Multiclass Classification

Wei Xu

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

This Lecture

- Multiclass fundamentals
- Feature extraction
- Multiclass logistic regression
- Optimization

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.

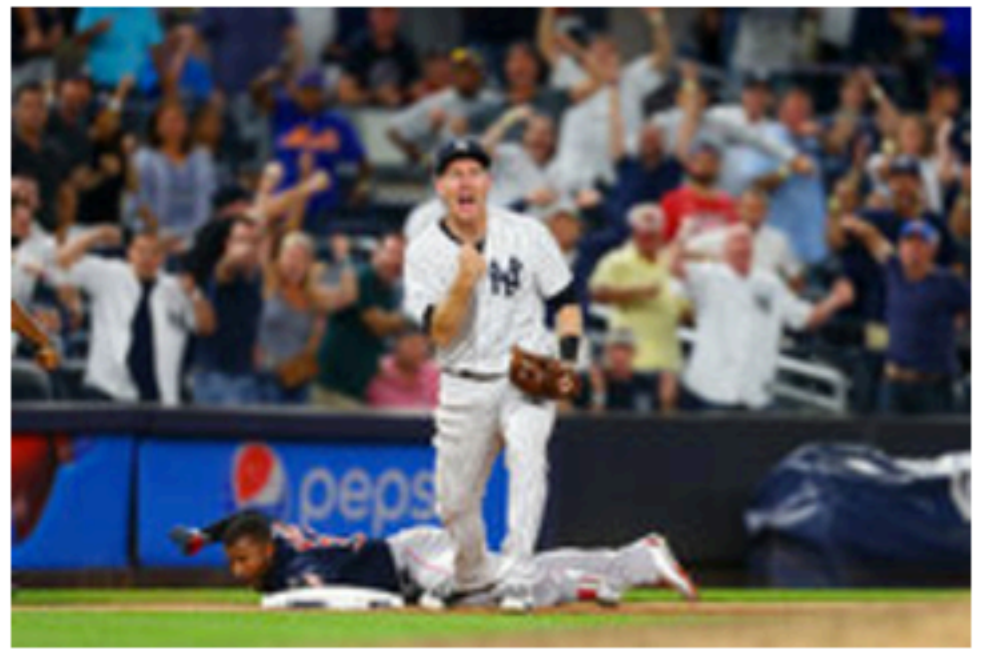
By GINA KOLATA

→ 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

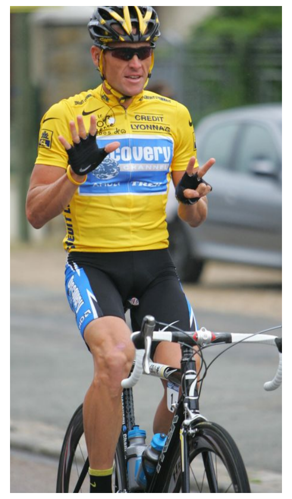
→ Dog

→ 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.



Lance Edward Armstrong is an American former professional road cyclist

Armstrong County is a county in Pennsylvania…

?

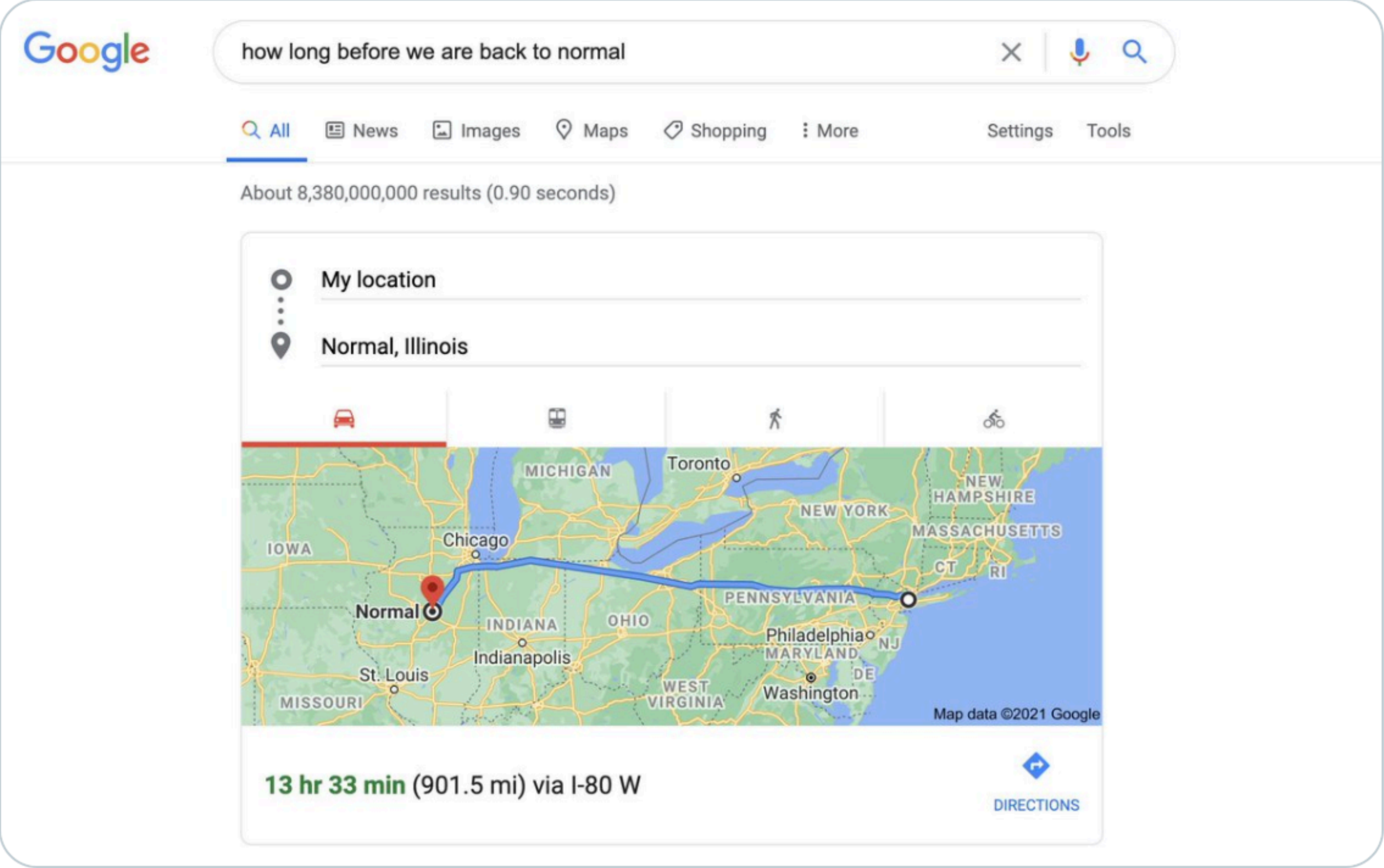
?

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

Entity Linking

Kara Schechtman
@karaschechtman

this is just decidedly not what I meant

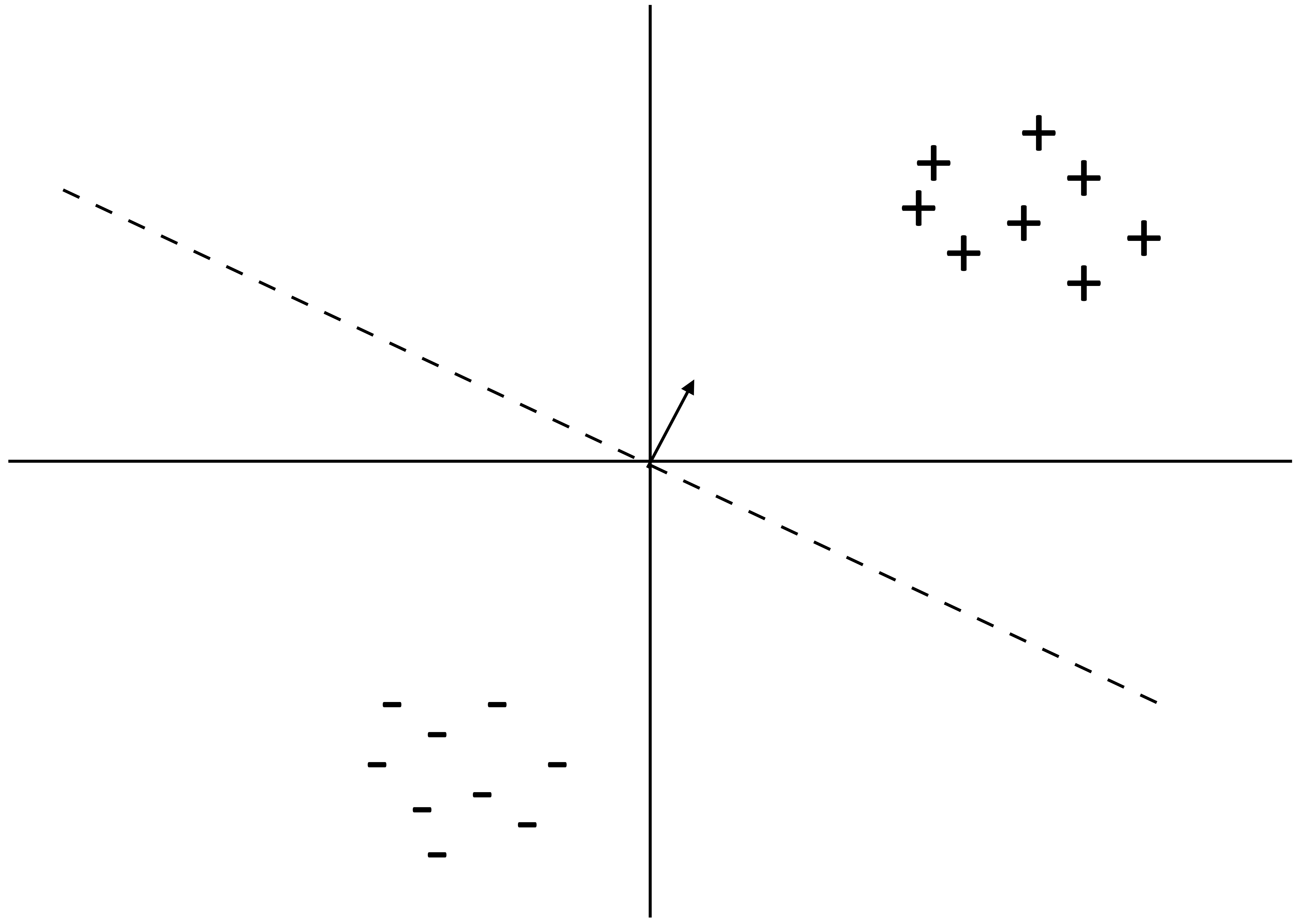


8:58 PM · Jan 30, 2021 · Twitter Web App

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

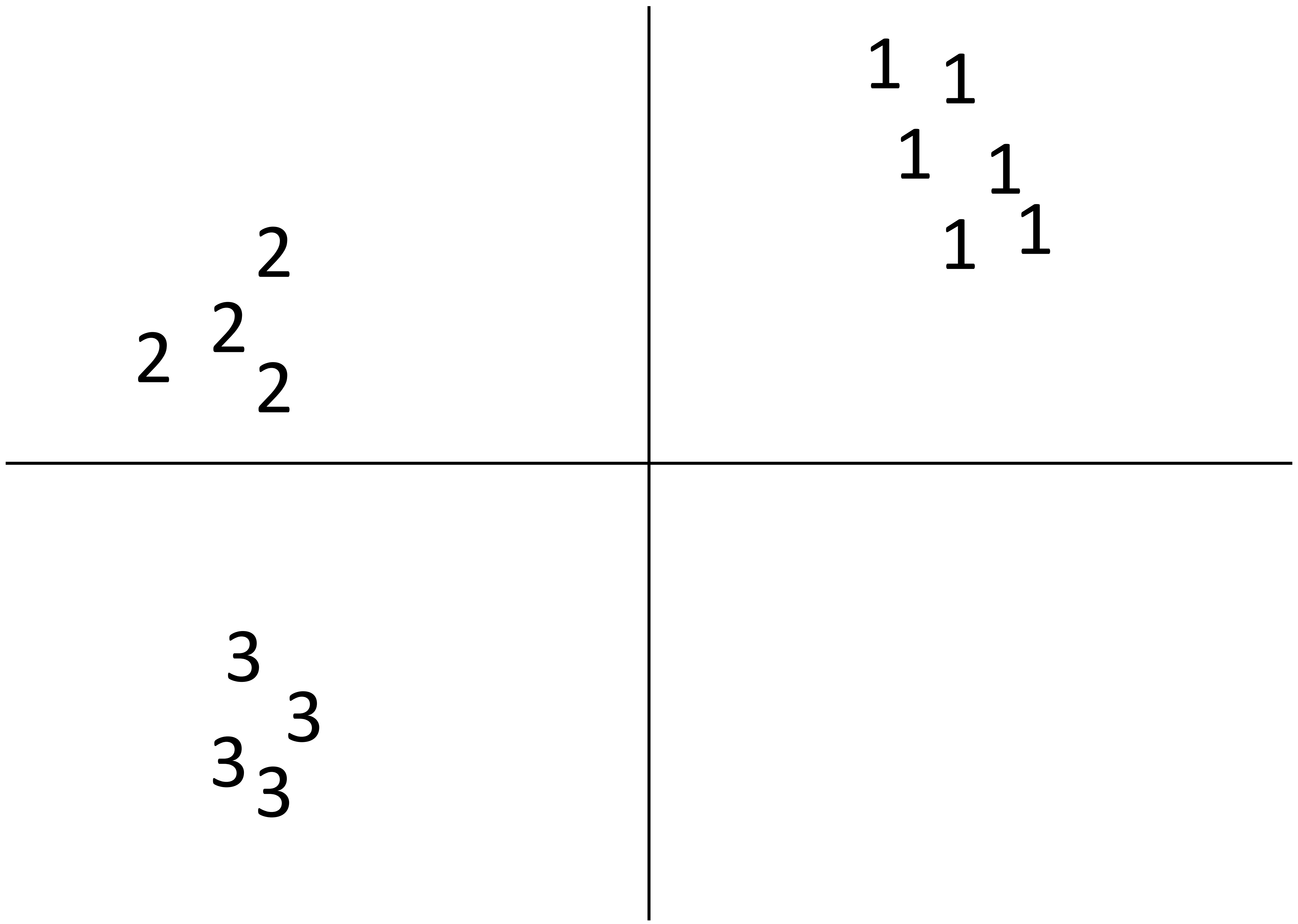
Binary Classification

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



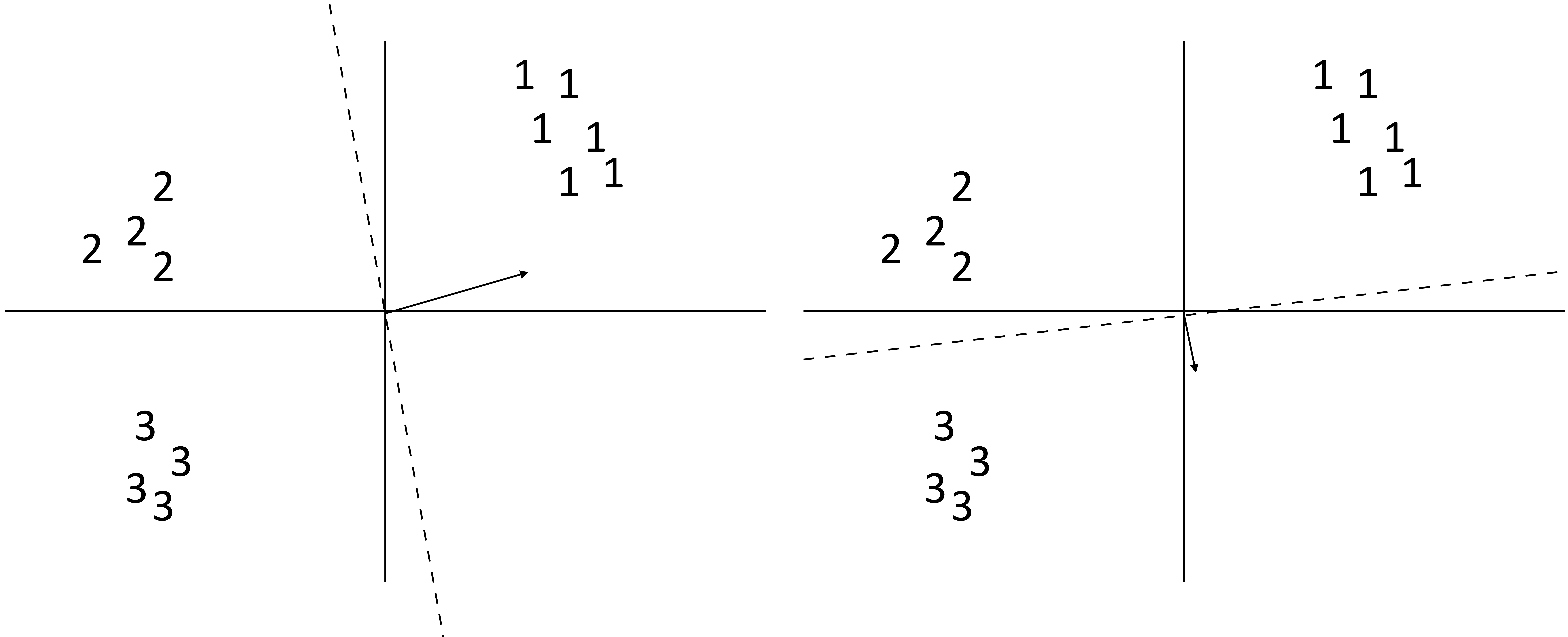
Multiclass Classification

- Can we just use binary classifiers here?



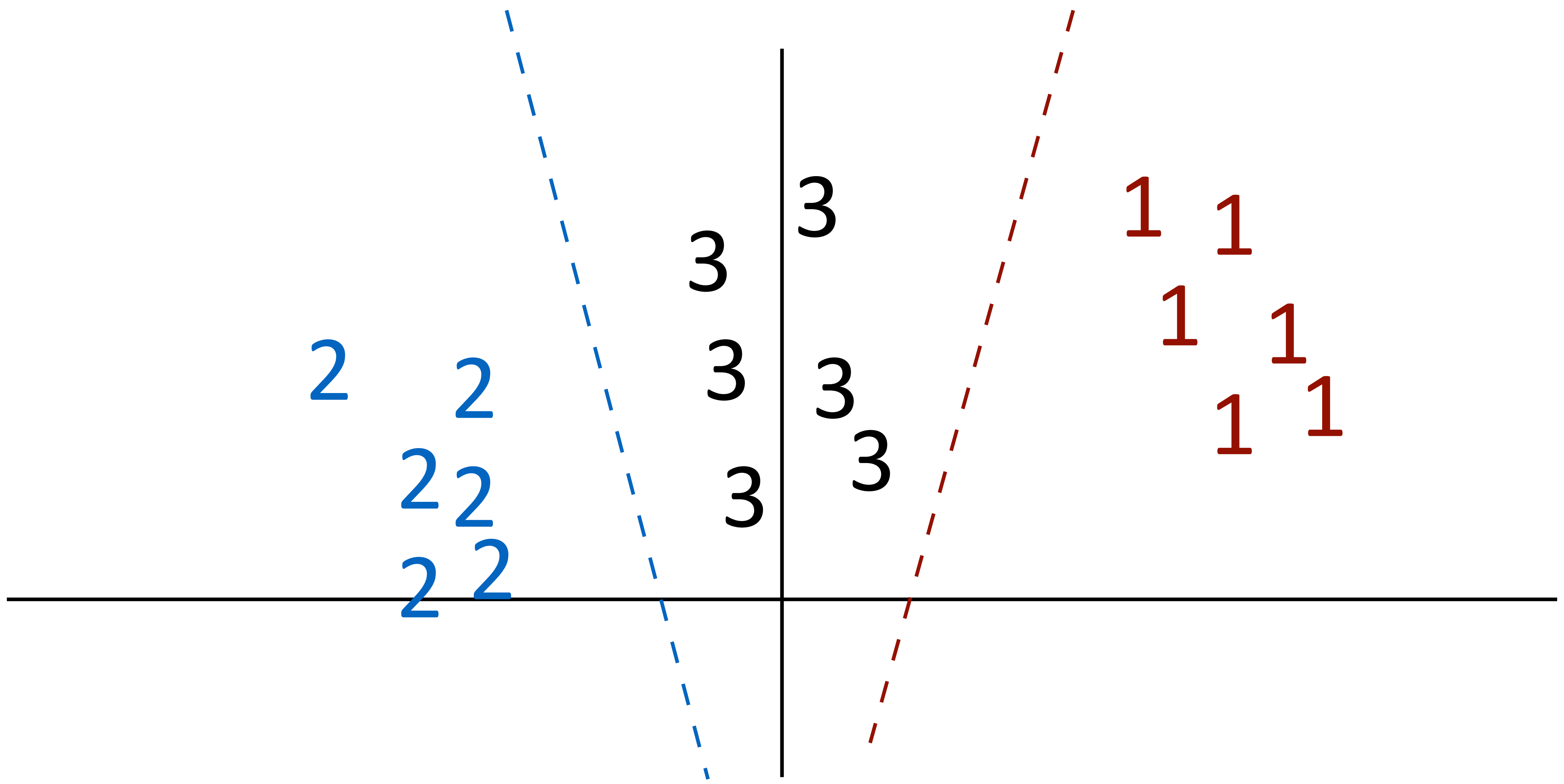
Multiclass Classification

- 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

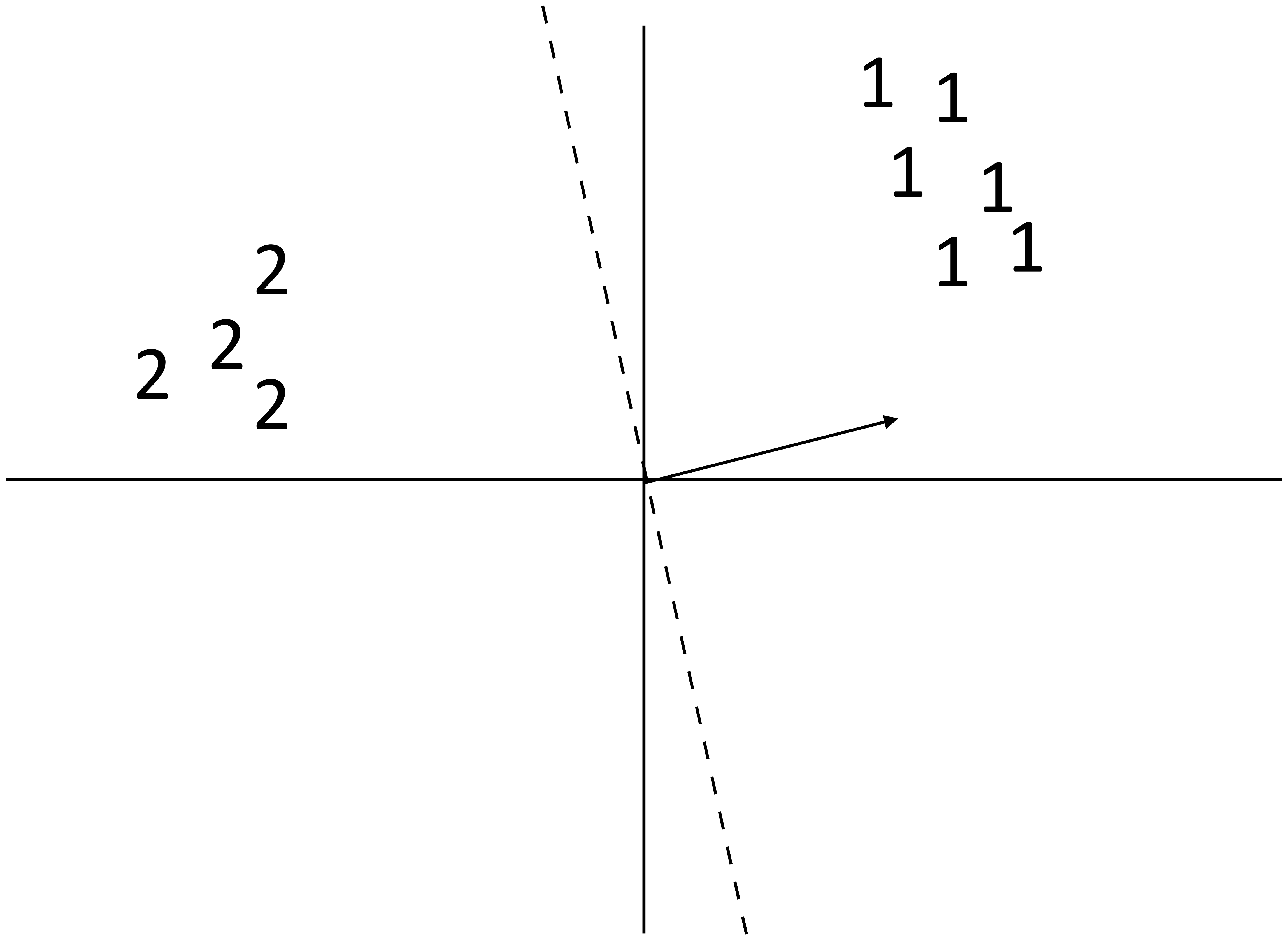
- Not all classes may even be separable using this approach

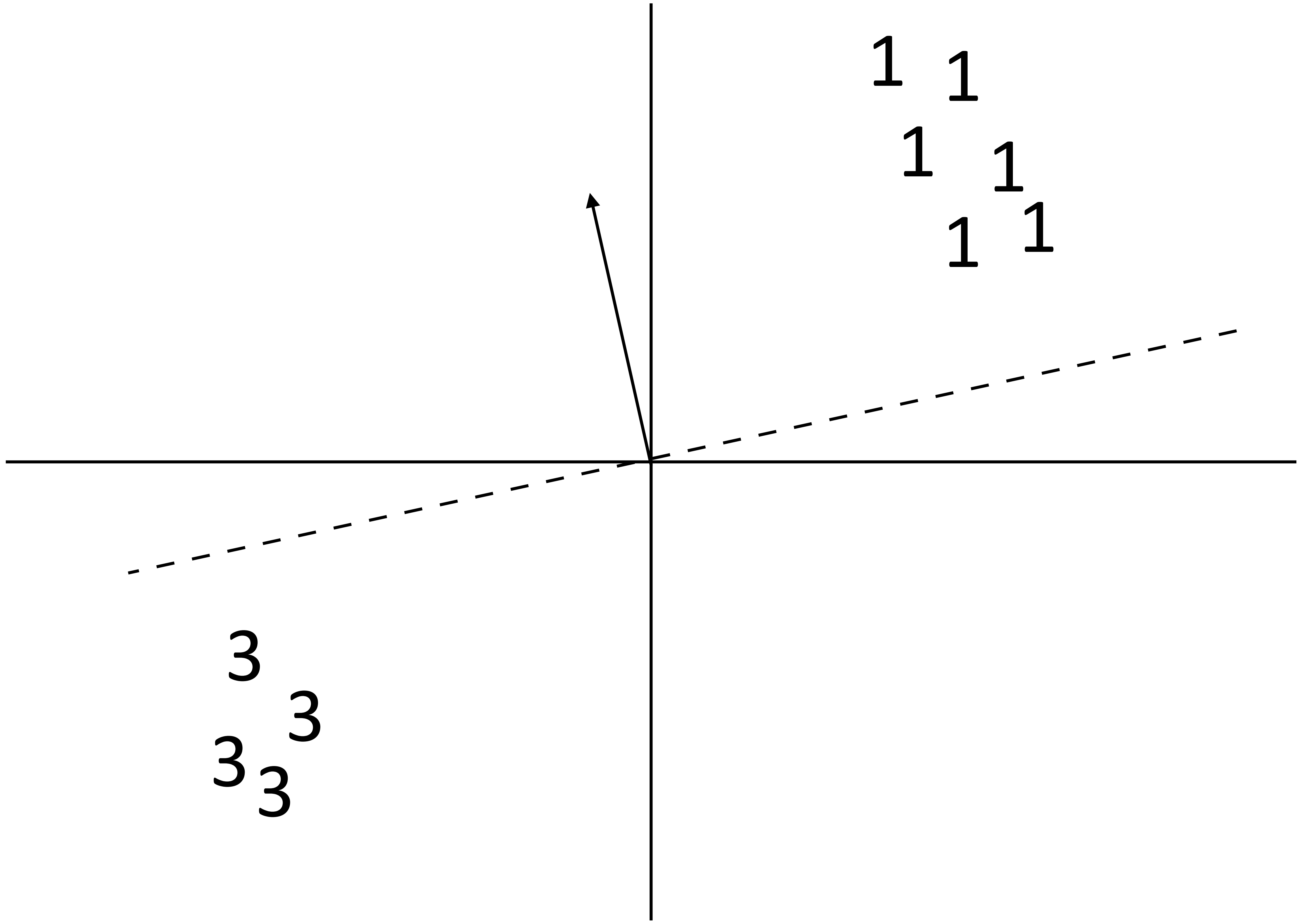


- Can separate 1 from 2+3 and 2 from 1+3 but not 3 from the others (with these features)

Multiclass Classification

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





Multiclass Classification

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Administrivia

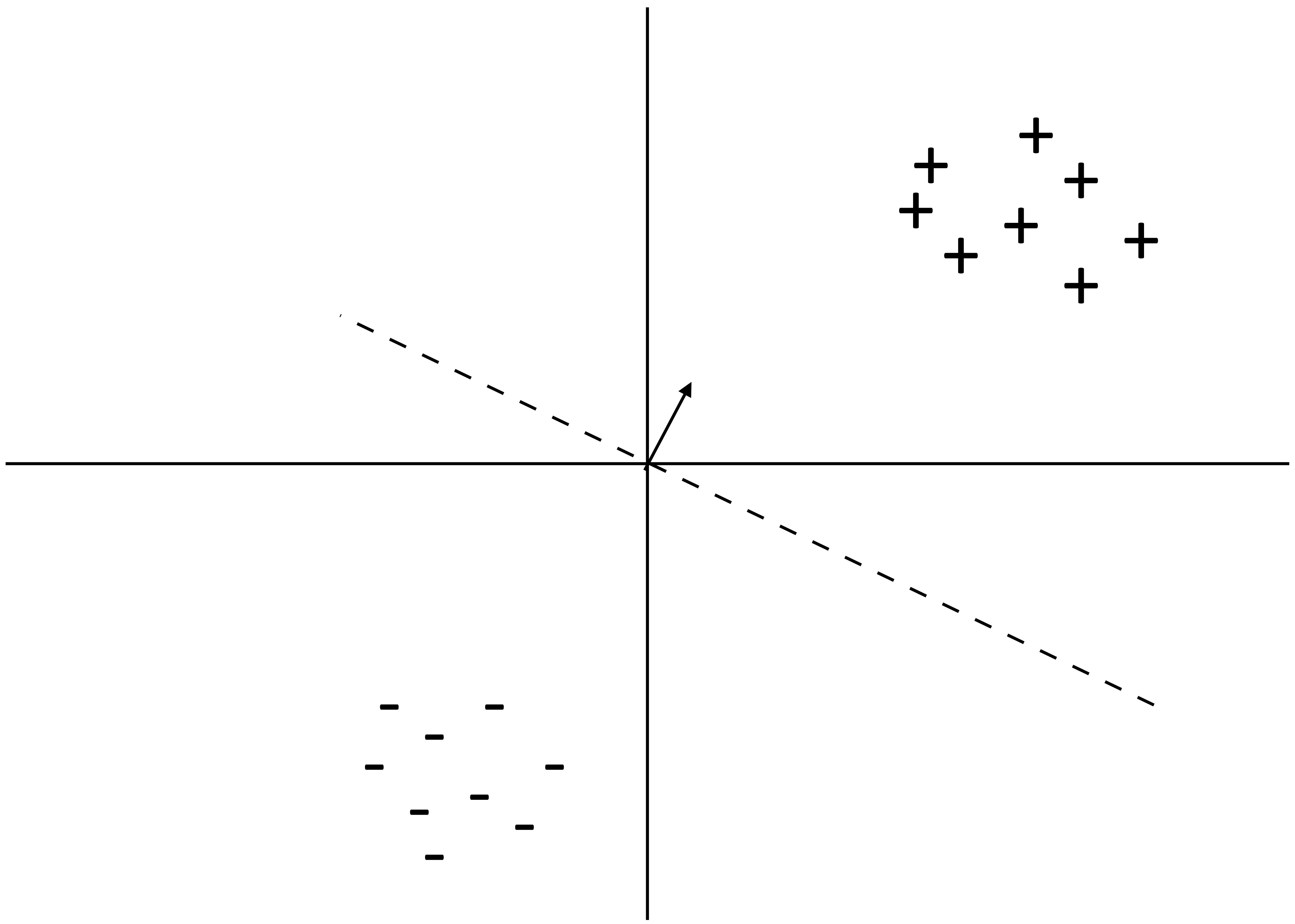
- Problem Set 1 Graded (on Gradescope)
- Programming Project 1 is released (due 9/20)
- Reading: Eisenstein 2.0-2.5, 4.1, 4.3-4.5
- Optional readings related to Project 1 were posted by TA on Piazza

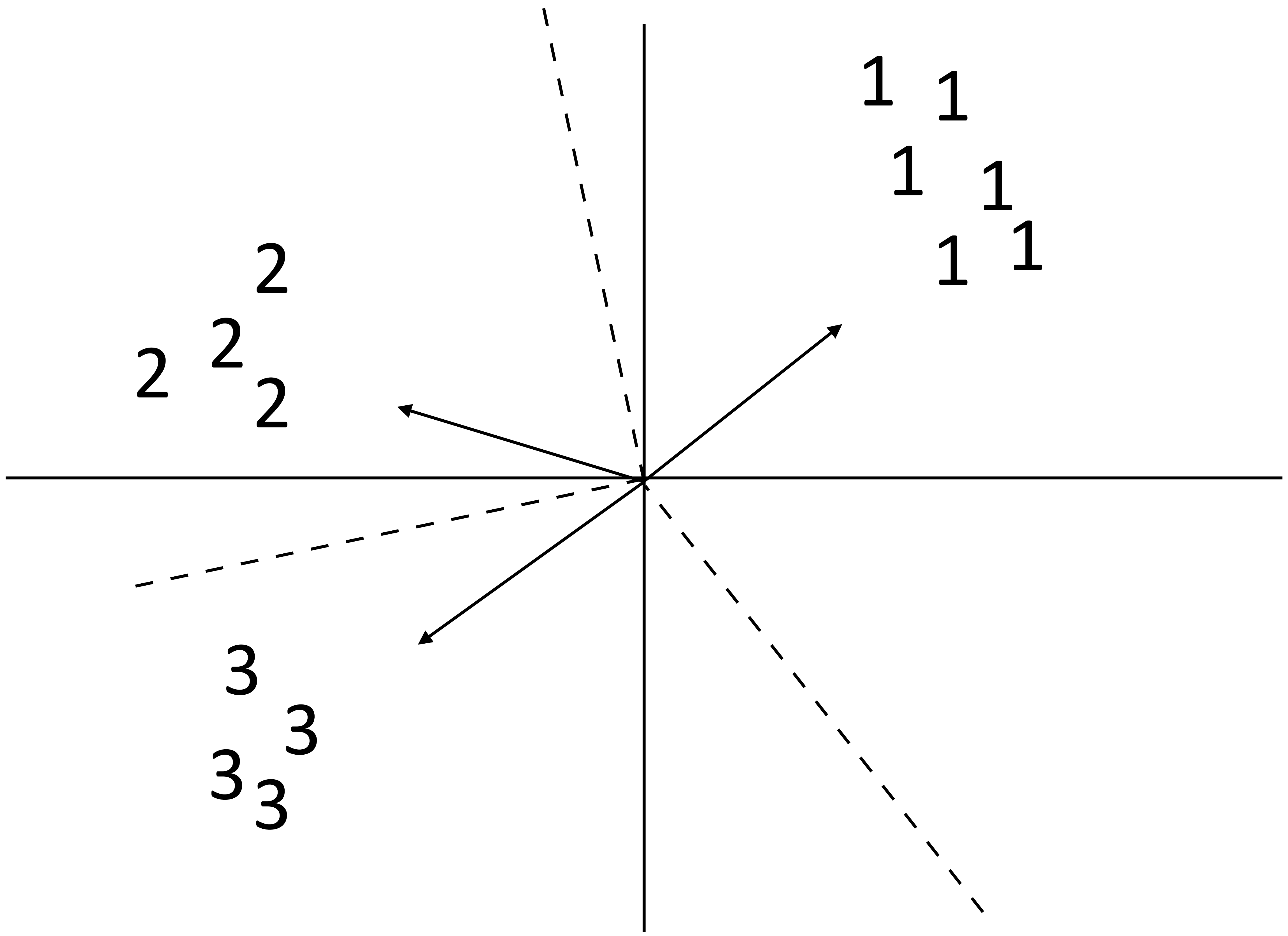
This Lecture

- Multiclass fundamentals
- Feature extraction
- Multiclass logistic regression
- Optimization

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

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

$f(x, y =$ Health $) =$ [1, 1, 0, 0, 0, 0, 0, 0, 0]   I[contains *drug* & label = Health]

$f(x, y =$ Sports $) =$ [0, 0, 0, 1, 1, 0, 0, 0, 0]

$f(x, y =$ Science$) =$ [0, 0, 0, 0, 0, 0, 1, 1, 0]

- Equivalent to having three weight vectors in this case

Making Decisions

too many drug trials, too few patients → Health

→ Sports

→ Science

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

$f(x, y =$ Health $) =$ [1, 1, 0, 0, 0, 0, 0, 0, 0]

$f(x, y =$ Sports $) =$ [0, 0, 0, 1, 1, 0, 0, 0, 0]

$f(x, y =$ 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

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:

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

negative class implicitly had $f(x, y=0)$ = the zero vector

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

$w^\top f(x,y)$		probabilities must be >= 0 (unnormalized probabilities)		probabilities must sum to 1 ($P_w(y|x)$)
Health: +2.2	exp →	6.05	normalize →	0.21
Sports: +3.1		22.2		0.77
Science: -0.6		0.55		0.02

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

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

index of data points (j)

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

Q: max/min of log prob.?

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

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

too many drug trials, too few patients

y^* = Health

$f(x, y =$ Health $) =$ [1, 1, 0, 0, 0, 0, 0, 0, 0]
$f(x, y =$ Sports $) =$ [0, 0, 0, 1, 1, 0, 0, 0, 0]
$f(x, y =$ 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: $P_w(y|x) = \dfrac{\exp\left(w^\top f(x,y)\right)}{\sum_{y' \in \mathcal{Y}} \exp\left(w^\top f(x,y')\right)}$
- 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"

Multiclass SVM

Soft Margin SVM

Minimize $\lambda\|w\|_2^2 + \sum_{j=1}^{m} \xi_j$ ← slack variables > 0 iff example is support vector

s.t. $\forall j \quad \xi_j \geq 0$

$\forall j \quad (2y_j - 1)(w^\top x_j) \geq 1 - \xi_j$

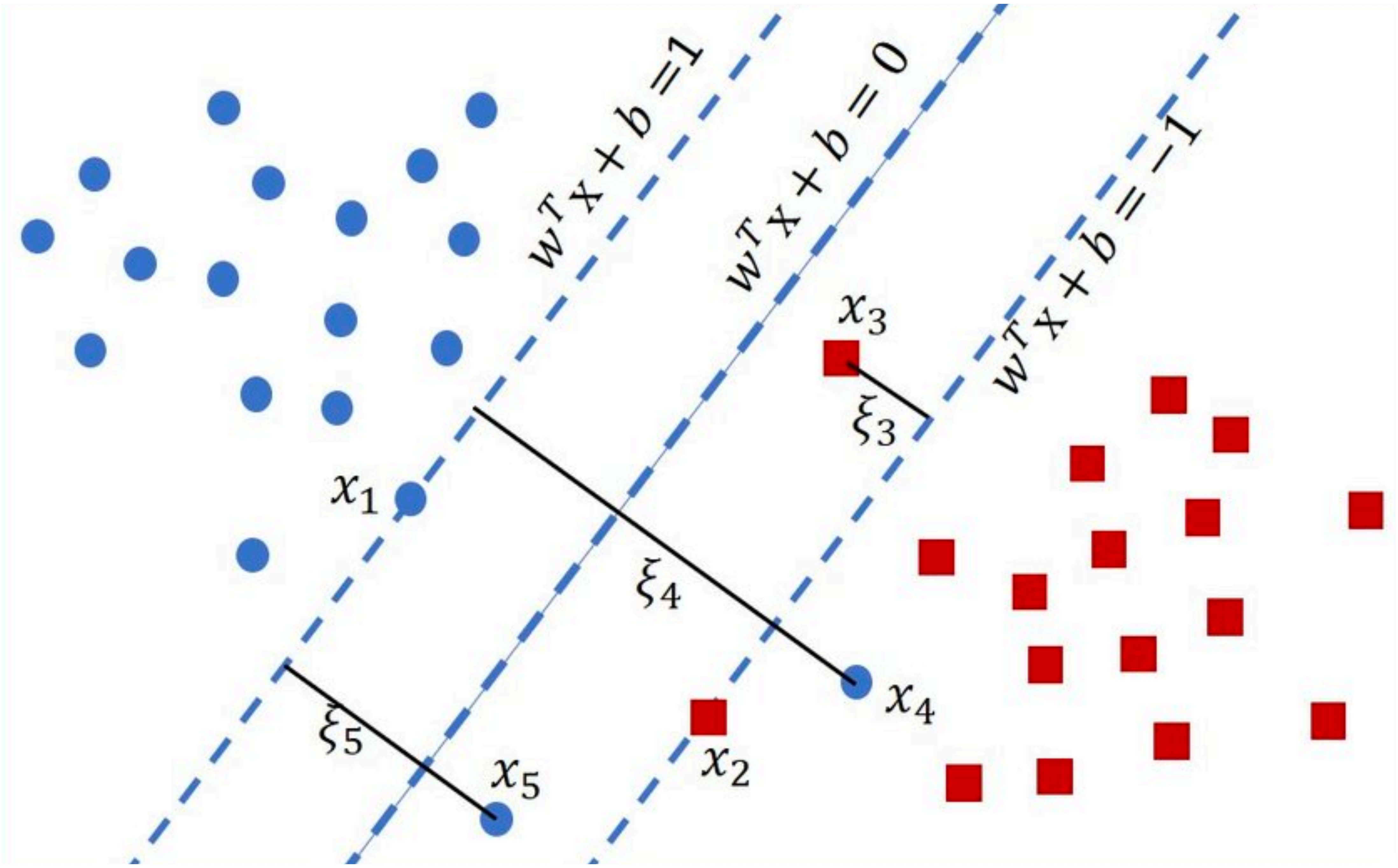


Image credit: Lang Van Tran

Multiclass SVM

Minimize $\lambda\|w\|_2^2 + \sum_{j=1}^{m} \xi_j$ ← slack variables > 0 iff example is support vector

s.t. $\forall j \quad \xi_j \geq 0$

~~$\forall j \quad (2y_j - 1)(w^\top x_j) \geq 1 - \xi_j$~~

$\forall j \forall y \in \mathcal{Y} \quad w^\top f(x_j, y_j^*) \geq w^\top f(x_j, y) + \ell(y, y_j^*) - \xi_j$

Correct prediction now has to beat every other class

Score comparison is more explicit now

The 1 that was here is replaced by a loss function

Training (loss-augmented)

- Are all decisions equally costly?

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

Predicted Sports: bad error

Predicted Science: not so bad

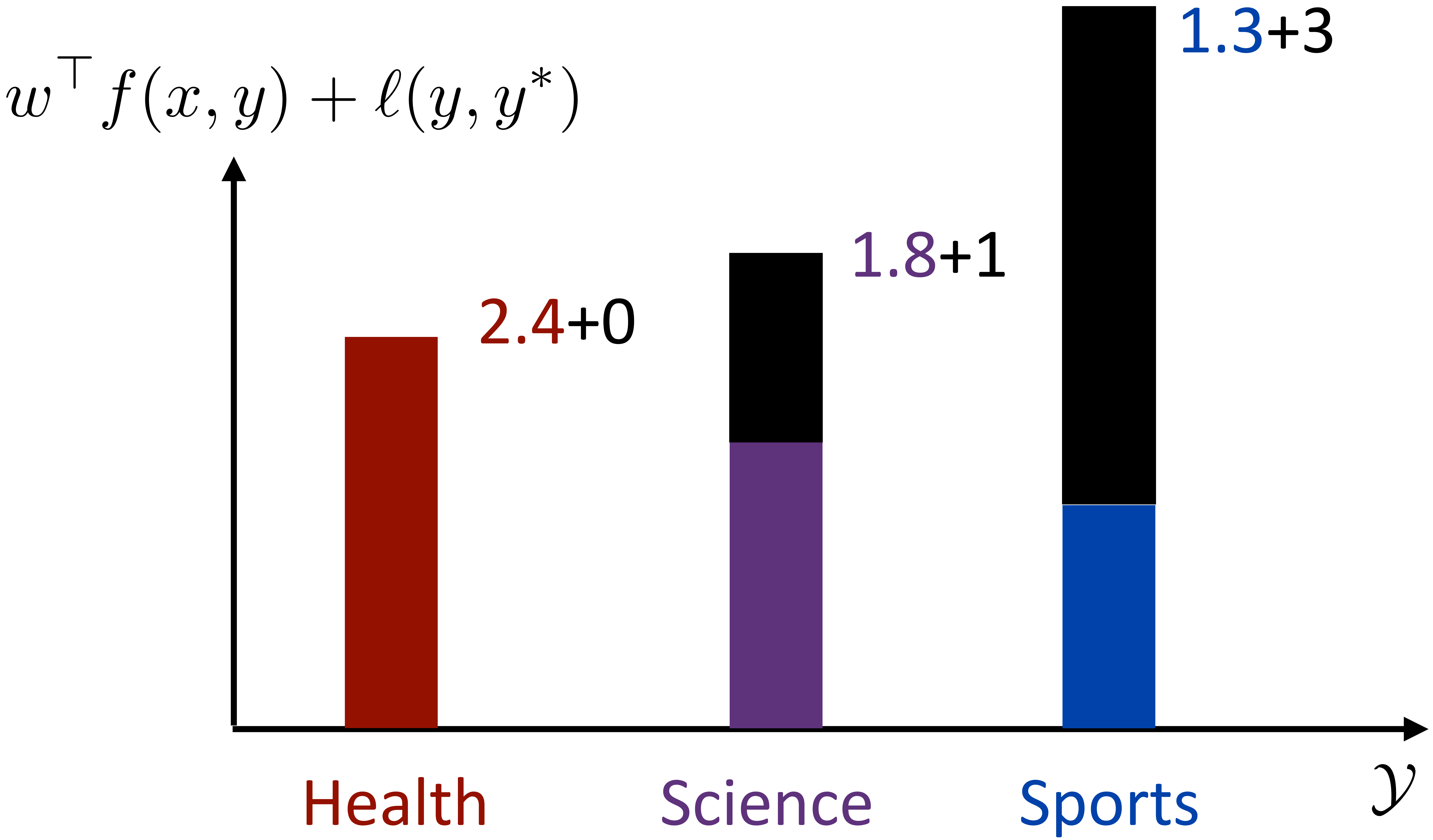
- We can define a loss function $\ell(y, y^*)$

$$\ell(\text{Sports}, \text{Health}) = 3$$

$$\ell(\text{Science}, \text{Health}) = 1$$

Loss-Augmented Decoding

$$\forall j \forall y \in \mathcal{Y} \quad w^\top f(x_j, y_j^*) \geq w^\top f(x_j, y) + \ell(y, y_j^*) - \xi_j$$



- Does gold beat every label + loss? No!
- Most violated constraint is Sports; what is ξ_j ?
- ξ_j = 4.3 - 2.4 = 1.9
- Perceptron would make no update here

Loss-Augmented Decoding

$$\xi_j = \max_{y \in \mathcal{Y}} \boxed{w^\top f(x_j, y) + \ell(y, y_j^*)} - w^\top f(x_j, y_j^*)$$

too many drug trials, too few patients Health

	$w^\top f(x,y)$	Loss	Total	
Health	+2.4	0	2.4	
Sports	+1.3	3	4.3	← argmax
Science	+1.8	1	2.8	

- Sports is most violated constraint, slack = 4.3 — 2.4 = 1.9
- Perceptron would make no update, regular SVM would pick Science

Multiclass SVM

Minimize $\lambda\|w\|_2^2 + \sum_{j=1}^{m} \xi_j$

s.t. $\forall j \quad \xi_j \geq 0$

$\forall j \forall y \in \mathcal{Y} \quad w^\top f(x_j, y_j^*) \geq w^\top f(x_j, y) + \ell(y, y_j^*) - \xi_j$

- One slack variable per example, so it's set to be whatever the *most violated constraint* is for that example

$$\xi_j = \max_{y \in \mathcal{Y}} \boxed{w^\top f(x_j, y) + \ell(y, y_j^*)} - w^\top f(x_j, y_j^*)$$

- Plug in the gold *y* and you get 0, so slack is always nonnegative!

Computing the Subgradient

$$\text{Minimize } \lambda\|w\|_2^2 + \sum_{j=1}^{m} \xi_j$$

s.t. $\forall j \quad \xi_j \geq 0$

$$\forall j \forall y \in \mathcal{Y} \quad w^\top f(x_j, y_j^*) \geq w^\top f(x_j, y) + \ell(y, y_j^*) - \xi_j$$

- If $\xi_j = 0$, the example is not a support vector, gradient is zero
- Otherwise, $\xi_j = \max_{y \in \mathcal{Y}} w^\top f(x_j, y) + \ell(y, y_j^*) - w^\top f(x_j, y_j^*)$

$$\frac{\partial}{\partial w_i} \xi_j = f_i(x_j, y_{\max}) - f_i(x_j, y_j^*)$$

← (update looks backwards — we're minimizing here!)

- Perceptron-like, but we update away from *loss-augmented* prediction

Putting it Together

Minimize $\lambda\|w\|_2^2 + \sum_{j=1}^{m} \xi_j$

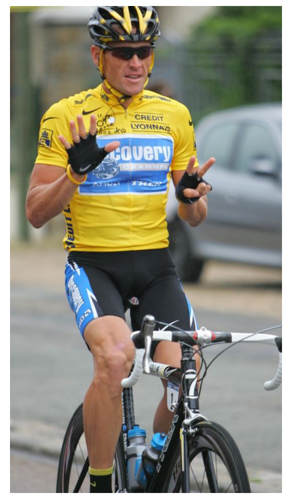
s.t. $\forall j \quad \xi_j \geq 0$

$\forall j \forall y \in \mathcal{Y} \quad w^\top f(x_j, y_j^*) \geq w^\top f(x_j, y) + \ell(y, y_j^*) - \xi_j$

- (Unregularized) gradients:
  - SVM: $f(x, y^*) - f(x, y_{\max})$ (loss-augmented max)
  - Log reg: $f(x, y^*) - \mathbb{E}_y[f(x, y)] = f(x, y^*) - \sum_y [P_w(y|x) f(x, y)]$
- SVM: max over ys to compute gradient. LR: need to sum over ys

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 is an American former professional road cyclist

Armstrong County is a county in Pennsylvania…

? ?

- 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

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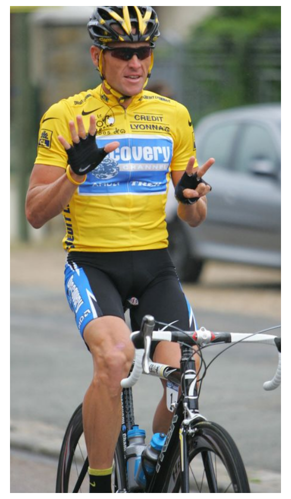


Lance Edward Armstrong

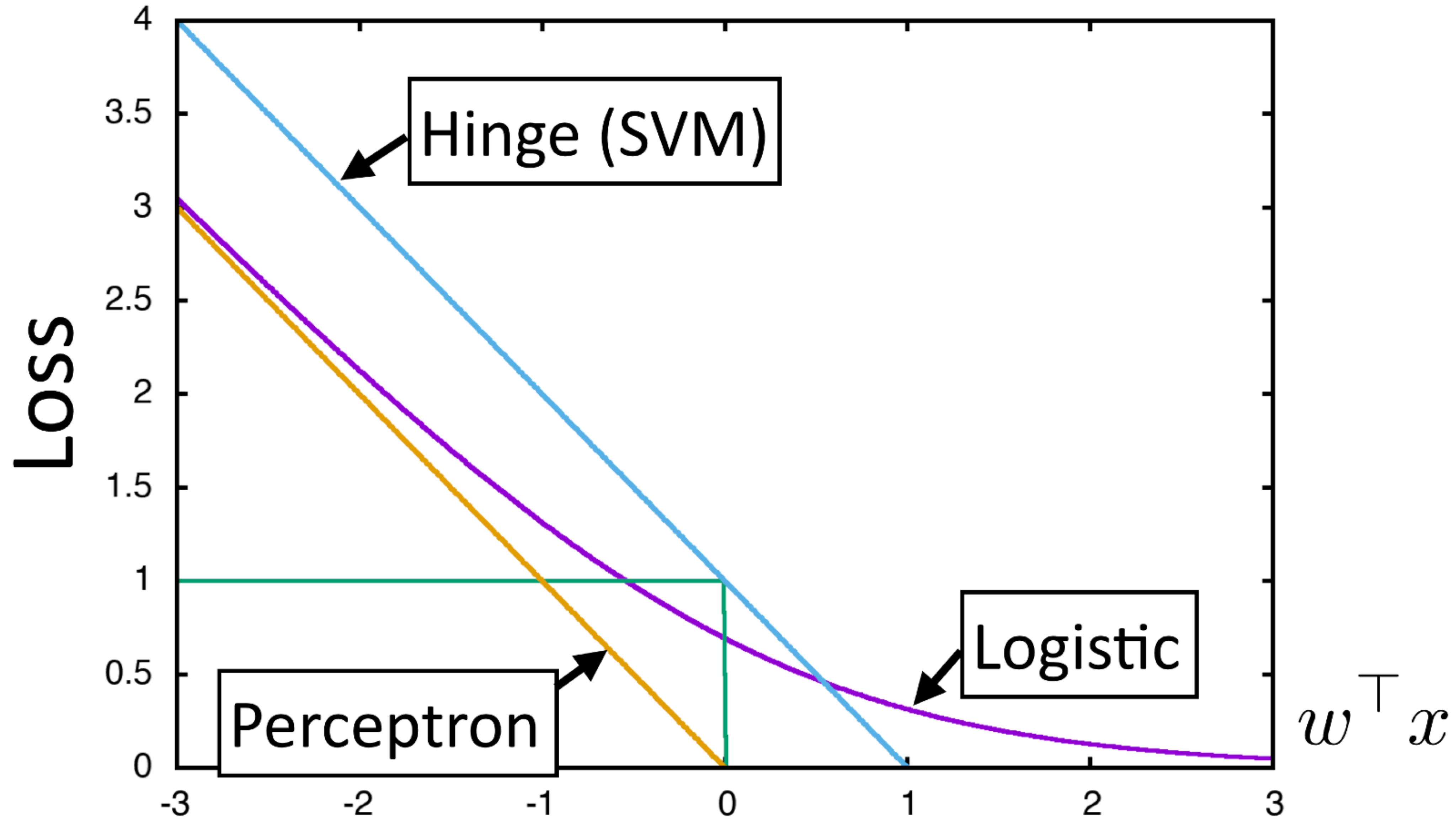
Armstrong County

- 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 * log10(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]

Optimization

Recap

- Four elements of a machine learning method:
  - Model: probabilistic, max-margin, deep neural network
  - Objective:



  - Inference: just maxes and simple expectations so far, but will get harder
  - Training: gradient descent?

Optimization

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

Multiclass Logistic Regression

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

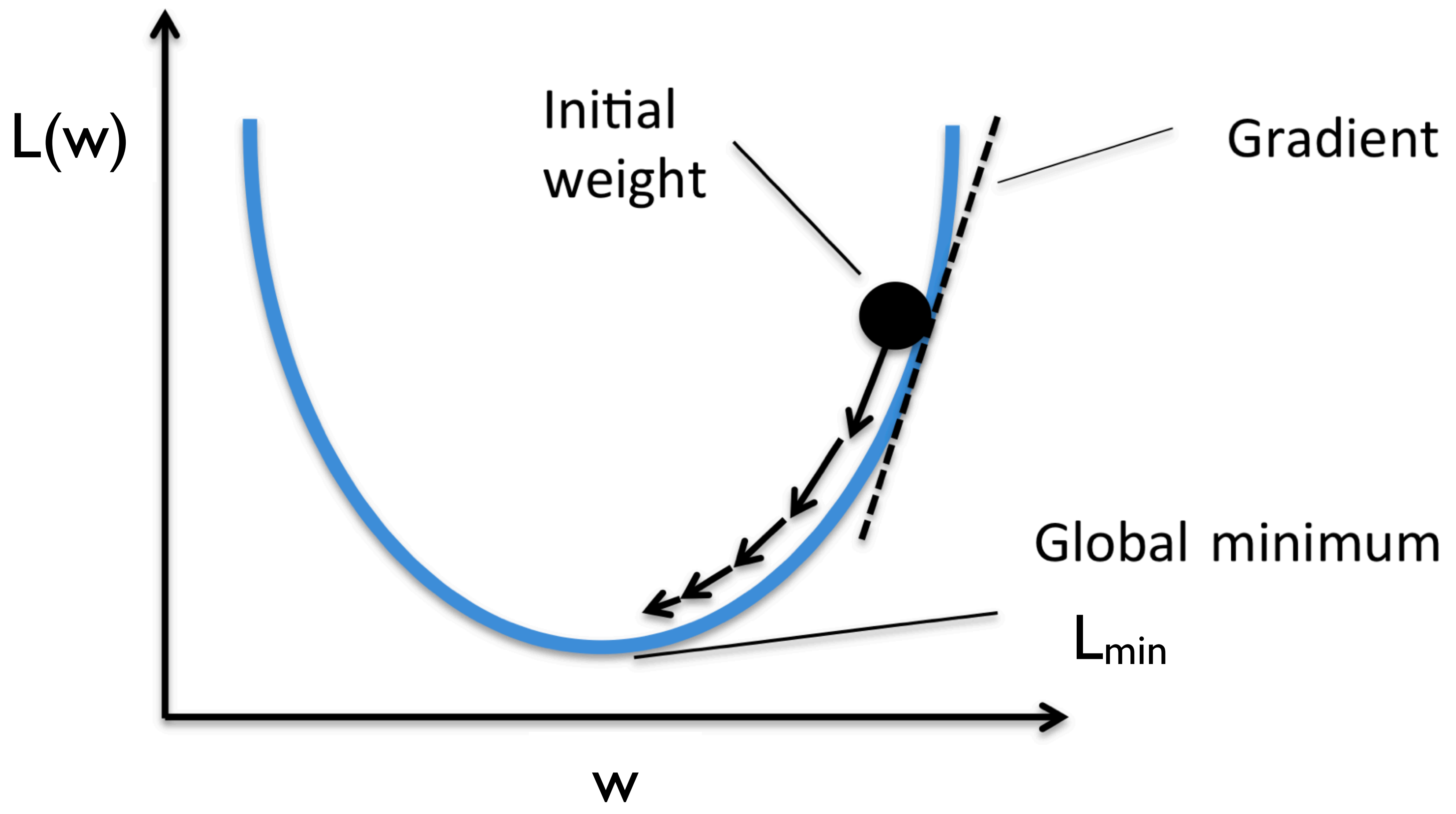
sum over output space to normalize

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

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

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

index of data points (j)



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index of data points (j)

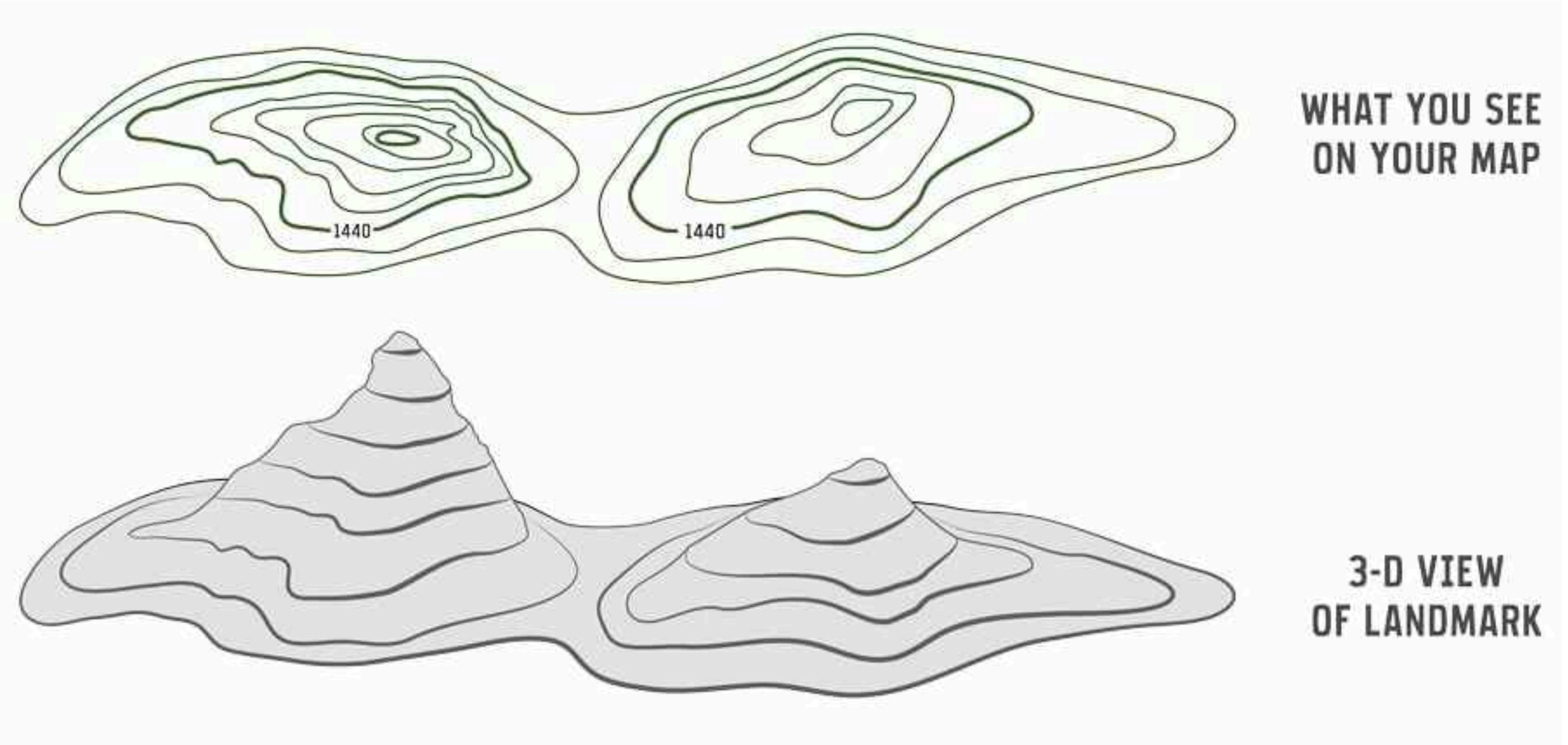
i.e. minimize negative log likelihood or cross-entropy loss

- 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
```

Optimization

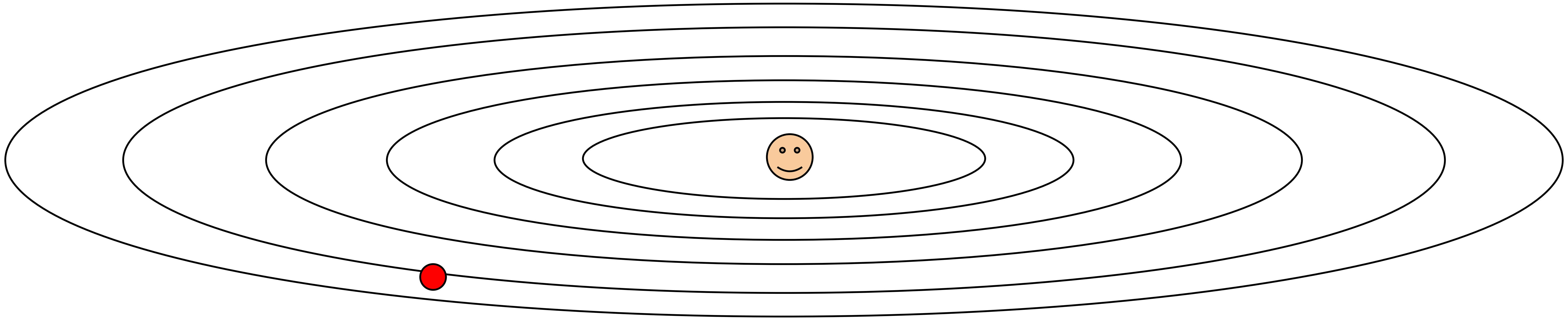


- **Stochastic** gradient descent

$$w \leftarrow w - \alpha g, \quad g = \frac{\partial}{\partial w}\mathcal{L}$$

  - Approx. gradient is computed on a single instance

Q: What if loss changes quickly in one direction and slowly in another direction?



contour plot

Optimization

- **Stochastic** gradient descent

$$w \leftarrow w - \alpha g, \quad g = \frac{\partial}{\partial w}\mathcal{L}$$

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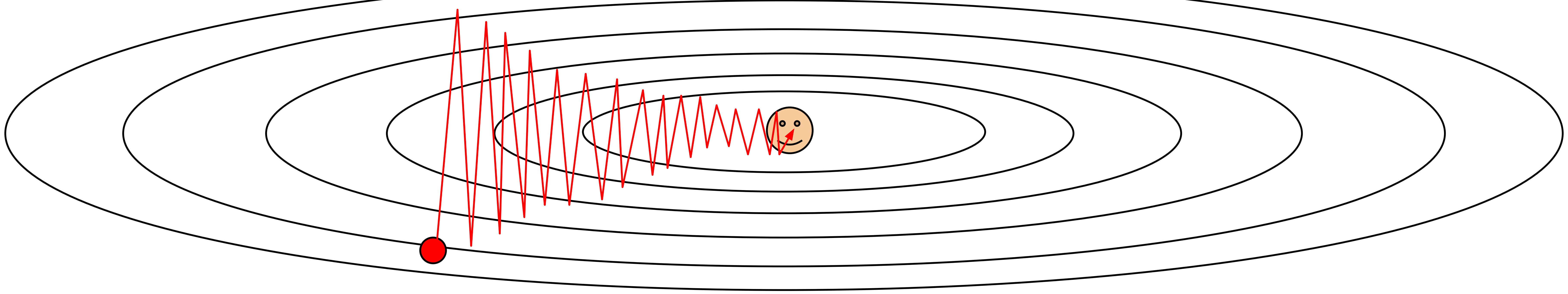
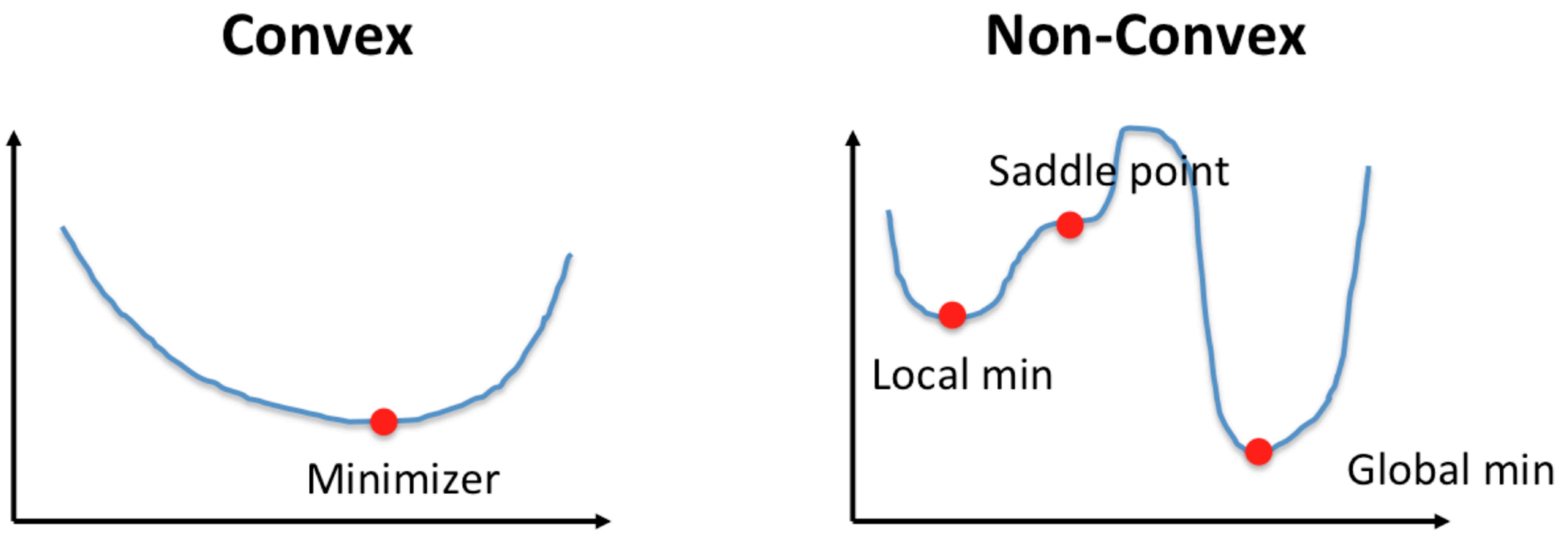


Optimization

- **Stochastic** gradient descent
  - Very simple to code up
  - What if the loss function has a local minima or saddle point?

$$w \leftarrow w - \alpha g, \quad g = \frac{\partial}{\partial w}\mathcal{L}$$

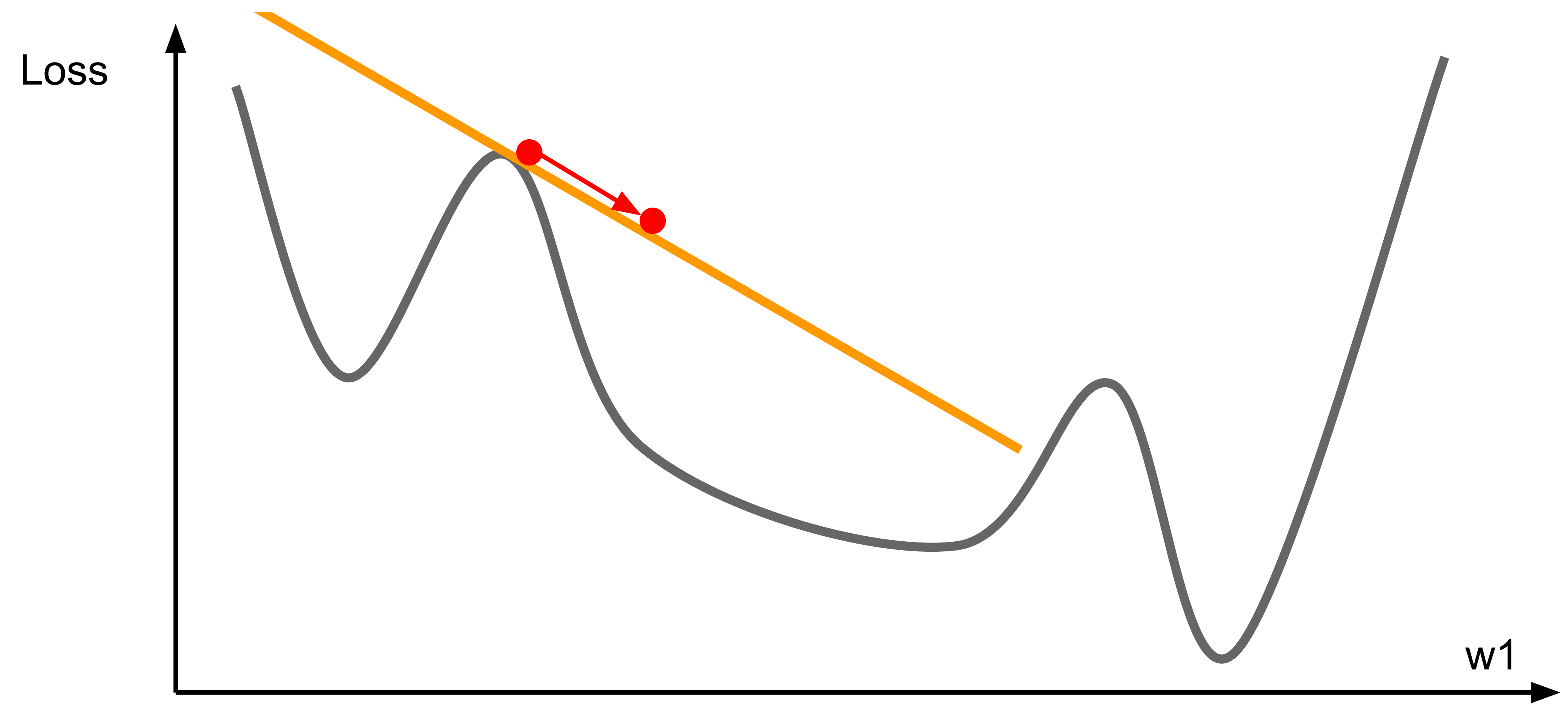


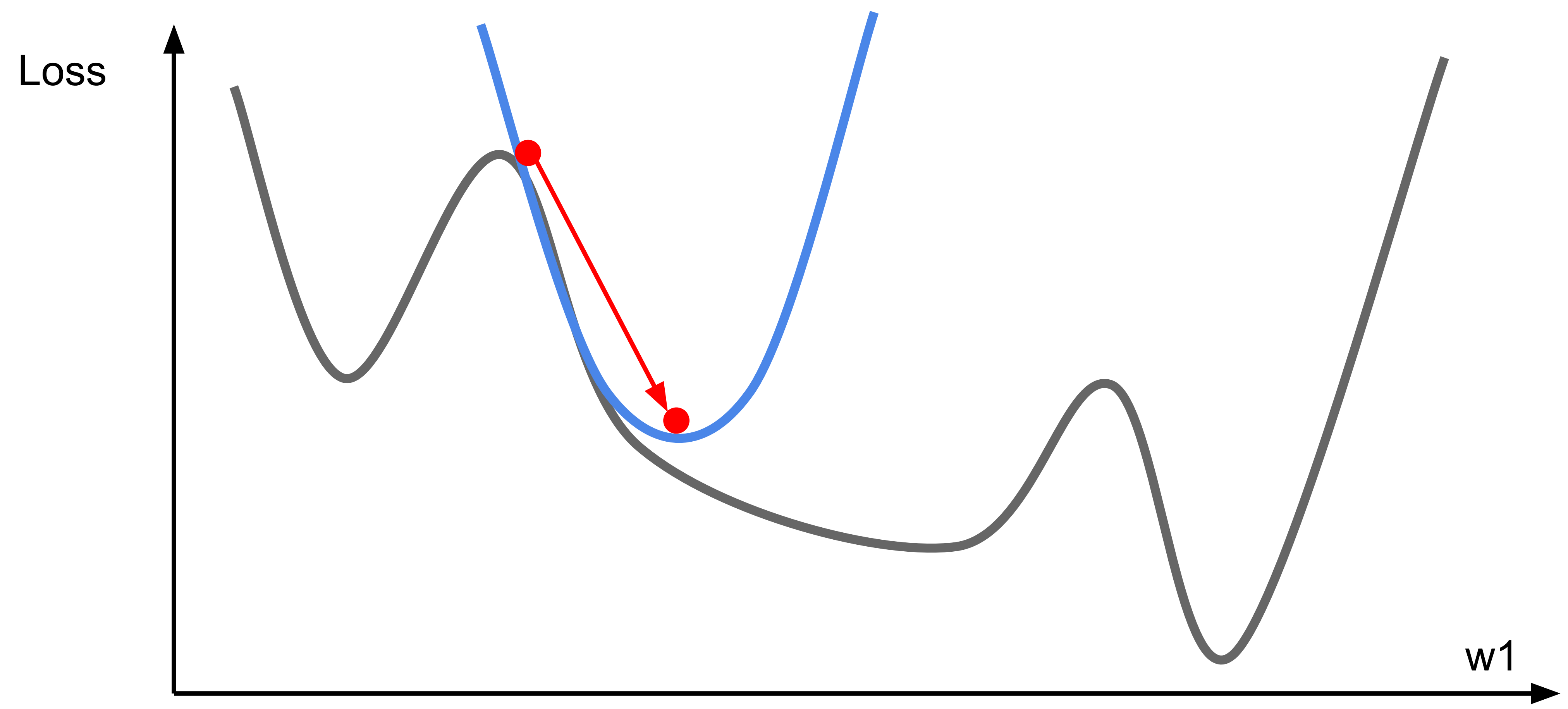
"Identifying and attacking the saddle point problem in high-dimensional non-convex optimization"
Dauphin et al. (2014)

Optimization

- Stochastic gradient descent
  - Very simple to code up
  - "First-order" technique: only relies on having gradient

$$w \leftarrow w - \alpha g, \quad g = \frac{\partial}{\partial w}\mathcal{L}$$





Optimization (extracurricular)

- Stochastic gradient descent
  - Very simple to code up
  - "First-order" technique: only relies on having gradient
  - Setting step size is hard (decrease when held-out performance worsens?)

$$w \leftarrow w - \alpha g, \quad g = \frac{\partial}{\partial w}\mathcal{L}$$

- Newton's method
  - Second-order technique
  - Optimizes quadratic instantly

$$w \leftarrow w - \left(\frac{\partial^2}{\partial w^2}\mathcal{L}\right)^{-1} g$$

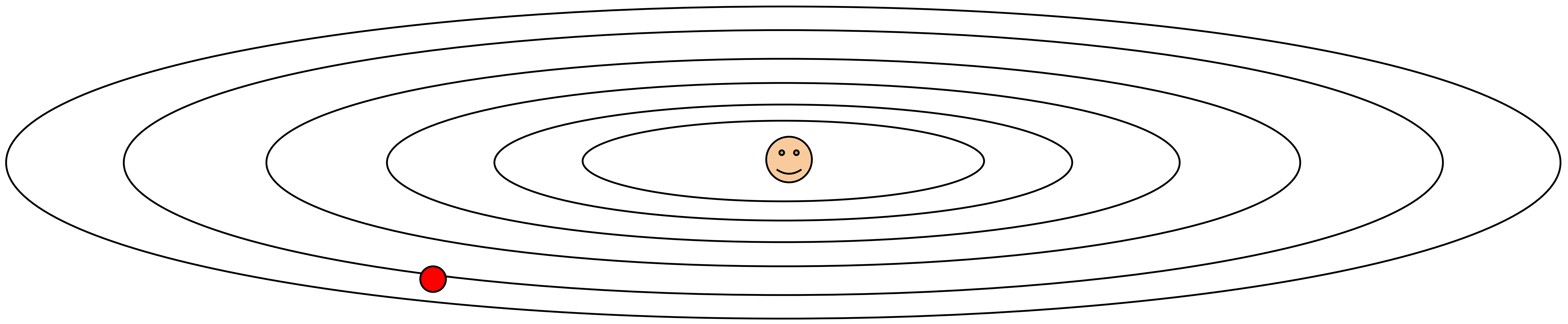
Inverse Hessian: *n* x *n* mat, expensive!

- Quasi-Newton methods: L-BFGS, etc. approximate inverse Hessian

AdaGrad

- Optimized for problems with sparse features
- Per-parameter learning rate: smaller updates are made to parameters that get updated frequently

```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```



Duchi et al. (2011)

AdaGrad

- Optimized for problems with sparse features
- Per-parameter learning rate: smaller updates are made to parameters that get updated frequently

$$w_i \leftarrow w_i + \alpha \frac{1}{\sqrt{\epsilon + \sum_{\tau=1}^{t} g_{\tau,i}^2}} g_{t_i}$$

← (smoothed) sum of squared gradients from all updates

- Generally more robust than SGD, requires less tuning of learning rate
- Other techniques for optimizing deep models — more later!

Duchi et al. (2011)

Summary

- Design tradeoffs need to reflect interactions:
  - Model and objective are coupled: probabilistic model <-> maximize likelihood
  - …but not always: a linear model or neural network can be trained to minimize any differentiable loss function
  - Inference governs what learning: need to be able to compute expectations to use logistic regression

Next Up

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