Machine Learning Recap (multiclass classification)

Wei Xu

(many slides from Greg Durrett, Vivek Srikumar, Stanford CS231n)

Multiclass Fundamentals

Text Classification

A Cancer Conundrum: Too Many Drug Trials, Too Few Patients

Breakthroughs in immunotherapy and a rush to develop profitable new treatments have brought a crush of clinical trials scrambling for patients.

By GINA KOLATA

→ Health

Yankees and Mets Are on Opposite Tracks This Subway Series

As they meet for a four-game series, the Yankees are playing for a postseason spot, and the most the Mets can hope for is to play spoiler.

By FILIP BONDY

→ Sports

~20 classes

Image Classification

Dog

Car

- Thousands of classes (ImageNet)

Entity Linking

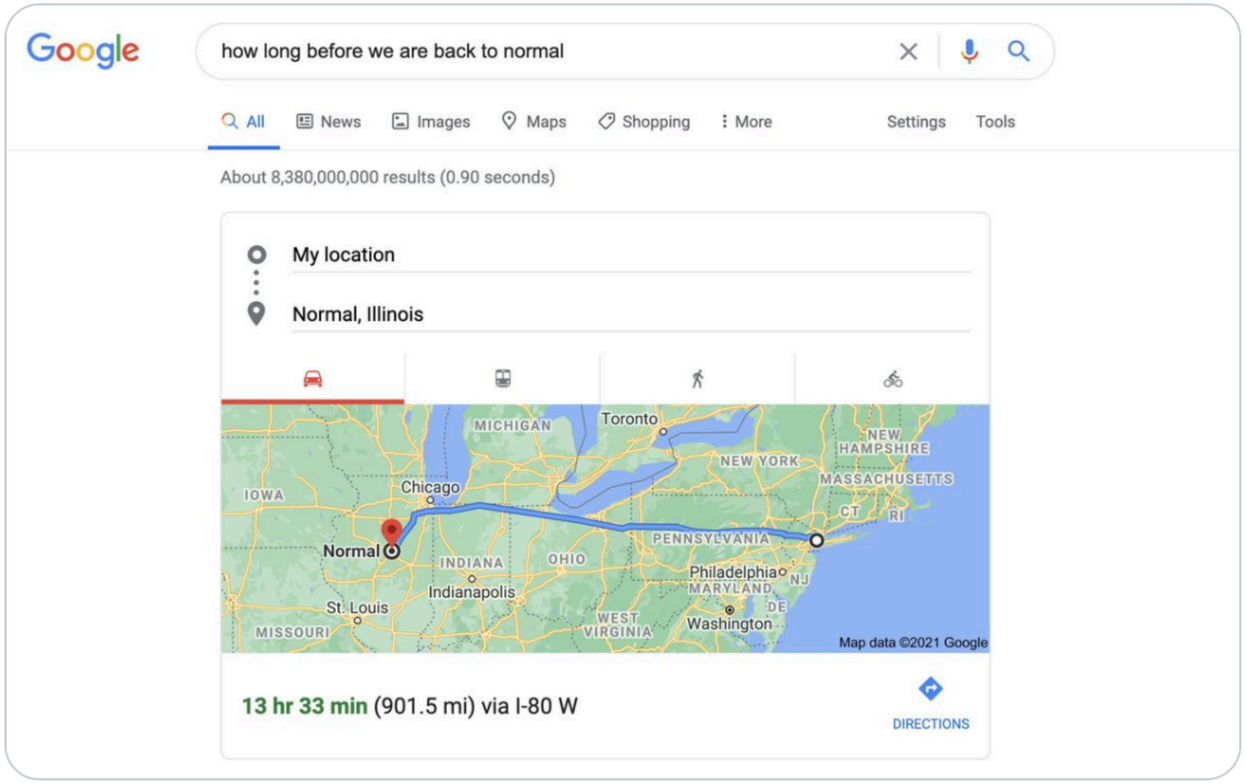
Although he originally won the event, the United States Anti-Doping Agency announced in August 2012 that they had disqualified **Armstrong** from his seven consecutive Tour de France wins from 1999–2005.

- 4,500,000 classes (all articles in Wikipedia)

Entity Linking

Kara Schechtman
@karaschechtman

this is just decidedly not what I meant

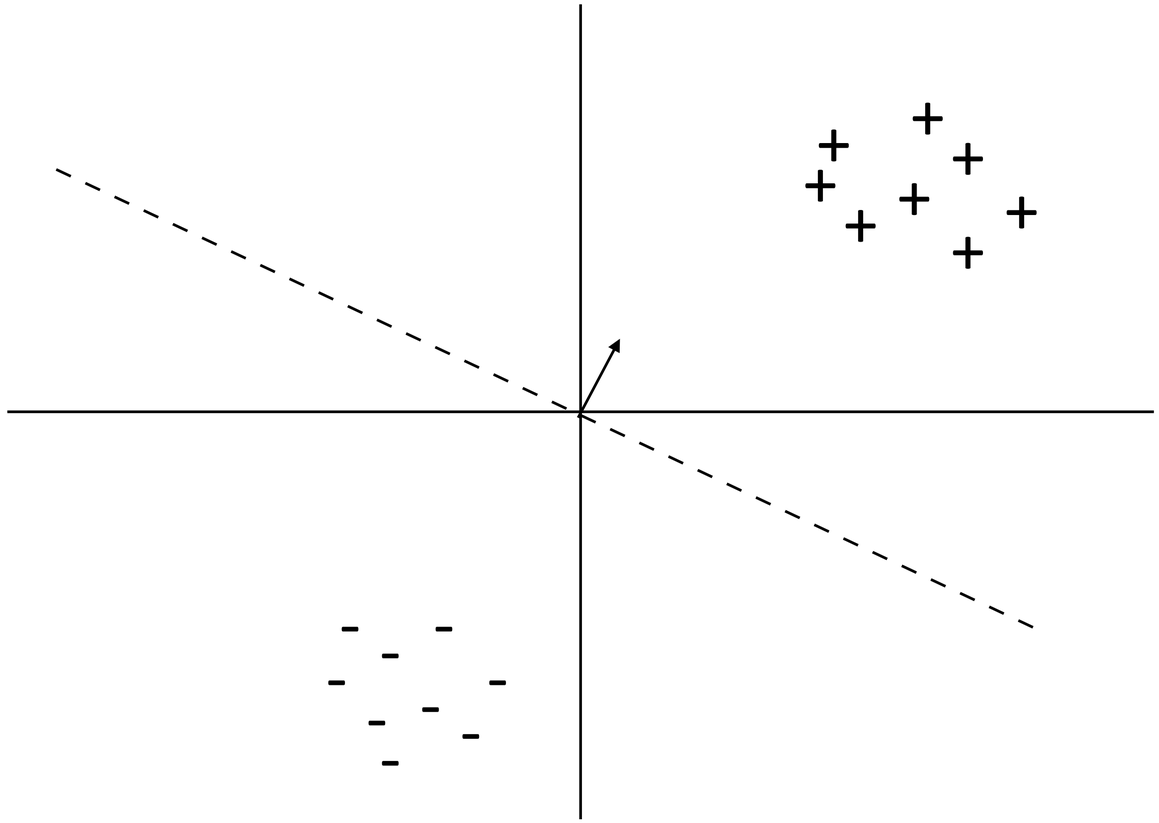


8:58 PM · Jan 30, 2021 · Twitter Web App

80 Retweets **16** Quote Tweets **700** Likes

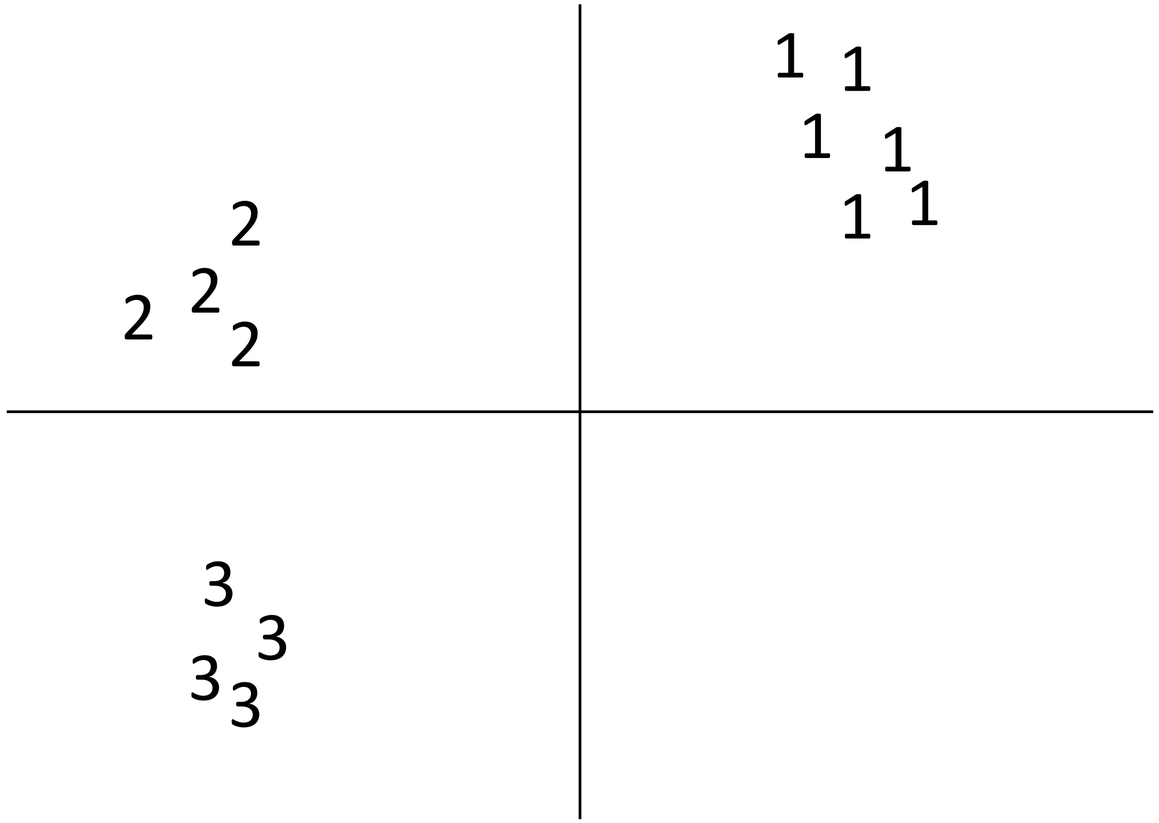
Binary Classification

- Binary classification: one weight vector defines positive and negative classes



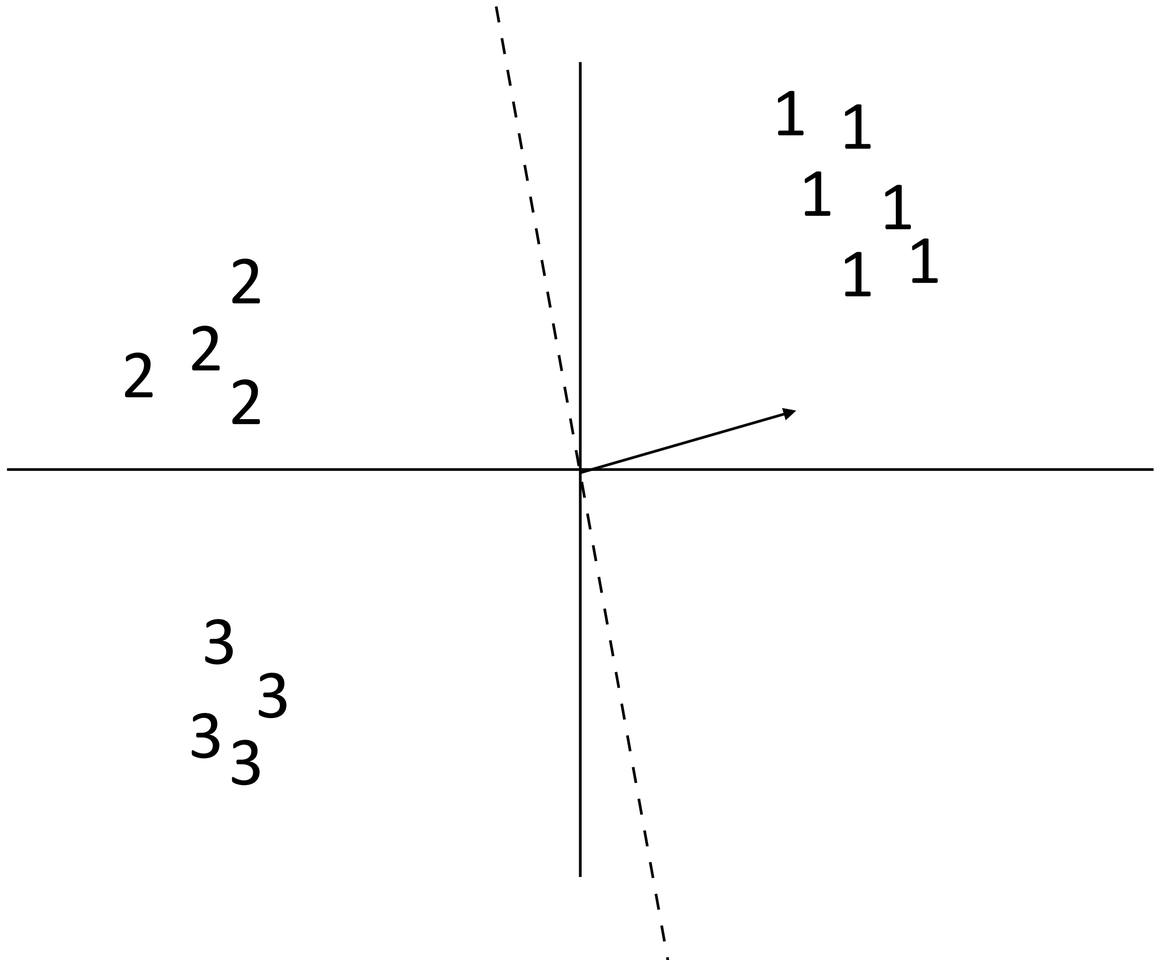
Multiclass Classification

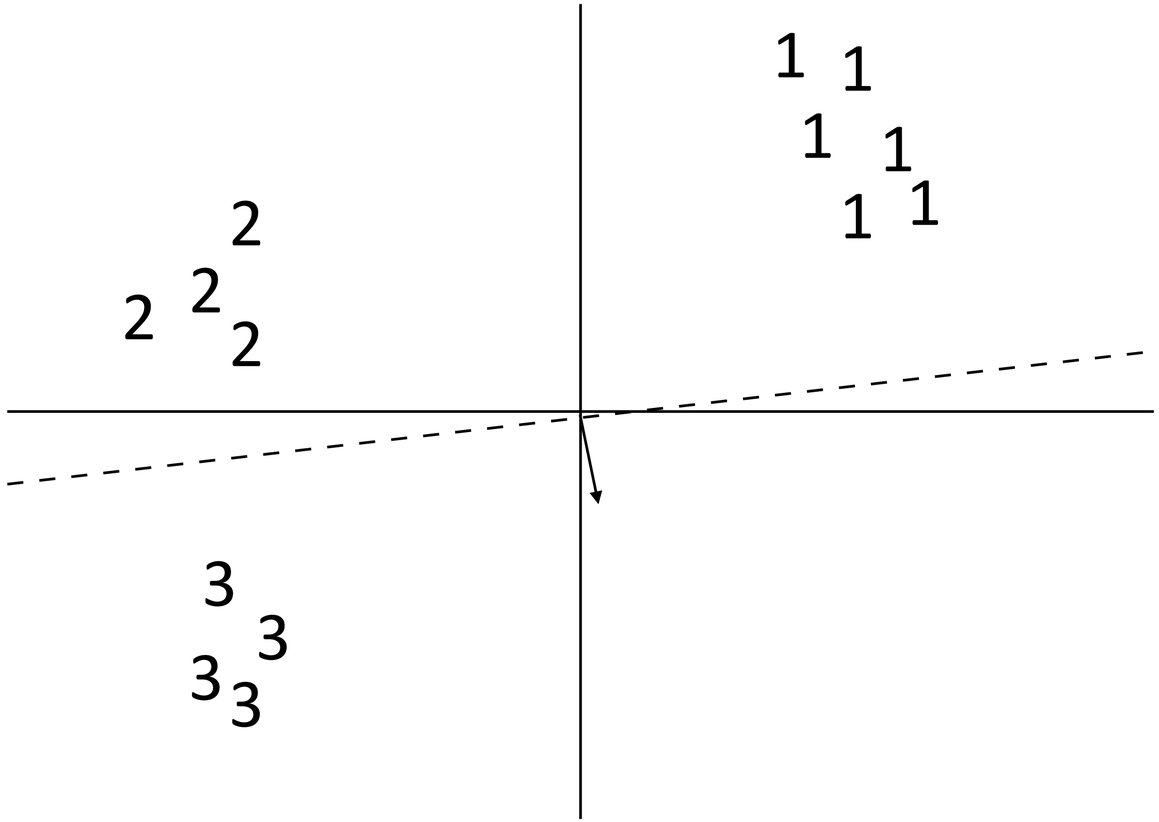
- Can we just use binary classifiers here?



Multiclass Classification

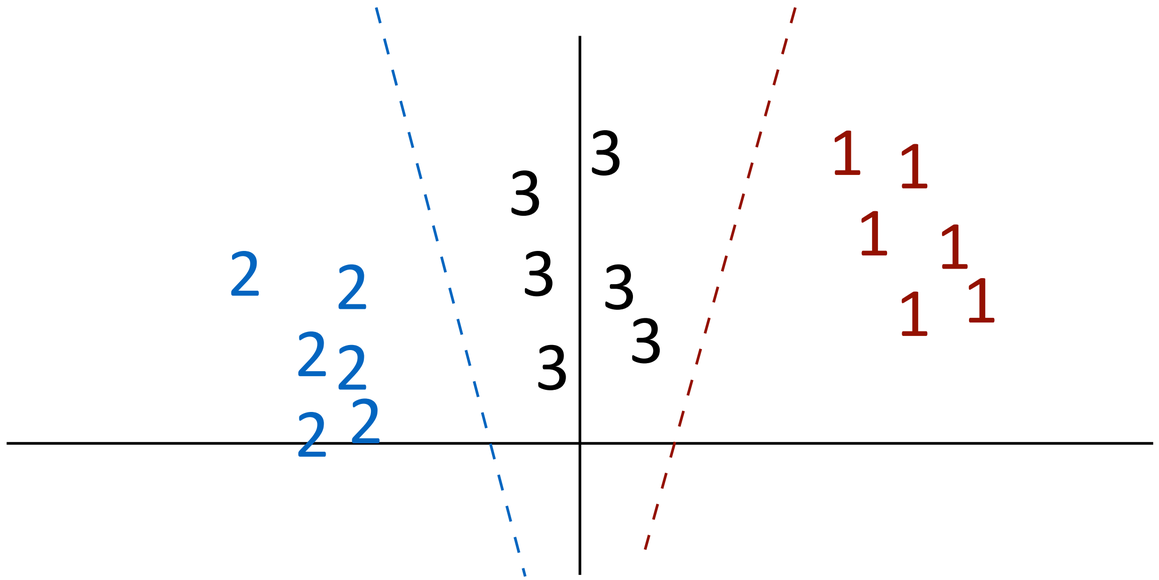
- One-vs-all: train *k* classifiers, one to distinguish each class from all the rest
- How do we reconcile multiple positive predictions? Highest score?





Multiclass Classification

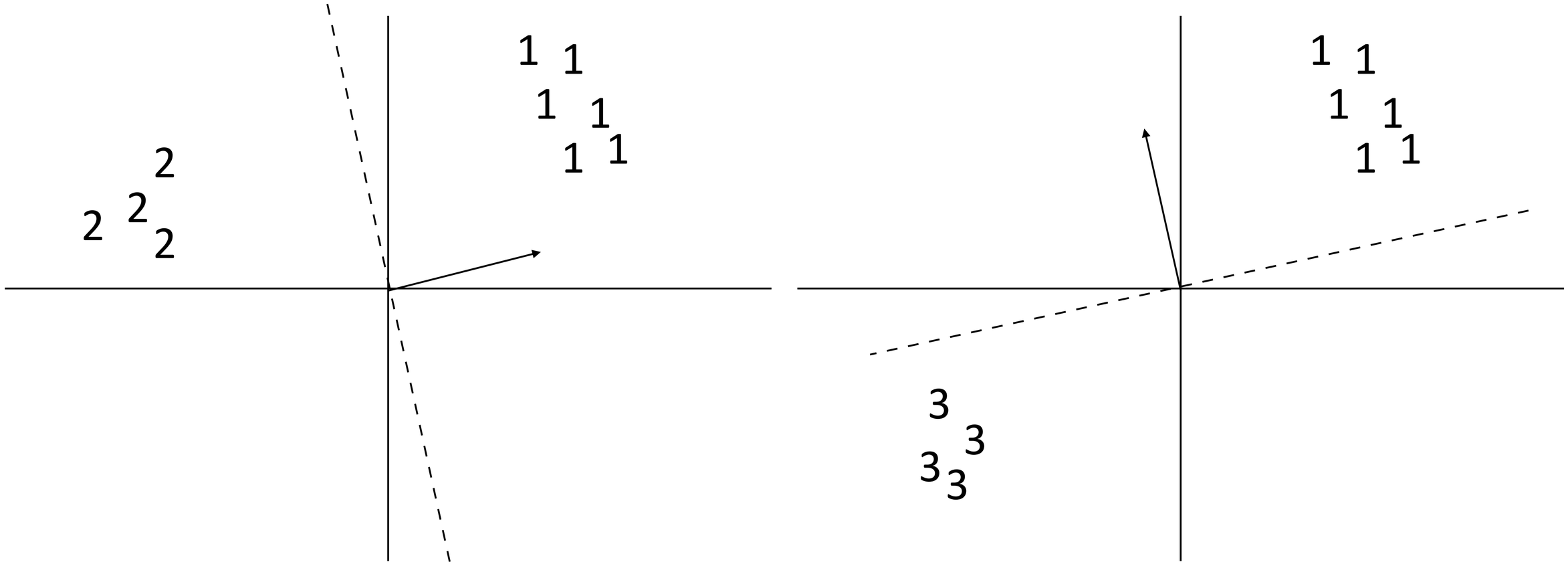
- Not all classes may even be separable using this approach



- Can separate 1 from 2+3 and 2 from 1+3 but not 3 from the others (with these features)

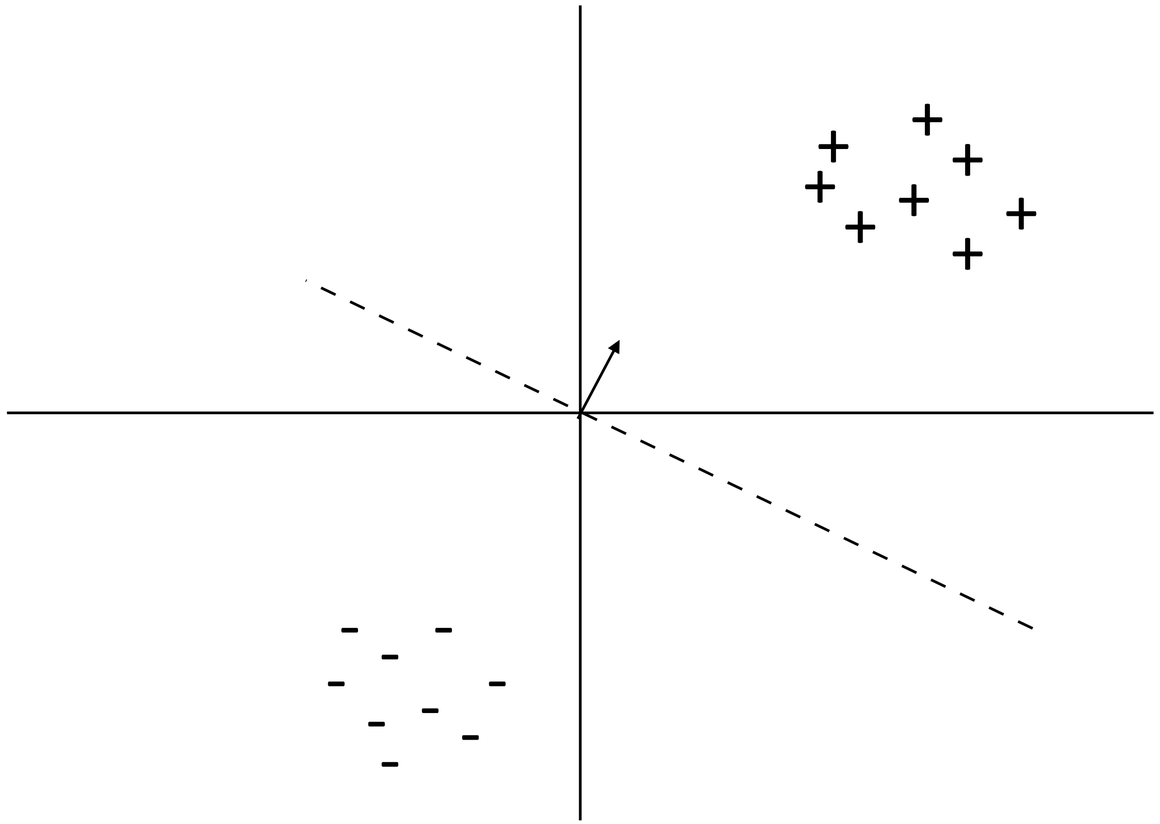
Multiclass Classification

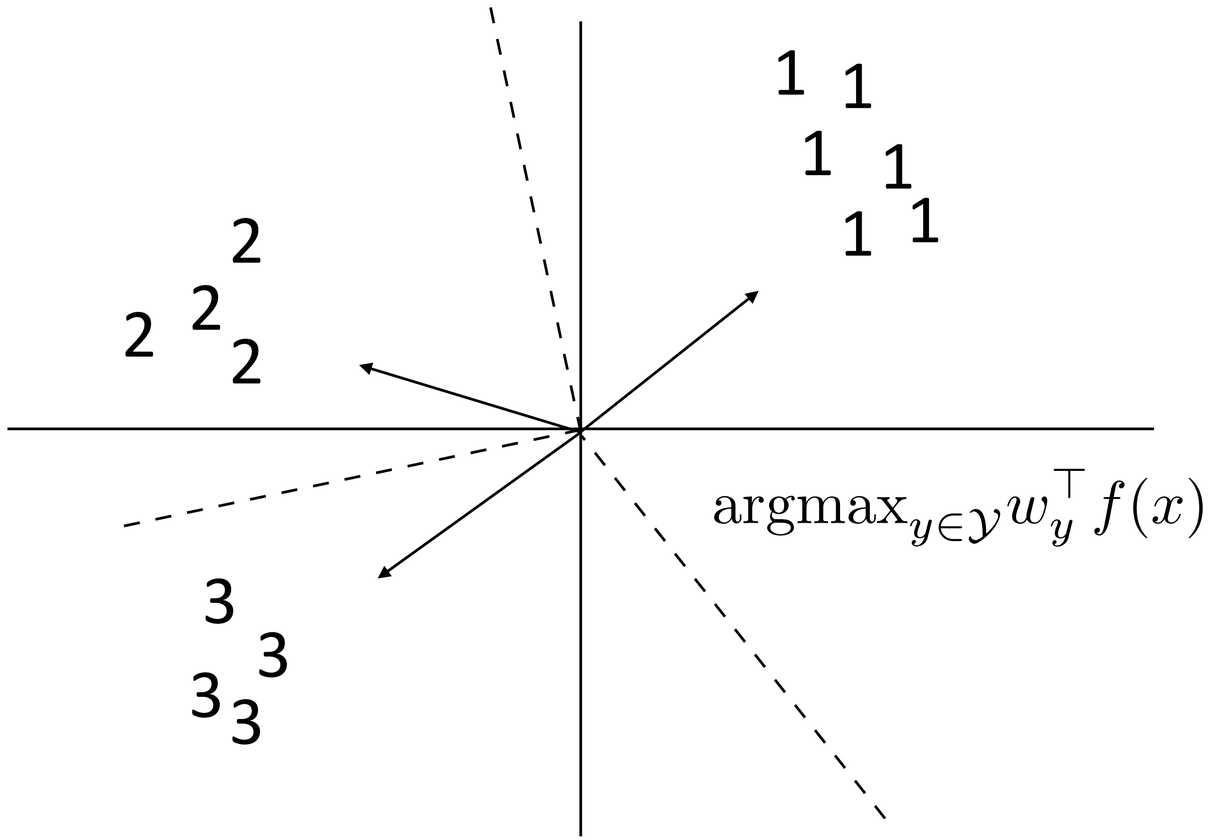
- All-vs-all: train n(n-1)/2 classifiers to differentiate each pair of classes
- Again, how to reconcile?



Multiclass Classification

- Binary classification: one weight vector defines both classes
- Multiclass classification: different weights and/or features per class





Multiclass Classification

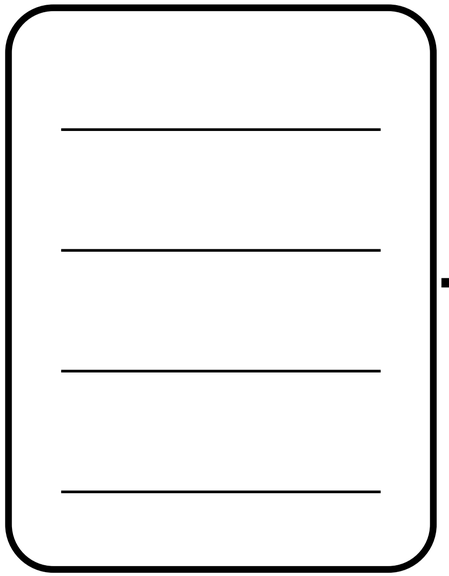
- Formally: instead of two labels, we have an output space $\mathcal{Y}$ containing a number of possible classes
  - Same machinery that we'll use later for exponentially large output spaces, including sequences and trees
- Decision rule: $\text{argmax}_{y \in \mathcal{Y}} w^\top f(x, y)$

features depend on choice of label now! note: this isn't the gold label

  - Multiple feature vectors, one weight vector
  - Can also have one weight vector per class: $\text{argmax}_{y \in \mathcal{Y}} w_y^\top f(x)$
  - The single weight vector approach will generalize to structured output spaces, whereas per-class weight vectors won't

Structured Prediction

Text



Labels

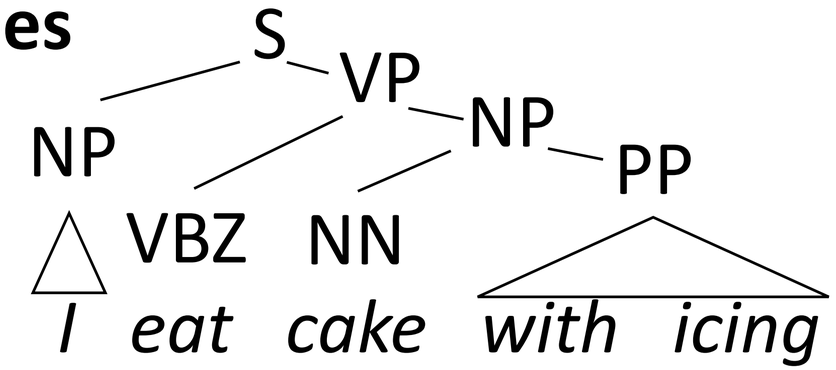
the movie was good +

Beyoncé had one of the best videos of all time **subjective**

Sequences/tags

PERSON *Tom Cruise* *stars in the new* **MOVIE** *Mission Impossible* *film*

Trees



$\lambda x.\ flight(x) \wedge dest(x)=Miami$

flights to Miami

Part-of-speech (POS) Tags

CC	conjunction, coordinating	and both but either or
CD	numeral, cardinal	mid-1890 nine-thirty 0.5 one
DT	determiner	a all an every no that the
EX	existential there	there
FW	foreign word	gemeinschaft hund ich jeux
IN	preposition or conjunction, subordinating	among whether out on by if
JJ	adjective or numeral, ordinal	third ill-mannered regrettable
JJR	adjective, comparative	braver cheaper taller
JJS	adjective, superlative	bravest cheapest tallest
MD	modal auxiliary	can may might will would
NN	noun, common, singular or mass	cabbage thermostat investment subhumanity
NNP	noun, proper, singular	Motown Cougar Yvette Liverpool
NNPS	noun, proper, plural	Americans Materials States
NNS	noun, common, plural	undergraduates bric-a-brac averages
POS	genitive marker	' 's
PRP	pronoun, personal	hers himself it we them
PRP$	pronoun, possessive	her his mine my our ours their thy your
RB	adverb	occasionally maddeningly adventurously
RBR	adverb, comparative	further gloomier heavier less-perfectly
RBS	adverb, superlative	best biggest nearest worst
RP	particle	aboard away back by on open through
TO	"to" as preposition or infinitive marker	to
UH	interjection	huh howdy uh whammo shucks heck
VB	verb, base form	ask bring fire see take
VBD	verb, past tense	pleaded swiped registered saw
VBG	verb, present participle or gerund	stirring focusing approaching erasing
VBN	verb, past participle	dilapidated imitated reunifed unsettled
VBP	verb, present tense, not 3rd person singular	twist appear comprise mold postpone
VBZ	verb, present tense, 3rd person singular	bases reconstructs marks uses
WDT	WH-determiner	that what whatever which whichever
WP	WH-pronoun	that what whatever which who whom
WP$	WH-pronoun, possessive	whose
WRB	Wh-adverb	however whenever where why

Slide credit: Yoav Artzi

Feature Extraction

Block Feature Vectors

- Decision rule: $\text{argmax}_{y \in \mathcal{Y}} w^\top f(x, y)$

too many drug trials, too few patients → Health / Sports / Science

- Base feature function:

$f(x)$ = I[contains *drug*], I[contains *patients*], I[contains *baseball*] = [1, 1, 0]

feature vector blocks for each label

$f(x, y = \text{Health}) =$ [1, 1, 0, 0, 0, 0, 0, 0, 0]

I[contains *drug* & label = Health]

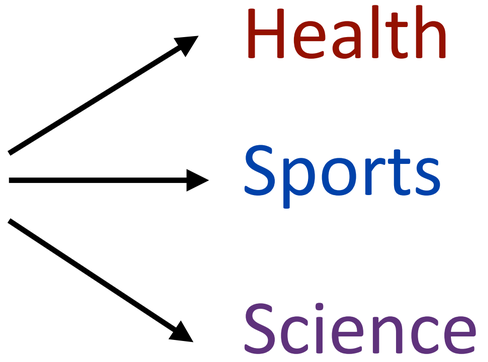
$f(x, y = \text{Sports}) =$ [0, 0, 0, 1, 1, 0, 0, 0, 0]

$f(x, y = \text{Science}) =$ [0, 0, 0, 0, 0, 0, 1, 1, 0]

- Equivalent to having three weight vectors in this case $\text{argmax}_{y \in \mathcal{Y}} w_y^\top f(x)$

Making Decisions

too many drug trials, too few patients



$f(x)$ = I[contains *drug*], I[contains *patients*], I[contains *baseball*]

$f(x, y = \text{Health}) = [1, 1, 0, 0, 0, 0, 0, 0, 0]$

$f(x, y = \text{Sports}) = [0, 0, 0, 1, 1, 0, 0, 0, 0]$

$f(x, y = \text{Science}) = [0, 0, 0, 0, 0, 0, 1, 1, 0]$

"word drug in Science article" = +1.1

$w = [+2.1, +2.3, -5, -2.1, -3.8, 0, +1.1, -1.7, -1.3]$

$w^\top f(x, y)$ = Health: +4.4 Sports: -5.9 Science: -0.6

↖ argmax

Another example: POS tagging

- Classify *blocks* as one of 33 POS tags
- Example *x*: sentence with a word (in this case, *blocks*) highlighted
- Extract features with respect to this word:

$f(x, y=\text{VBZ}) = \text{I}[\text{curr\_word}=\textit{blocks} \;\&\; \text{tag} = \text{VBZ}],$
$\text{I}[\text{prev\_word}=\textit{router} \;\&\; \text{tag} = \text{VBZ}]$
$\text{I}[\text{next\_word}=\textit{the} \;\&\; \text{tag} = \text{VBZ}]$
$\text{I}[\text{curr\_suffix}=\textit{s} \;\&\; \text{tag} = \text{VBZ}]$

- Later lectures: sequence labeling!

the router *blocks* *the packets*

NNS
VBZ
NN
DT
…

not saying that *the* is tagged as VBZ! saying that *the* follows the VBZ word

Multiclass Logistic Regression

Multiclass Logistic Regression

Softmax function

$$P_w(y|x) = \frac{\exp\left(w^\top f(x,y)\right)}{\sum_{y' \in \mathcal{Y}} \exp\left(w^\top f(x,y')\right)}$$

sum over output

space to normalize

- Compare to binary:

$$P(y=1|x) = \frac{\exp(w^\top f(x))}{1+\exp(w^\top f(x))}$$

Multiclass Logistic Regression

$$P_w(y|x) = \frac{\exp\left(w^\top f(x,y)\right)}{\sum_{y' \in \mathcal{Y}} \exp\left(w^\top f(x,y')\right)}$$

sum over output space to normalize

Why? Interpret raw classifier scores as **probabilities**

too many drug trials, too few patients

Health: +2.2

Sports: +3.1

Science: -0.6

$w^\top f(x,y)$

exp

probabilities must be >= 0

6.05

22.2

0.55

unnormalized probabilities

normalize

probabilities must sum to 1

0.21

0.77

0.02

$P_w(y|x)$

Multiclass Logistic Regression

$$P_w(y|x) = \frac{\exp\left(w^\top f(x,y)\right)}{\sum_{y' \in \mathcal{Y}} \exp\left(w^\top f(x,y')\right)}$$

sum over output space to normalize

i.e. minimize negative log likelihood or cross-entropy loss

- Training: maximize $\mathcal{L}(x,y) = \sum_{j=1}^{m} \log P(y_j^*|x_j)$

index of data points (j)

$$= \sum_{j=1}^{m} \left(w^\top f(x_j, y_j^*) - \log \sum_y \exp(w^\top f(x_j, y)) \right)$$

Multiclass Logistic Regression

$$P_w(y|x) = \frac{\exp\left(w^\top f(x,y)\right)}{\sum_{y' \in \mathcal{Y}} \exp\left(w^\top f(x,y')\right)}$$

sum over output space to normalize

too many drug trials, too few patients

Health: +2.2

Sports: +3.1

Science: -0.6

$w^\top f(x,y)$

exp

probabilities must be >= 0

6.05

22.2

0.55

unnormalized probabilities

normalize

probabilities must sum to 1

0.21

0.77

0.02

$P_w(y|x)$

log(0.21) = - 1.56

compare

$\mathcal{L}(x_j, y_j^*) = \log P(y_j^*|x_j)$

1.00

0.00

0.00

correct (gold) probabilities

Training

- Multiclass logistic regression $P_w(y|x) = \frac{\exp\left(w^\top f(x,y)\right)}{\sum_{y' \in \mathcal{Y}} \exp\left(w^\top f(x,y')\right)}$

- Likelihood $\mathcal{L}(x_j, y_j^*) = w^\top f(x_j, y_j^*) - \log \sum_y \exp(w^\top f(x_j, y))$

$$\frac{\partial}{\partial w_i}\mathcal{L}(x_j, y_j^*) = f_i(x_j, y_j^*) - \frac{\sum_y f_i(x_j, y) \exp(w^\top f(x_j, y))}{\sum_y \exp(w^\top f(x_j, y))}$$

$$\frac{\partial}{\partial w_i}\mathcal{L}(x_j, y_j^*) = f_i(x_j, y_j^*) - \sum_y f_i(x_j, y) P_w(y|x_j)$$

$$\frac{\partial}{\partial w_i}\mathcal{L}(x_j, y_j^*) = f_i(x_j, y_j^*) - \mathbb{E}_y[f_i(x_j, y)]$$

gold feature value

model's expectation of feature value

Training

gold feature value

$$\frac{\partial}{\partial w_i}\mathcal{L}(x_j, y_j^*) = f_i(x_j, y_j^*) - \sum_y f_i(x_j, y) P_w(y|x_j)$$

← model's expectation of feature value

too many drug trials, too few patients

y^* = Health

$f(x, y = \text{Health}) = [1, 1, 0, 0, 0, 0, 0, 0, 0]$
$f(x, y = \text{Sports}) = [0, 0, 0, 1, 1, 0, 0, 0, 0]$
$f(x, y = \text{Science}) = [0, 0, 0, 0, 0, 0, 1, 1, 0]$

$P_w(y|x)$ = [0.21, 0.77, 0.02]

gradient: [1, 1, 0, 0, 0, 0, 0, 0, 0] — 0.21 [1, 1, 0, 0, 0, 0, 0, 0, 0]
— 0.77 [0, 0, 0, 1, 1, 0, 0, 0, 0] — 0.02 [0, 0, 0, 0, 0, 0, 1, 1, 0]

= [0.79, 0.79, 0, -0.77, -0.77, 0, -0.02, -0.02, 0]

update $w^\top$:

[1.3, 0.9, -5, 3.2, -0.1, 0, 1.1, -1.7, -1.3] + [0.79, 0.79, 0, -0.77, -0.77, 0, -0.02, -0.02, 0]
= [2.09, 1.69, 0, 2.43, -0.87, 0, 1.08, -1.72, 0]

↘ new $P_w(y|x)$ = [0.89, 0.10, 0.01]

Multiclass Logistic Regression: Summary

- Model: $P_w(y|x) = \frac{\exp\left(w^\top f(x,y)\right)}{\sum_{y' \in \mathcal{Y}} \exp\left(w^\top f(x,y')\right)}$
- Inference: $\text{argmax}_y P_w(y|x)$
- Learning: gradient ascent on the discriminative log-likelihood

$$f(x,y^*) - \mathbb{E}_y[f(x,y)] = f(x,y^*) - \sum_y [P_w(y|x) f(x,y)]$$

"towards gold feature value, away from expectation of feature value"

Optimization

- Gradient descent (or ascent)
  - **Batch update** for logistic regression
  - Each update is based on a computation over the entire dataset

Multiclass Logistic Regression

$$P_w(y|x) = \frac{\exp\left(w^\top f(x,y)\right)}{\sum_{y' \in \mathcal{Y}} \exp\left(w^\top f(x,y')\right)}$$

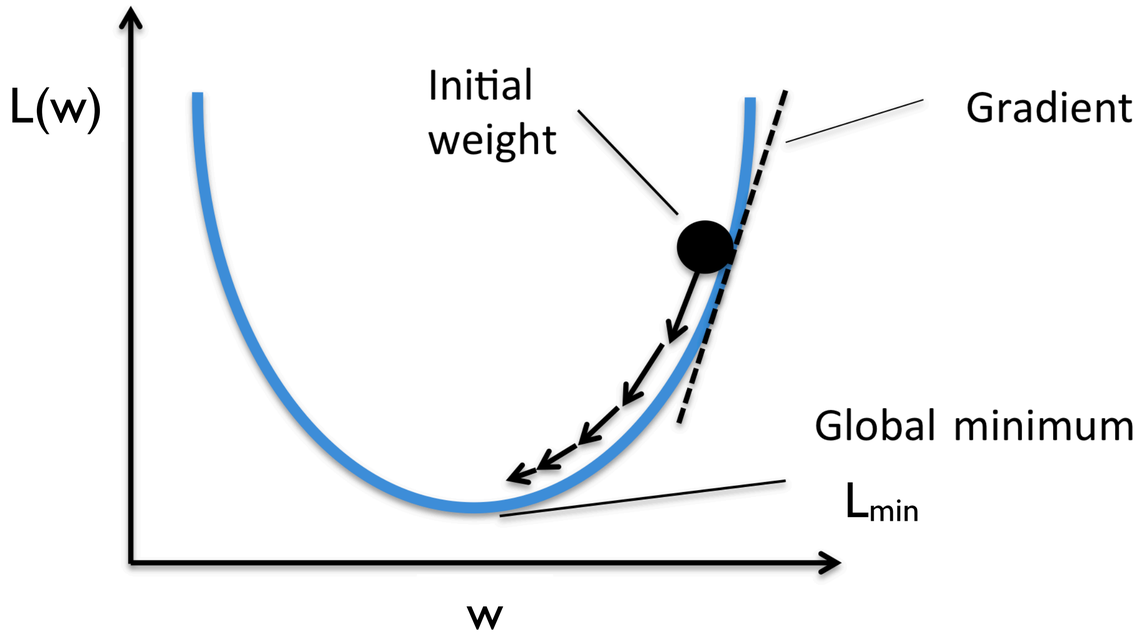
sum over output space to normalize

i.e. minimize negative log likelihood or cross-entropy loss

- Training: maximize $\mathcal{L}(x,y) = \sum_{j=1}^{m} \log P(y_j^*|x_j)$

index of data points (*j*)

$$= \sum_{j=1}^{m} \left(w^\top f(x_j, y_j^*) - \log \sum_y \exp(w^\top f(x_j, y)) \right)$$



Optimization

- Gradient descent
  - **Batch update** for logistic regression
  - Each update is based on a computation over the entire dataset

Multiclass Logistic Regression

$$P_w(y|x) = \frac{\exp\left(w^\top f(x,y)\right)}{\sum_{y' \in \mathcal{Y}} \exp\left(w^\top f(x,y')\right)}$$

sum over output space to normalize

i.e. minimize negative log likelihood or cross-entropy loss

- Training: maximize $\mathcal{L}(x,y) = \sum_{j=1}^{m} \log P(y_j^*|x_j)$

index of data points (*j*)

$$= \sum_{j=1}^{m} \left(w^\top f(x_j, y_j^*) - \log \sum_y \exp(w^\top f(x_j, y)) \right)$$

- Very simple to code up

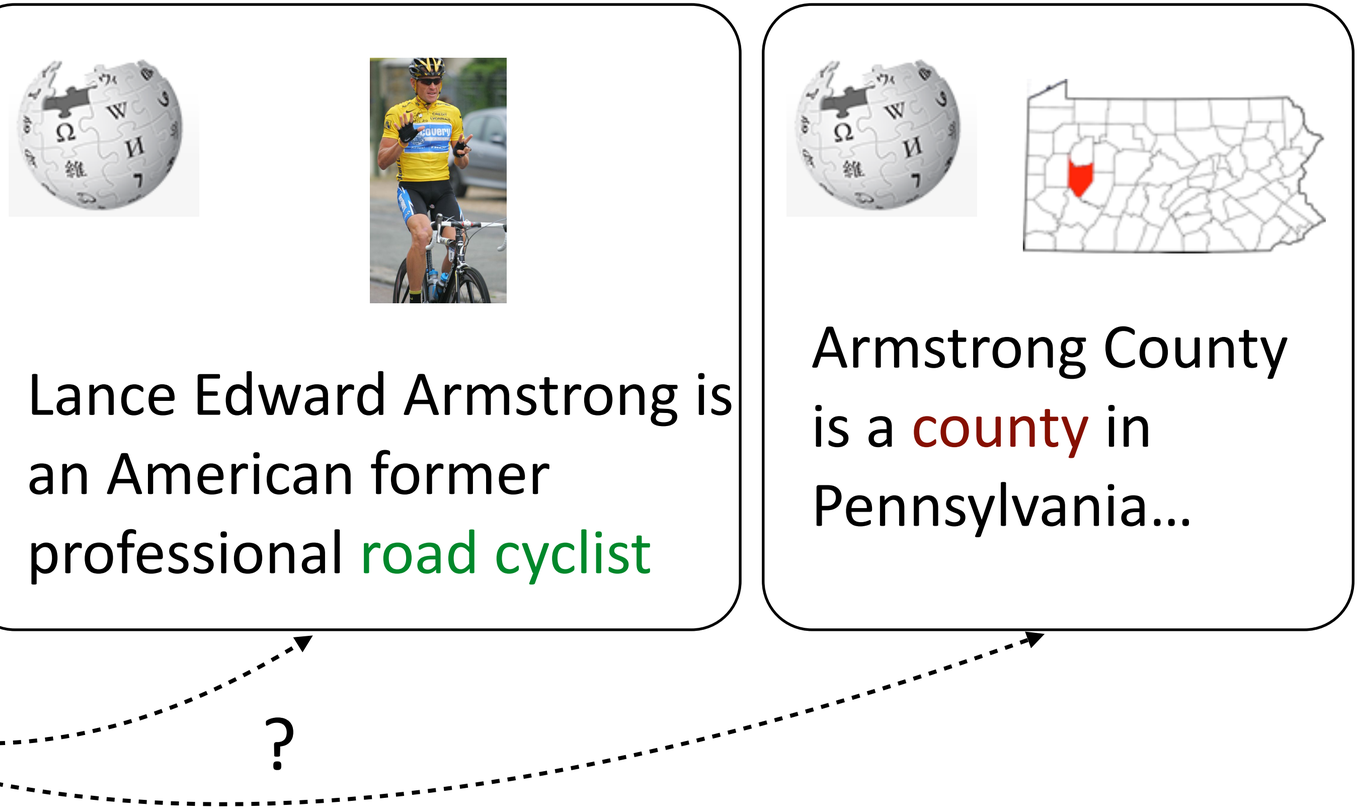
```
# Vanilla Gradient Descent

while True:
  weights_grad = evaluate_gradient(loss_fun, data, weights)
  weights += - step_size * weights_grad # perform parameter update
```

Another Example: Entity Linking

Entity Linking

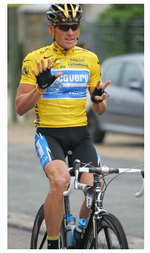
Although he originally won the event, the United States Anti-Doping Agency announced in August 2012 that they had disqualified **Armstrong** from his seven consecutive Tour de France wins from 1999–2005.



- 4.5M classes, not enough data to learn features like “Tour de France <-> en/wiki/Lance_Armstrong”
- Instead, features $f(x, y)$ look at the actual article associated with y

Entity Linking

Although he originally won the event, the United States Anti-Doping Agency announced in August 2012 that they had disqualified **Armstrong** from his seven consecutive Tour de France wins from 1999–2005.

Lance Edward Armstrong


Armstrong County

- tf-idf(doc, *w*) = freq of *w* in doc * log(4.5M/# Wiki articles *w* occurs in)
  - *the*: occurs in every article, tf-idf = 0
  - *cyclist*: occurs in 1% of articles, tf-idf = # occurrences * $\log_{10}(100)$
- tf-idf(doc) = vector of tf-idf(doc, *w*) for all words in vocabulary (50,000)
- *f*(*x*,*y*) = [cos(tf-idf(*x*), tf-idf(*y*)), … other features]

Entity Linking

Baseline Feature: $P(t\|m), P(t)$
Local Features: $\phi_i(t, m)$
cosine-sim(Text(t),Text(m)) : Naive/Reweighted
cosine-sim(Text(t),Context(m)): Naive/Reweighted
cosine-sim(Context(t),Text(m)): Naive/Reweighted
cosine-sim(Context(t),Context(m)): Naive/Reweighted
Global Features: $\psi_i(t_i, t_j)$
$I_{[t_i-t_j]}$*PMI(InLinks(t_i),InLinks(t_j)) : avg/max*
$I_{[t_i-t_j]}$*NGD(InLinks(t_i),InLinks(t_j)) : avg/max*
$I_{[t_i-t_j]}$*PMI(OutLinks(t_i),OutLinks(t_j)) : avg/max*
$I_{[t_i-t_j]}$*NGD(OutLinks(t_i),OutLinks(t_j)) : avg/max*
$I_{[t_i\leftrightarrow t_j]}$ *: avg/max*
$I_{[t_i\leftrightarrow t_j]}$*PMI(InLinks($t_i$),InLinks($t_j$)) : avg/max*
$I_{[t_i\leftrightarrow t_j]}$*NGD(InLinks($t_i$),InLinks($t_j$)) : avg/max*
$I_{[t_i\leftrightarrow t_j]}$*PMI(OutLinks($t_i$),OutLinks($t_j$)) : avg/max*
$I_{[t_i\leftrightarrow t_j]}$*NGD(OutLinks($t_i$),OutLinks($t_j$)) : avg/max*

Table 1: Ranker features. $I_{[t_i-t_j]}$ is an indicator variable which is 1 iff t_i links to t_j or vise-versa. $I_{[t_i\leftrightarrow t_j]}$ is 1 iff the titles point to each other.

Wikipedia titles. We are aware of two previous methods for estimating the relatedness between two Wikipedia concepts: (Strube and Ponzetto, 2006), which uses category overlap, and (Milne and Witten, 2008a), which uses the incoming link structure. Previous work experimented with two relatedness measures: NGD, and Specificity-weighted Cosine Similarity. Consistent with previous work, we found NGD to be the better-performing of the two. Thus we use only NGD along with a well-known Pontwise Mutual Information (PMI) relatedness measure. Given a Wikipedia title collection W, titles t_1 and t_2 with a set of incoming links L_1, and L_2 respectively, PMI and NGD are defined as follows:

$$NGD(L_1, L_2) = \frac{Log(Max(|L_1|, |L_2|)) - Log(|L_1 \cap L_2|)}{Log(|W|) - Log(Min(|L_1|, |L_2|))}$$

$$PMI(L_1, L_2) = \frac{|L_1 \cap L_2|/|W|}{|L_1|/|W||L_2|/|W|}$$

The NGD and the PMI measures can also be computed over the set of *outgoing* links, and we include these as features as well. We also included a fea-

- $f(x,y)$ = [cos(tf-idf(x), tf-idf(y)), … other features]

Ratinov et al. (2011)

Next Up

- You've now seen everything you need to implement multi-class classification models
- Next up: Neural Network Basics!
- In 2 weeks: Sequential Models (HMM, CRF, …) for POS tagging, NER

QA Time