University of Colorado **Boulder**

Department of Computer Science

CSCI 5622: Machine Learning

Chenhao Tan

Lecture 10: Evaluation metrics and multi-class classification

Slides adapted from Chris Ketelsen, Jordan Boyd-Graber, and Noah Smith

Administrivia

- HW2 due on Friday
- Final project information
- Final project team formation
- Hands on lecture on Wednesday

Learning Objectives

- Understand evaluation metrics for classification
- Understand inherent multi-class classifiers
- Understand techniques to convert binary classifiers to multi-class classifiers
- Understanding regularization (bonus)

Outline

- Evaluation metrics
- Inherent multi-class classifiers
- From binary classifiers to multi-class classifiers
- Regularization

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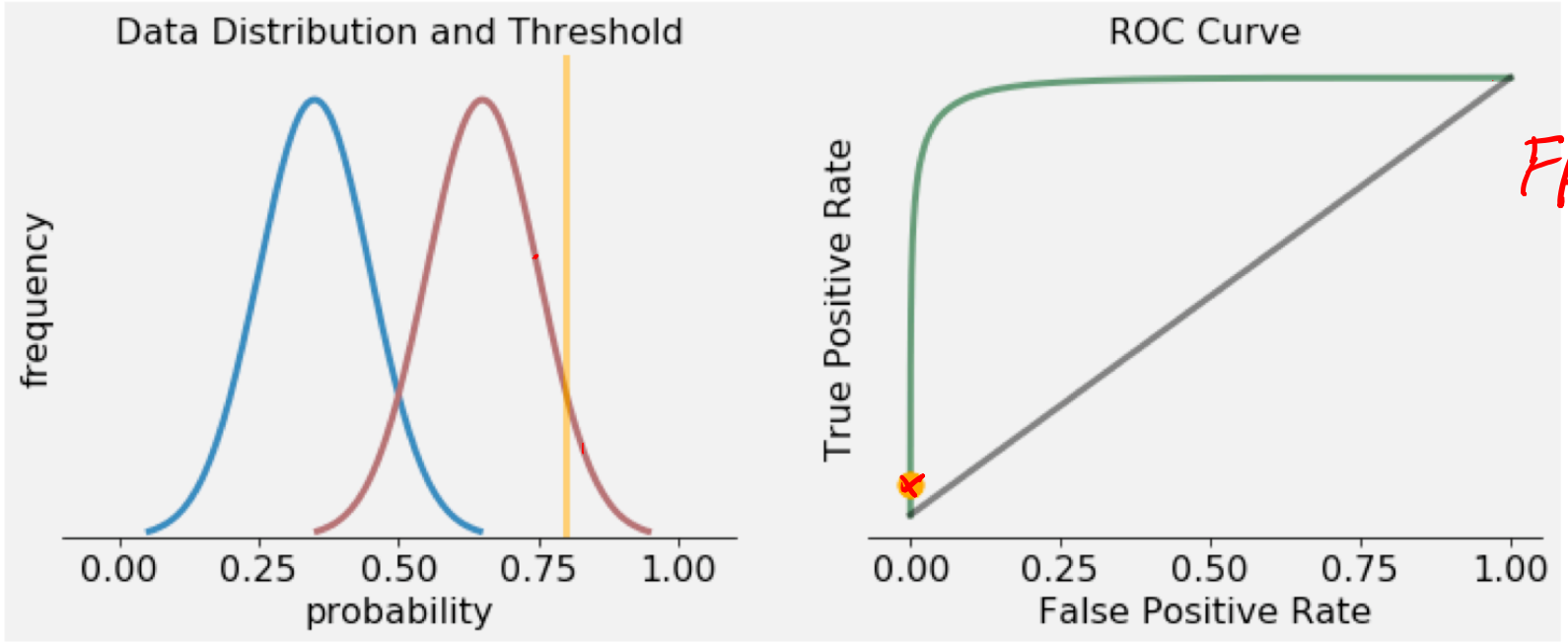
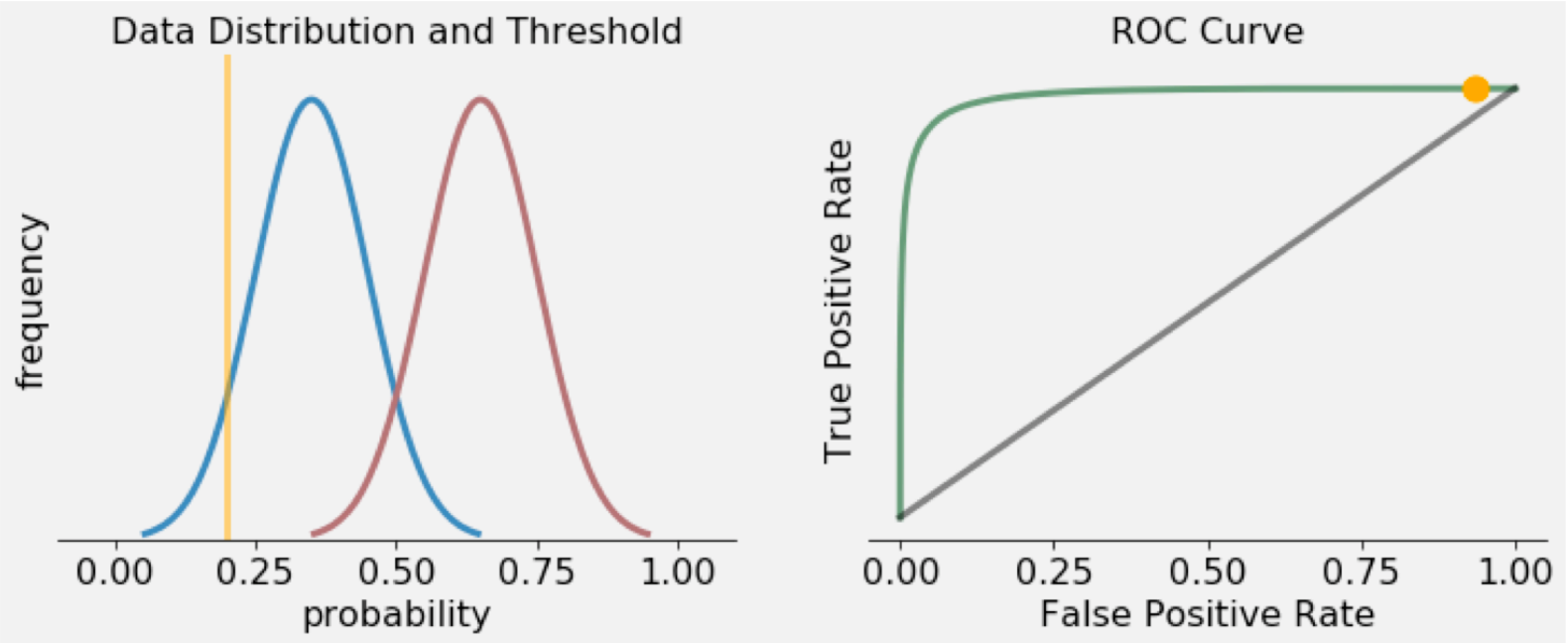
The ROC curve



A ROC Curve is a plot of FPR (horizontal) vs. TPR (vertical) for all possible threshold values.

Convenient to see how a model would perform at all thresholds simultaneously, rather than looking at misclassification rate for each threshold individually.

The ROC curve



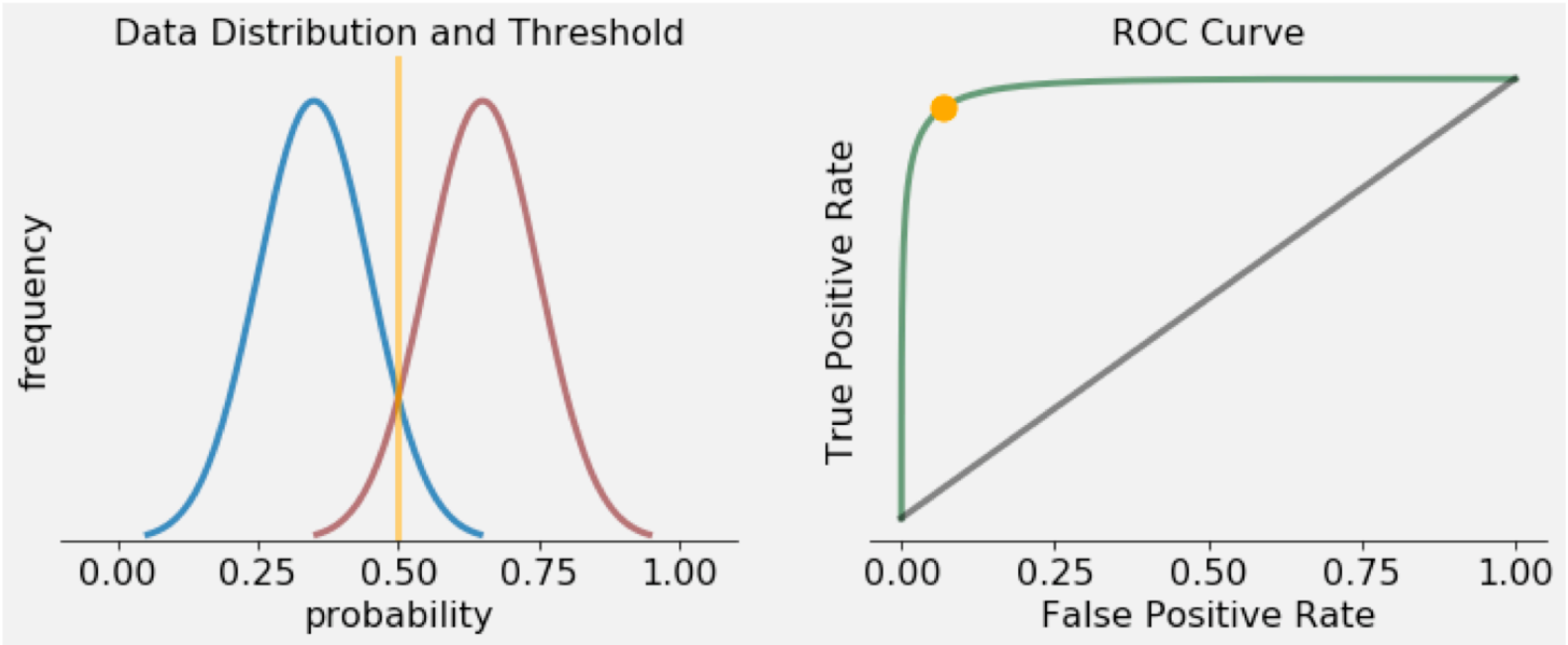
$TPR = \frac{TP}{TP+FN}$

$FPR = \frac{FP}{FP+TN}$

A ROC Curve is a plot of FPR (horizontal) vs. TPR (vertical) for all possible threshold values.

Convenient to see how a model would perform at all thresholds simultaneously, rather than looking at misclassification rate for each threshold individually.

The ROC curve



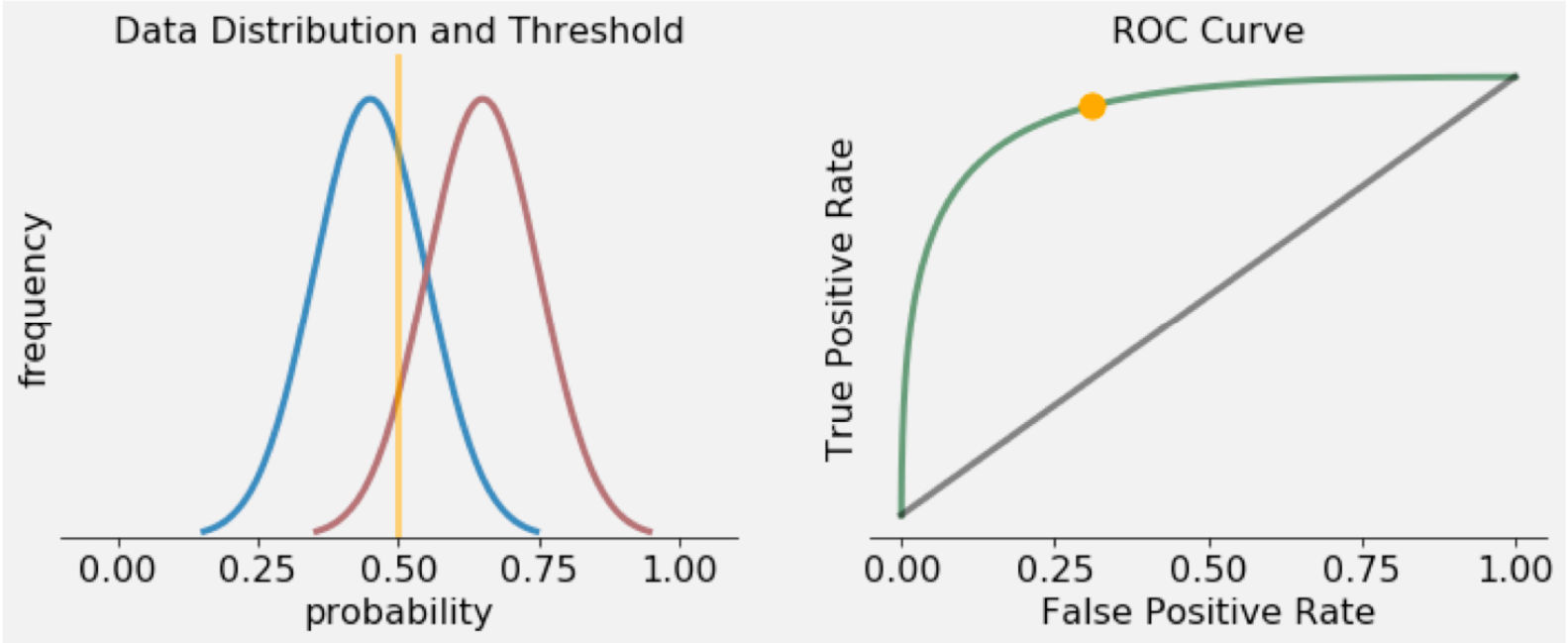
$\hat{P}(y=1|x)$

The threshold gives the parameterization of the ROC curve (i.e., it moves the dot).

When the threshold separates the two classes fairly well, the curve is far away from the diagonal.

What happens if we can't separate the classes very well?

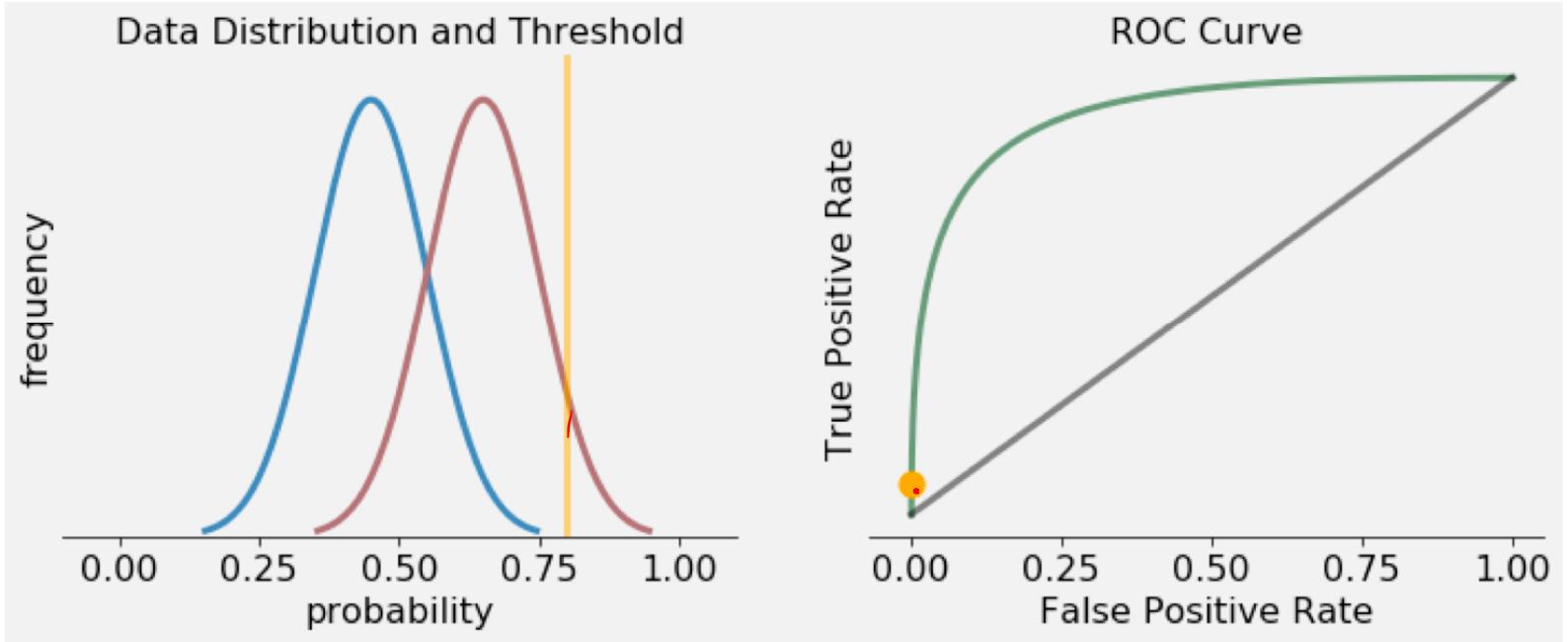
The ROC curve



Now we're not doing so well at separating the classes.

The ROC curve starts bending towards the center.

The ROC curve



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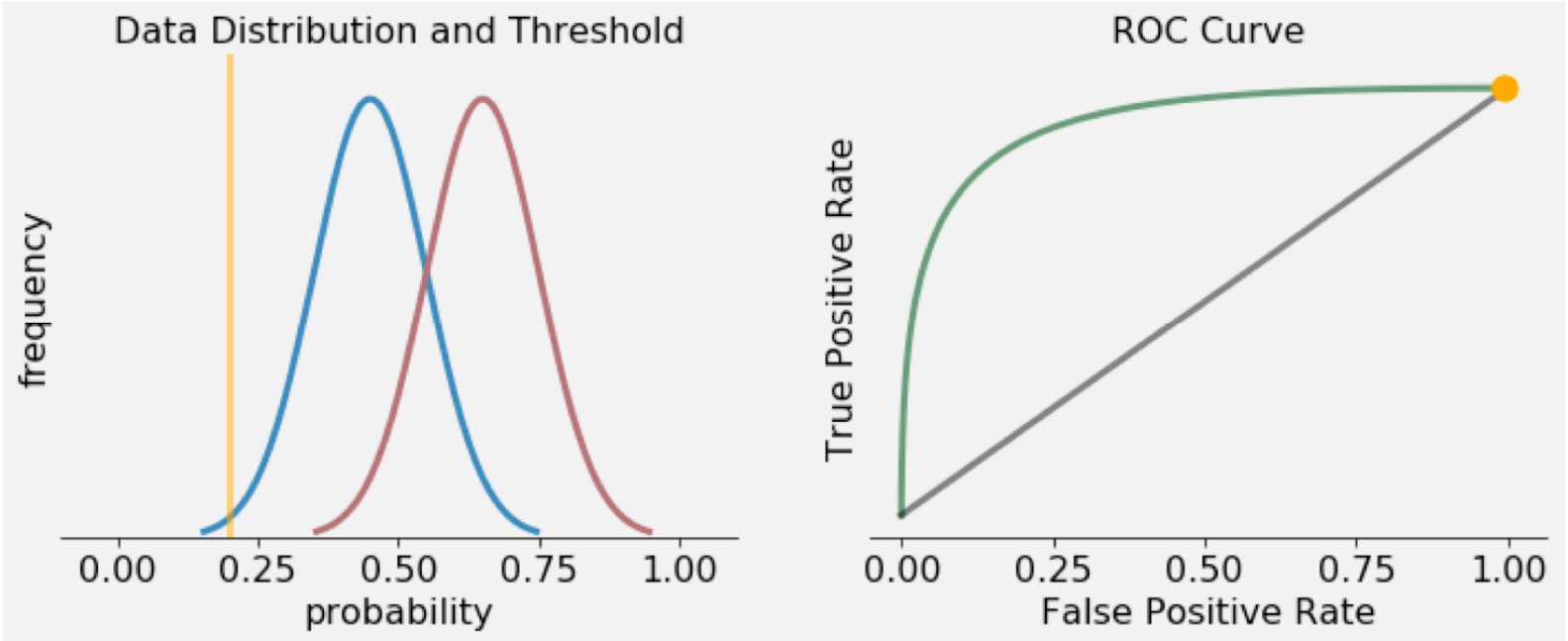

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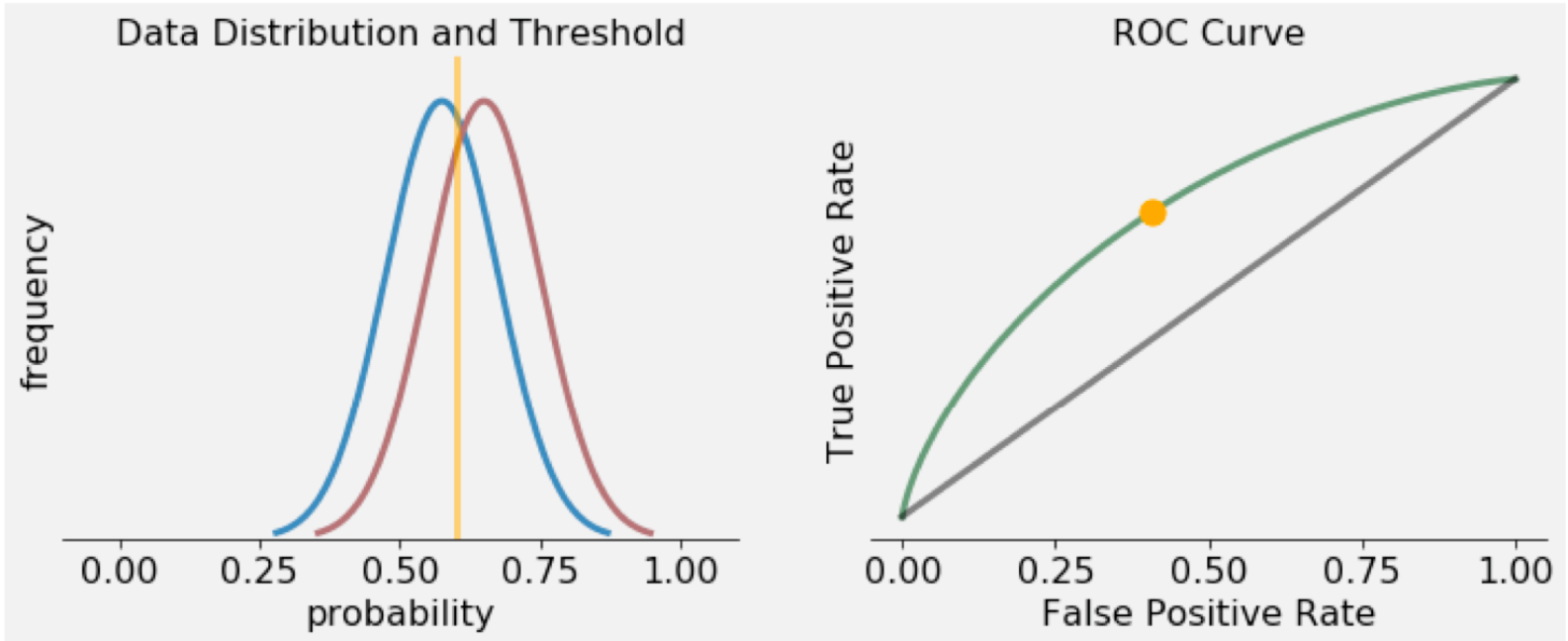
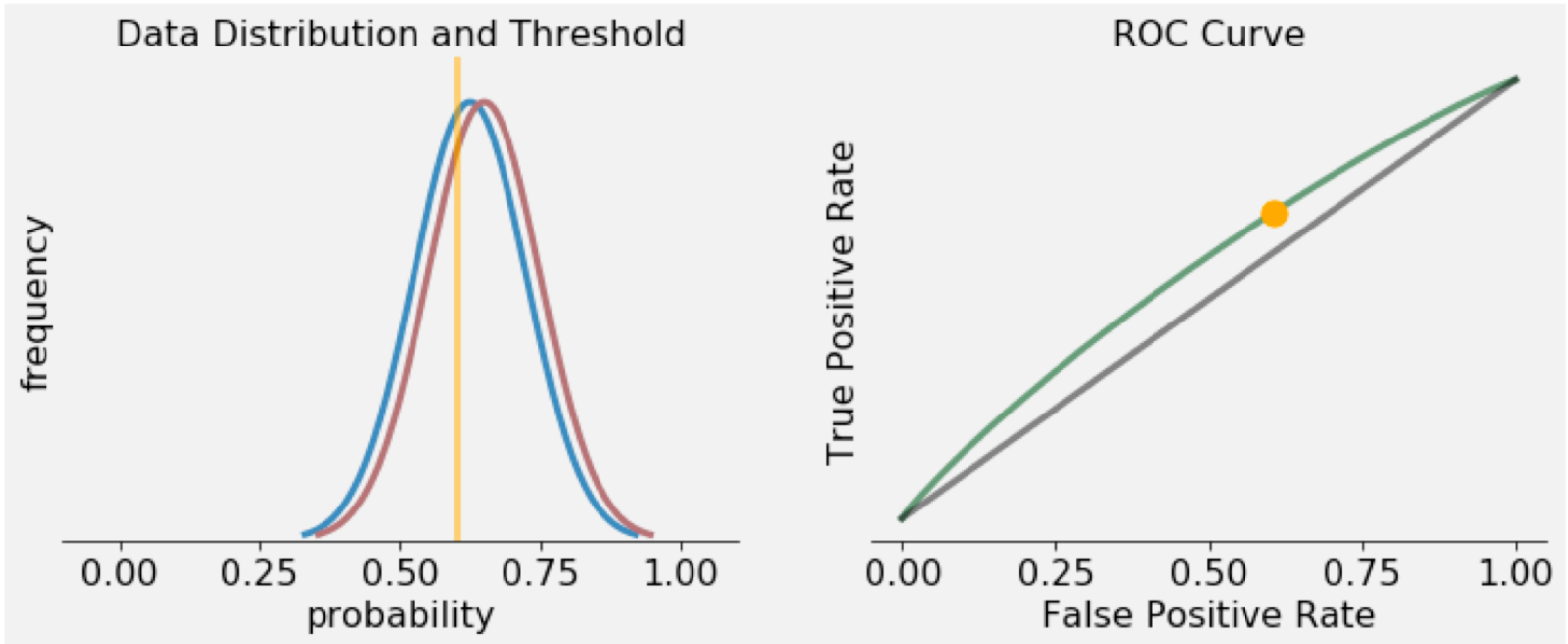
The ROC curve



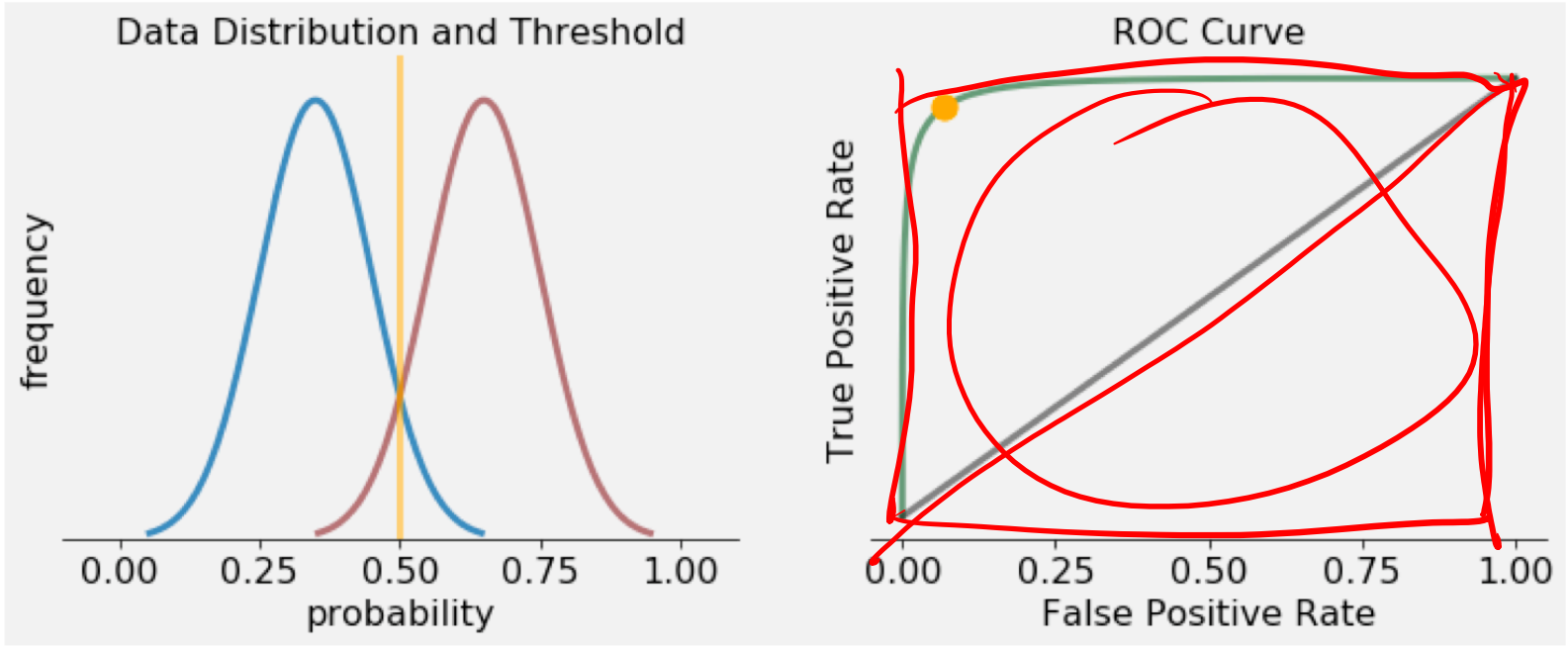
And as we do a poorer job of separating the classes, the curve continues to bend.

The ROC curve



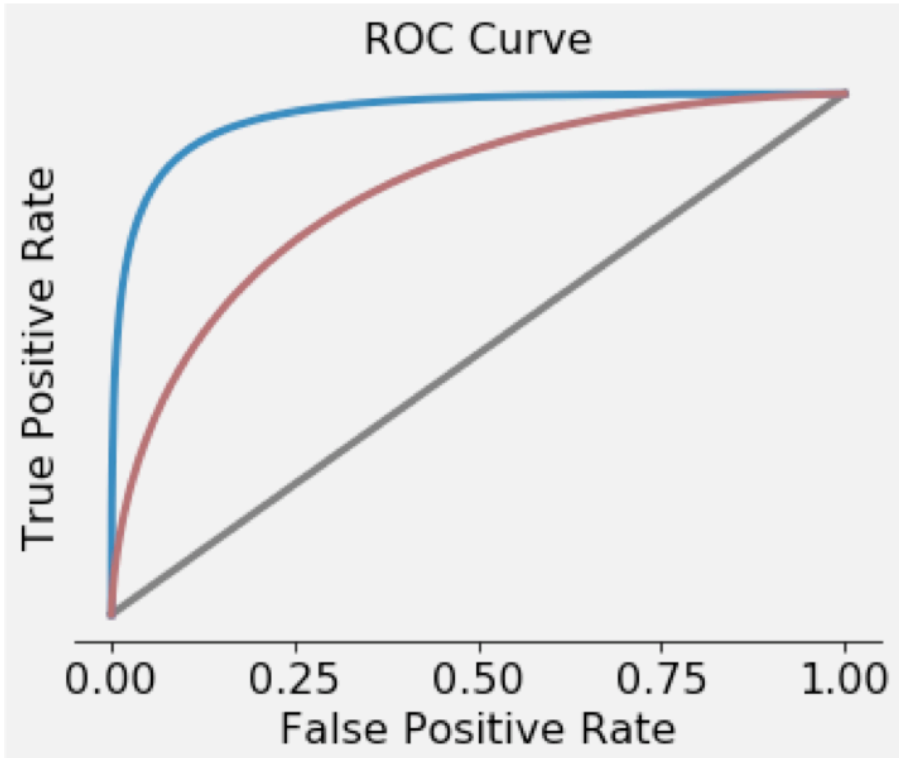
And if we do a terrible job, the curve approaches the random chance line, indicating that our classifier is not much better than a random guess.

The ROC curve



The ROC curve addresses the cases when we're worried about FPs and TPs simultaneously.
But, if you want a single number, evaluating how the model will do in all cases You can compute the AUC (Area under the ROC curve).

ROC-AUC comparisons



To compare two models, plot their ROC curves on the same axes.
If one encloses the other, then it's better on both ends of the spectrum, and has higher AUC.

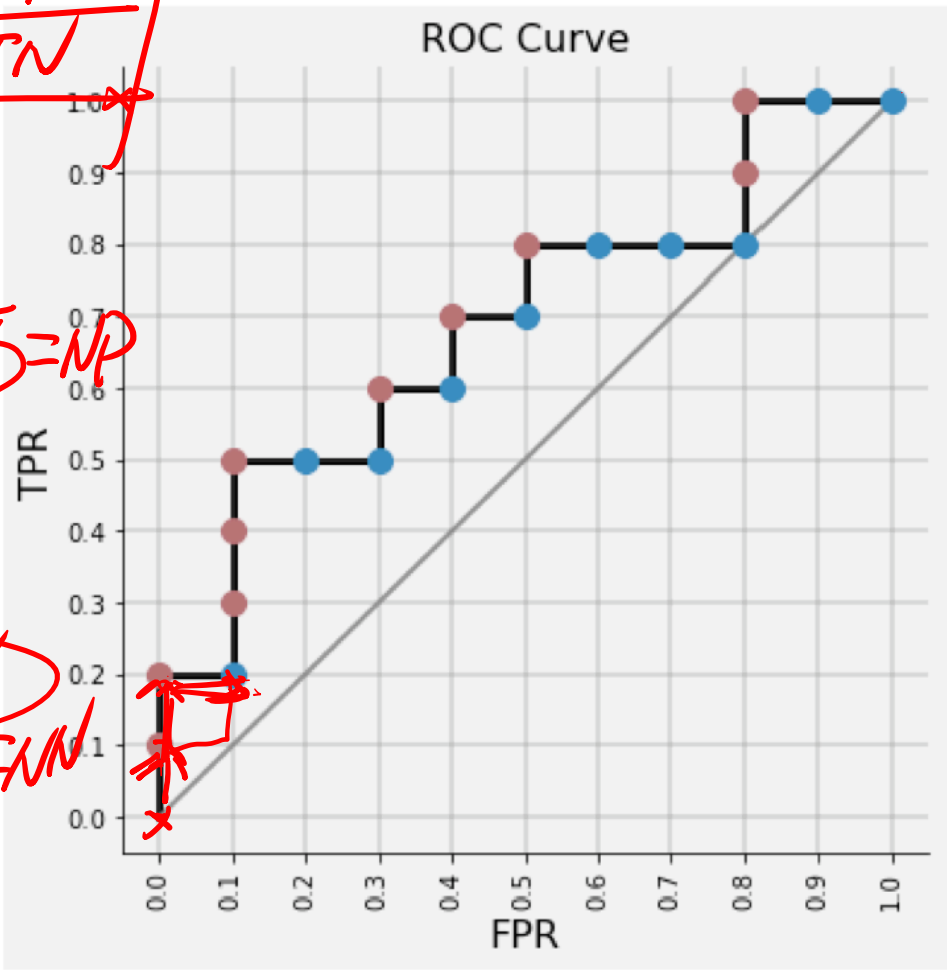
Constructing a ROC curve

You need a classifier that is able to rank examples by predicted score.

- Order all examples by prediction confidence
- Move threshold to each point, one at a time
- If point is true positive, move vertically (1/NP)
- If point is true negative, move horizontally (1/NN)

#	c	$\hat{p}$	#	c	$\hat{p}$
1	P	0.90	11	P	0.40
2	P	0.80	12	N	0.39
3	N	0.70	13	P	0.38
4	P	0.60	14	N	0.37
5	P	0.55	15	N	0.36
6	P	0.54	16	N	0.35
7	N	0.53	17	P	0.34
8	N	0.52	18	P	0.33
9	P	0.51	19	N	0.30
10	N	0.50	20	N	0.10

Constructing a ROC curve



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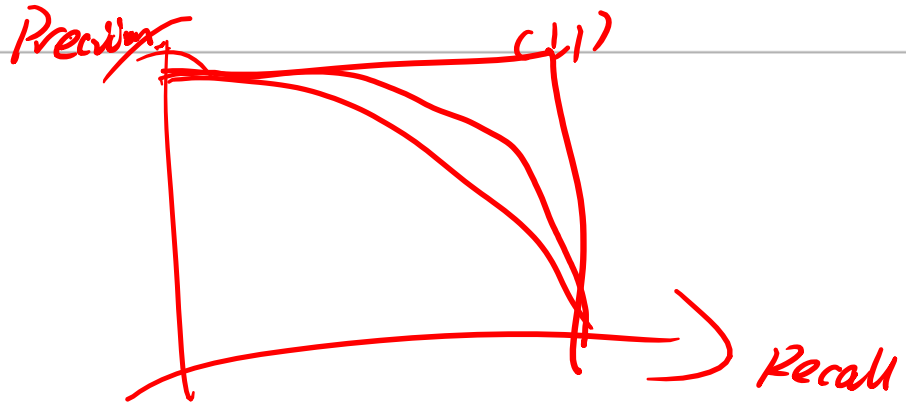
ROC curve



ROC cares both about TPR and FPR, so it values both positive examples and negative examples.

If only positive examples are important, one can plot precision and recall curve.

Outline

- Evaluation metrics
- Inherent multi-class classifiers
- From binary classifiers to multi-class classifiers
- Regularization

Multi-class classification

- Binary examples
  - Spam classification
  - Sentiment classification

Multi-class classification

- Binary examples
  - Spam classification
  - Sentiment classification
- Multi-class examples
  - Star-ratings classification 1, 2, 3, 4, 5
  - Part-of-speech tagging
  - Image classification

Binary vs. multi-class classification

Given: $S_{\text{train}} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^{m}$ training examples, $\boldsymbol{x}_i \in \mathbb{R}^d$, $y_i \in \{-1, 1\}$
Goal: Find hypothesis function $h : X \to Y$

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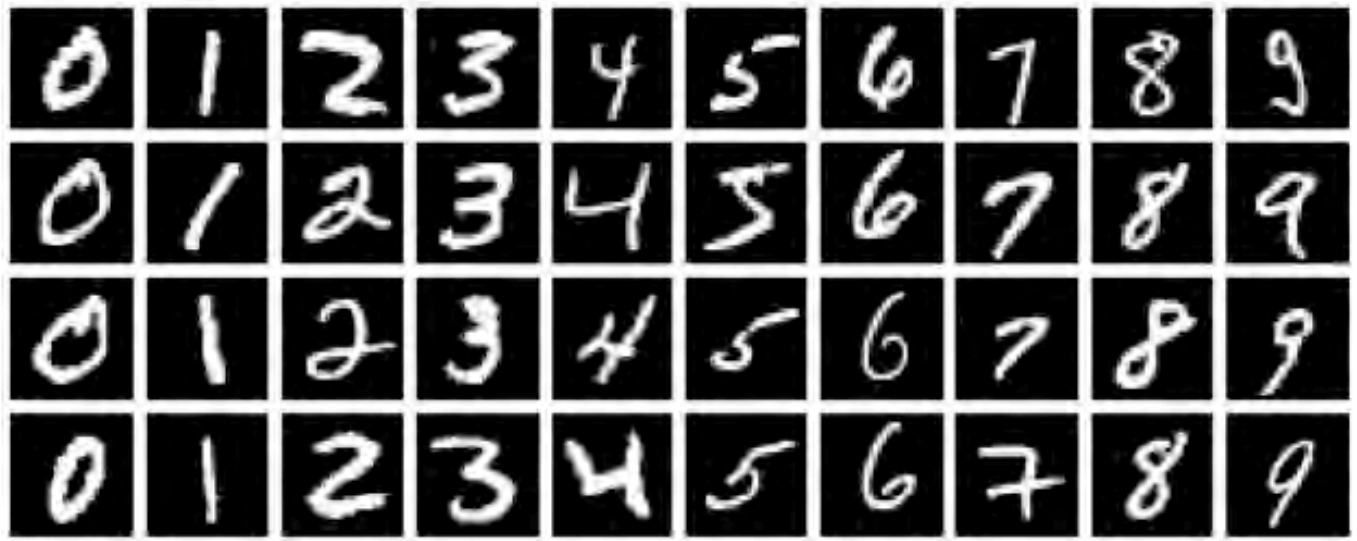
Given: $S_{\text{train}} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^{m}$ training examples, $\boldsymbol{x}_i \in \mathbb{R}^d$, $y_i \in \{0, 1, \ldots, C-1\}$, $C > 2$
Goal: Find hypothesis function $h : X \to Y$

What we have learned so far

- Decision tree
- K-nearest neighbor
- Perceptron
- Logistic regression
- Naïve Bayes

Inherent multi-class classifiers

K-nearest neighbor: Find the K-nearest neighbors of x in training data and predict the majority label of those K points.



Inherent multi-class classifiers

Naïve Bayes:

$$P(c \mid \boldsymbol{x}) \propto P(c, \boldsymbol{x}) = P(c) \prod_{j} P(\boldsymbol{x}_j \mid c)$$

Inherent multi-class classifiers

Naïve Bayes:

$$P(c \mid \boldsymbol{x}) \propto P(c, \boldsymbol{x}) = P(c) \prod_{j} P(\boldsymbol{x}_j \mid c)$$

As long as we can estimate $P(\boldsymbol{x}_j \mid c)$ for each class, we can infer

$$\hat{y} = argmax_c P(y = c|\boldsymbol{x}).$$

Inherent multi-class classifiers

Logistic regression:

$$P(y = 1 \mid \boldsymbol{x}) = \sigma(\beta_0 + \sum_j \beta_j \boldsymbol{x}_j)$$

$$P(y = 0 \mid \boldsymbol{x}) = 1 - \sigma(\beta_0 + \sum_j \beta_j \boldsymbol{x}_j),$$

where $\sigma(z) = \frac{1}{1+exp[-z]}$

Inherent multi-class classifiers

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P(y=c|x)

where $\sigma(z) = \frac{1}{1+exp[-z]}$

In the odds view,

$$\beta_0 + \sum_j \beta_j \boldsymbol{x}_j = \log \frac{P(y = 1|\boldsymbol{x})}{P(y = 0 \mid \boldsymbol{x})}$$

Inherent multi-class classifiers

Logistic regression with more than two classes:

$$\beta_{10} + \sum_j \beta_{1j} x_j = \log \frac{P(y=1|\boldsymbol{x})}{P(y=C \mid \boldsymbol{x})}$$

$$\beta_{20} + \sum_j \beta_{2j} x_j = \log \frac{P(y=2|\boldsymbol{x})}{P(y=C \mid \boldsymbol{x})}$$

$$\vdots$$

$$\beta_{C-1,0} + \sum_j \beta_{C-1,j} x_j = \log \frac{P(y=C-1|\boldsymbol{x})}{P(y=C \mid \boldsymbol{x})}$$

P(y=c|x)

Inherent multi-class classifiers

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$$P(y=c \mid \boldsymbol{x}) = \frac{\exp(\beta_c^T \boldsymbol{x})}{1 + \sum_{c'=1}^{C-1} \exp(\beta_{c'}^T \boldsymbol{x})}, P(y=C \mid \boldsymbol{x}) = \frac{1}{1 + \sum_{c'=1}^{C-1} \exp(\beta_{c'}^T \boldsymbol{x})}$$

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Classifiers

Now we are left with classifiers that are basically binary

- Perceptron

Is there anything that we can do?

Reduction

Multiclass Data

⟨name=Cindy , age=5 , sex=F⟩,
⟨name=Marcia, age=15, sex=F⟩, 
⟨name=Bobby , age=6 , sex=M⟩, 
⟨name=Jan , age=12, sex=F⟩, 
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Reduction

Multiclass Data

⟨name=Cindy , age=5 , sex=F⟩, ■ 9
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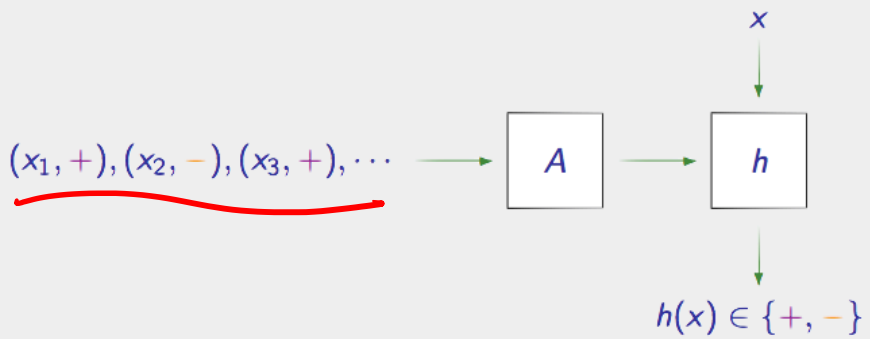
⟨name=Peter , age=13, sex=M⟩, ■ 3

Binary Classifier



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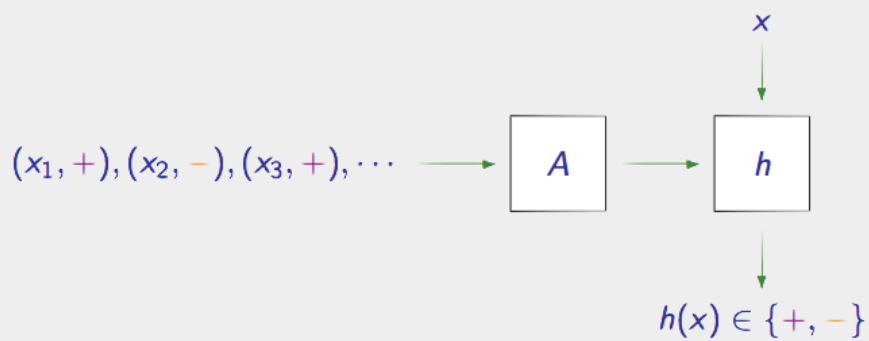
Binary Classifier



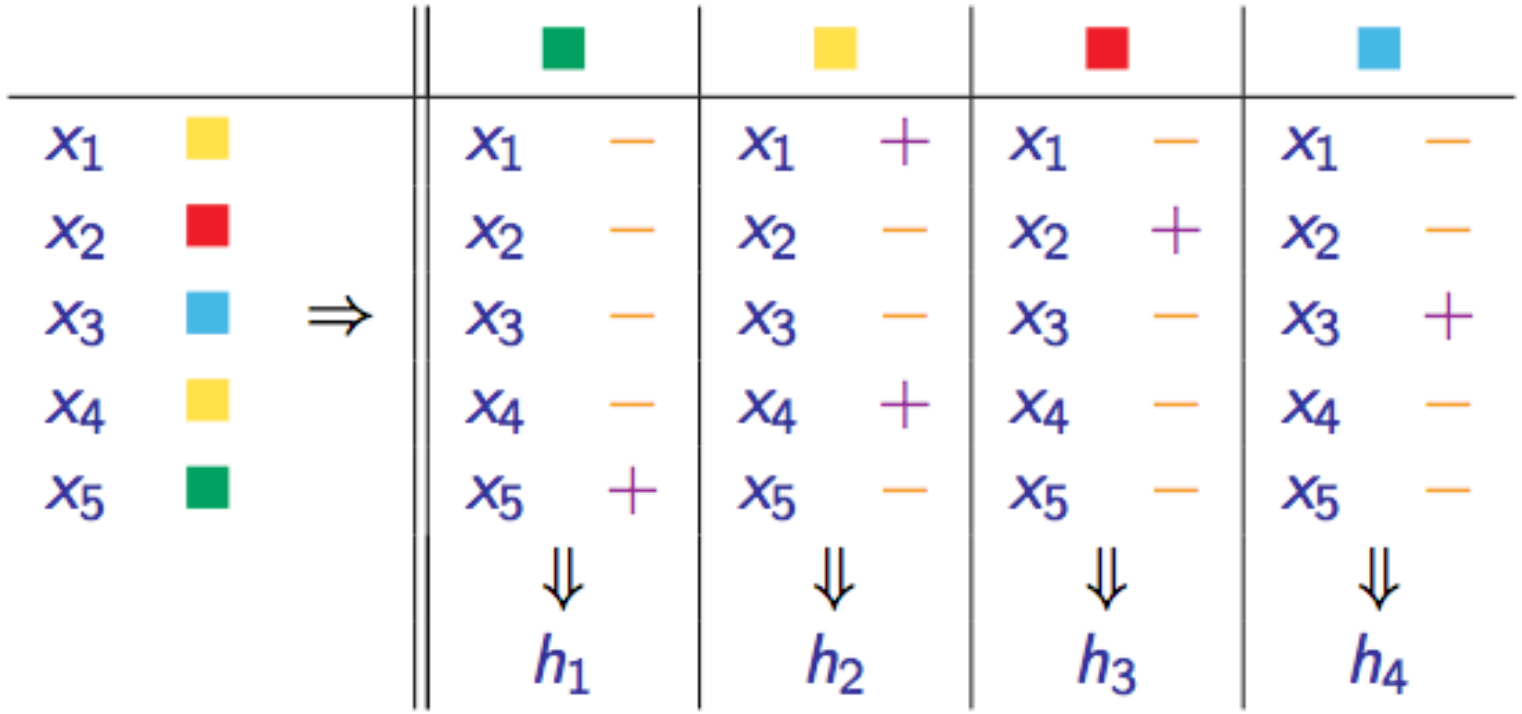
Goal: Multiclass Classifier

Reduction

Two strategies

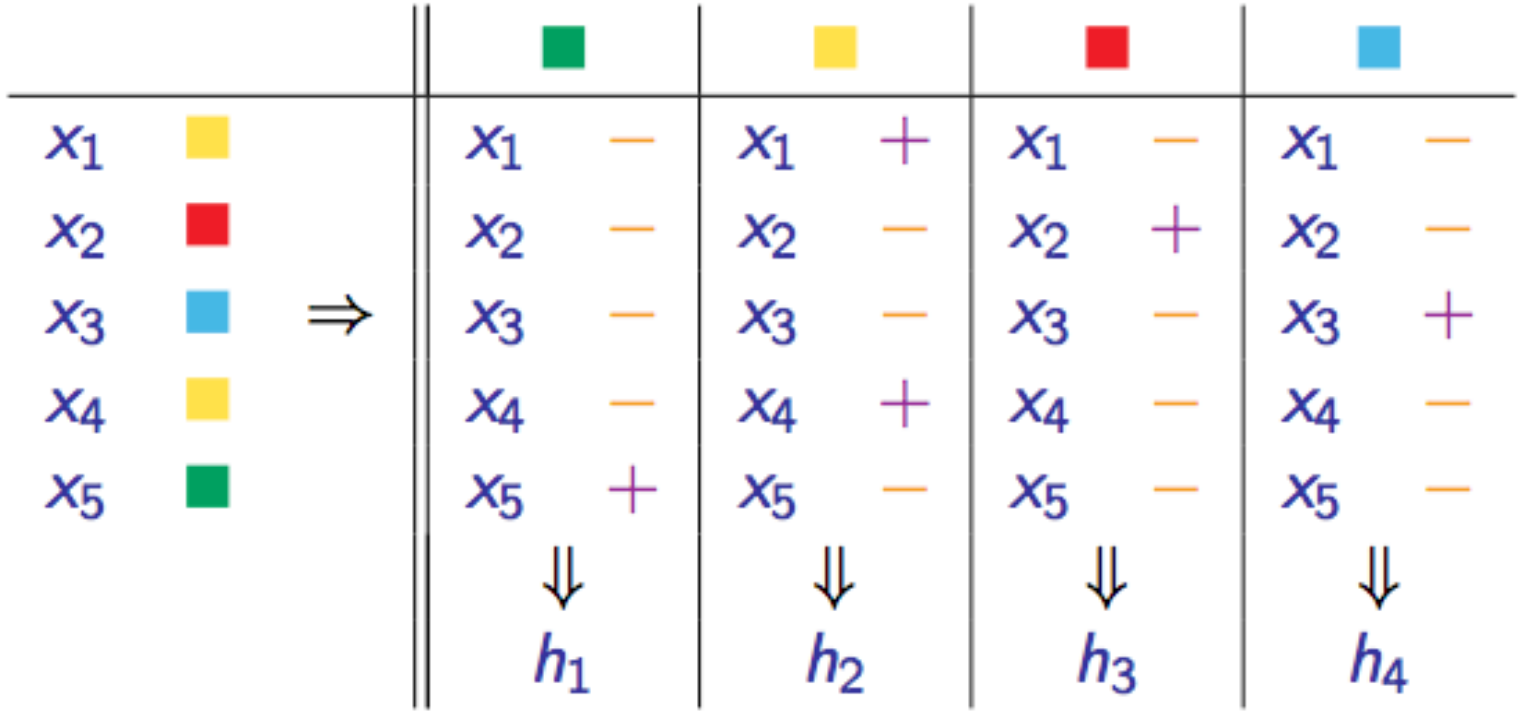
- One against all
- All pairs

One against all



- Break k-class problem into k binary problems and solve separately
- Combine predictions: evaluate all h's, hope exactly one is $+$ (otherwise, take highest confidence)

One against all



$$h(x) = \arg\max_{c \in C} h_c(\boldsymbol{x})$$

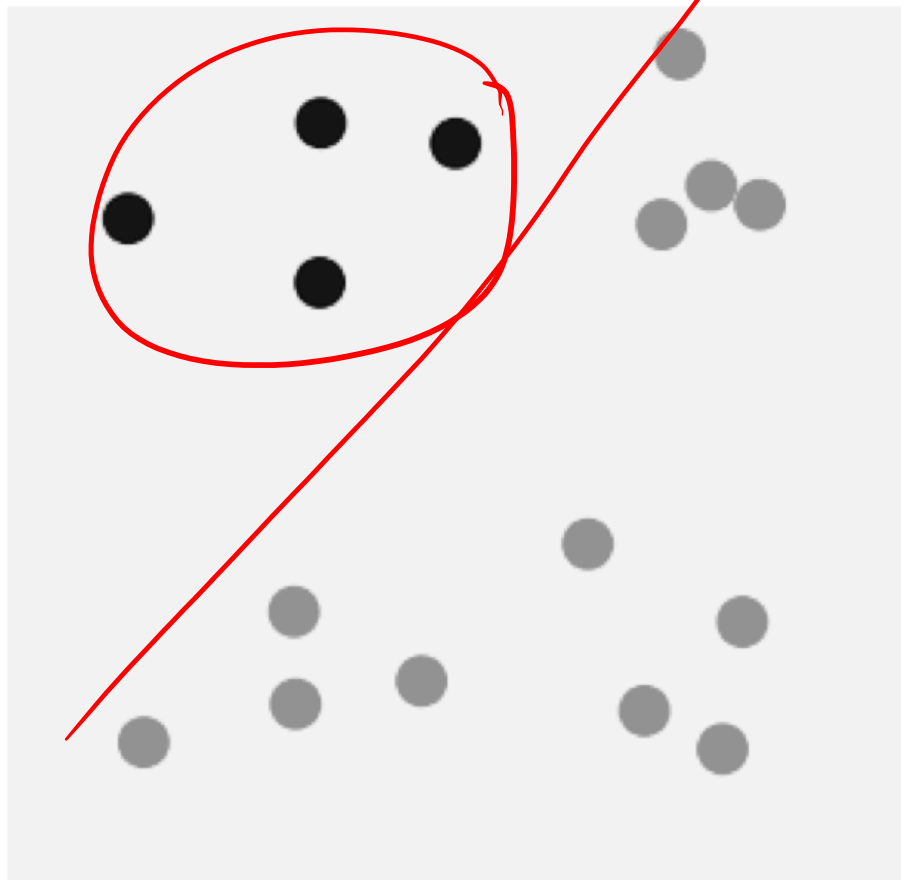
One against all

Build C binary classifiers of the form Class c vs Class $\neg c$

One against all

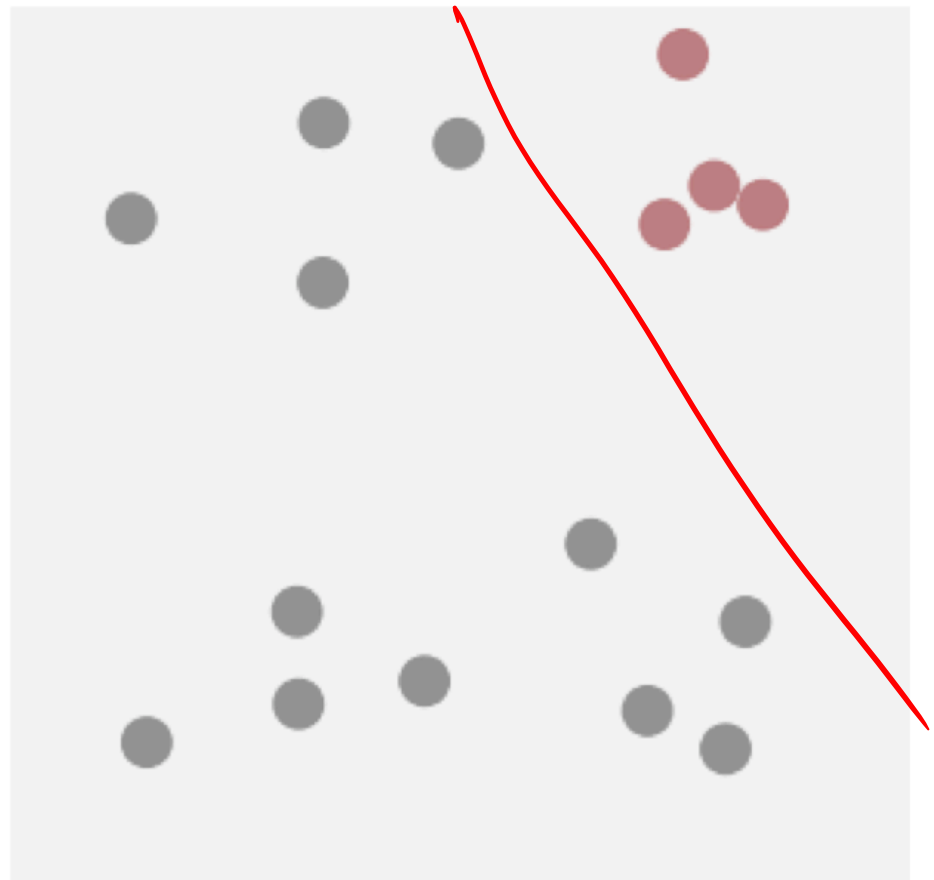
Build C binary classifiers of the form Class c vs Class $\neg c$

Black vs. not black



One against all

Build C binary classifiers of the form Class c vs Class $\neg c$
Red vs. not red



One against all

Build C binary classifiers of the form Class c vs Class $\neg c$
Yellow vs. not yellow

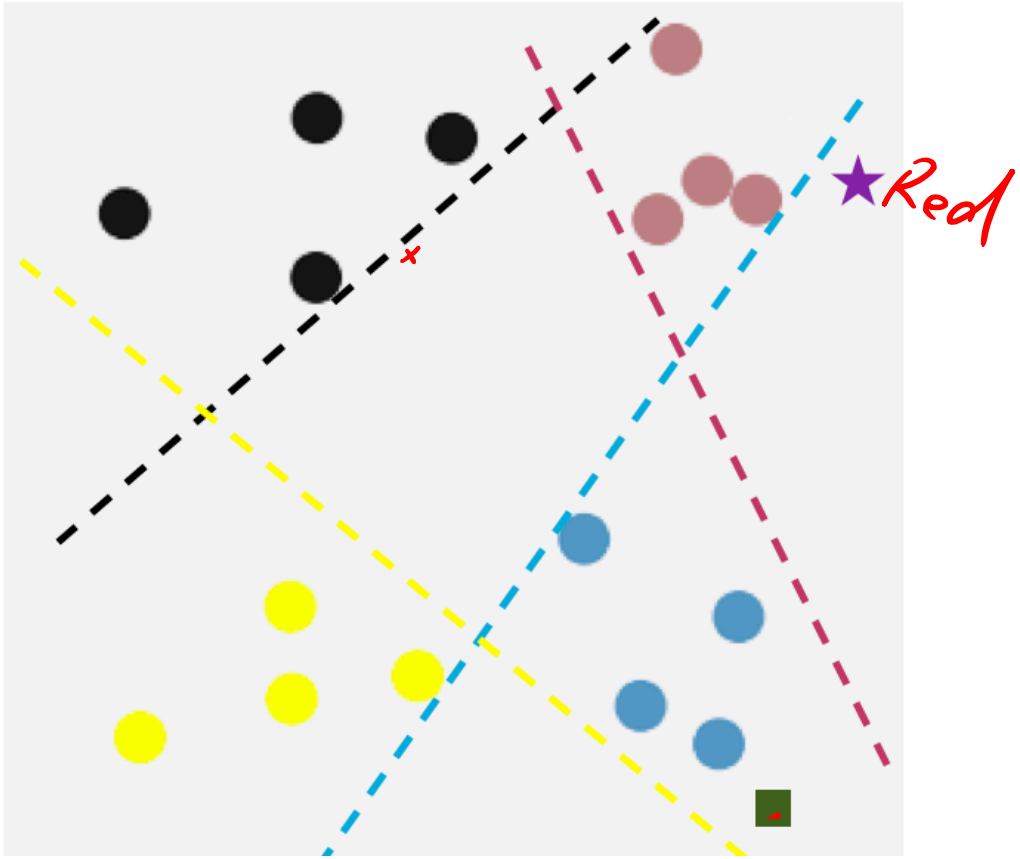
One against all

Build C binary classifiers of the form Class c vs Class $\neg c$
Blue vs. not blue

One against all

Build C binary classifiers of the form Class c vs Class $\neg c$
Predict class with highest confidence

- Predict green square
- Predict purple star



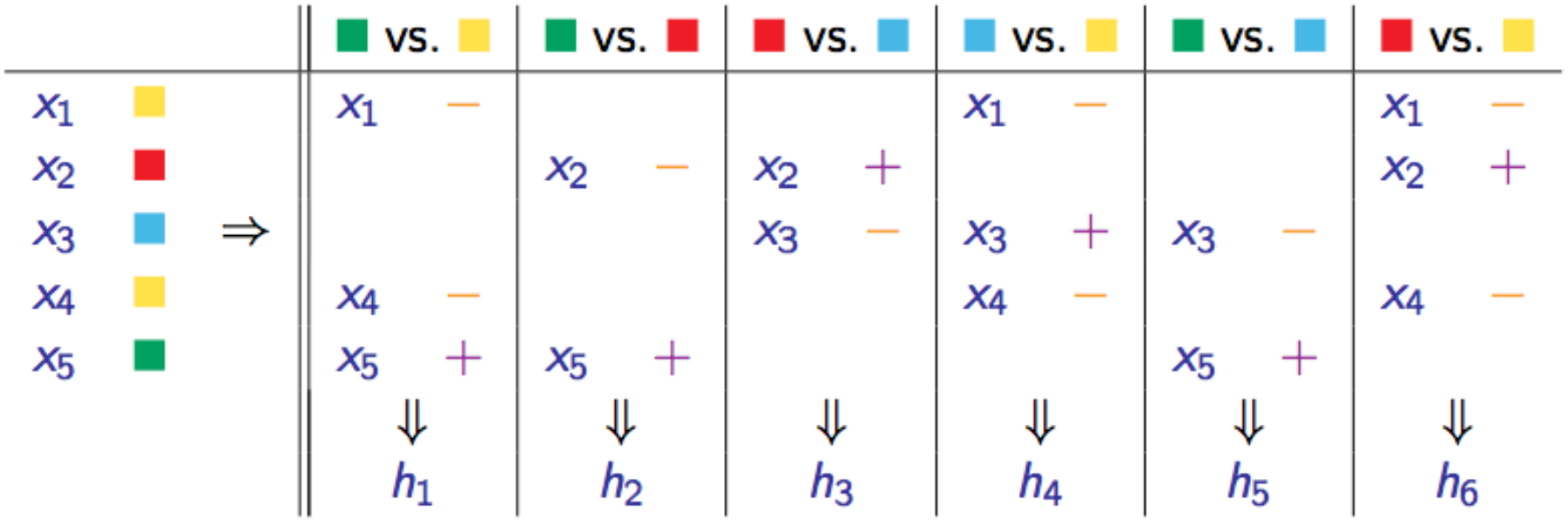
One against all

Can you see any pitfalls of the one-against-all method?

One against all

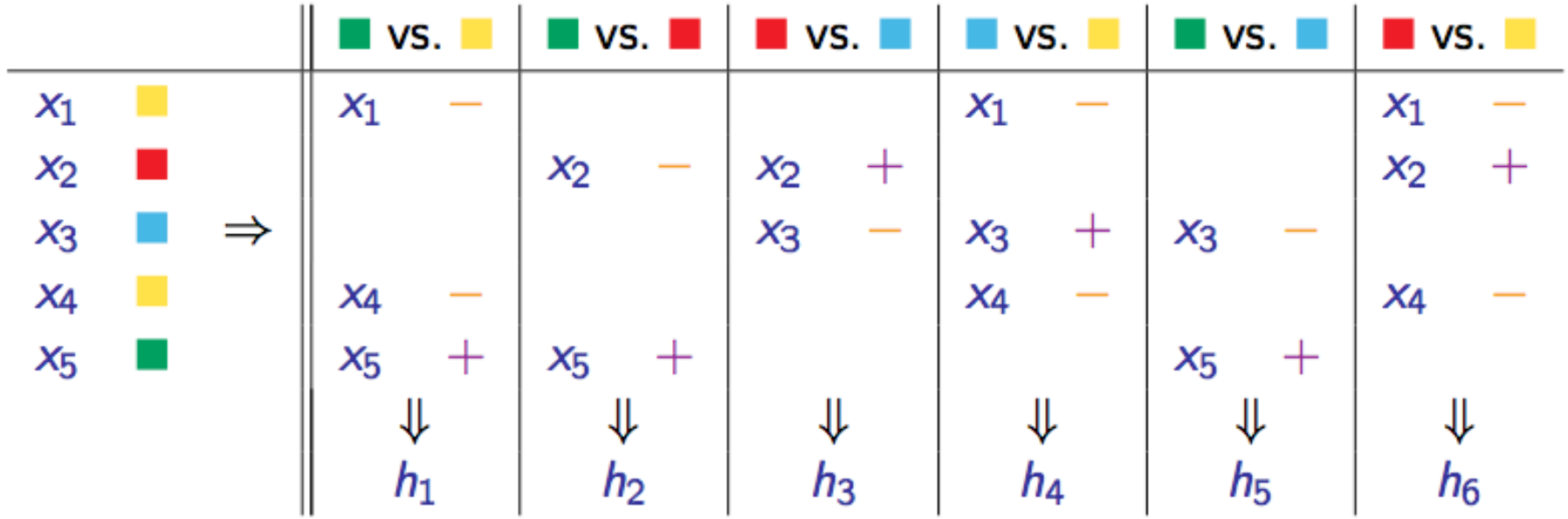
Can you see any pitfalls of the one-against-all method?
A big one is that if you start with a balanced training data, you immediately create imbalanced data.

All pairs



- Break k-class problem into $k(k-1)/2$ binary problems and solve separately
- Combine predictions: evaluate all h's, take the one with highest sum confidence

All pairs



$$h(x) = \arg\max_{c \in C} \sum_{c' \neq c} h_{c'c}(\boldsymbol{x})$$

Time Comparison

Assume training time is $\mathcal{O}(m^\alpha)$ and test time is $\mathcal{O}(c_t)$

	train	test
One vs all	$O(km^\alpha)$	$O(kc_t)$
All pairs	$O(k^2(\frac{m}{k})^\alpha)$ $O(k^{2-\alpha}m^\alpha)$	$O(k^2c_t)$

$\alpha > 1$

Time Comparison

Assume training time is $\mathcal{O}\left(m^{\alpha}\right)$ and test time is $\mathcal{O}\left(c_t\right)$

	Training	Testing
One-against-all	$\mathcal{O}\left(Cm^{\alpha}\right)$	$\mathcal{O}\left(Cc_t\right)$
All-pairs	$\mathcal{O}\left(C^2\left(\frac{m}{C}\right)^{\alpha}\right)$	$\mathcal{O}\left(C^2c_t\right)$

T

Time Comparison

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- One-against-all better for testing time
- All-pairs better for training (usually)
- All-pairs usually better for performance

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Ridge vs. Lasso

Ridge Regression or ℓ_2-Regularization:

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 + \lambda \sum_{k=1}^{D} w_k^2$$

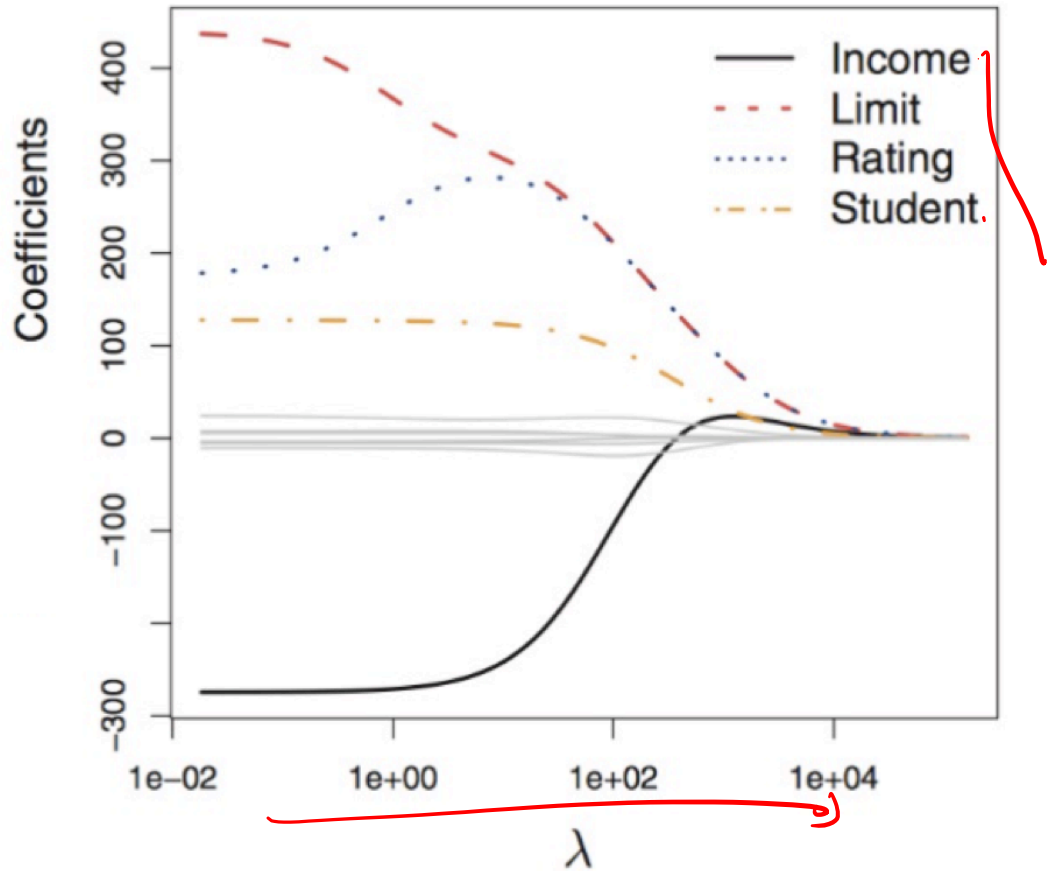
Lasso Regression or ℓ_1-Regularization:

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 + \lambda \sum_{k=1}^{D} |w_k|$$

Different penalty terms lead to different character of models

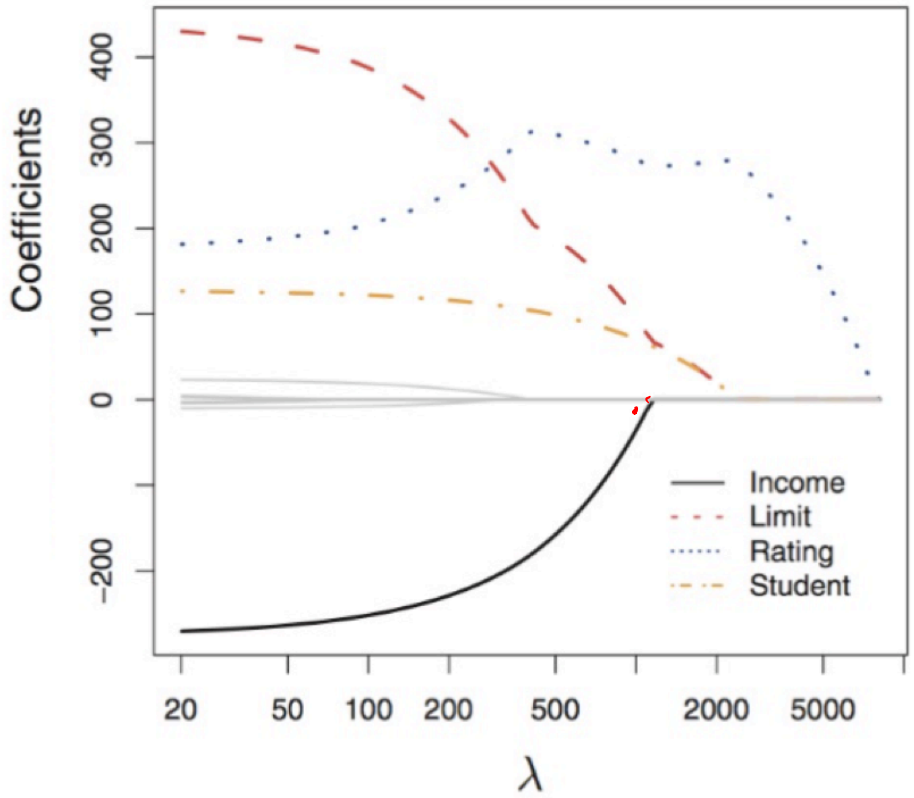
Ridge

Coefficients shrink to zero uniformly smoothly



Lasso

Some coefficients shrink to zero very fast



The constrained optimization explanation

Consider the minimizer of

$$\min_{\mathbf{w}} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 + \lambda \sum_{k=1}^{D} w_k^2 \quad \text{or} \quad \min_{\mathbf{w}} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 + \lambda \sum_{k=1}^{D} |w_k|$$

For each objective function, can show that for a given λ there is an equivalent s such that the usual solution also solves

$$\text{Ridge:} \quad \min_{\mathbf{w}} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 \quad \text{s.t.} \quad \sum_{k=1}^{D} w_k^2 \leq s$$

$$\text{Lasso:} \quad \min_{\mathbf{w}} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 \quad \text{s.t.} \quad \sum_{k=1}^{D} |w_k| \leq s$$

The constrained optimization explanation

Think of the constraint as a budget on the size of the parameters
For a given budget s (corresponding to a given λ), find the $\mathbf{w}$ that minimizes the residual sum of squares (RSS) while staying inside the constrained region
Lasso Region for Two Features: Diamond

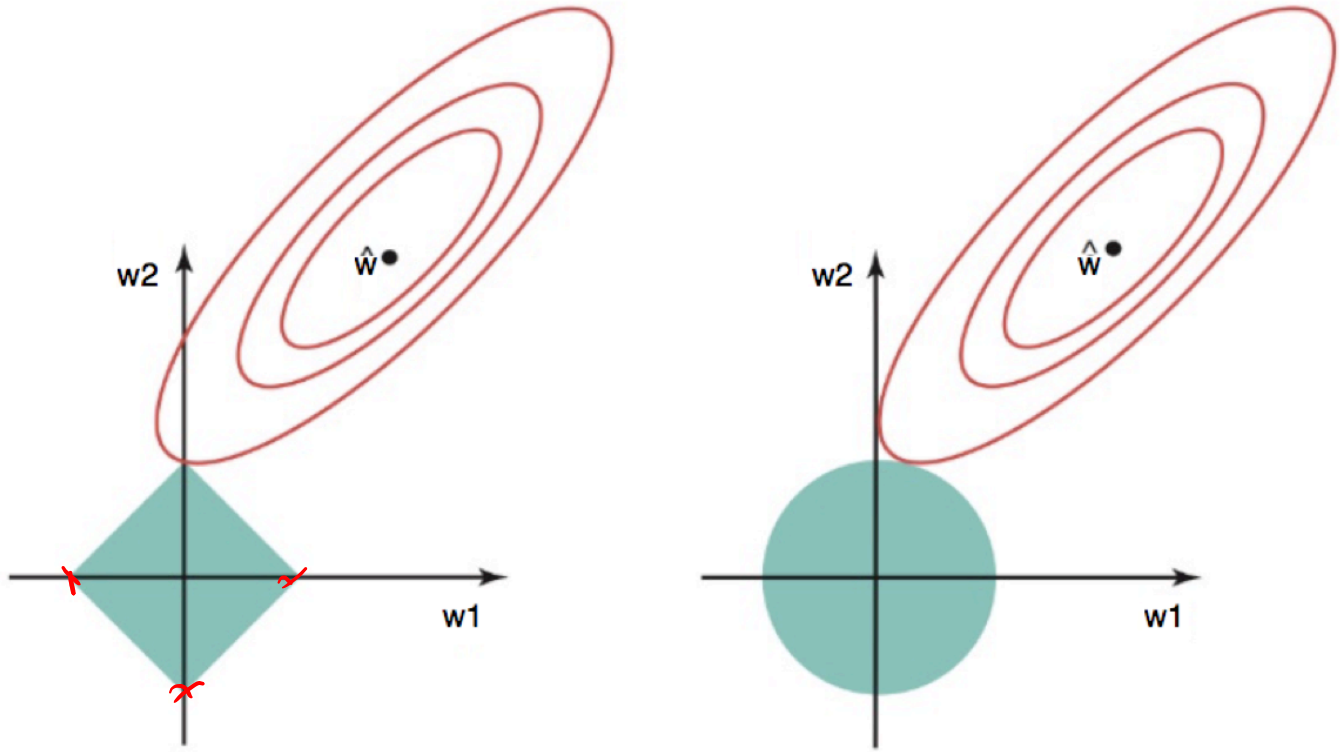
$$|w_1| + |w_2| \leq s$$

Ridge Region for Two Features: Circle

$$w_1^2 + w^2 \leq s$$

The constrained optimization explanation

Minimum is more likely to be at point of diamond with Lasso, causing some feature weights to be set to zero.



Recap

- AUC can be used for evaluating imbalanced datasets
- Many classifiers that we learned so far are inherently multi-class
- We can build multi-class classifiers using binary classifiers