Lecture 13: Boosting & Multi-class methods

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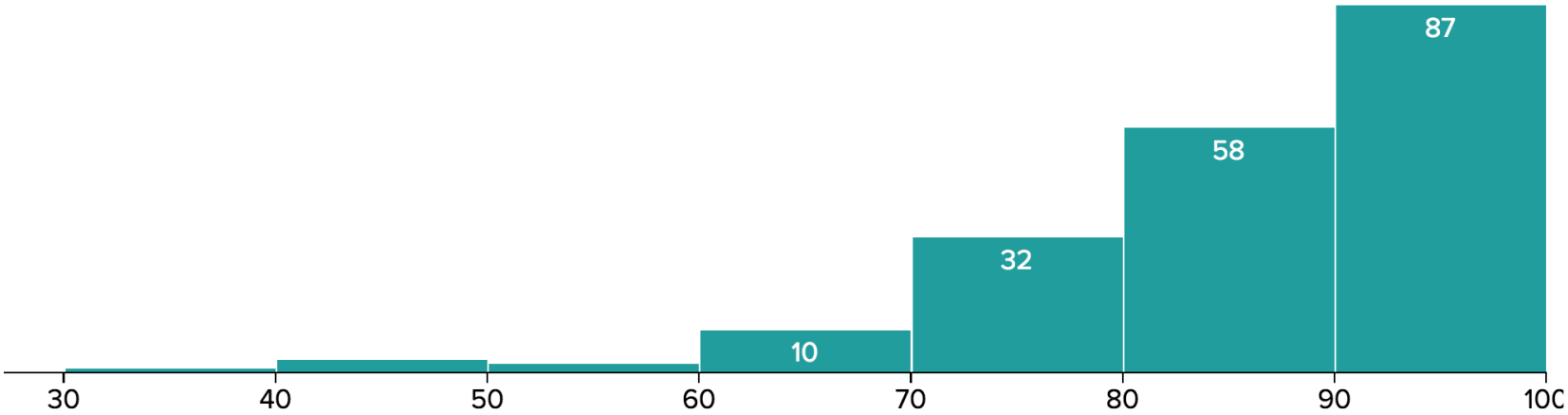
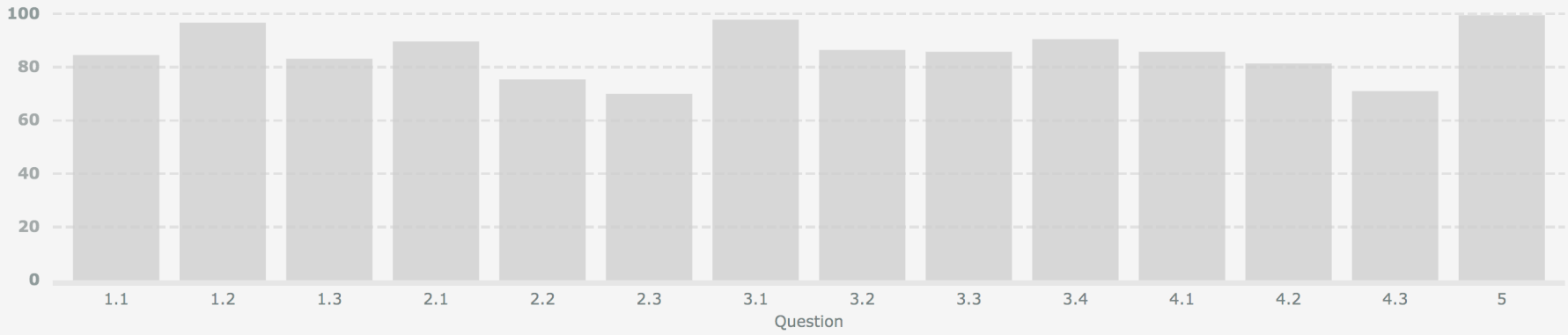
Midterm Exam

MEDIAN	MAXIMUM	MEAN	STD DEV
88.0%	100.0% (11)	85.0%	13.13%





Feedback

1. (1) I am keeping up with the course material

- (0) Strongly Disagree:	2 (2.82 %)
- (1) Disagree:	7 (9.86 %)
- (2) Neutral:	16 (22.54 %)
- (3) Agree:	29 (40.85 %)
- (4) Strongly Agree:	17 (23.94 %)

Average: 2.73

2. (2) The level of difficulty of the material is

- (0) Too Easy:	1 (1.41 %)
- (1) Easy:	4 (5.63 %)
- (2) Okay:	28 (39.44 %)
- (3) Difficult:	33 (46.48 %)
- (4) Too Difficult:	5 (7.04 %)

Average: 2.52

3. (3) The lectures help me understand the course concept

- (0) Not at all:	3 (4.23 %)
- (1) Sometimes:	14 (19.72 %)
- (2) Usually:	17 (23.94 %)
- (3) Mostly:	28 (39.44 %)
- (4) Always:	9 (12.68 %)

Average: 2.37

4. (4) The assignments help me understand the course concepts

- (0) Not at all:	3 (4.23 %)
- (1) Sometimes:	15 (21.13 %)
- (2) Usually:	14 (19.72 %)
- (3) Mostly:	24 (33.80 %)
- (4) Always:	15 (21.13 %)

Average: 2.46

5. (5) The pace of the course is

- (0) Too Slow:	0
- (1) Slow:	10 (14.08 %)
- (2) Just Right:	35 (49.30 %)
- (3) Fast:	23 (32.39 %)
- (4) Too Fast:	3 (4.23 %)

Average: 2.27

6. I feel the time spent on homework problems is well-spent on learning

- (0) Strongly Disagree:	2 (2.82 %)
- (1) Disagree:	13 (18.31 %)
- (2) Neutral:	21 (29.58 %)
- (3) Agree:	27 (38.03 %)
- (4) Strongly Agree:	8 (11.27 %)

Average: 2.37

7. (7) The exam is

- (0) Too Easy:	0
- (1) Easy:	5 (7.04 %)
- (2) Just the Right Difficulty:	49 (69.01 %)
- (3) Difficult:	15 (21.13 %)
- (4) Too Difficult:	2 (2.82 %)

Average: 2.20

Kernel Perceptron Algorithm

Given a training set $\mathcal{D} = \{(\boldsymbol{x}, y)\}^{m}_{i=1}$, $\boldsymbol{\phi(.)}$

1. Initialize $\boldsymbol{\alpha} \leftarrow \mathbf{0} \in \mathbb{R}^{\boldsymbol{m}}$
2. For $(\boldsymbol{x_j}, y_j)$ in $\mathcal{D}$: $(\mathrm{j} = 1 \ldots m)$
3. if $y_j\left(\sum_{1..m} \alpha_i \, y_i K(x_i, x_j)\right) \leq \mathbf{0}$
4. $\alpha_j \leftarrow \alpha_j + 1$
5. Return $\boldsymbol{\alpha}$
6.

$$w = \sum_{1..m} \alpha_i \, y_i \phi(x_i)$$

Let $K(x_i, x_j) = \phi(x_i)^T \phi(x_j)$

Prediction: $y^{\text{test}} \leftarrow \text{sgn}\left(\sum_{1..m} \alpha_i \, y_i K(x_i, x^{Test})\right)$

Example

- Kernel Perceptron for XOR data in 2D space (1: true, -1: false
- Kernel: $\mathrm{K}(\mathrm{x}, z) = (x^T z)^2$
- What is the kernel matrix?
- What are α learned from Perceptron
- What is the implicit separator

	x_1	x_2	y
I1	-1	1	1
I2	1	-1	1
I3	-1	-1	-1
I4	1	1	-1

	I1	I2	I3	I4
I1	4	4	0	0
I2	4	4	0	0
I3	0	0	4	4
I4	0	0	4	4

Kernel Perceptron Algorithm

Given a training set $\mathcal{D} = \{(\boldsymbol{x}, y)\}_{i=1}^{m}$, $\boldsymbol{\phi(.)}$

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	x_1	x_2	y
I1	-1	1	1
I2	1	-1	1
I3	-1	-1	-1
I4	1	1	-1

	I1	I2	I3	I4
I1	4	4	0	0
I2	4	4	0	0
I3	0	0	4	4
I4	0	0	4	4

Let $K(x_i, x_j) = \phi(x_i)^T \phi(x_j)$

$w = \sum_{1..m} \alpha_i \, y_i \phi(x_i)$

Prediction: $y^{\text{test}} \leftarrow \text{sgn}\left(\sum_{1..m} \alpha_i \, y_i K(x_i, x^{Test})\right)$

Kernel Perceptron Algorithm

Given a training set $\mathcal{D} = \{(\boldsymbol{x}, y)\}_{i=1}^{m}$, $\boldsymbol{\phi(.)}$

1. Initialize $\boldsymbol{\alpha} \leftarrow \mathbf{0} \in \mathbb{R}^{\boldsymbol{m}}$
2. For $(\boldsymbol{x_j}, y_j)$ in $\mathcal{D}$: (j= $1 \ldots m$)
3. if $y_j\left(\sum_{1..m} \alpha_i \, y_i K(x_i, x_j)\right) \leq \mathbf{0}$
4. $\alpha_j \leftarrow \alpha_j + 1$
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6.

	x_1	x_2	y
I1	-1	1	1
I2	1	-1	1
I3	-1	-1	-1
I4	1	1	-1

Let $K(x_i, x_j) = \phi(x_i)^T \phi(x_j)$

	I1	I2	I3	I4
I1	4	4	0	0
I2	4	4	0	0
I3	0	0	4	4
I4	0	0	4	4

$w = \sum_{1..m} \alpha_i \, y_i \phi(x_i)$

Prediction: $y^{\text{test}} \leftarrow \text{sgn}\left(\sum_{1..m} \alpha_i \, y_i K(x_i, x^{Test})\right)$

Exercise

- Kernel Perceptron for XOR data in 2D space (1: true, -1: false
- Kernel: $\mathrm{K}(\mathrm{x}, z) = (1 + x^T z)^2$
- What is the kernel matrix?
- What are α learned from Perceptron
- What is the implicit separator

	x_1	x_2	y
I1	-1	1	1
I2	1	-1	1
I3	-1	-1	-1
I4	1	1	-1

	I1	I2	I3	I4
I1				
I2				
I3				
I4				

Recap: Dual SVM problem

- w may be infinite variables
- We can derive the Lagrangian dual problem

$$\begin{aligned} \min_{\boldsymbol{\alpha}} \quad & \frac{1}{2}\boldsymbol{\alpha}^T Q\boldsymbol{\alpha} - \mathbf{e}^T\boldsymbol{\alpha} \\ \text{subject to} \quad & 0 \le \alpha_i \le C, i = 1, \ldots, l \\ & \mathbf{y}^T\boldsymbol{\alpha} = 0, \end{aligned}$$

where $Q_{ij} = y_i y_j \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$ and $\mathbf{e} = [1, \ldots, 1]^T$

$$Q_{ij} = y_i y_j K(x_i, x_j)$$

	I1	I2	I3	I4
I1	4	4	0	0
I2	4	4	0	0
I3	0	0	4	4
I4	0	0	4	4

https://www.csie.ntu.edu.tw/~cjlin/talks/MLSS.pdf

Boosting

How to?

Given a training set $(x_1, y_1), \cdots, (x_m, y_m)$

- Instances $x_i \in X$ labeled with $y_i \in \{-1, +1\}$

- For t = 1, 2, ⋯, T:
  - Construct a distribution D_t on {1, 2, ⋯, m}
  - Find a weak hypothesis (rule of thumb) h_t such that it has a small *weighted* error ϵ_t on D_t

How to?

How to?

- Construct a final output H_{final}

How to?

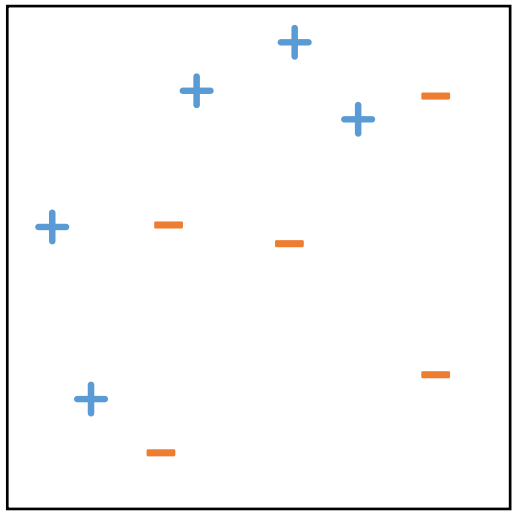
Advanced topic: (not covered in the exam) Boosting: Theoretical Motivation

- Strong PAC algorithm
  - For any distribution over examples,
  - For any $\delta > 0$, $\epsilon > 0$,
  - Given a polynomially many random examples
  - Finds a hypothesis with error ϵ with probability, $1 - \delta$

- Weak PAC algorithm
  - Same, but only for $\epsilon \leq \frac{1}{2} - \gamma \quad \gamma > 0$ is a small value
- Question [Kearns and Valiant '88]:
  - Does weak learnability imply strong learnability?

A toy example

$$D_1(i) = \frac{1}{m}$$

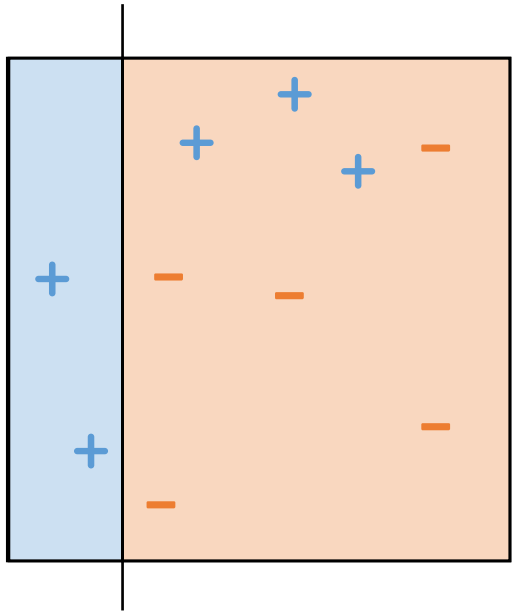


Our weak learner: An axis parallel line

Or

Initially all examples are equally important

A toy example



Our weak learner: An axis parallel line

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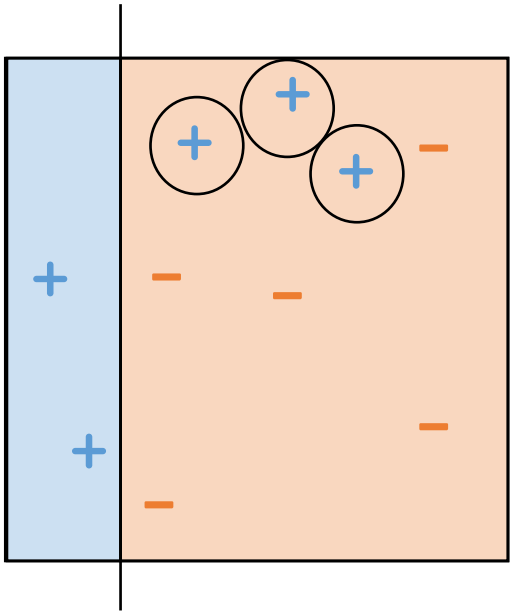
Initially all examples are equally important

h_1 = The best classifier on this data

A toy example



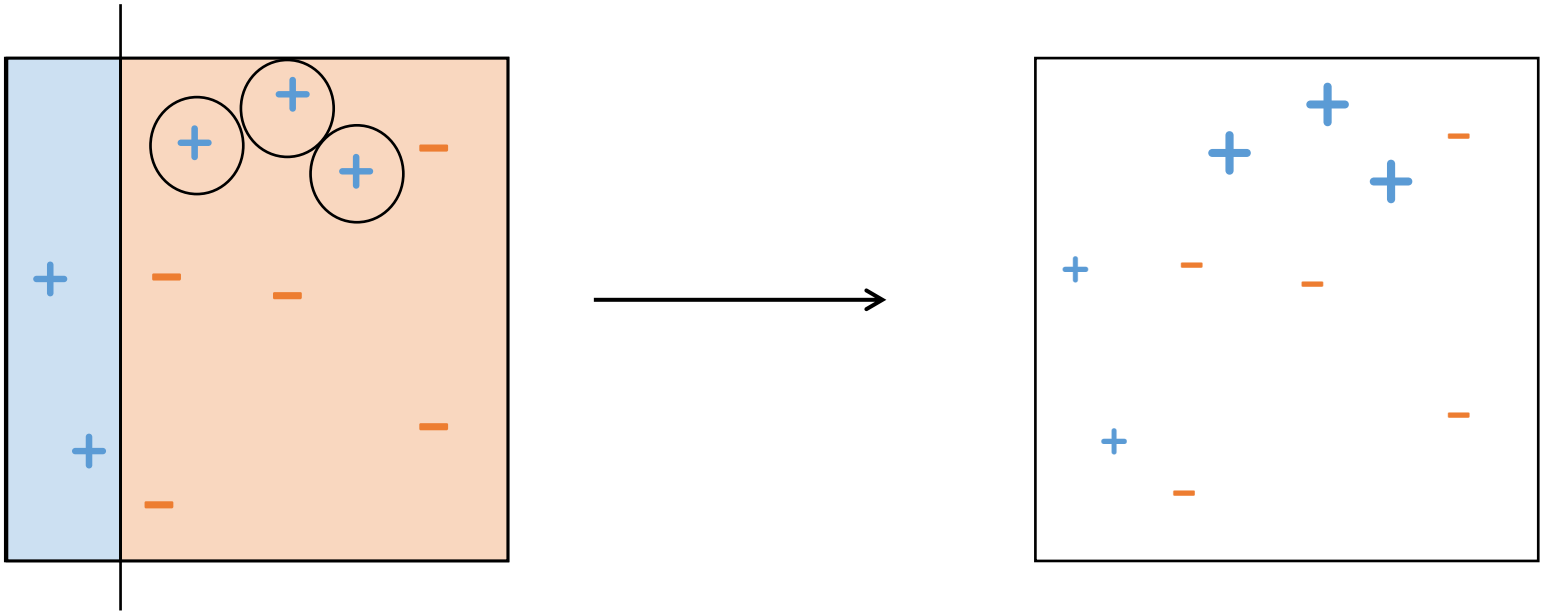
Our weak learner: An axis parallel line

Or

Initially all examples are equally important

h_1 = The best classifier on this data
Clearly there are mistakes. Error ϵ_1 = 0.3

A toy example



Initially all examples are equally important

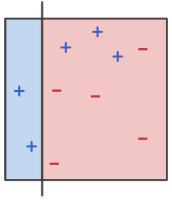
h_1 = The best classifier on this data
Clearly there are mistakes. Error ϵ_2 = 0.3

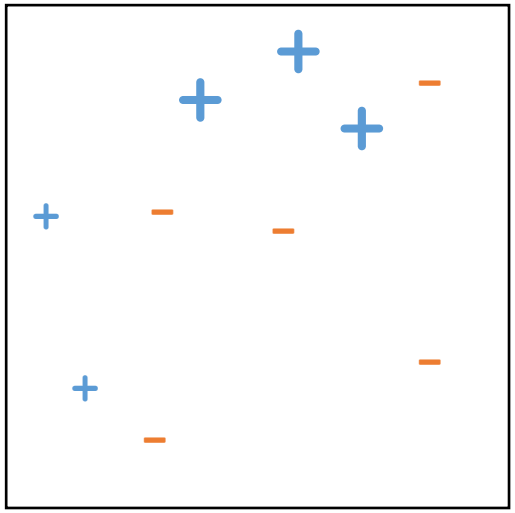
$$D_{t+1}(i) = \frac{D_t(i)}{Z_t} \begin{cases} e^{-\alpha_t} & \text{if } y_i = h_t(x_i) \\ e^{\alpha_t} & \text{if } y_i \neq h_t(x_i) \end{cases}$$

$$= \frac{D_t(i)}{Z_t} \cdot \exp\left(-\alpha_t \cdot y_i h_t(x_i)\right)$$

For the next round, increase the importance of the examples with mistakes and down-weight the examples that h_1 got correctly

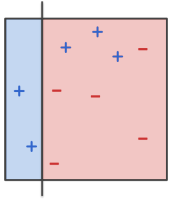
A toy example



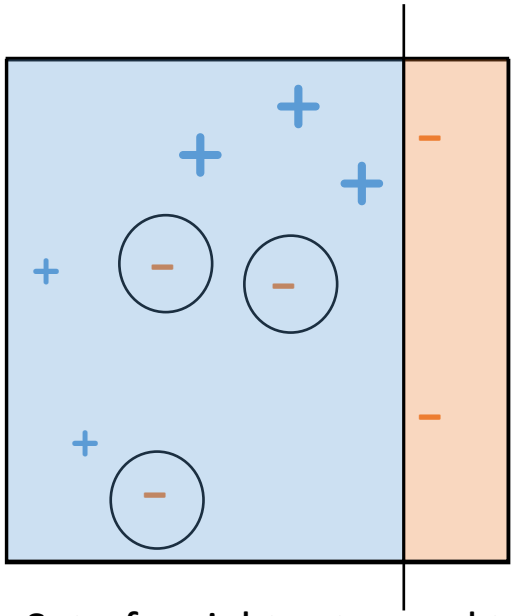


D_t = Set of weights at round t, one for each example. Think "How much should the weak learner care about this example in its choice of the classifier?"

A toy example



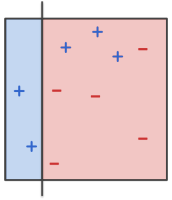
h_1



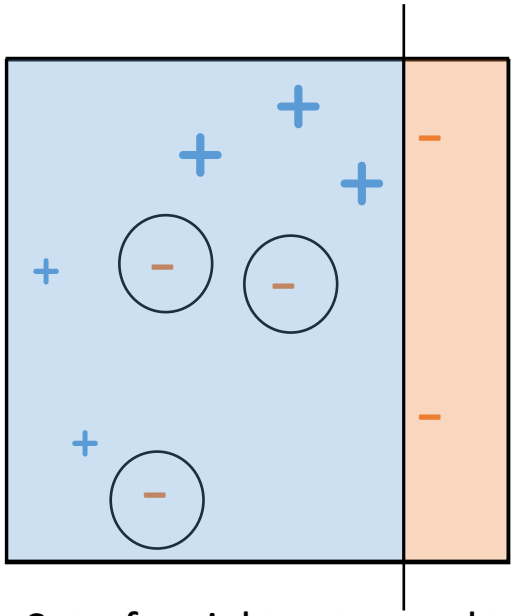
D_t = Set of weights at round t, one for each example. Think "How much should the weak learner care about this example in its choice of the classifier?"

h_2 = A classifier learned on this data. *Has an error* $\epsilon_2 = 0.21$

A toy example



h_1



$$\alpha_t = \frac{1}{2} \ln \left(\frac{1 - \epsilon_t}{\epsilon_t} \right)$$

$$D_{t+1}(i) = \frac{D_t(i)}{Z_t} \begin{cases} e^{-\alpha_t} & \text{if } y_i = h_t(x_i) \\ e^{\alpha_t} & \text{if } y_i \neq h_t(x_i) \end{cases}$$

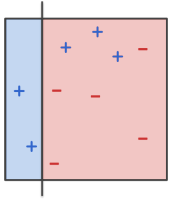
$$= \frac{D_t(i)}{Z_t} \cdot \exp\left(-\alpha_t \cdot y_i h_t(x_i)\right)$$

D_t = Set of weights at round t, one for each example. Think "How much should the weak learner care about this example in its choice of the classifier?"

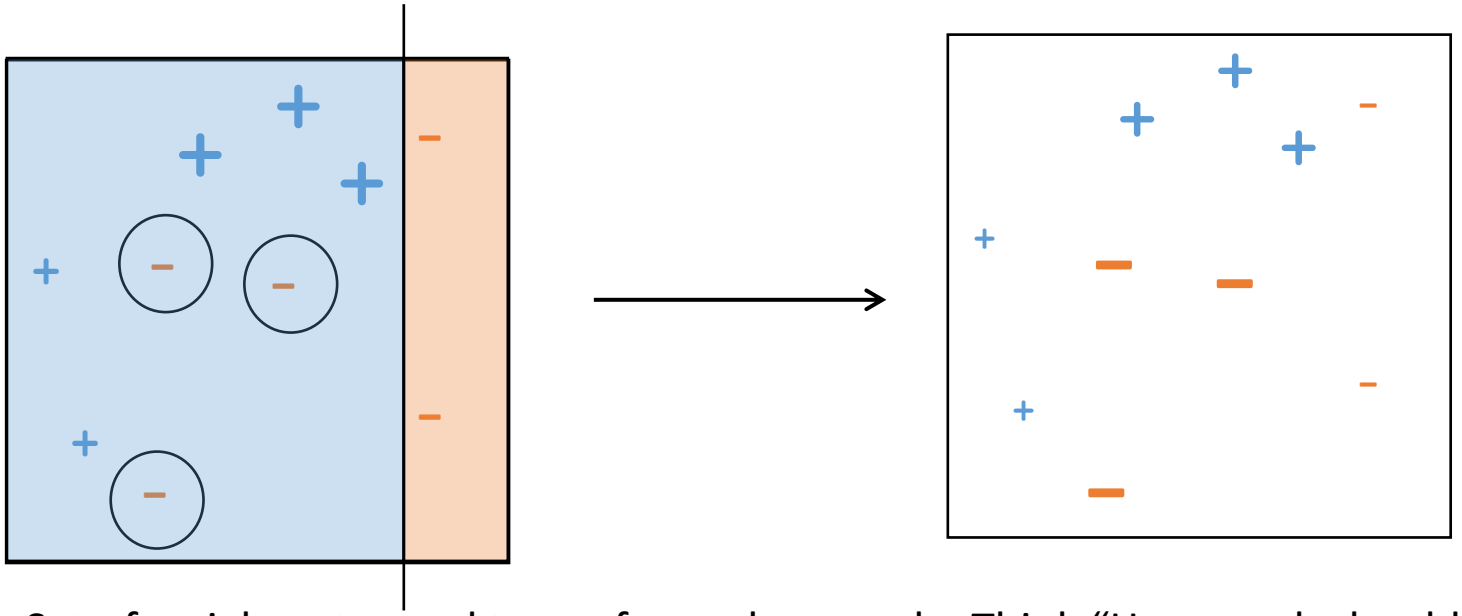
h_2 = A classifier learned on this data. *Has an error* $\epsilon_2 = 0.21$

Why not 0.3? Because while computing error, we will weight each example x_i by its $D_t(i)$

A toy example



h_1

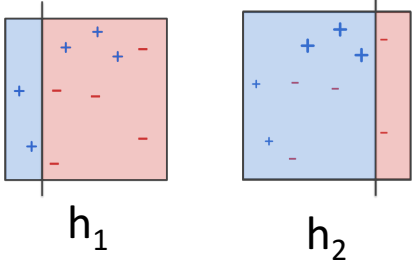


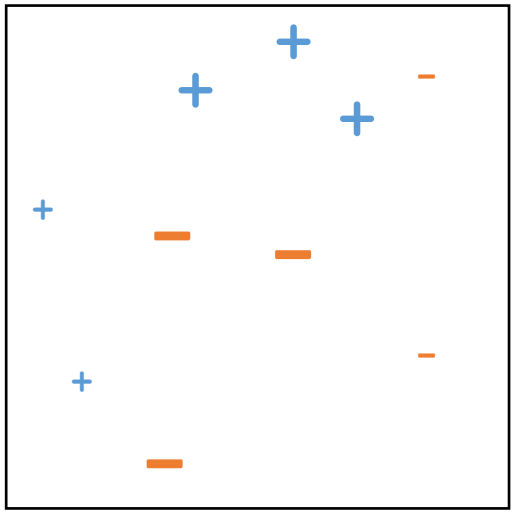
D_t = Set of weights at round t, one for each example. Think "How much should the weak learner care about this example in its choice of the classifier?"

h_2 = A classifier learned on this data. *Has an error* $\epsilon_2 = 0.21$

For the next round, increase the importance of the mistakes and down-weight the examples that h_2 got correctly

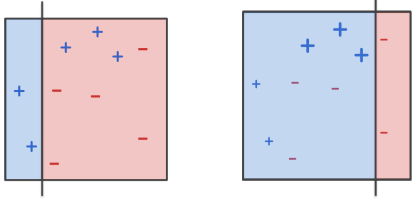
A toy example

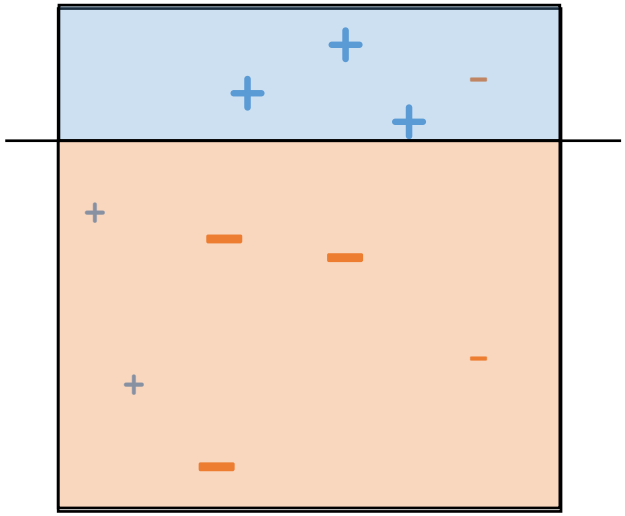




D_t = Set of weights at round t, one for each example. Think "How much should the weak learner care about this example in its choice of the classifier?"

A toy example





D_t = Set of weights at round t, one for each example. Think "How much should the weak learner care about this example in its choice of the classifier?"

h_3 = A classifier learned on this data. *Has an error* $\epsilon_3 = 0.14$

Why not 0.3? Because while computing error, we will weight each example x_i by its $D_t(i)$

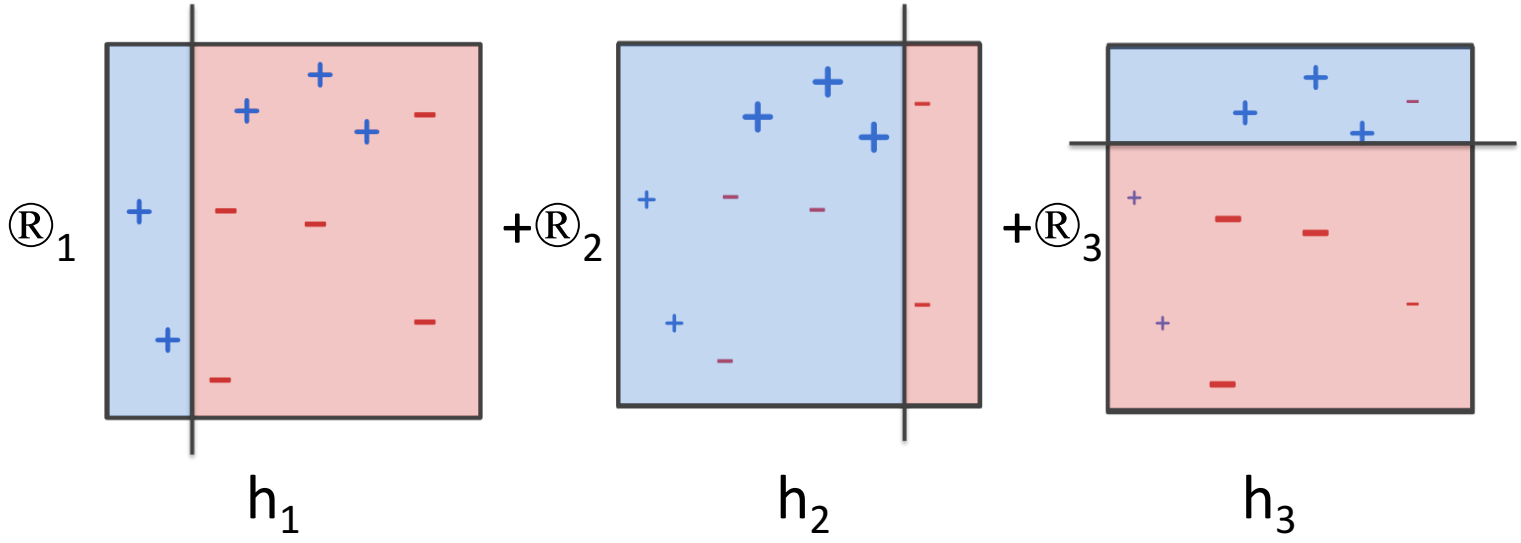
A toy example

$$\alpha_t = \frac{1}{2}\ln\left(\frac{1-\epsilon_t}{\epsilon_t}\right)$$

The final hypothesis is a combination of all the h_i's we have seen so far

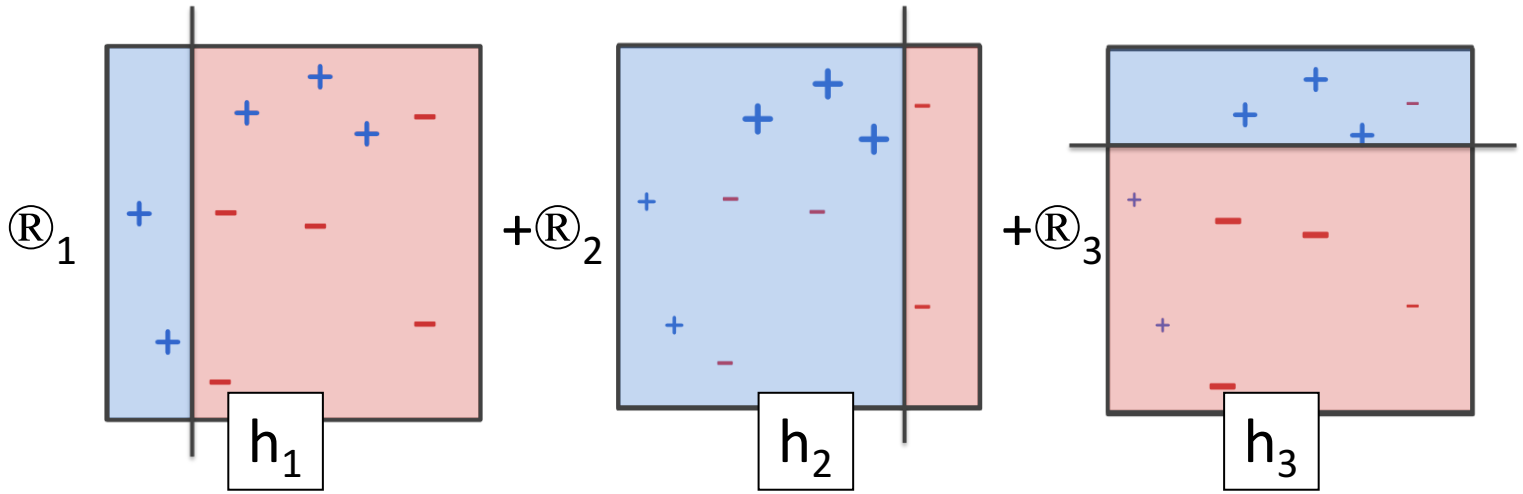
$$H_{final}(x) = \text{sgn}\left(\sum_t \alpha_t h_t(x)\right)$$

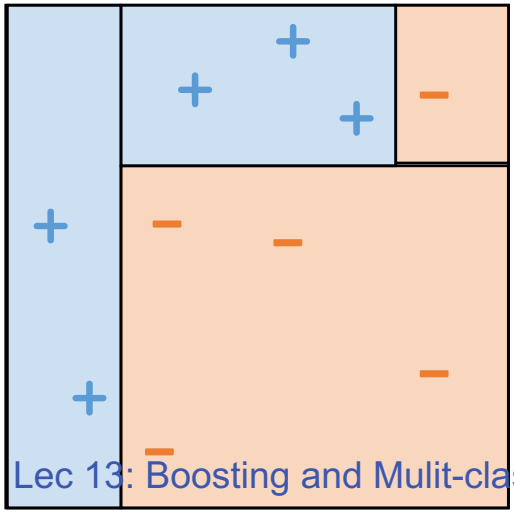
H_{final} =



A toy example: final classifier:

$H_{final} =$





AdaBoost: The full algorithm

Given a training set $(x_1, y_1), \cdots, (x_m, y_m)$

Instances $x_i \in X$ labeled with $y_i \in \{-1, +1\}$

T: a parameter to the learner

1. Initialize $D_1(i) = 1/m$ for all $i = 1, 2, \cdots, m$
2. For $t = 1, 2, \cdots T$:
   1. Find a classifier h_t whose *weighted classification error* is better than chance
   2. Compute its vote

$$\alpha_t = \frac{1}{2} \ln \left(\frac{1 - \epsilon_t}{\epsilon_t} \right)$$

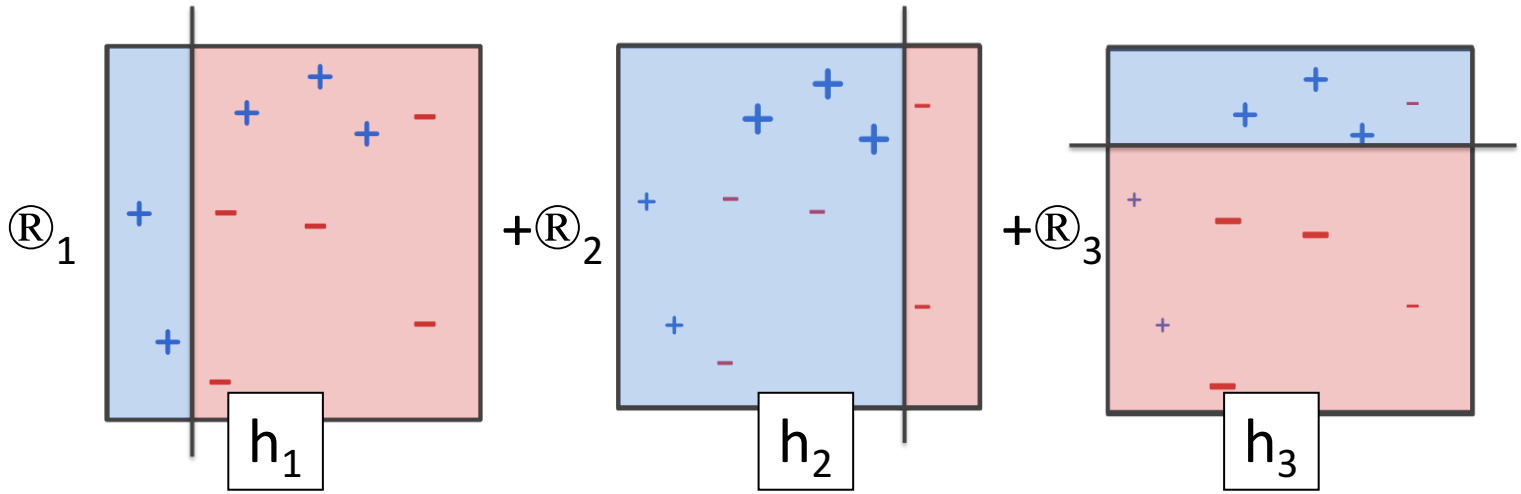
   3. Update the values of the weights for the training examples

$$D_{t+1}(i) = \frac{D_t(i)}{Z_t} \cdot \exp\left(-\alpha_t \cdot y_i h_t(x_i)\right)$$

3. Return the final hypothesis

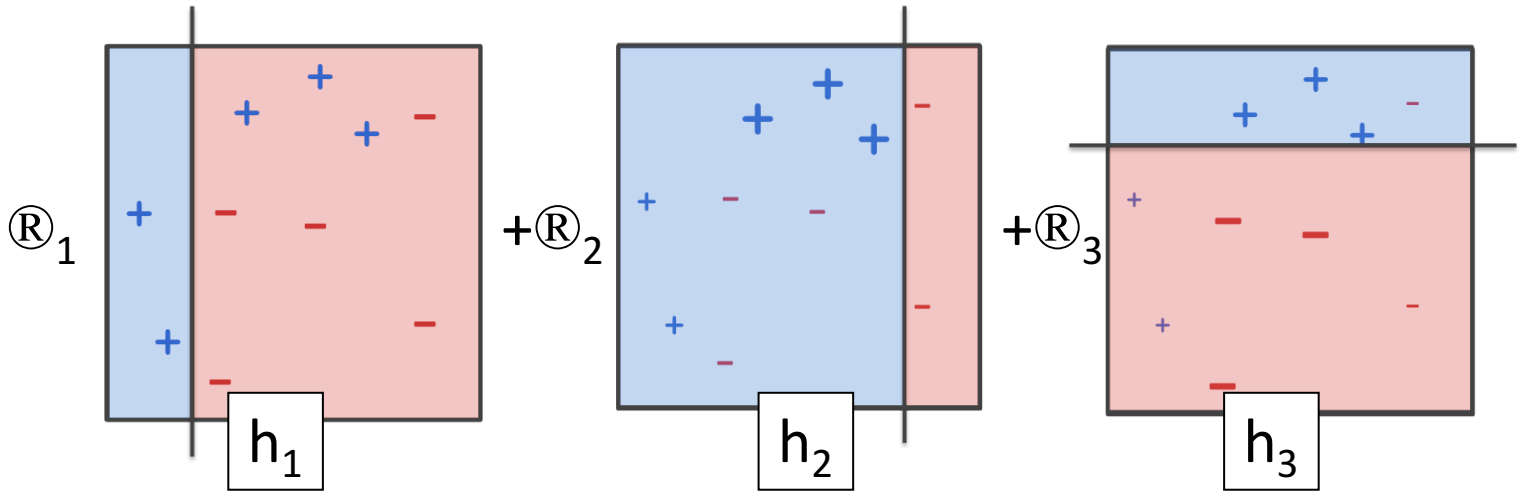
Back to the toy example

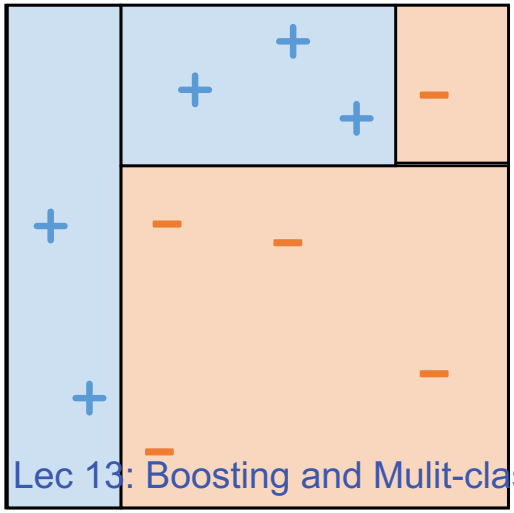
$H_{final} =$



Back to the toy example

$H_{final} =$





Analyzing the training error

Theorem:

- Run AdaBoost for T rounds
- Let ϵ_t = ½ - γ_t
- Let 0 < $\gamma \leq \gamma_t$ for all t
- Then,

$$\text{Training error}(\mathrm{H}_{\text{final}}) \leq e^{-2\gamma^2 T}$$

Analyzing the training error

Theorem:

- Run AdaBoost for T rounds
- Let $\epsilon_t = ½ - \gamma_t$
- Let $0 < \gamma \leq \gamma_t$ for all t
- Then,

We have a weak learner

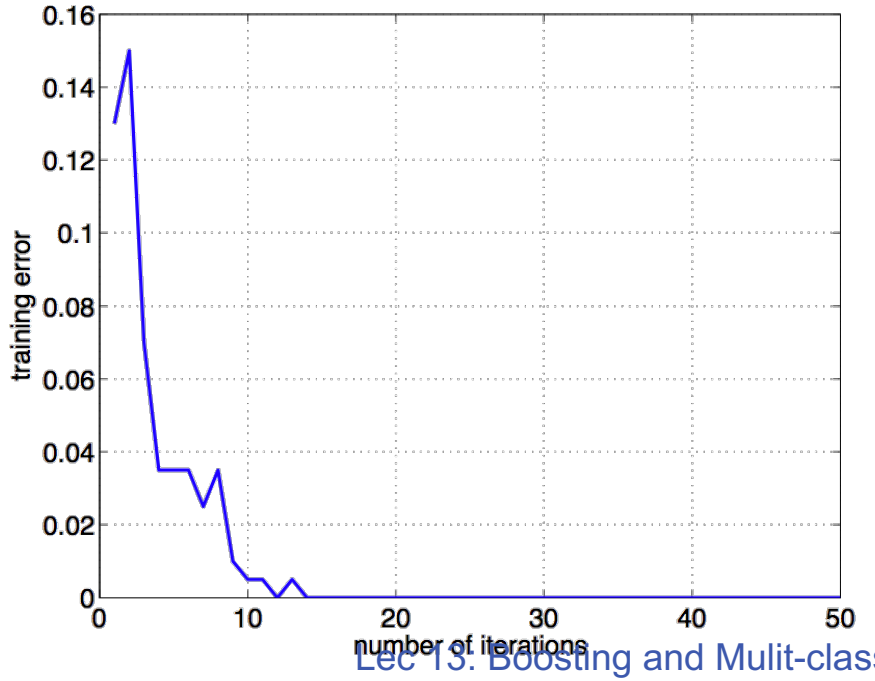
As T increases, the training error drops exponentially

$$\text{Training error}(H_{\text{final}}) \leq e^{-2\gamma^2 T}$$

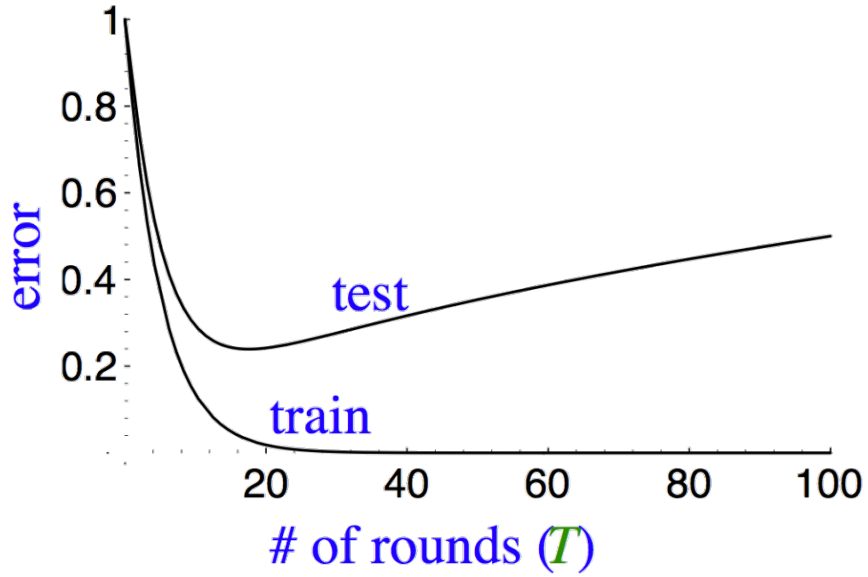
See the note at: https://svivek.com/teaching/machine-learning/fall2017/readings/boosting.pdf

Adaboost: Training error

The training error of the combined classifier decreases exponentially fast if the errors of the weak classifiers (the ϵ_t) are strictly better than chance



What about the test error?



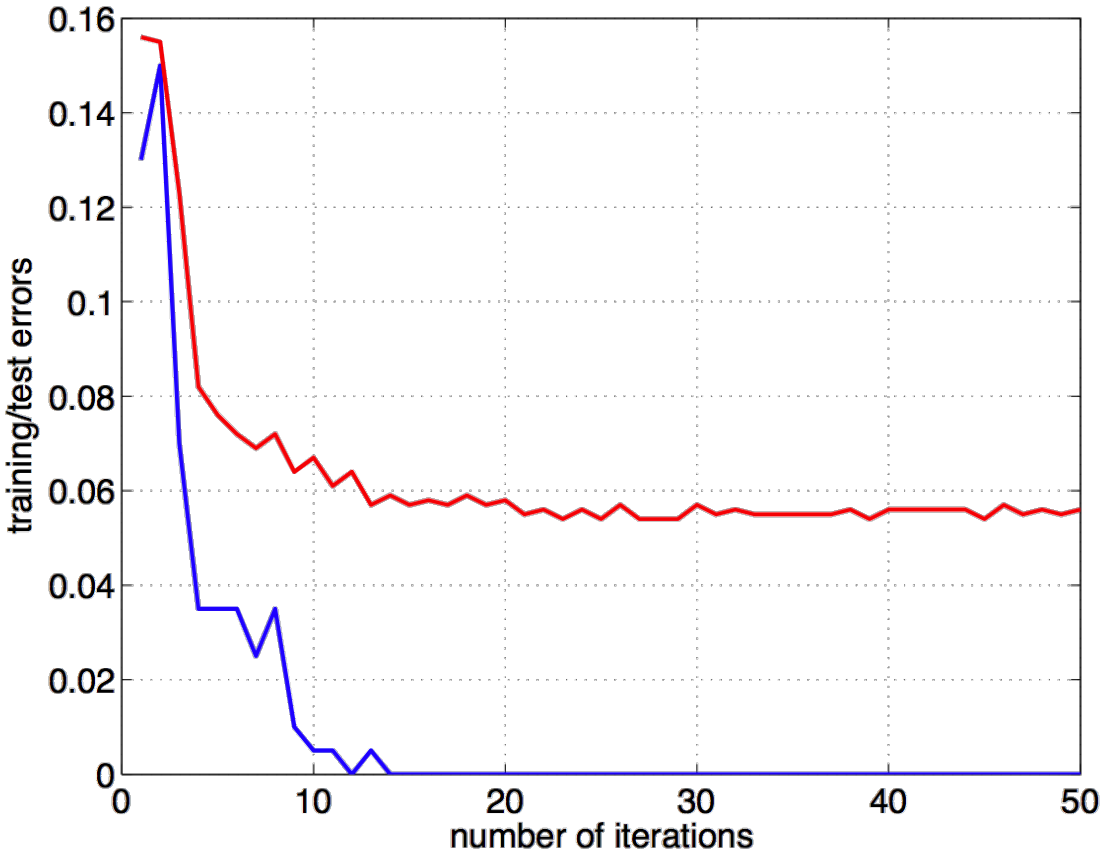
What the theory tells us:

Training error will keep decreasing or reach zero (the AdaBoost theorem)

Test error will increase after the H_{final} becomes too "complex"

- Overfitting

In practice


0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
training/test errors
0
10
20
30
40
50
number of iterations

Multi-class classification

What we have seen so far

- Binary linear classification models
  - Perceptron, SVMs, Logistic regression
- Prediction is simple:
  - Given an example x, prediction is $sgn(w^T \mathrm{x})$
  - Note that all these linear classifier have the same inference rule
  - In logistic regression, we can further estimate the probability

$$P(y = 1|\mathbf{x}, \mathbf{w}) = \frac{e^{\mathbf{w}^T\mathbf{x}}}{1 + e^{\mathbf{w}^T\mathbf{x}}} = \frac{1}{1 + e^{-\mathbf{w}^T\mathbf{x}}}$$

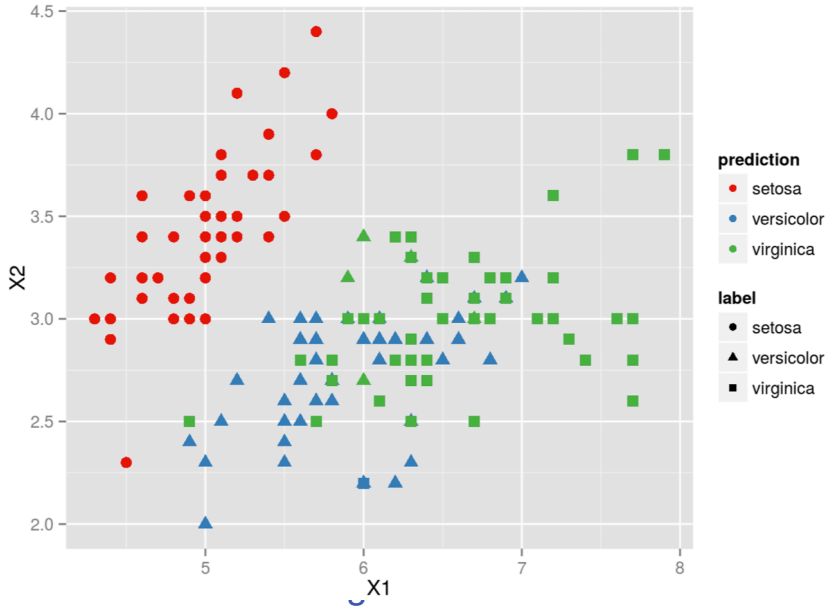
- KNN/Decision tree can easily handle multiclass

This Lecture

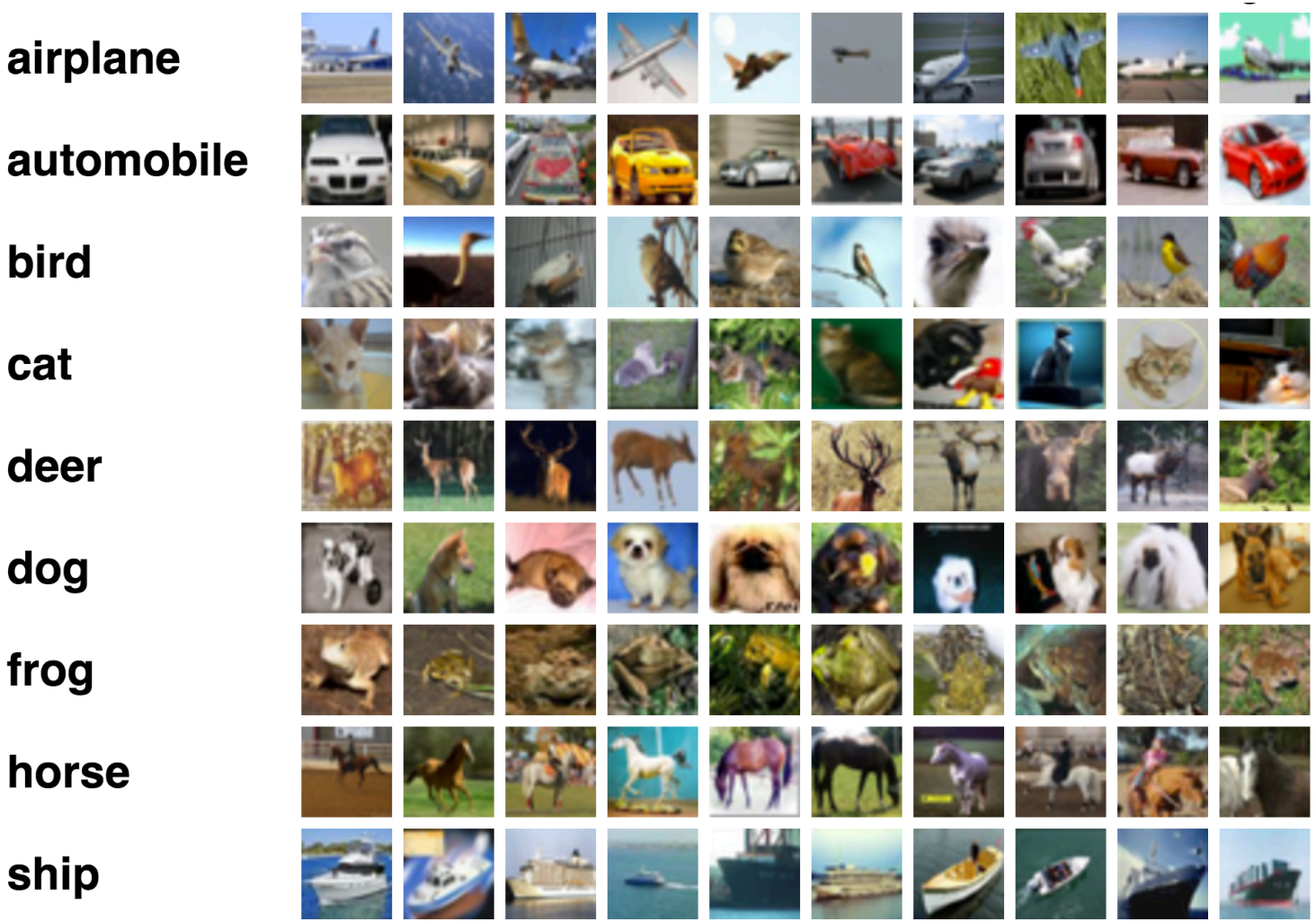
- Multiclass classification overview
- Reducing multiclass to binary
  - One-against-all & One-vs-one
- Training a single classifier
  - Multiclass Perceptron

What is multiclass

- Output $\in \{1,2,3, \ldots K\}$
  - In some cases, output space can be very large (i.e., K is very large)
- Each input belongs to exactly one class (c.f. in multilabel, input belongs to many classes)



Example applications



Two key ideas to solve multiclass

- Reducing multiclass to binary
  - Decompose the multiclass prediction into multiple binary decisions
  - Make final decision based on multiple binary classifiers
- Training a single classifier
  - Minimize the empirical risk
  - Consider all classes simultaneously

Reduction v.s. single classifier

- Reduction
  - Future-proof: binary classification improved so does muti-class
  - Easy to implement
- Single classifier
  - Global optimization: directly minimize the empirical loss; easier for joint prediction
  - Easy to add constraints and domain knowledge

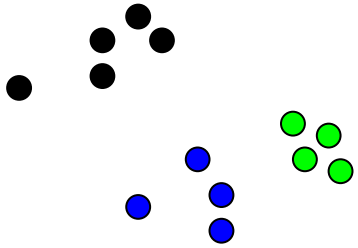
This Lecture

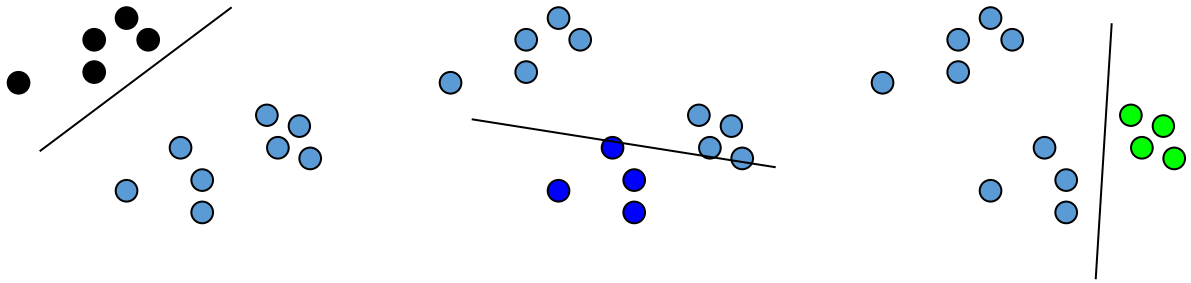
- Multiclass classification overview
- Reducing multiclass to binary
  - One-against-all & One-vs-one
- Training a single classifier
  - Multiclass Perceptron

One against all strategy

One against All learning

- Multiclass classifier
  - Function $f : R^n \rightarrow \{1,2,3,\ldots,k\}$
- Decompose into binary problems



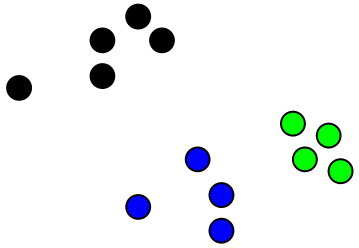


One-again-All learning algorithm

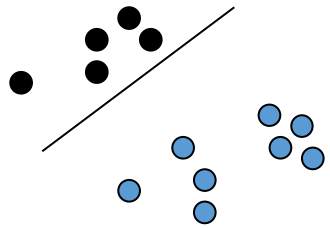
- Learning: Given a dataset $D = \{(x_i, y_i)\}$
  $x_i \in R^n, y_i \in \{1,2,3, \ldots K\}$
- Decompose into K binary classification tasks
  - Learn K models: $w_1, w_2, w_3, \ldots w_K$
  - For class k, construct a binary classification task as:
    - Positive examples: Elements of D with label k
    - Negative examples: All other elements of D
  - The binary classification can be solved by any algorithm we have seen

One against All learning

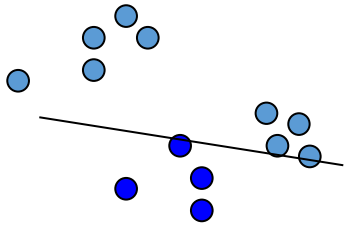
- Multiclass classifier
  - Function $f : R^n \rightarrow \{1,2,3,\ldots,k\}$
- Decompose into binary problems



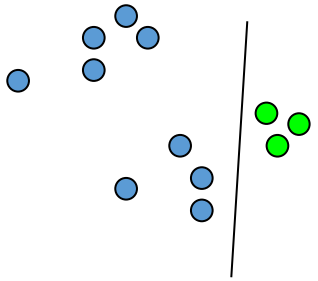
Ideal case: only the correct label will have a positive score



$w_{black}^T x > 0$



$w_{blue}^T x > 0$



$w_{green}^T x > 0$

One-again-All Inference

- Learning: Given a dataset $D = \{(x_i, y_i)\}$
  $x_i \in R^n, y_i \in \{1,2,3, \dots K\}$
- Decompose into K binary classification tasks
  - Learn K models: $w_1, w_2, w_3, \dots w_K$
- Inference: "Winner takes all"
  - $\hat{y} = \text{argmax}_{y \in \{1,2,\dots K\}} \, w_y^T \, x$

For example: $\text{y} = \text{argmax}(w_{black}^T \, x \, , \;\; w_{blue}^T \, x, \;\; w_{green}^T \;\; x)$

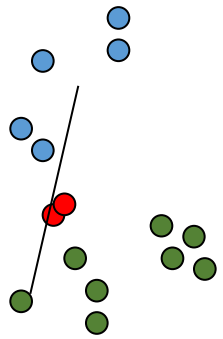
  - An instance of the general form

$$\hat{y} = \text{argmax}_{\boldsymbol{y} \in \mathcal{Y}} \, f(\boldsymbol{y}; \boldsymbol{w}, \boldsymbol{x})$$

$$w = \{w_1, w_2, \dots w_K\}, \; f(\boldsymbol{y}; \boldsymbol{w}, \boldsymbol{x}) = \boldsymbol{w}_y^T \, x$$

One-again-All analysis

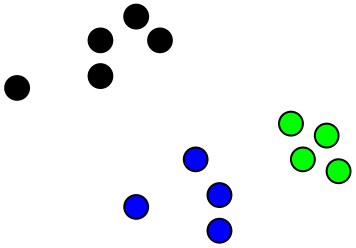
- Not always possible to learn
  - Assumption: each class individually separable from all the others
- No theoretical justification
  - Need to make sure the range of all classifiers is the same – we are comparing scores produced by K classifiers trained independently.
- Easy to implement; work well in practice

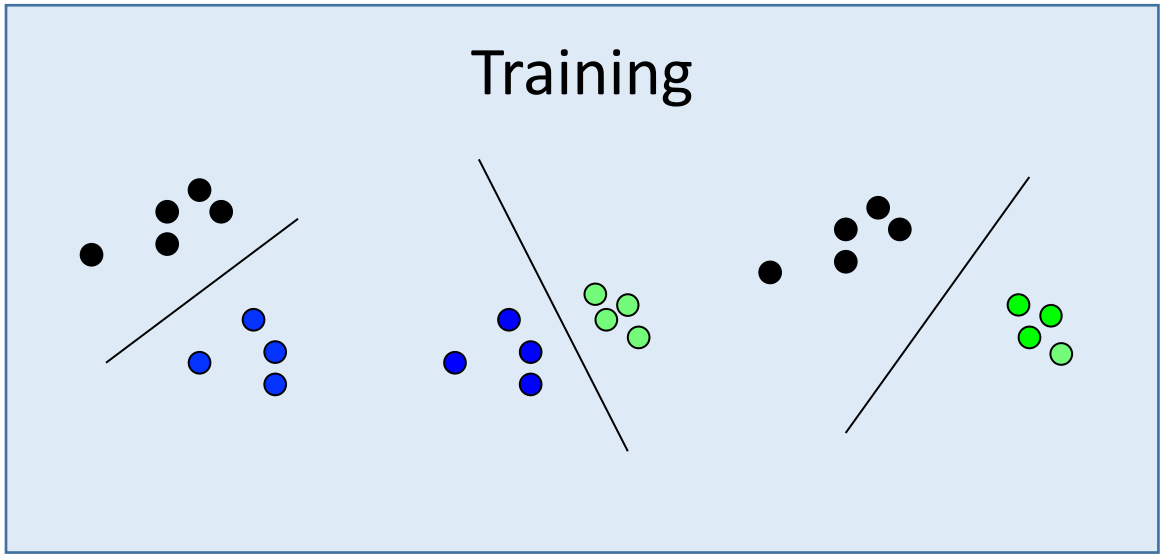


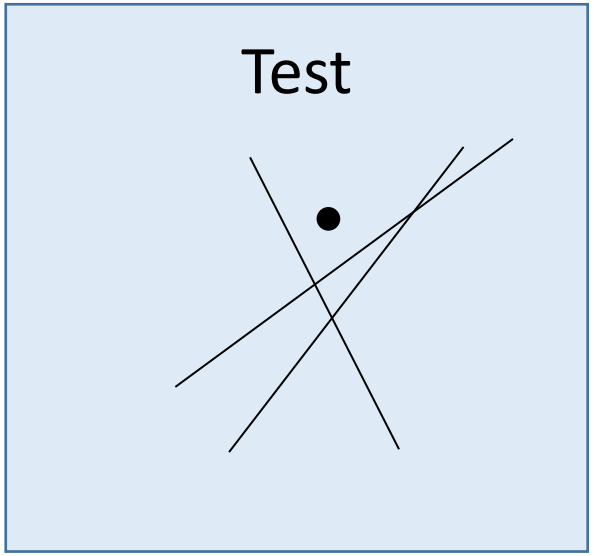
One v.s. One (All against All) strategy

One v.s. One learning

- Multiclass classifier
  - Function $f : R^n \rightarrow \{1,2,3,\ldots,k\}$
- Decompose into binary problems







One-v.s-One learning algorithm

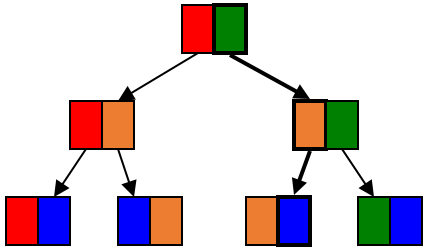
- Learning: Given a dataset $D = \{(x_i, y_i)\}$
  $x_i \in R^n, y_i \in \{1,2,3, \ldots K\}$
- Decompose into C(K,2) binary classification tasks
  - Learn C(K,2) models: $w_1, w_2, w_3, \ldots w_{K*(K-1)/2}$
  - For each class pair (i,j), construct a binary classification task as:
    - Positive examples: Elements of D with label i
    - Negative examples Elements of D with label j
    - The binary classification can be solved by any algorithm we have seen

One-v.s-One Inference algorithm

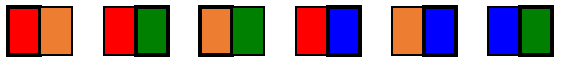
- Decision Options:
  - More complex; each label gets k-1 votes
  - Output of binary classifier may not cohere.
  - Majority: classify example x to take label i if i wins on x more often than j (j=1,…k)
  - A tournament: start with n/2 pairs; continue with winners

Classifying with One-vs-one

Tournament



Majority Vote



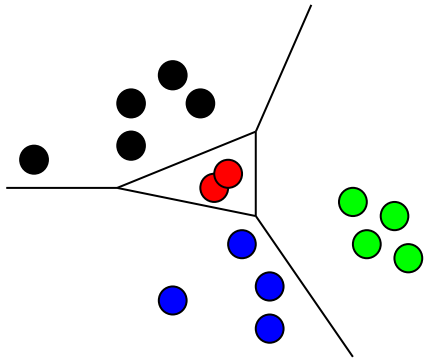
1 red, 2 yellow, 2 green

➔ ?

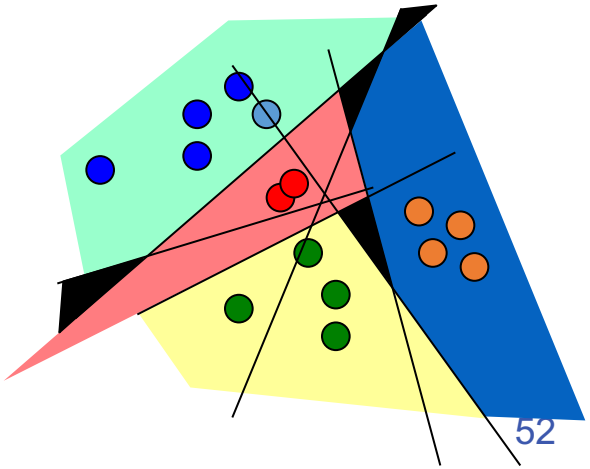
All are post-learning and *might* cause weird stuff

One-v.s.-one Assumption

- Every pair of classes is separable



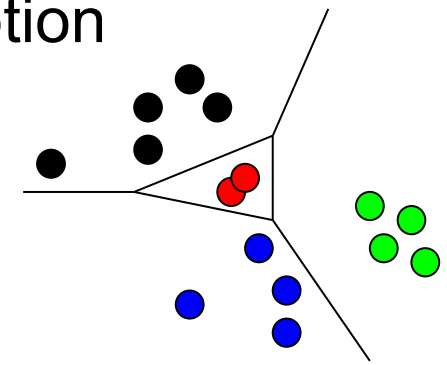
It is possible to separate all k classes with the $O(k^2)$ classifiers



Decision Regions

Comparisons

- One against all
  - O(K) weight vectors to train and store
  - Training set of the binary classifiers may unbalanced
  - Less expressive; make a strong assumption



- One v.s. One (All v.s. All)
  - O(K^2) weight vectors to train and store
  - Size of training set for a pair of labels could be small
    ⇒ overfitting of the binary classifiers
  - Need large space to store model

Problems with Decompositions

- Learning optimizes over *local* metrics
  - Does not guarantee good *global* performance
  - We don't care about the performance of the *local* classifiers
- Poor decomposition $\Rightarrow$ poor performance
  - Difficult local problems
  - Irrelevant local problems
- Efficiency: e.g., All vs. All vs. One vs. All
- Not clear how to generalize multi-class to problems with a very large # of output

Still an ongoing research direction

Key questions:

- How to deal with large number of classes
- How to select "right samples" to train binary classifiers

- Error-correcting tournaments
  [Beygelzimer, Langford, Ravikumar 09]
- Logarithmic Time One-Against-Some
  [Daume, Karampatziakis, Langford, Mineiro 16]
- Label embedding trees for large multi-class tasks.
  [Bengio, Weston, Grangier 10]
- …

Decomposition methods: Summary

- General Ideas:
  - Decompose the multiclass problem into many binary problems
  - Prediction depends on the decomposition
    - Constructs the multiclass label from the output of the binary classifiers
- Learning optimizes local correctness
  - Each binary classifier don't need to be globally correct and isn't aware of the prediction procedure

This Lecture

- Multiclass classification overview
- Reducing multiclass to binary
  - One-against-all & One-vs-one
- Training a single classifier
  - Multiclass Perceptron

Revisit One-again-All learning algorithm

- Learning: Given a dataset $D = \{(x_i, y_i)\}$
  $x_i \in R^n, y_i \in \{1,2,3, \ldots K\}$
- Decompose into K binary classification tasks
  - Learn K models: $w_1, w_2, w_3, \ldots w_K$
  - w_k: separate class k from others
- Prediction

$$\hat{y} = \text{argmax}_{y \in \{1,2,\ldots K\}} \; w_y^T \; x$$

Observation

- At training time, we require $w_i^T x$ to be positive for examples of class i.
- Really, all we need is for $w_i^T x$ to be more than all others ⇒ this is a weaker requirement

For examples with label i, we need

$$w_i^T x > w_j^T x \qquad \text{for all } j$$

Perceptron-style algorithm

For examples with label i, we need

$$w_i^T x > w_j^T x \quad \text{for all } j$$

- For each training example (x, y)
  - If for some y', $w_y^T x \leq w_{y'}^T x$ mistake!
    - $w_y \leftarrow w_y + \eta x$ update to promote y
    - $w_{y'} \leftarrow w_{y'} - \eta x$ update to demote y'

Why add ηx to w_y promote label y:

Before update $s(y) = < w_y^{old}, x >$

After update

$$\begin{aligned} s(y) &= < w_y^{new}, x > \\ &= < w_y^{old} + \eta x, x > \\ &= < w_y^{old}, x > + \eta < x, x > \end{aligned}$$

Note! $< x, x > = x^T x > 0$

A Perceptron-style Algorithm

Given a training set $\mathcal{D} = \{(\boldsymbol{x}, y)\}$

Initialize $\boldsymbol{w} \leftarrow \mathbf{0} \in \mathbb{R}^n$

For epoch $1 \ldots T$:

For $(\boldsymbol{x}, y)$ in $\mathcal{D}$:

For $y' \neq y$

if $w_y^T x < w_{y'}^T x$ make a mistake

$w_y \leftarrow w_y + \eta x$ promote y

$w_{y'} \leftarrow w_{y'} - \eta x$ demote y'

Return $\boldsymbol{w}$

How to analyze this algorithm and simplify the update rules?

Prediction: $\text{argmax}_y \; w_y^T x$

What you need to know

- Reducing multiclass to binary
  - One-against-all & One-vs-one
- Training a single classifier
  - Multiclass Perceptron