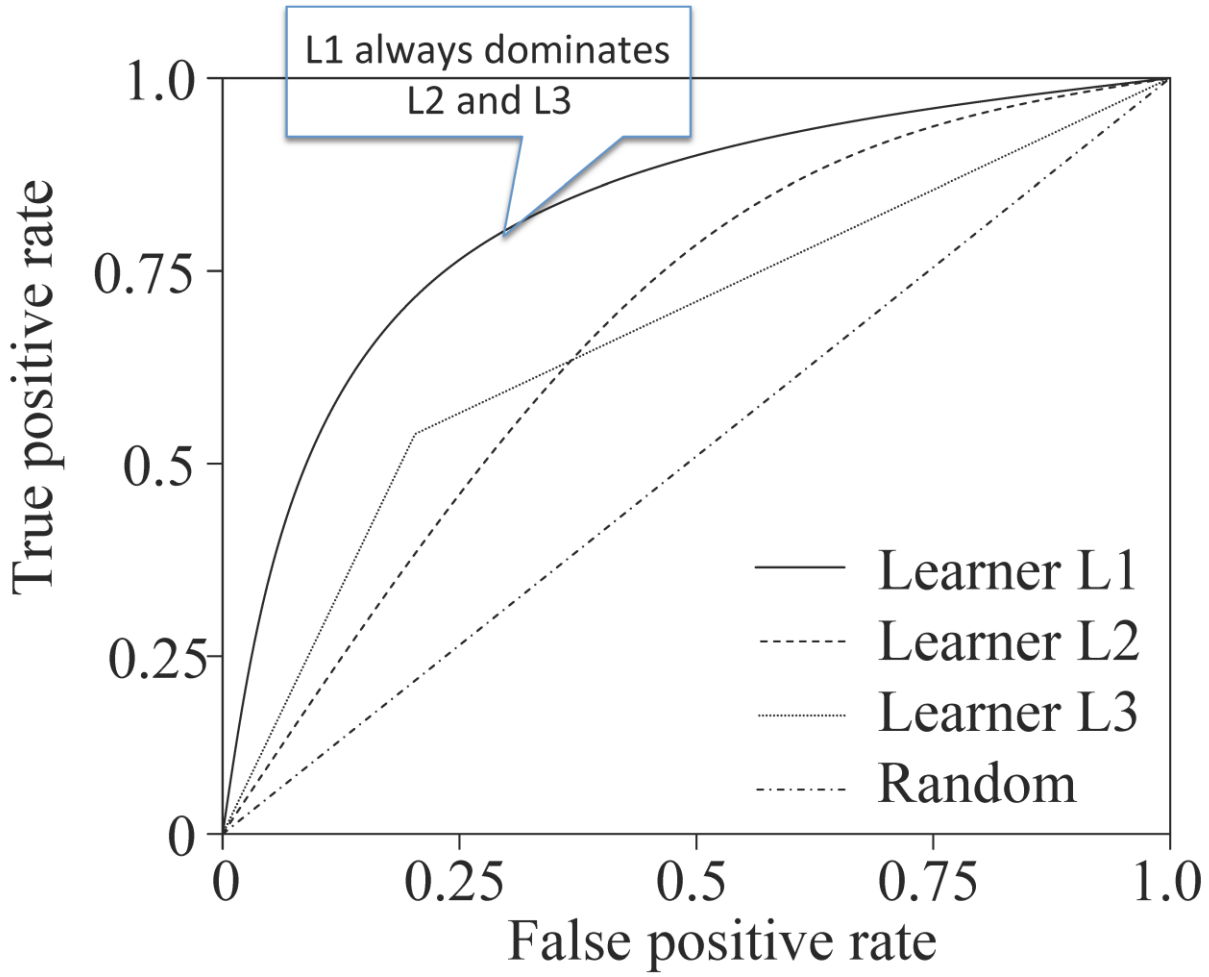
Receiver Operating Characteristic (ROC)



Receiver Operating Characteristic (ROC)



Receiver Operating Characteristic (ROC)



Area Under the ROC Curve (AUC)

- Can take area under the ROC curve to summarize performance as a single number