

Multiclass Classification

Alan Ritter

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

This Lecture

- ▶ Multiclass fundamentals
- ▶ Feature extraction
- ▶ Multiclass logistic regression
- ▶ Multiclass SVM
- ▶ 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

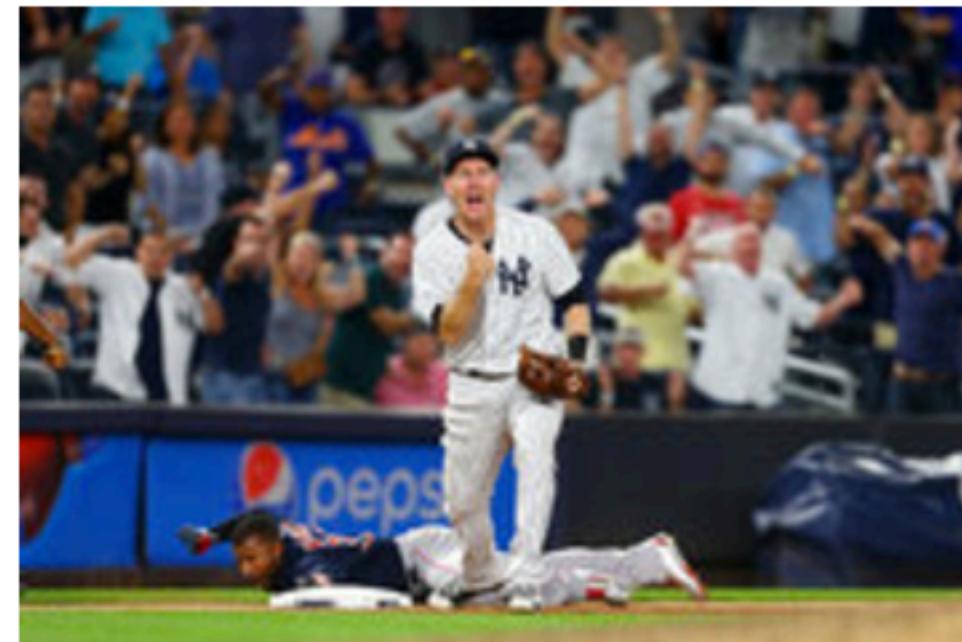
Yankees and Mets Are on Opposite Tracks This Subway Series

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



→ Health



→ Sports

~20 classes

Image Classification



→ Dog



→ Car

- ▶ Thousands of classes (ImageNet)

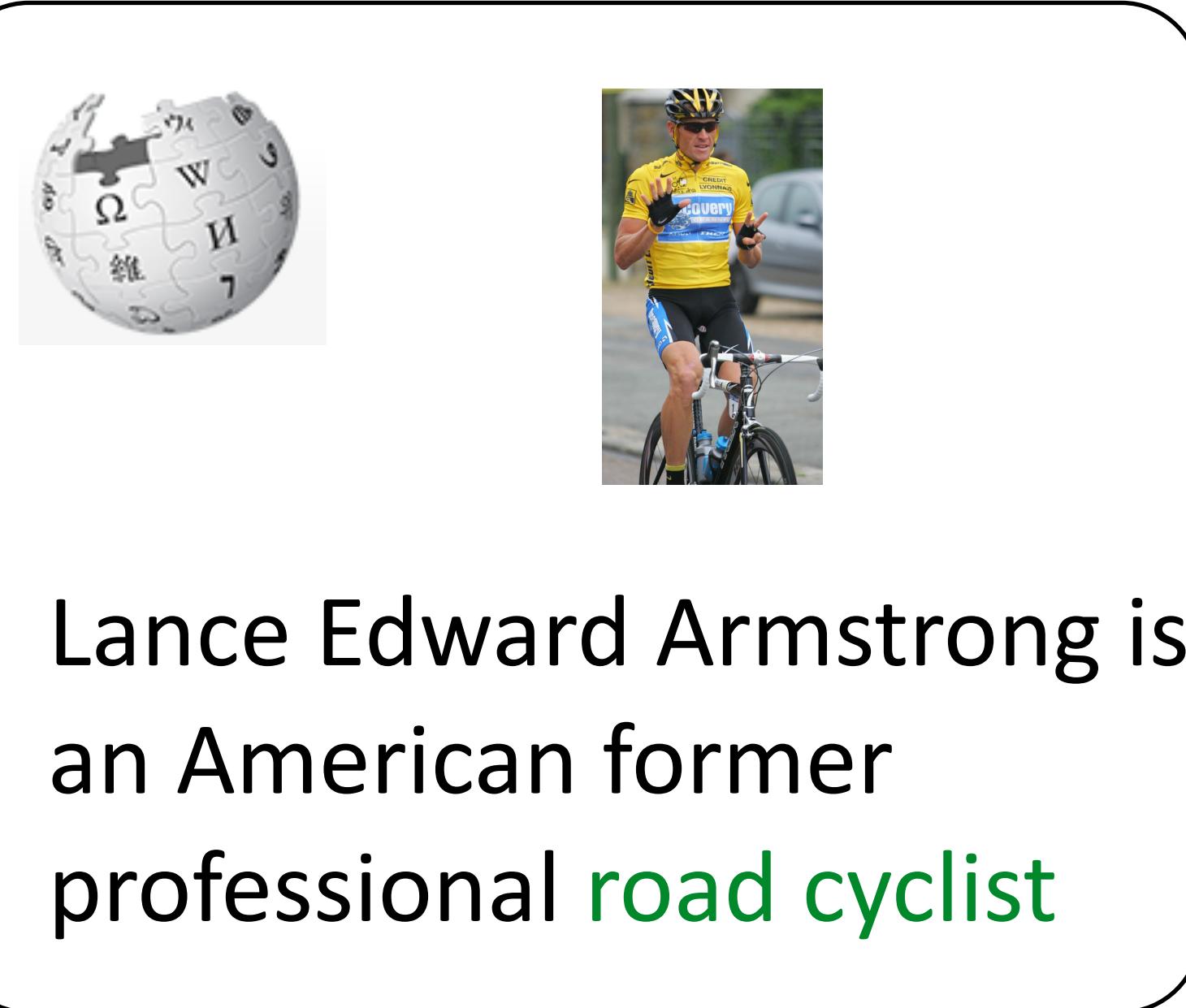
Entity Linking

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Armstrong County is a county in Pennsylvania...

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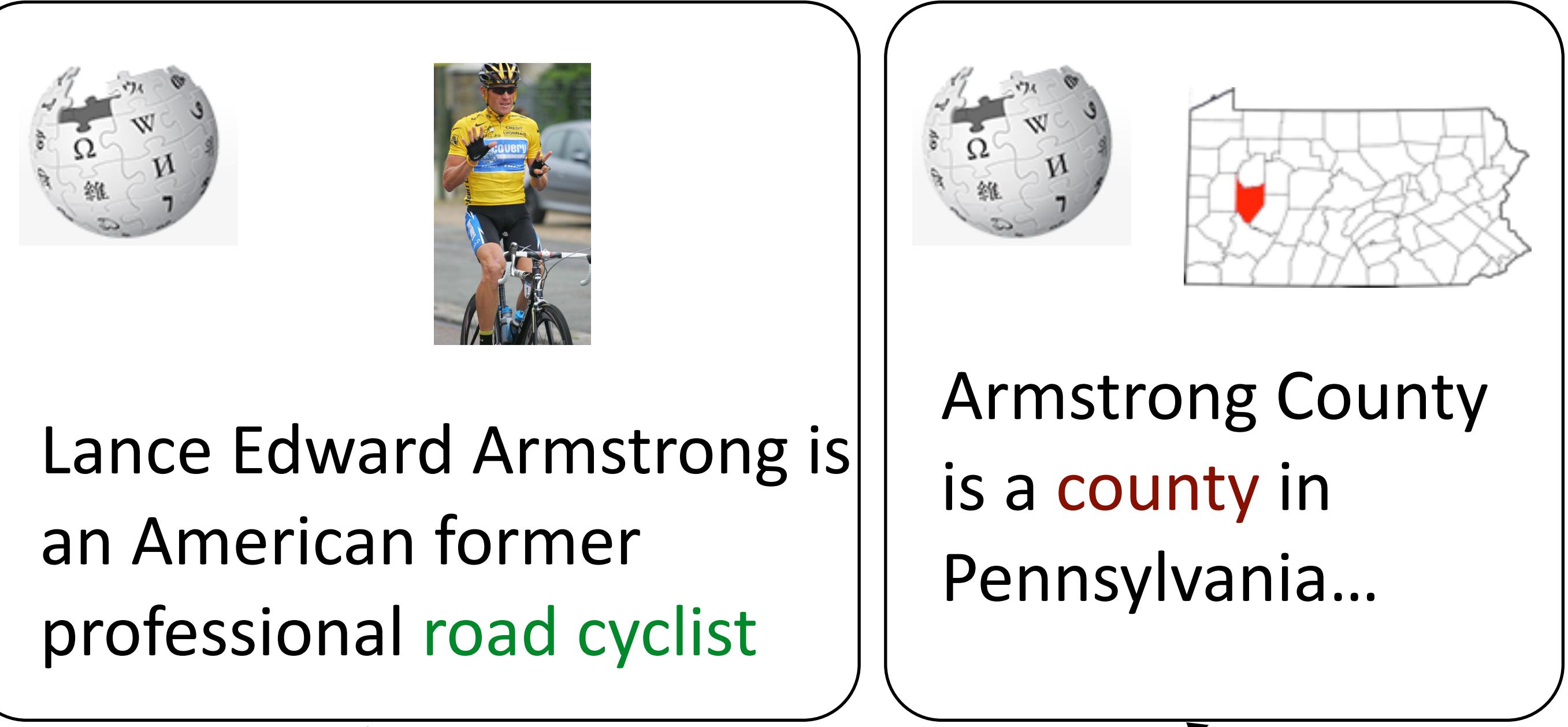
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- ▶ 4,500,000 classes (all articles in Wikipedia)

Reading Comprehension

One day, James thought he would go into town and see what kind of trouble he could get into. He went to the grocery store and pulled all the pudding off the shelves and ate two jars. Then he walked to the fast food restaurant and ordered 15 bags of fries. He didn't pay, and instead headed home.

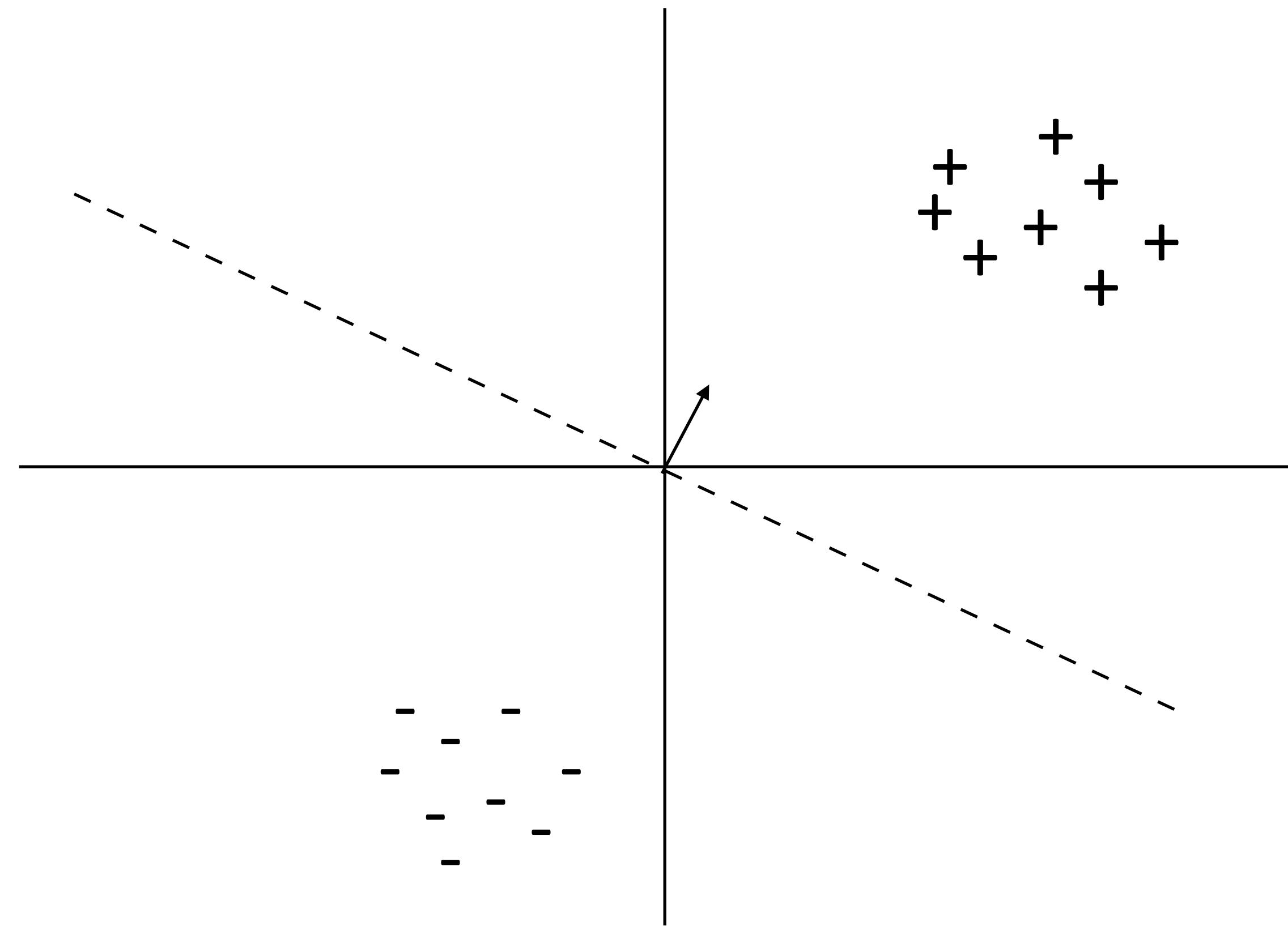
3) Where did James go after he went to the grocery store?

- A) his deck
- B) his freezer
- C) a fast food restaurant
- D) his room

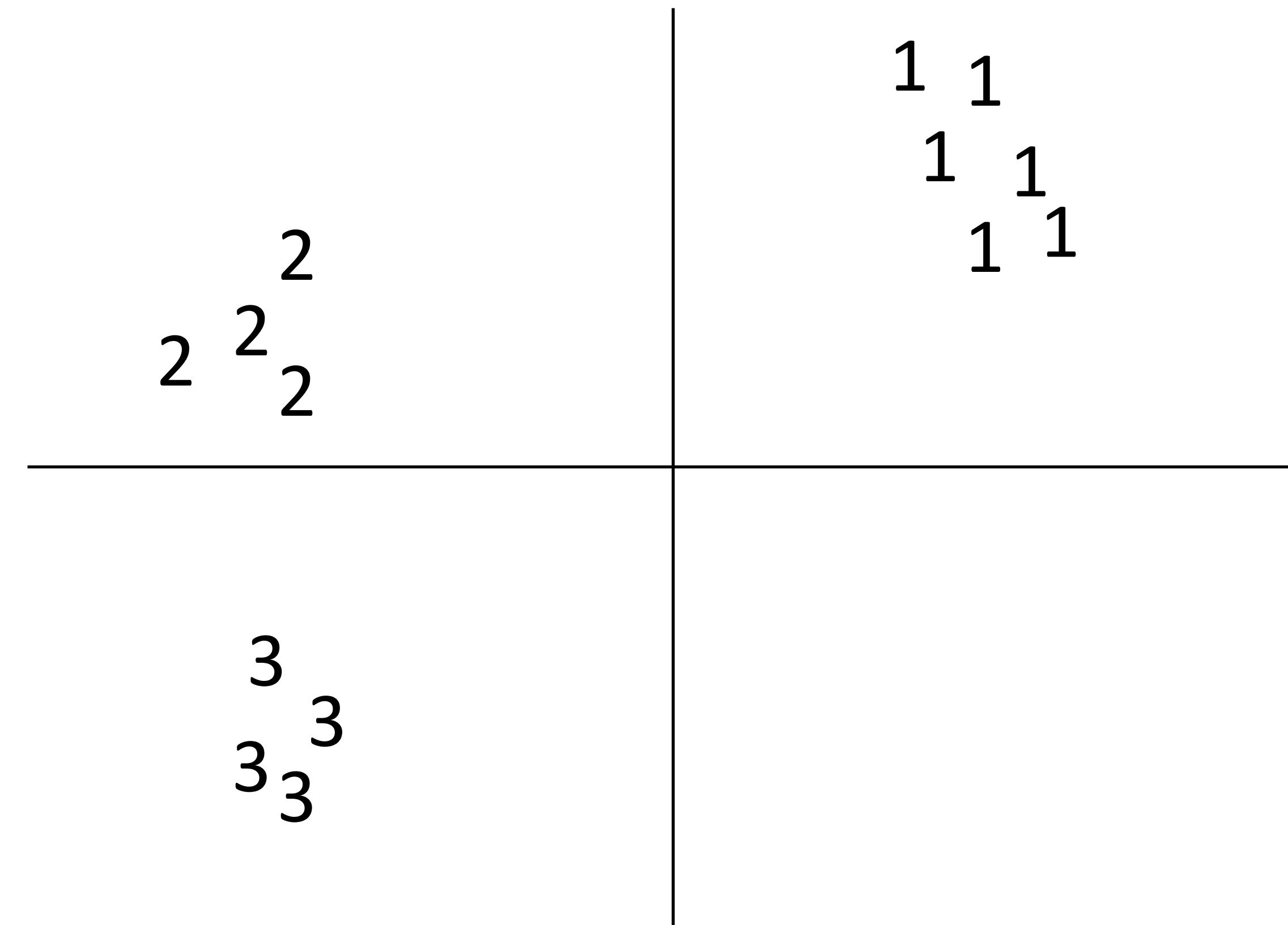
► Multiple choice questions, 4 classes (but classes change per example)

Binary Classification

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

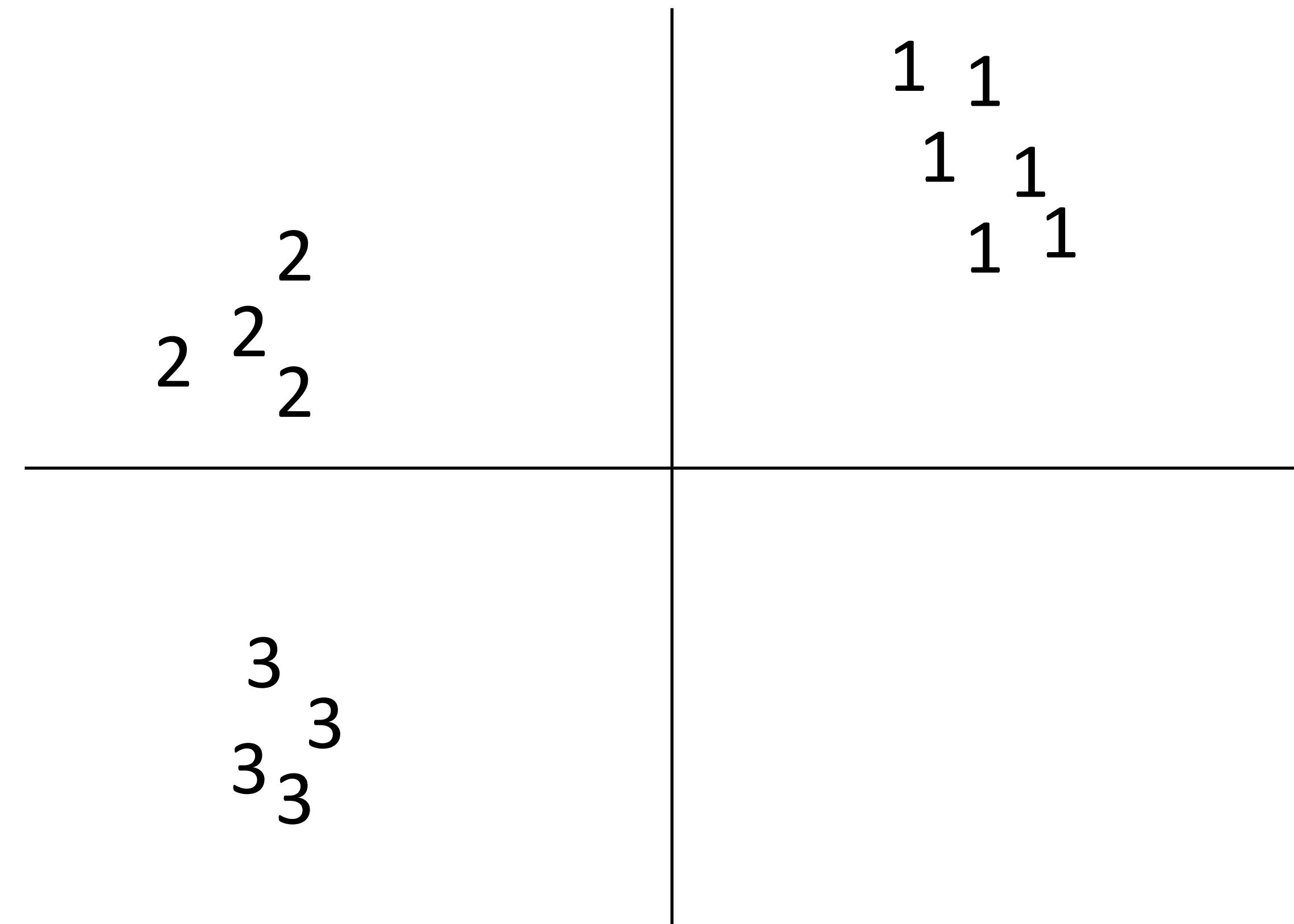


Multiclass Classification



Multiclass Classification

- ▶ Can we just use binary classifiers here?

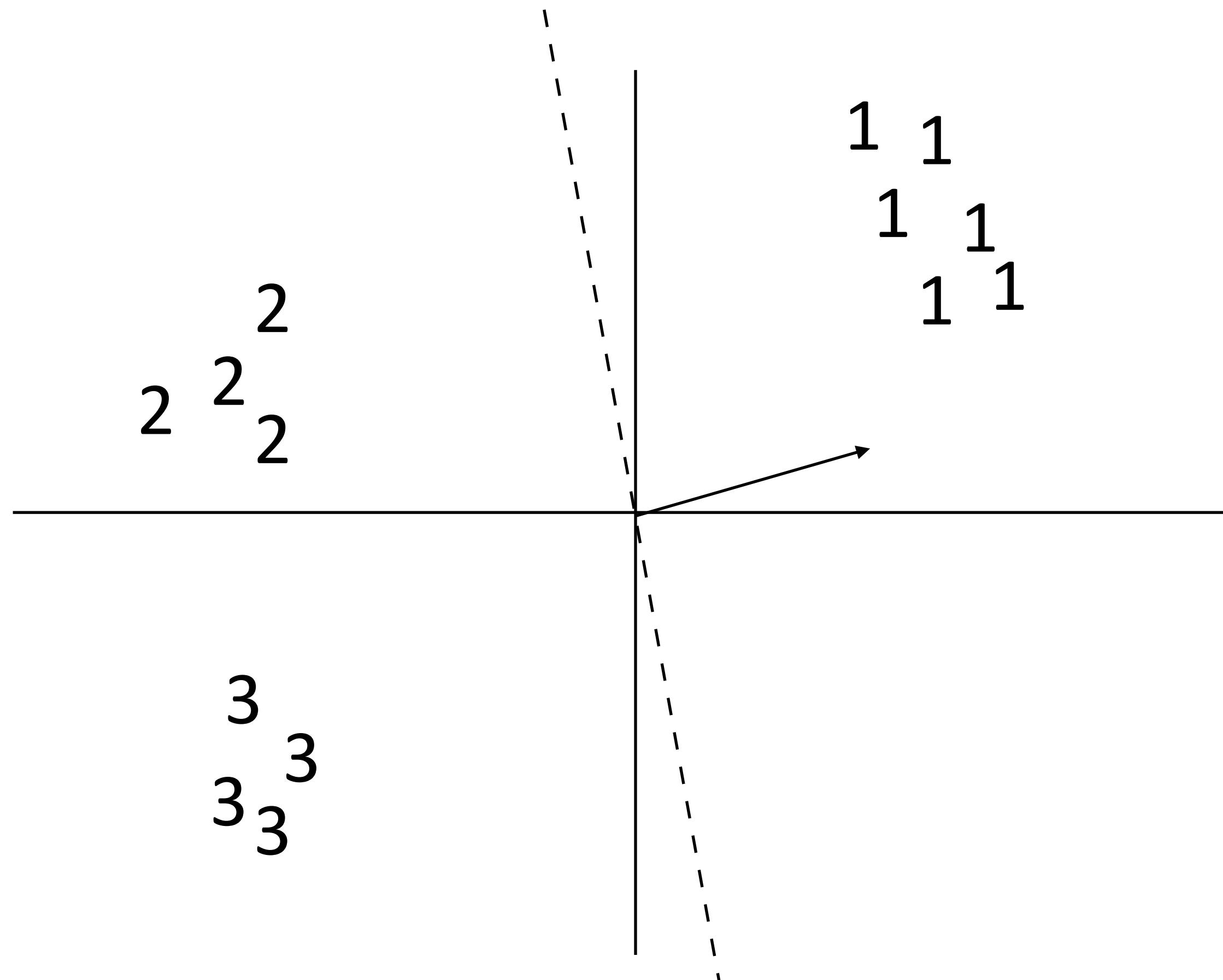


Multiclass Classification

- ▶ One-vs-all: train k classifiers, one to distinguish each class from all the rest

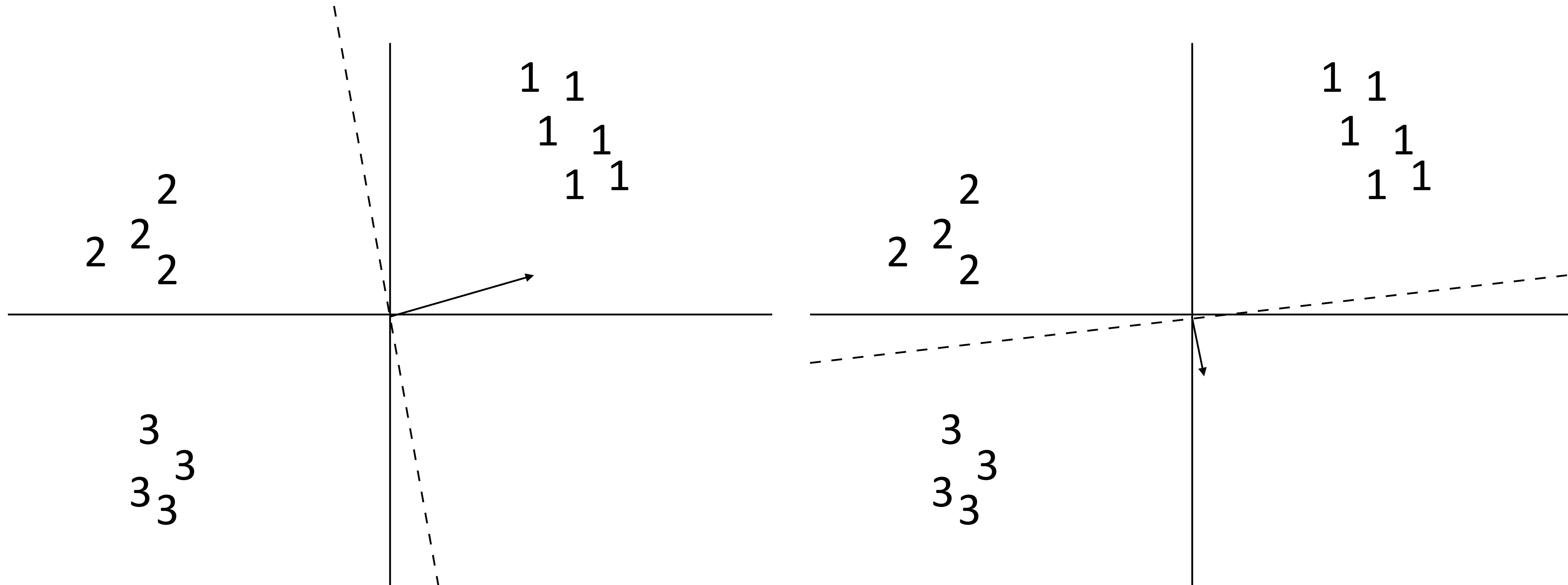
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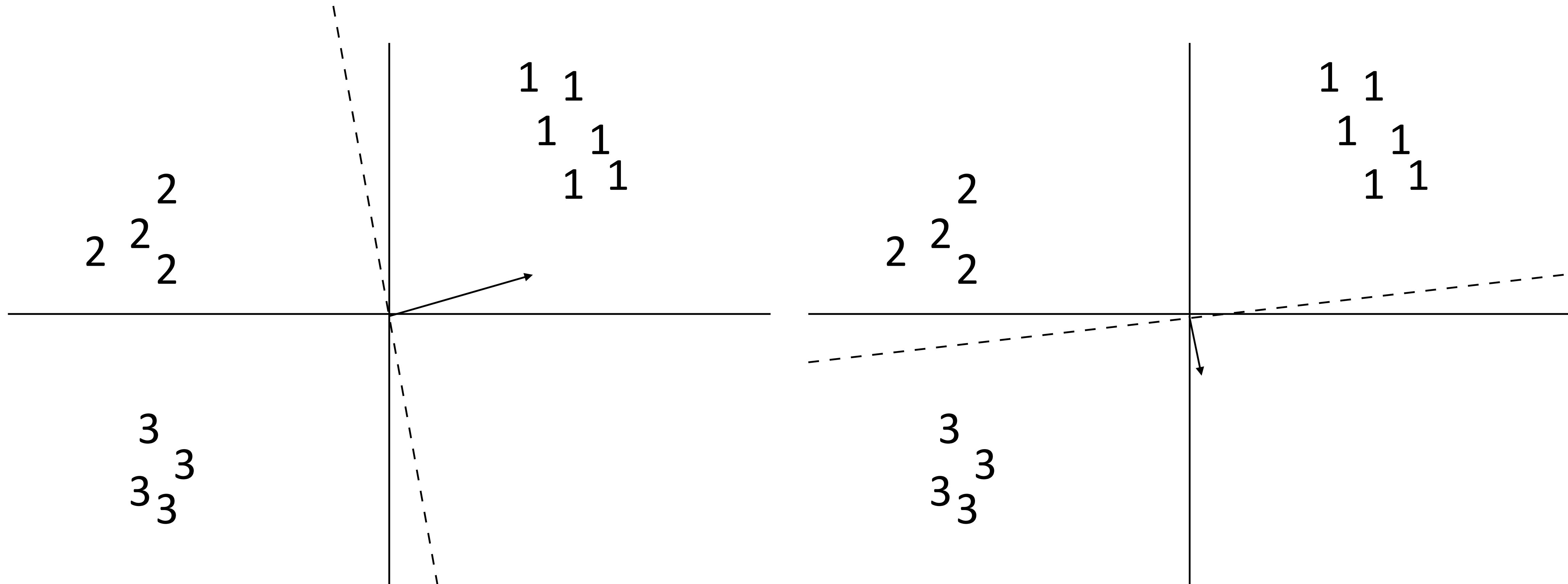
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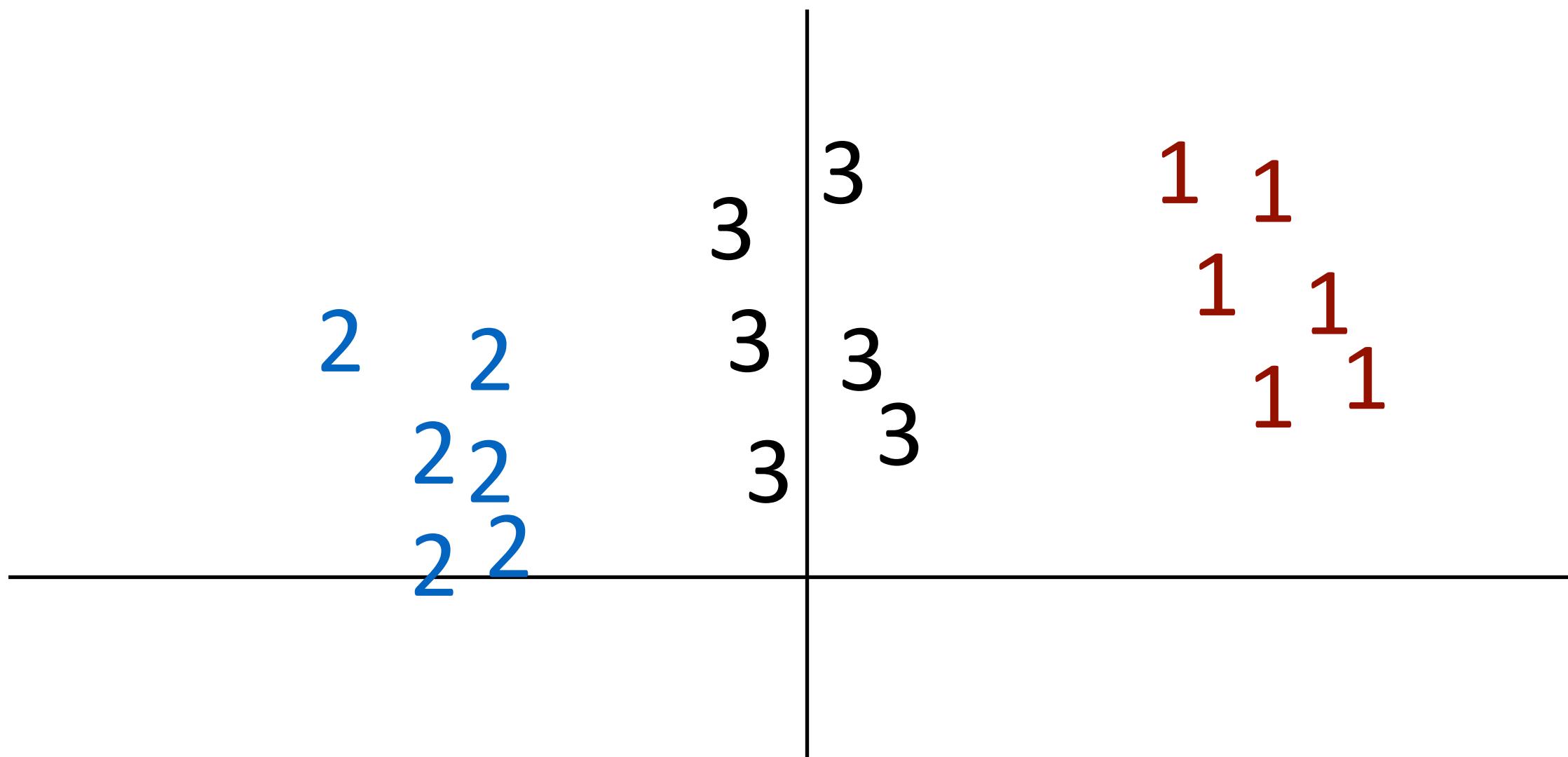
Multiclass Classification

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



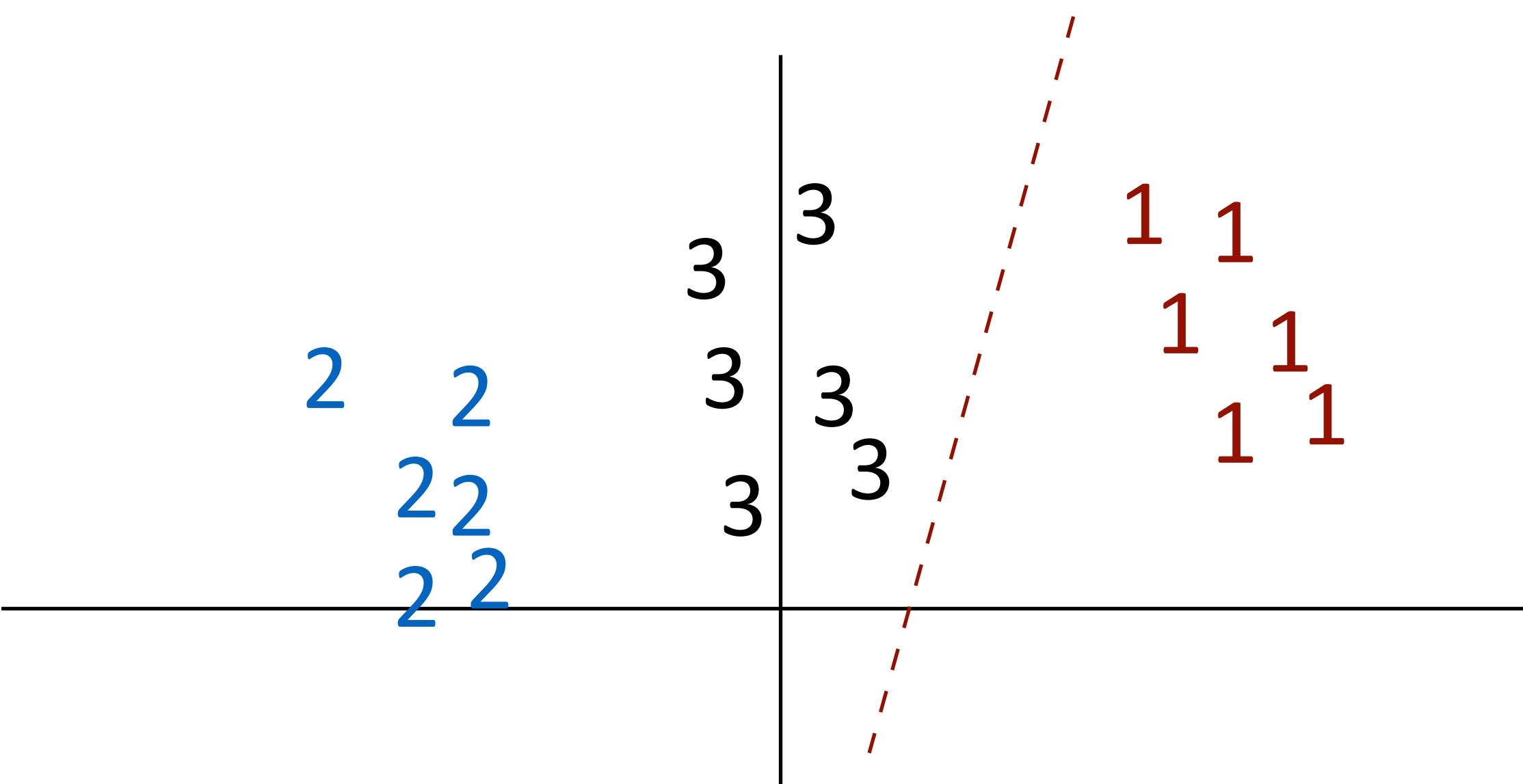
Multiclass Classification

- Not all classes may even be separable using this approach



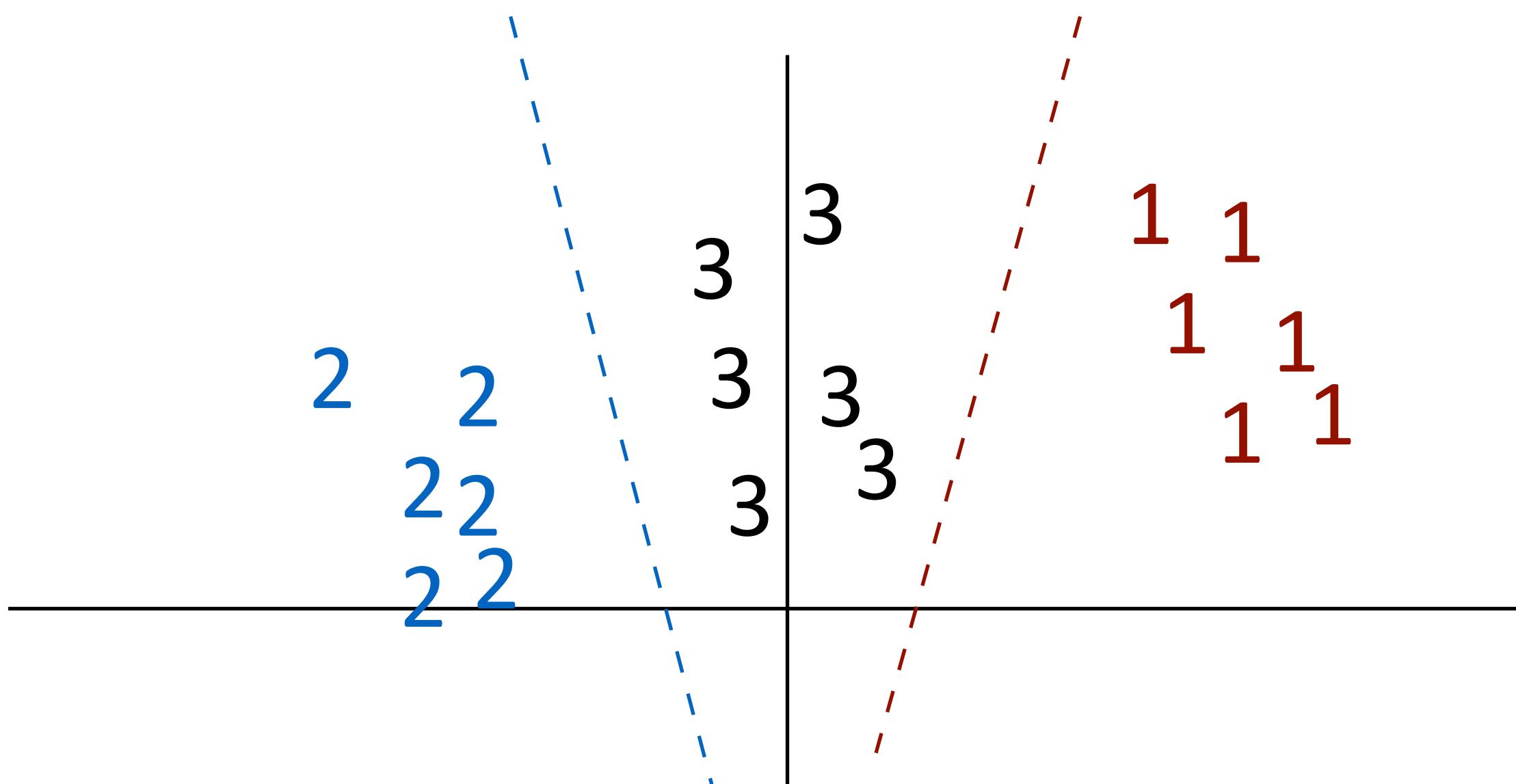
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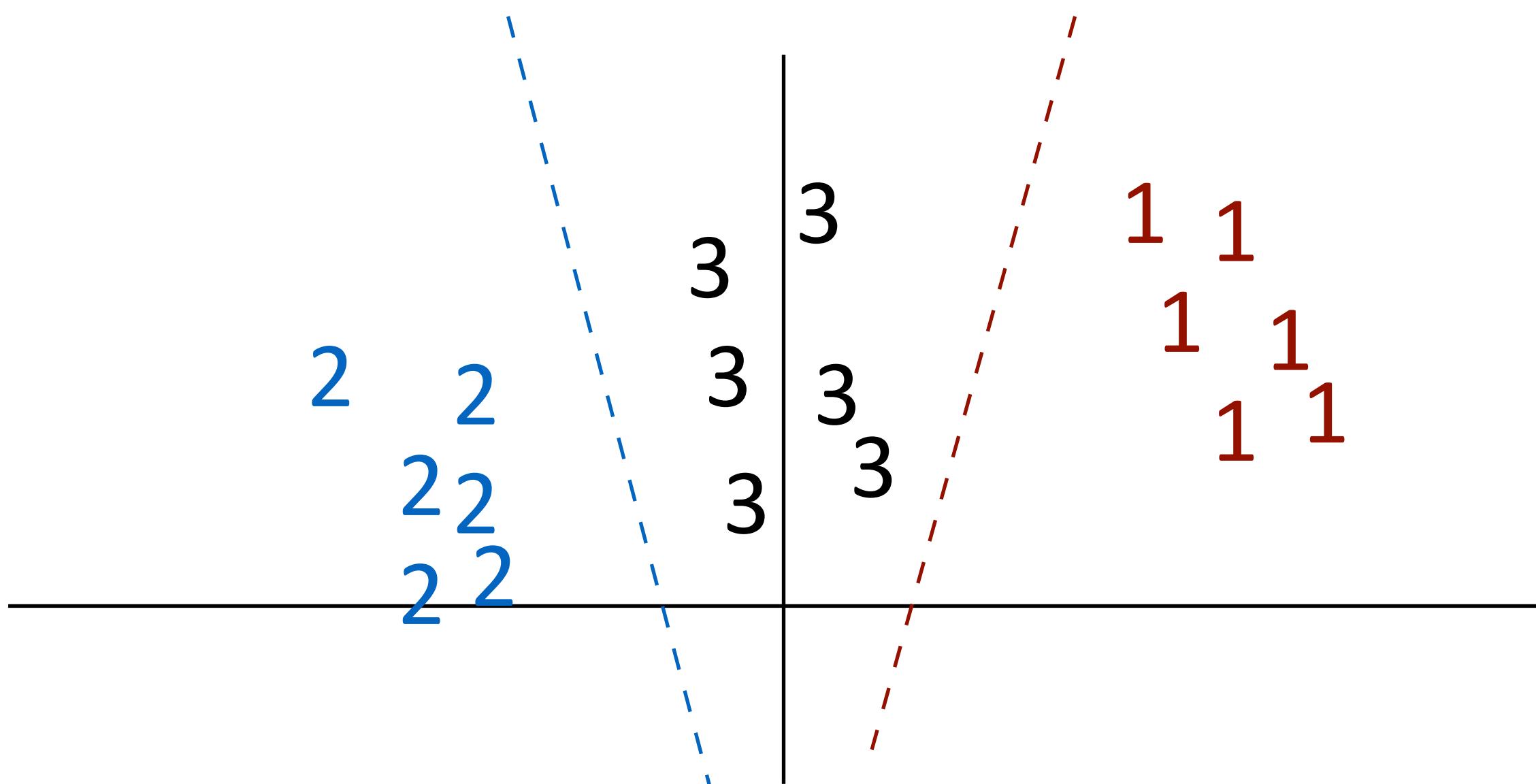
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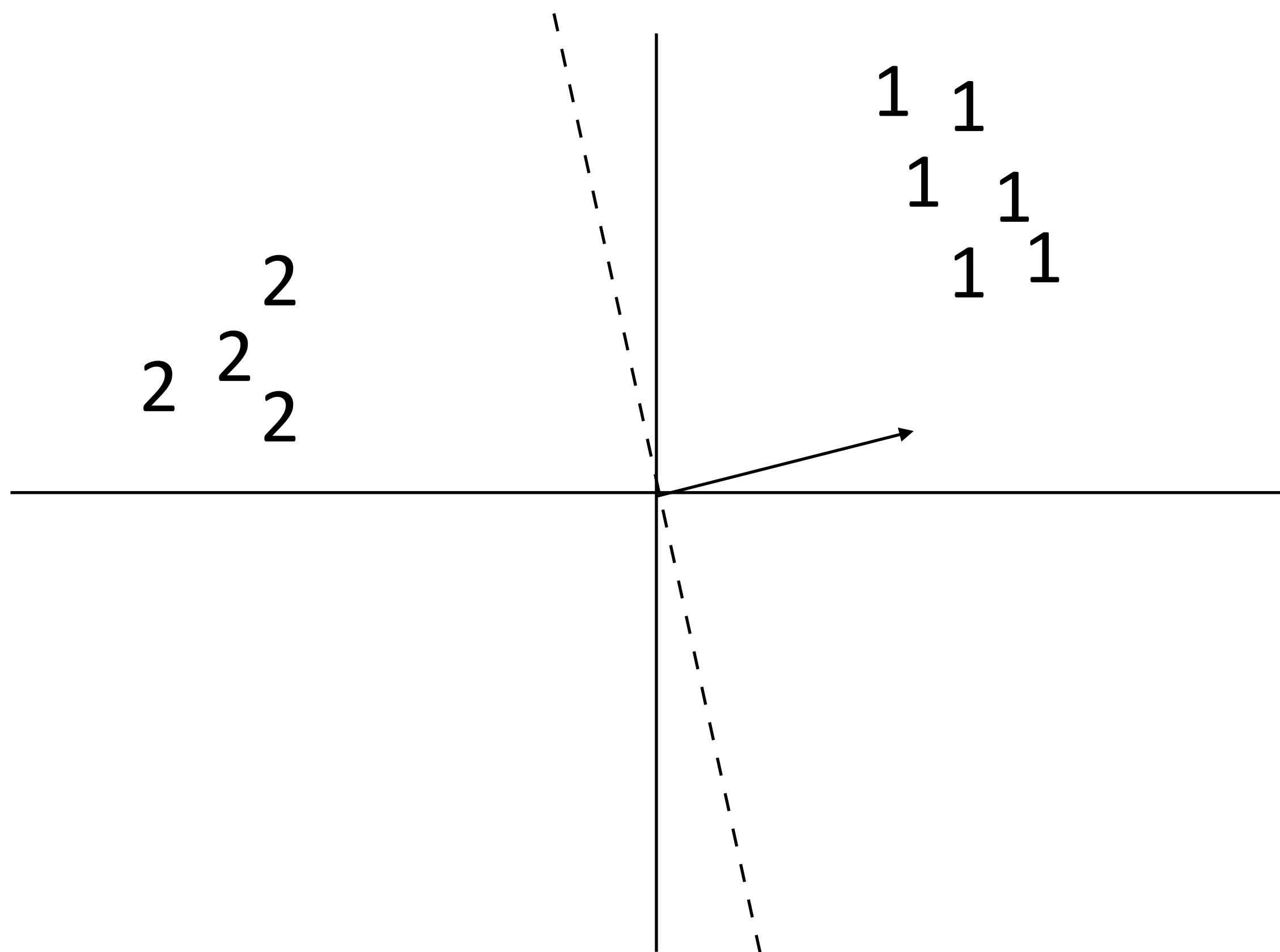
- ▶ Can separate 1 from 2+3 and 2 from 1+3 but not 3 from the others (with these features)

Multiclass Classification

- ▶ All-vs-all: train $n(n-1)/2$ classifiers to differentiate each pair of classes

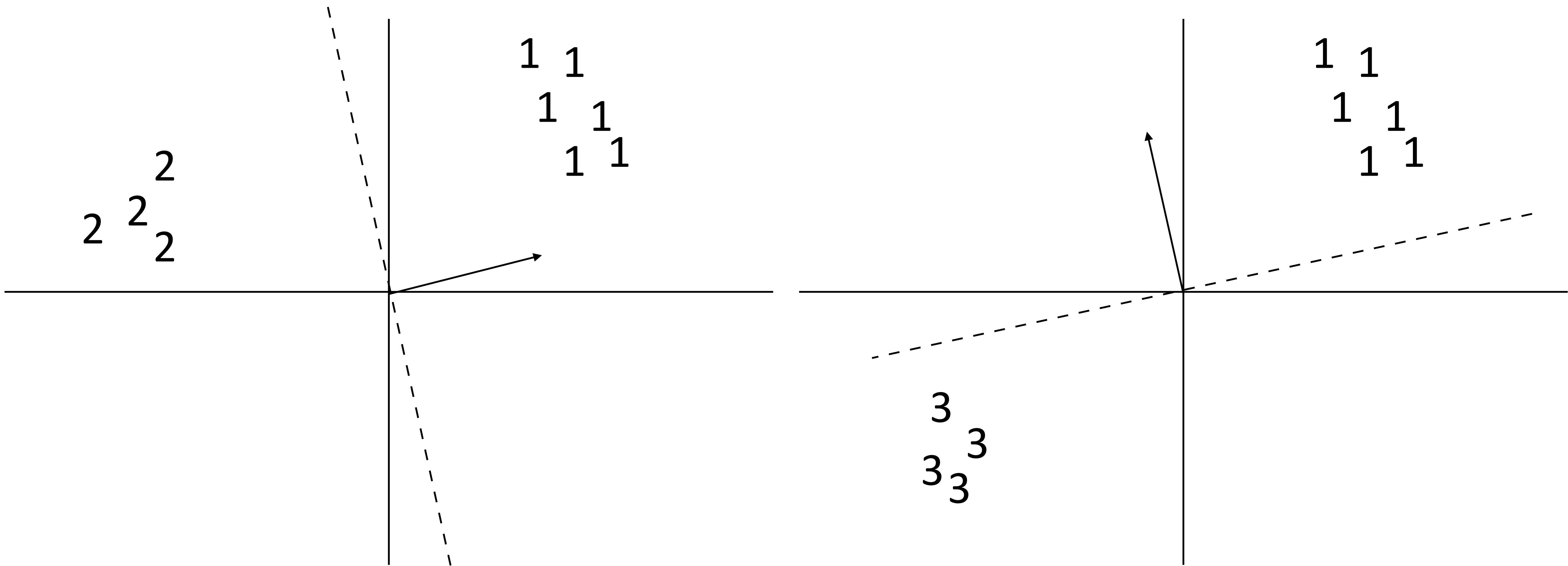
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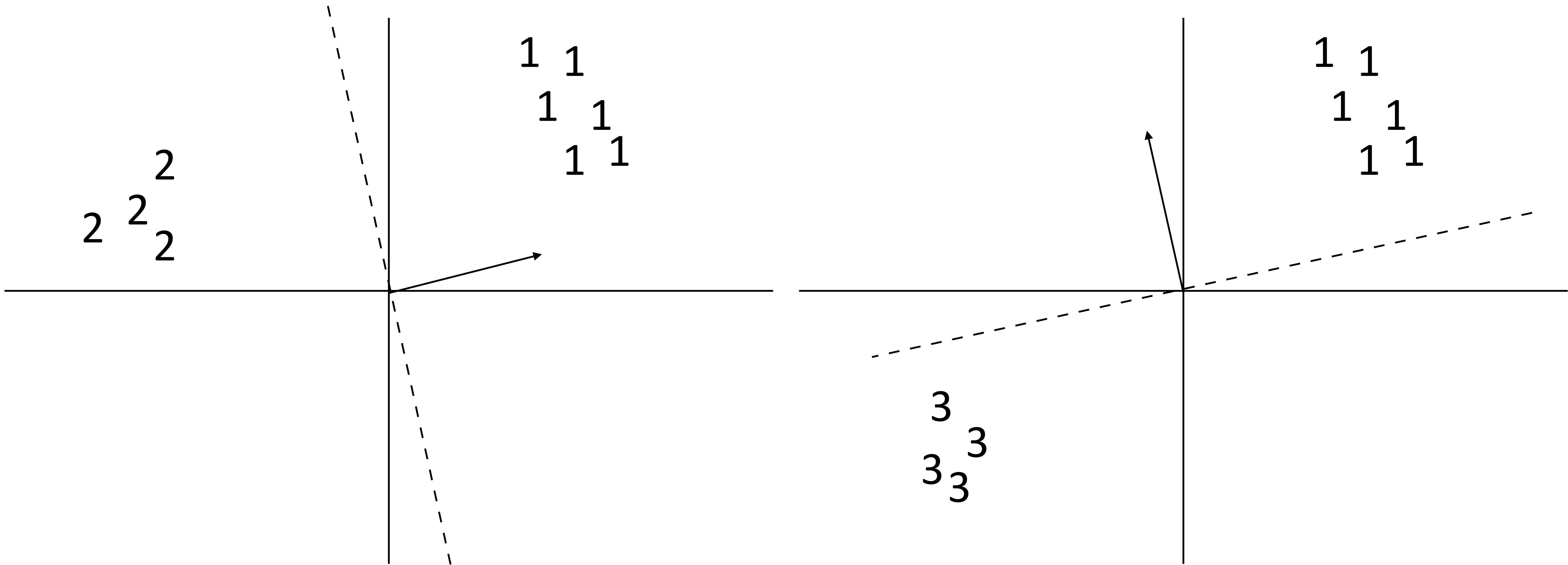
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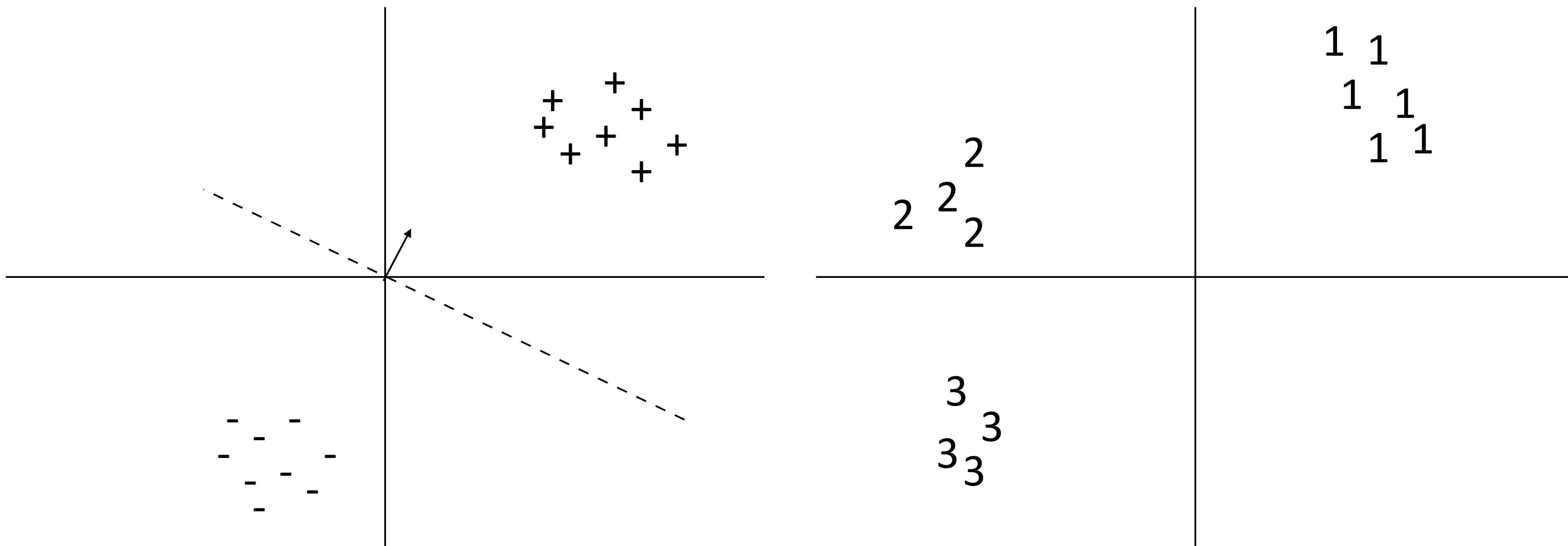
Multiclass Classification

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



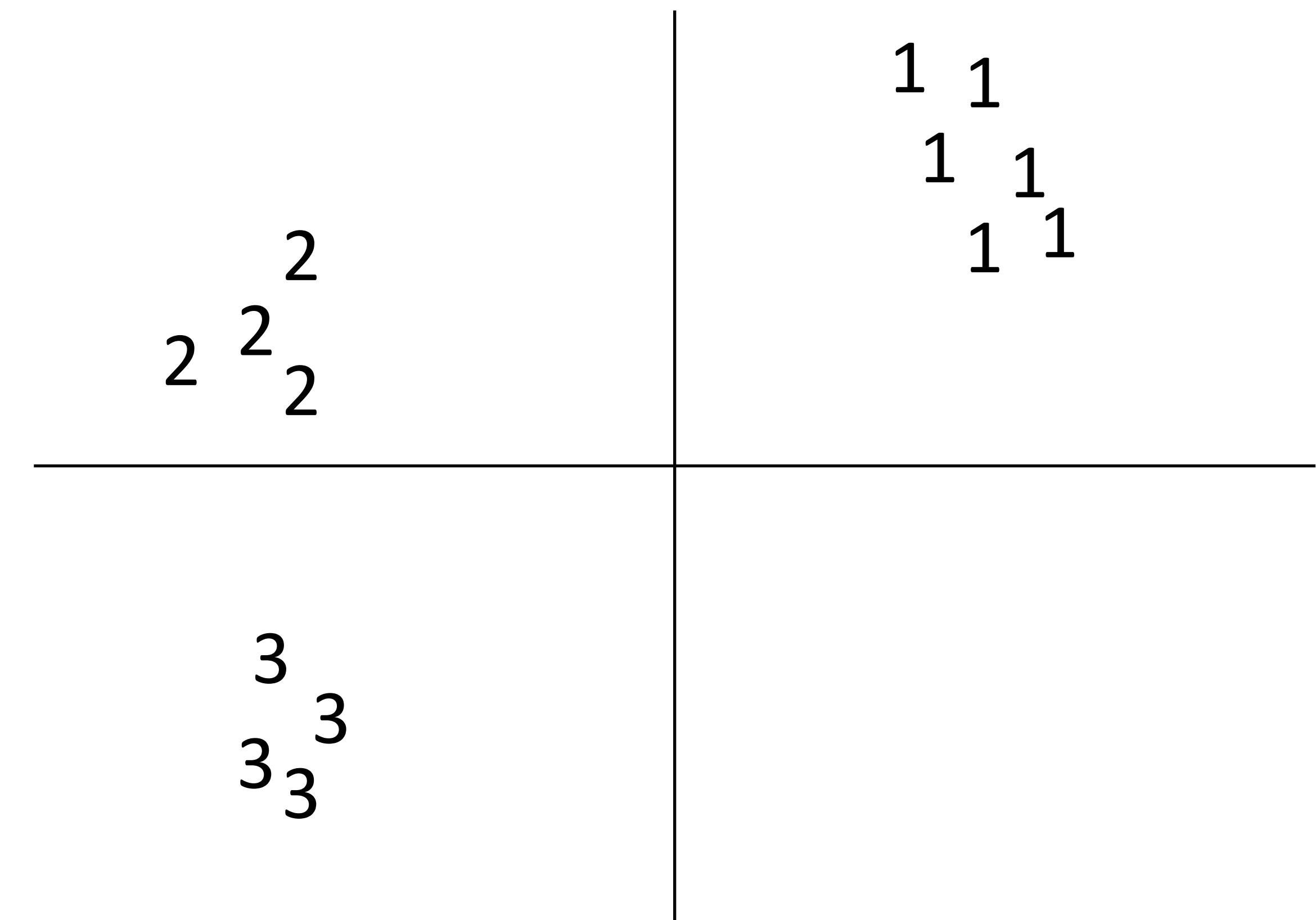
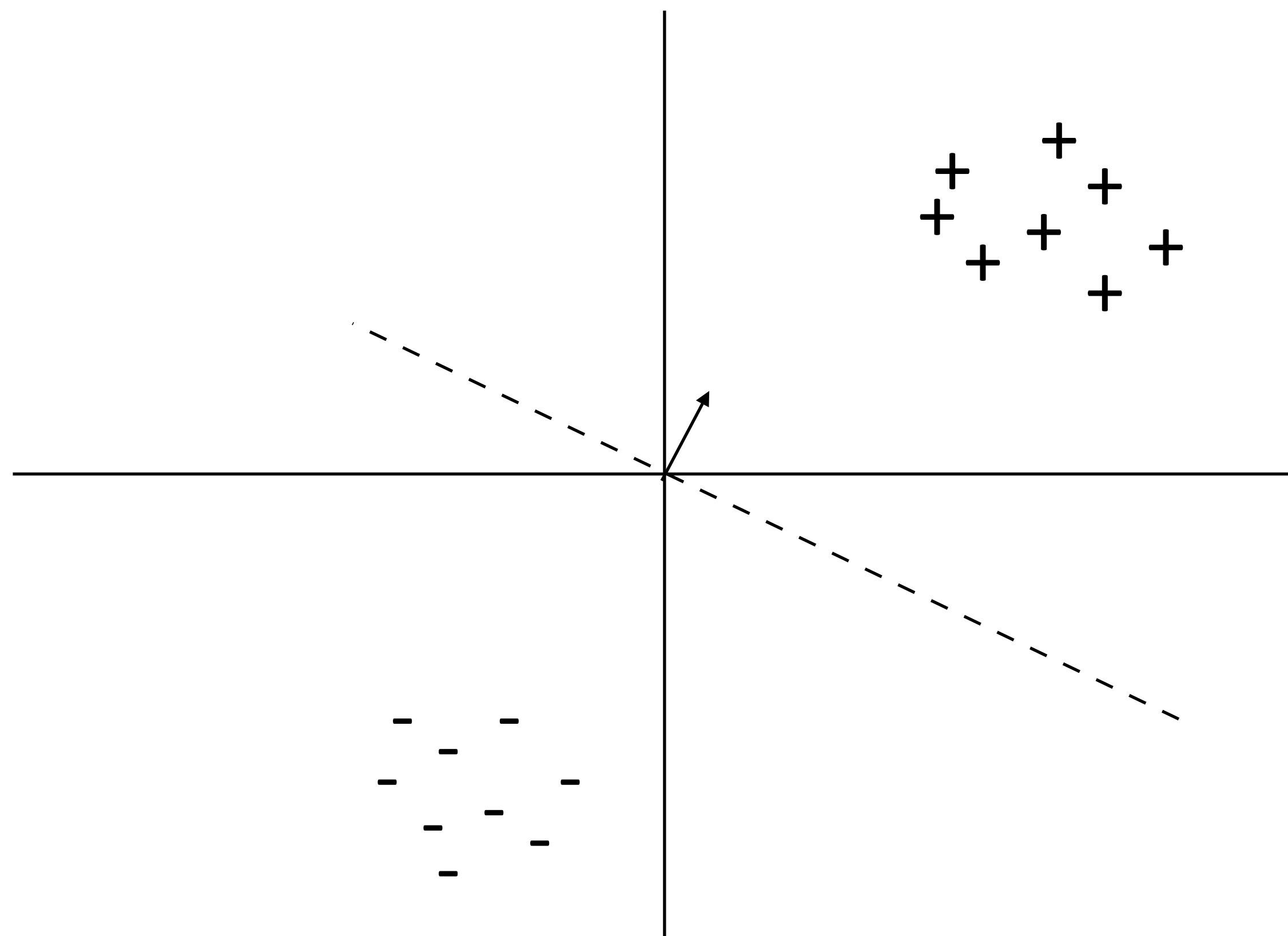
Multiclass Classification

- ▶ Binary classification: one weight vector defines both classes



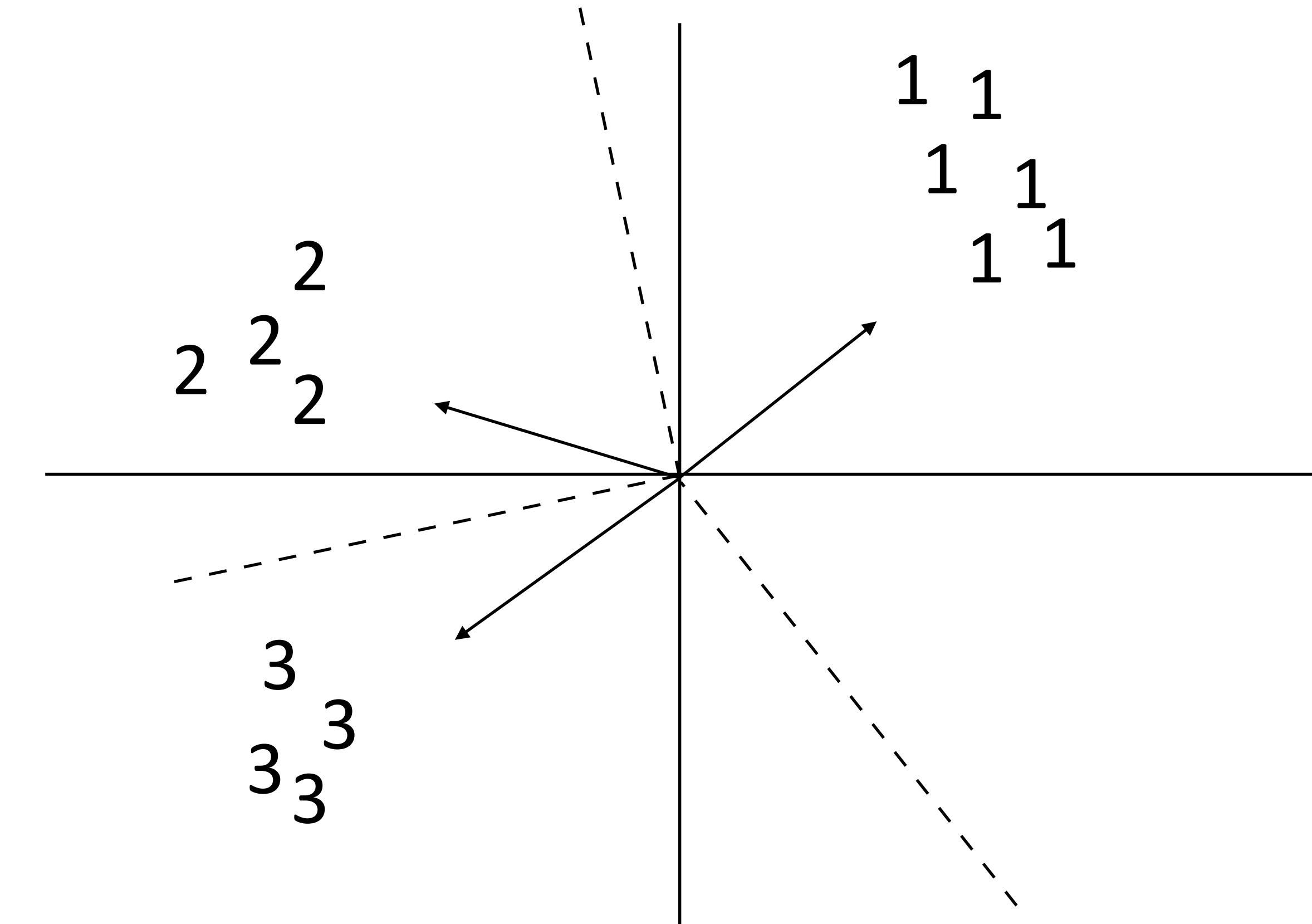
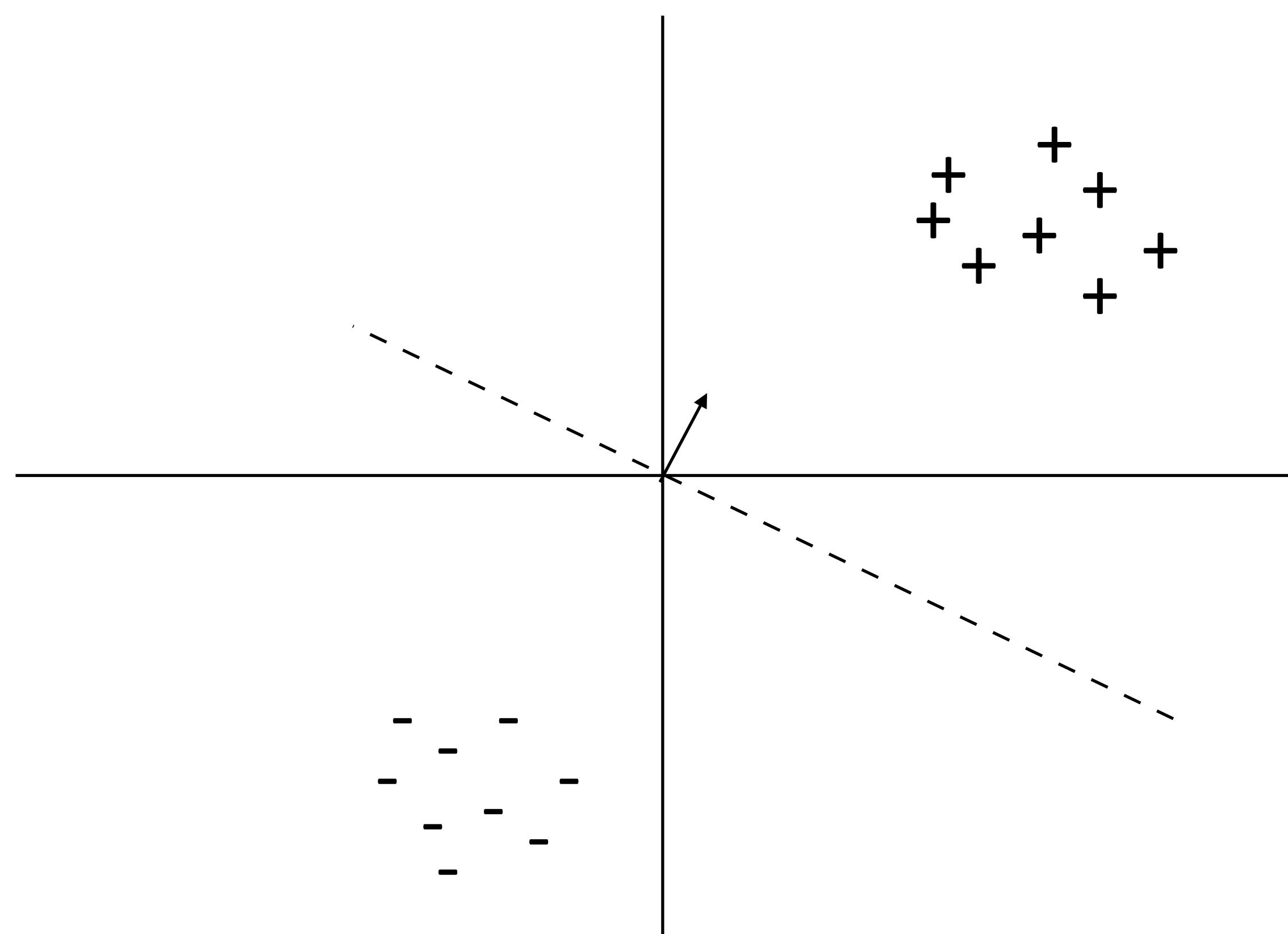
Multiclass Classification

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



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Multiclass Classification

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 - ▶ Same machinery that we'll use later for exponentially large output spaces, including sequences and trees

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

Feature Extraction

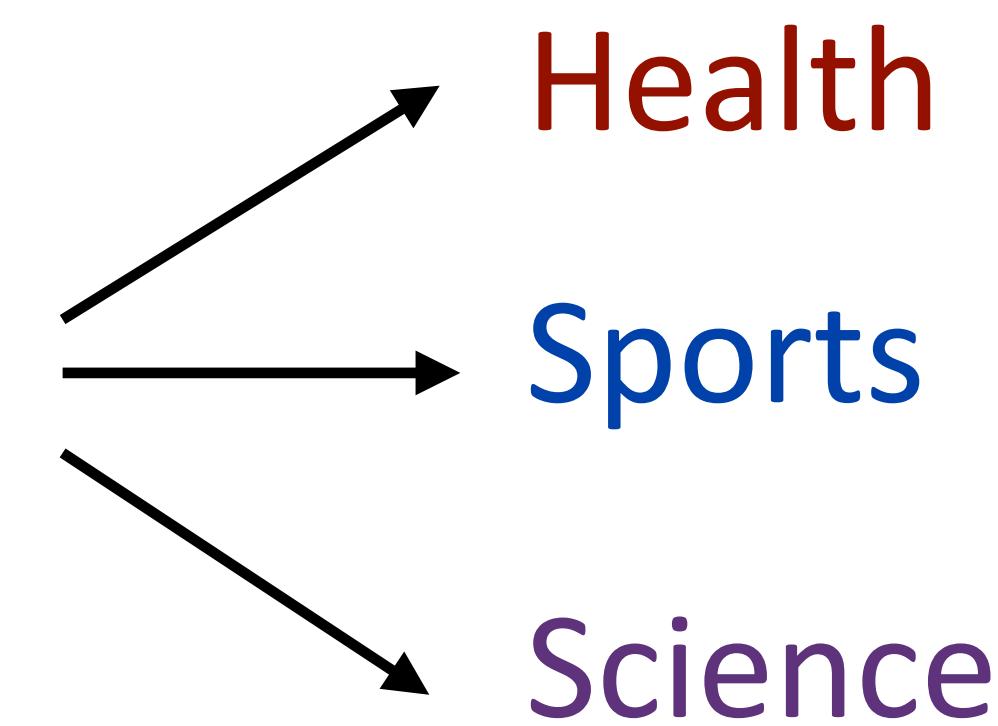
Block Feature Vectors

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

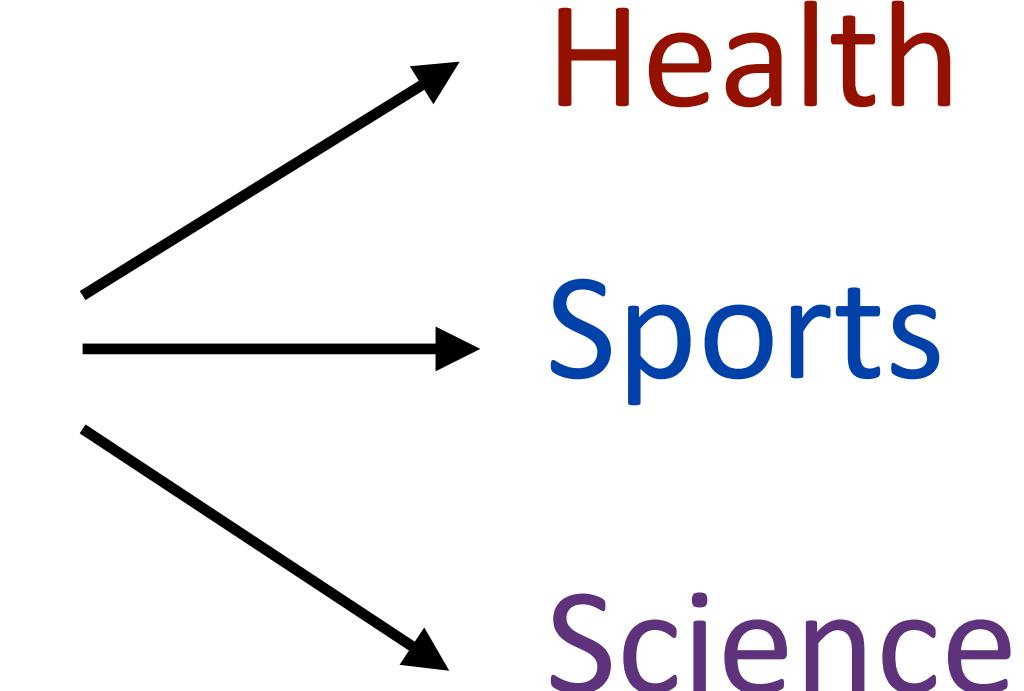
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too many drug trials, too few patients

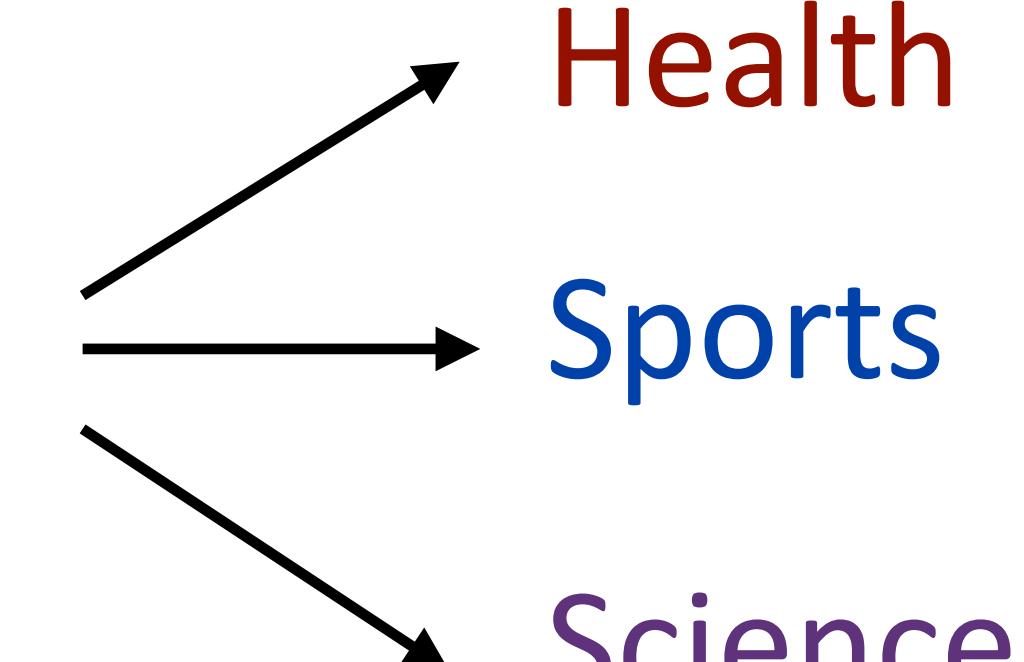


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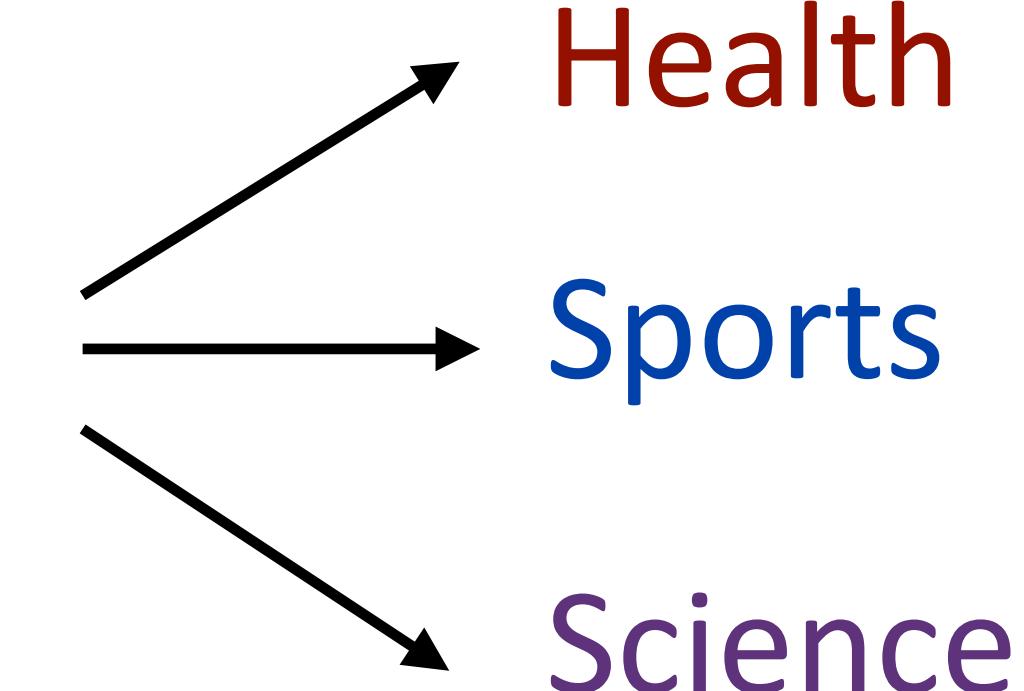
```
graph LR; A[too many drug trials, too few patients] --> B[Health]; A --> C[Sports]; A --> D[Science]
```
- ▶ Base feature function:

Block Feature Vectors

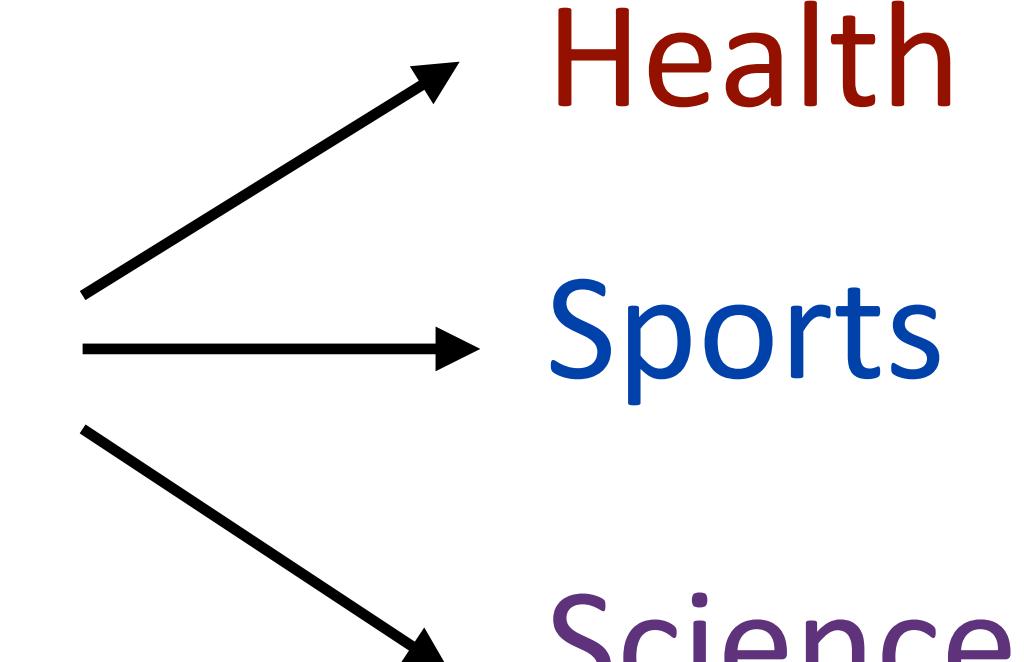
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- ▶ Base feature function:
 $f(x) = I[\text{contains } drug], I[\text{contains } patients], I[\text{contains } baseball]$

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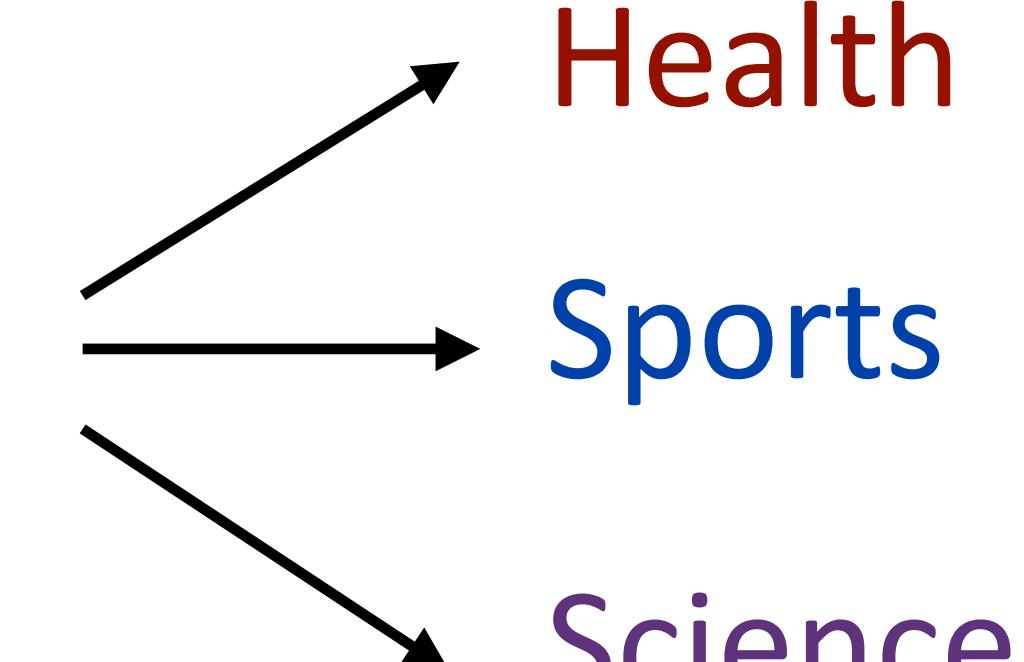
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$$f(x, y = \text{Health}) =$$

Block Feature Vectors

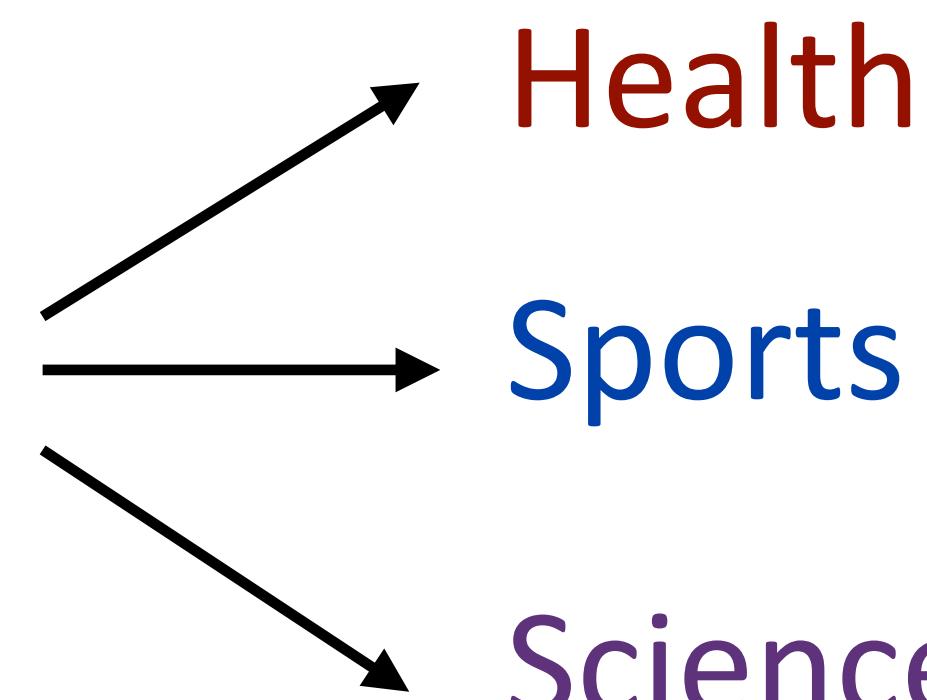
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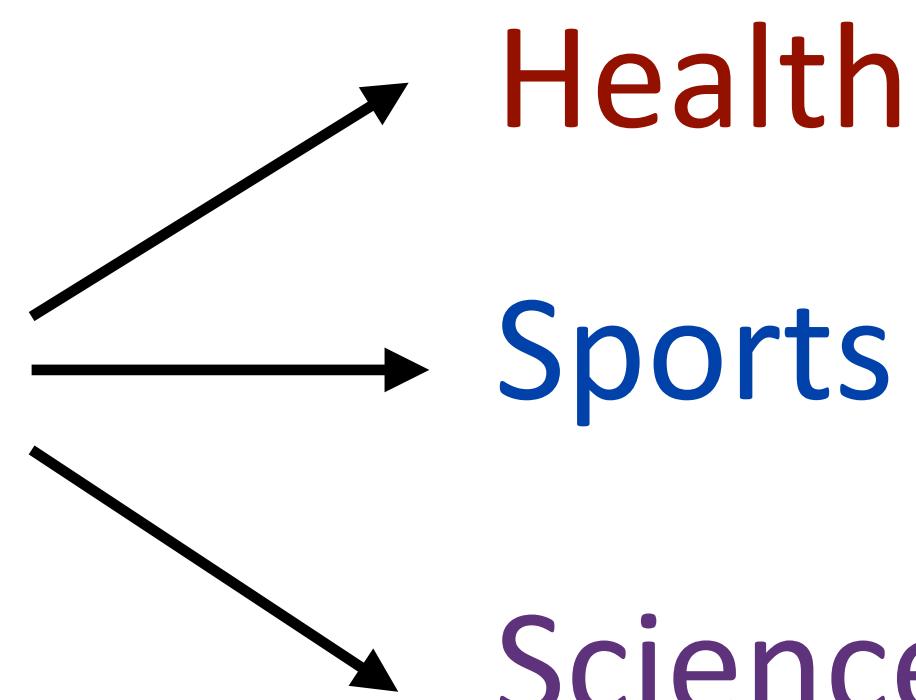
feature vector blocks for each label

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

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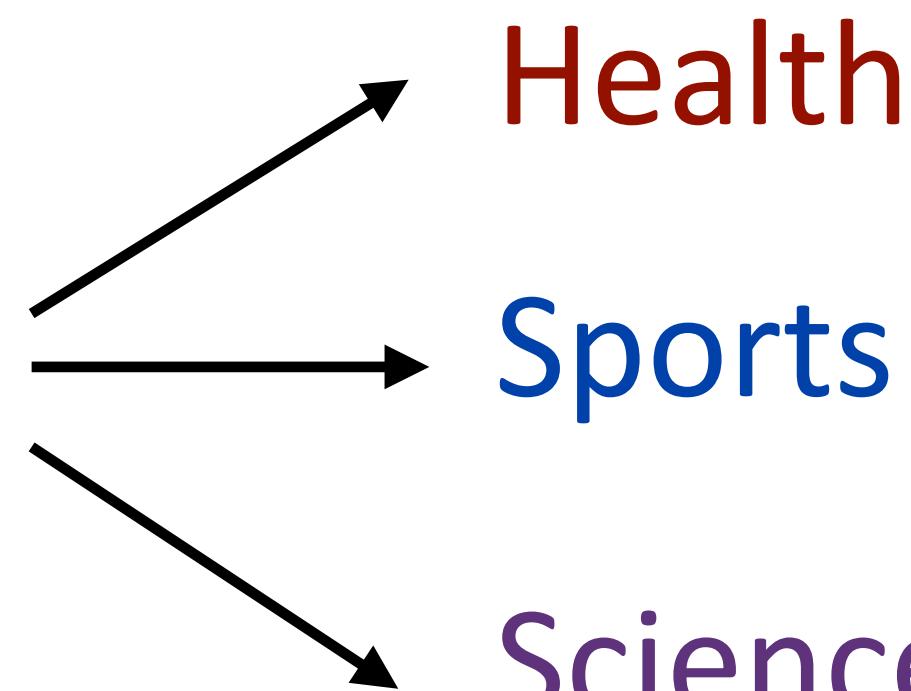
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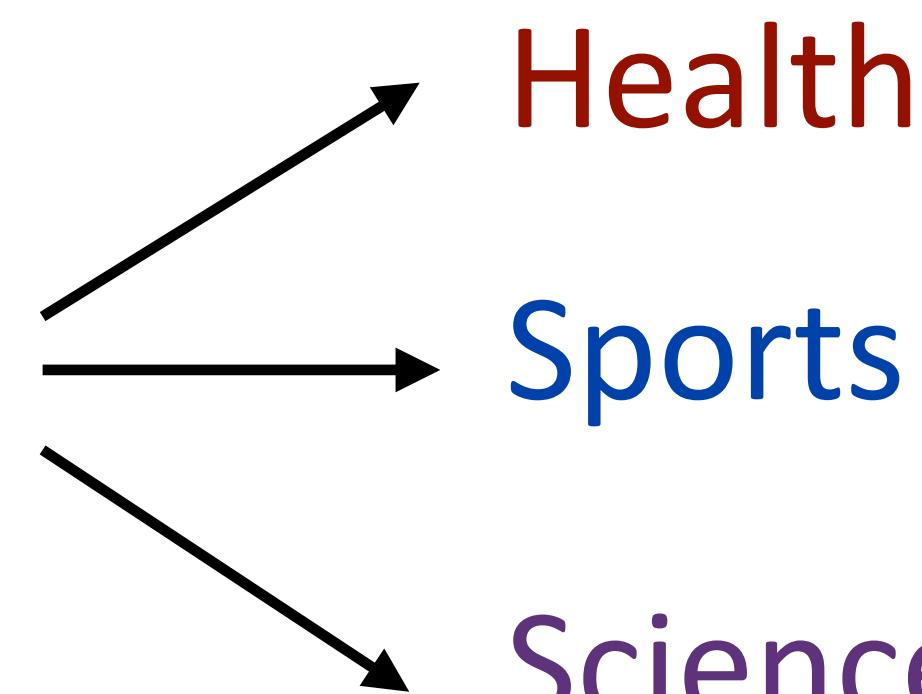
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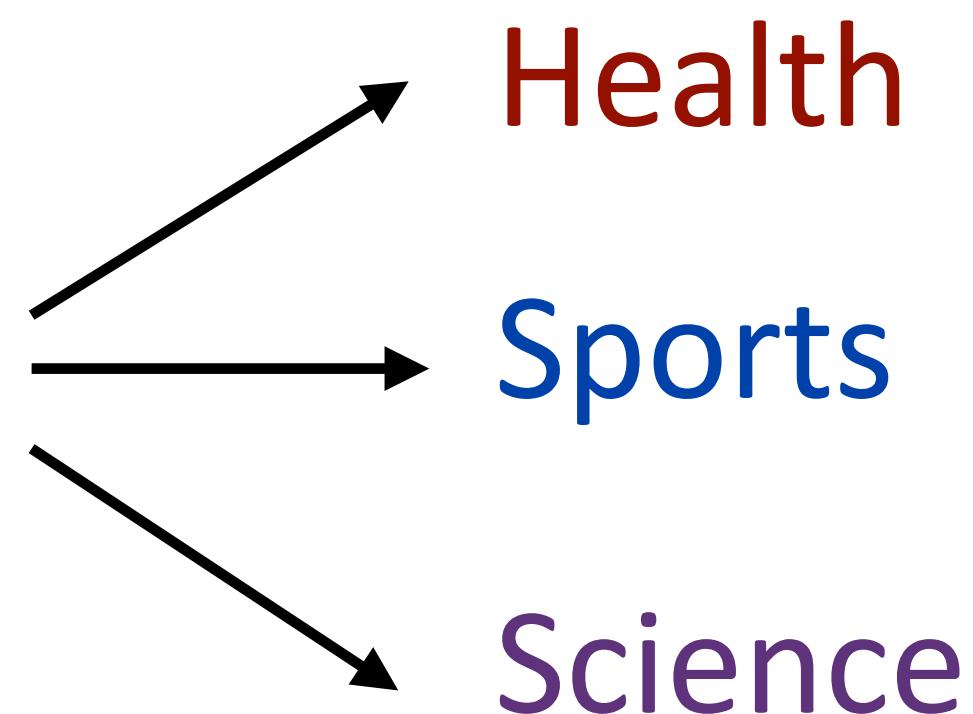
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- Equivalent to having three weight vectors in this case

Making Decisions

too many drug trials, too few patients



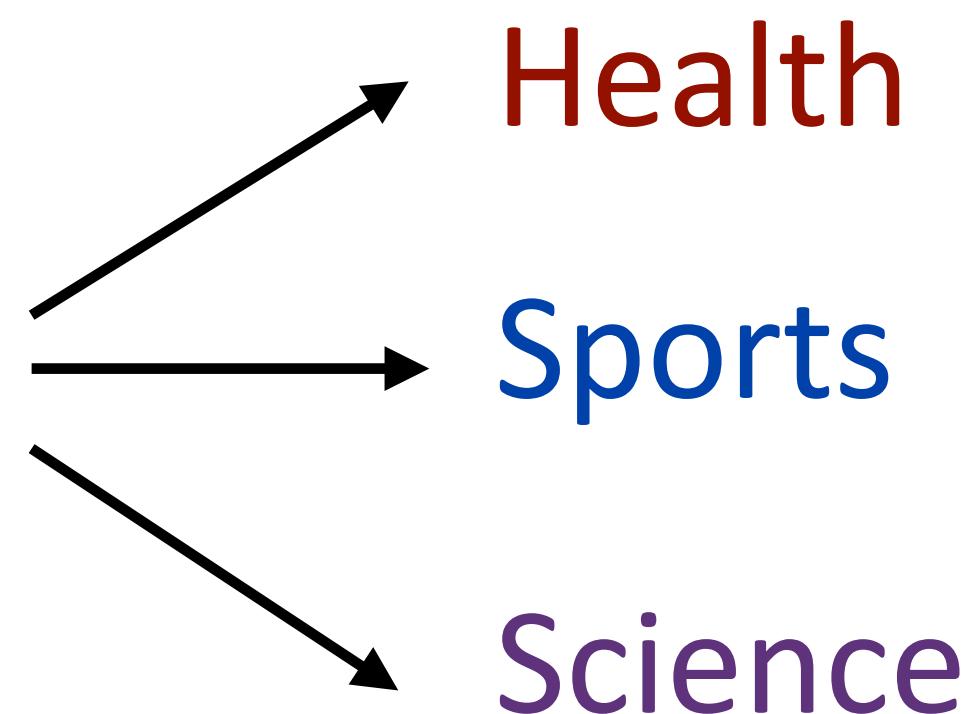
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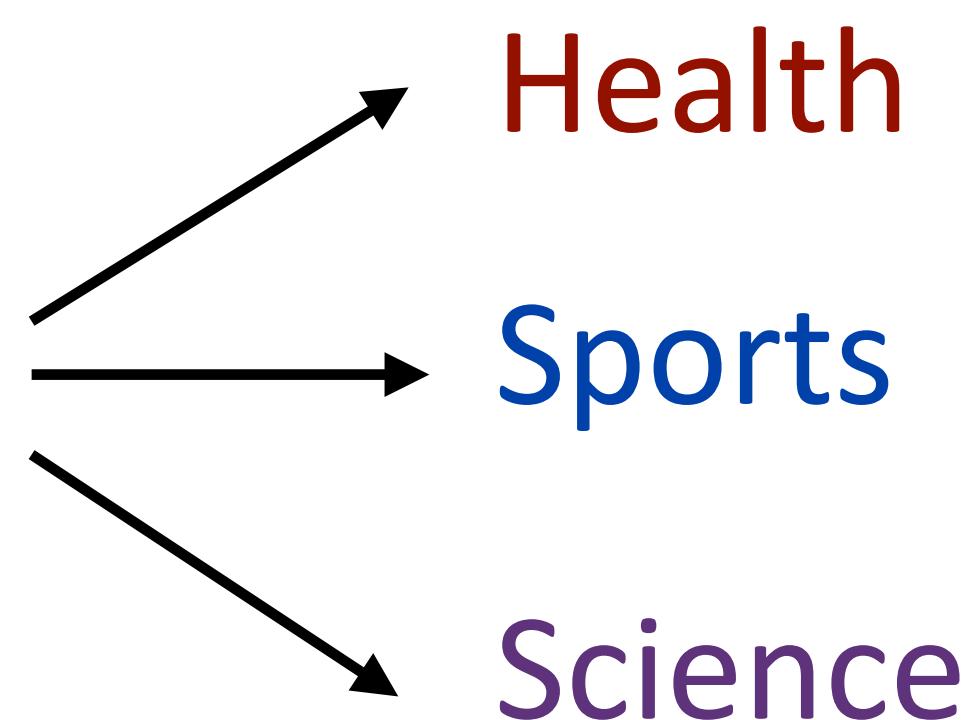
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$$w = [+2.1, +2.3, -5, -2.1, -3.8, 0, +1.1, -1.7, -1.3]$$

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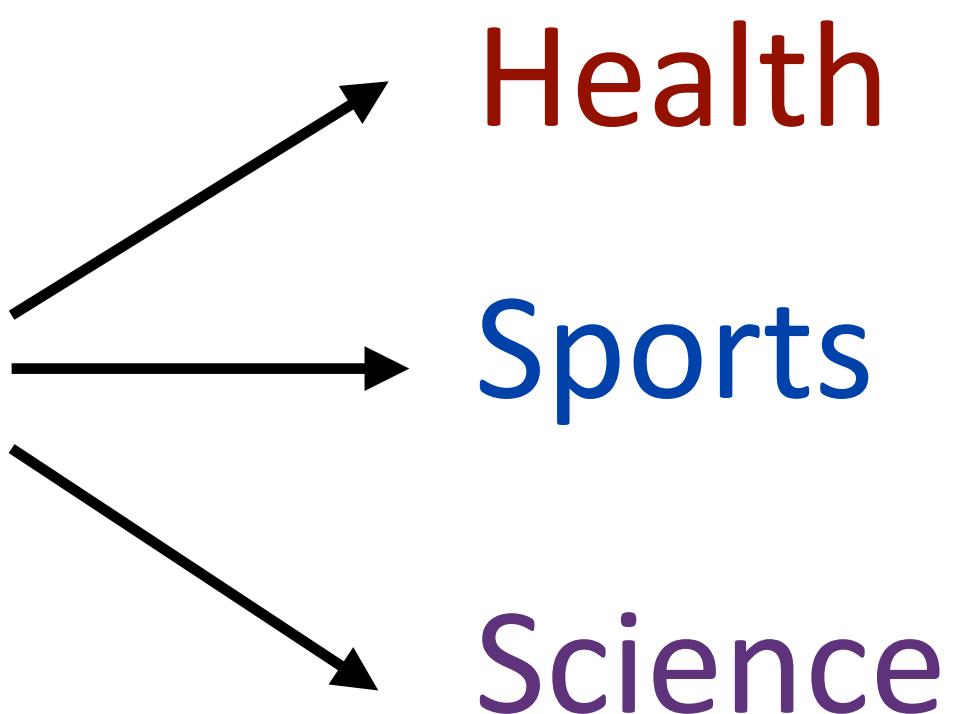
$$f(x, y = \text{Sports}) = [0, 0, 0, 1, 1, 0, 0, 0]$$

“word drug in Science article” = +1.1

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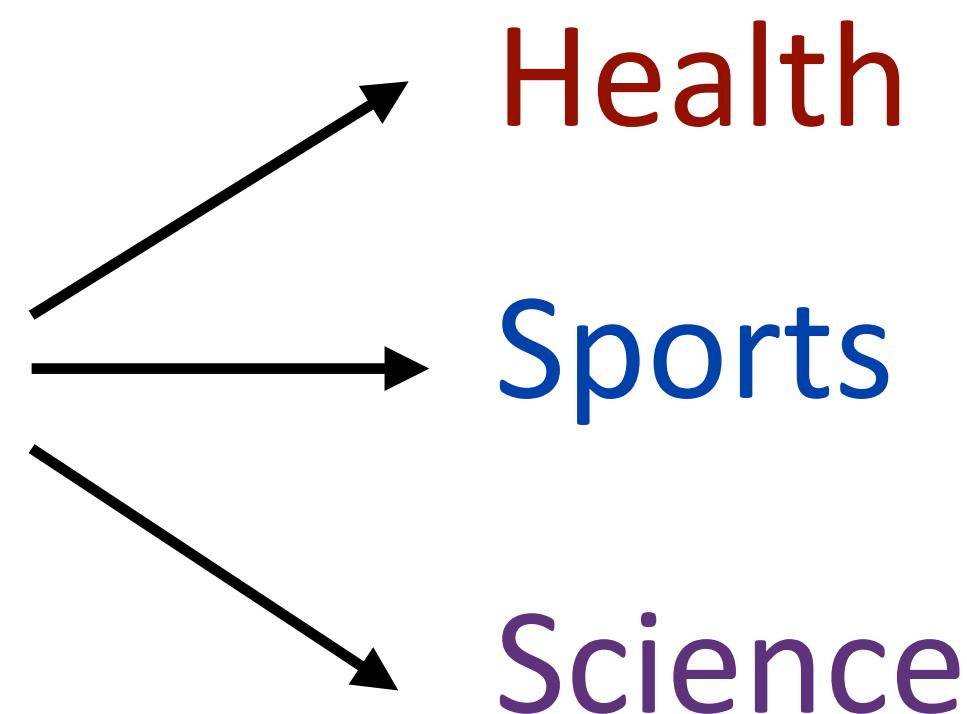
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$$w^\top f(x, y) =$$

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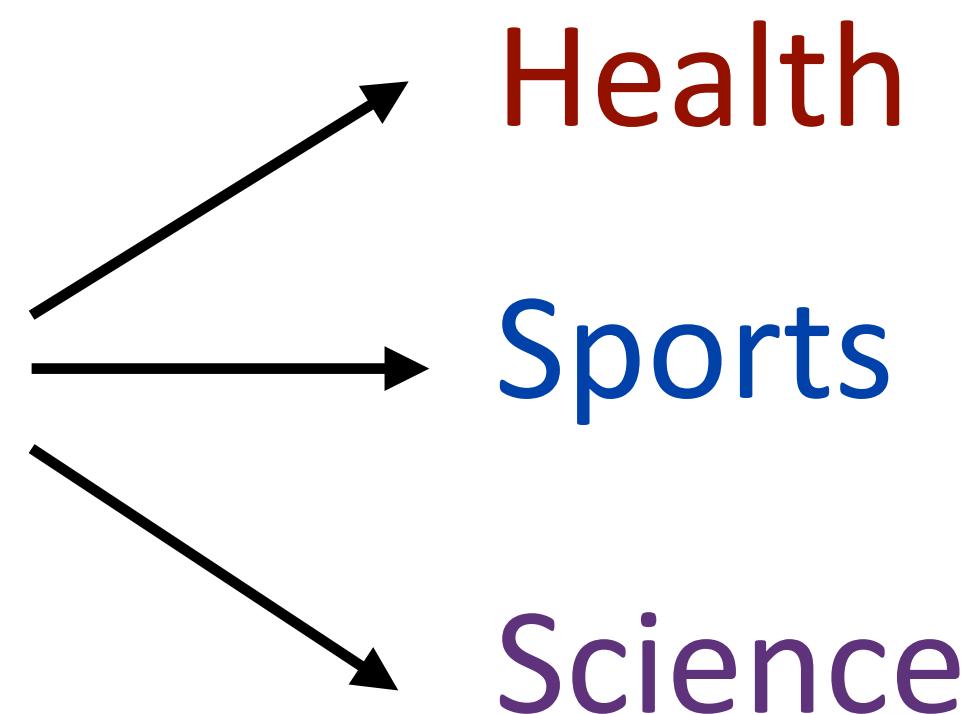
$$w^\top f(x, y) = \text{Health: } +4.4$$

$$\text{Sports: } -5.9$$

$$\text{Science: } -0.6$$

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↑ argmax

Another example: POS tagging

blocks

Another example: POS tagging

the router blocks the packets

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the router blocks the packets

NNS
VBZ
NN
DT
...

Another example: POS tagging

- ▶ Classify *blocks* as one of 36 POS tags

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- ▶ Example x: sentence with a word (in this case, *blocks*) highlighted

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- ▶ Extract features with respect to this word:

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$$f(x, y=\text{VBZ}) = I[\text{curr_word}=\text{blocks} \& \text{tag} = \text{VBZ}], \\ I[\text{prev_word}=\text{router} \& \text{tag} = \text{VBZ}] \\ I[\text{next_word}=\text{the} \& \text{tag} = \text{VBZ}] \\ I[\text{curr_suffix}=s \& \text{tag} = \text{VBZ}]$$

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- ▶ Extract features with respect to this word:

$$f(x, y=\text{VBZ}) = I[\text{curr_word}=\text{blocks} \& \text{tag} = \text{VBZ}], \\ I[\text{prev_word}=\text{router} \& \text{tag} = \text{VBZ}] \\ I[\text{next_word}=\text{the} \& \text{tag} = \text{VBZ}] \\ I[\text{curr_suffix}=s \& \text{tag} = \text{VBZ}]$$

<i>the router</i>	<i>'blocks'</i>	<i>the packets</i>
	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

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

↑
sum over output
space to normalize

Multiclass Logistic Regression

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

↗
sum over output
space to normalize

► Compare to binary:

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

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► 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

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Softmax
function

sum over output
space to normalize

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

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too few patients*

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

*too many drug trials,
too few patients*

Health: +2.2

Sports: +3.1

Science: -0.6

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

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probabilities
must be ≥ 0

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Science: -0.6

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

\exp

6.05
22.2
0.55
unnormalized
probabilities

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probabilities
must sum to 1

0.21
0.77
0.02

probabilities

Multiclass Logistic Regression

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Softmax
function

probabilities
must be ≥ 0

probabilities
must sum to 1

unnormalized
probabilities

probabilities

correct (gold)
probabilities

\exp

normalize

Multiclass Logistic Regression

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

sum over output space to normalize

Softmax function

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probabilities
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probabilities

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

1.00
0.00
0.00
correct (gold)
probabilities

Multiclass Logistic Regression

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0.21
0.77
0.02
probabilities

1.00
0.00
0.00
correct (gold)
probabilities

$\log(0.21) = -1.56$

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

compare

Multiclass Logistic Regression

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

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sum over output
space to normalize

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

Multiclass Logistic Regression

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sum over output
space to normalize

- ▶ Training: maximize $\mathcal{L}(x, y) = \sum_{j=1}^n \log P(y_j^*|x_j)$
 $= \sum_{j=1}^n \left(w^\top f(x_j, y_j^*) - \log \sum_y \exp(w^\top f(x_j, y)) \right)$

Training

- ▶ Multiclass logistic regression $P_w(y|x) = \frac{\exp(w^\top f(x, y))}{\sum_{y' \in \mathcal{Y}} \exp(w^\top f(x, y'))}$
- ▶ Likelihood $\mathcal{L}(x_j, y_j^*) = w^\top f(x_j, y_j^*) - \log \sum_y \exp(w^\top f(x_j, y))$

Training

- Multiclass logistic regression $P_w(y|x) = \frac{\exp(w^\top f(x, y))}{\sum_{y' \in \mathcal{Y}} \exp(w^\top f(x, y'))}$
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$$\frac{\partial}{\partial w_i} \mathcal{L}(x_j, y_j^*) = f_i(x_j, y_j^*) - \frac{\sum_y f_i(x_j, y) \exp(w^\top f(x_j, y))}{\sum_y \exp(w^\top f(x_j, y))}$$
$$\frac{\partial}{\partial w_i} \mathcal{L}(x_j, y_j^*) = f_i(x_j, y_j^*) - \sum_y f_i(x_j, y) P_w(y|x_j)$$

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gold feature value

Training

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

$$\frac{\partial}{\partial w_i} \mathcal{L}(x_j, y_j^*) = f_i(x_j, y_j^*) - \mathbb{E}_y[f_i(x_j, y)]$$
 model's expectation of
gold feature value

Training

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too many drug trials, too few patients $y^* = \text{Health}$

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

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

Training

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

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

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gradient:

Training

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$$\text{gradient: } [1, 1, 0, 0, 0, 0, 0, 0]$$

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$$\text{gradient: } [1, 1, 0, 0, 0, 0, 0, 0] - 0.21 [1, 1, 0, 0, 0, 0, 0, 0]$$

Training

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Training

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update w^\top :

Training

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

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update w^\top :

$$[1.3, 0.9, -5, 3.2, -0.1, 0, 1.1, -1.7, -1.3]$$

Training

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

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$$[1.3, 0.9, -5, 3.2, -0.1, 0, 1.1, -1.7, -1.3] + [0.79, 0.79, 0, -0.77, -0.77, 0, -0.02, -0.02, 0]$$

Training

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

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update w^\top :

$$\begin{aligned} & [1.3, 0.9, -5, 3.2, -0.1, 0, 1.1, -1.7, -1.3] + [0.79, 0.79, 0, -0.77, -0.77, 0, -0.02, -0.02, 0] \\ & = [2.09, 1.69, 0, 2.43, -0.87, 0, 1.08, -1.72, 0] \end{aligned}$$

Training

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

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update w^\top :

$$\begin{aligned} & [1.3, 0.9, -5, 3.2, -0.1, 0, 1.1, -1.7, -1.3] + [0.79, 0.79, 0, -0.77, -0.77, 0, -0.02, -0.02, 0] \\ & = [2.09, 1.69, 0, 2.43, -0.87, 0, 1.08, -1.72, 0] \end{aligned}$$

$$\curvearrowleft \text{new } P_w(y|x) = [0.89, 0.10, 0.01]$$

Logistic Regression: Summary

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

Logistic Regression: Summary

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- ▶ Inference: $\operatorname{argmax}_y P_w(y|x)$
- ▶ 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”

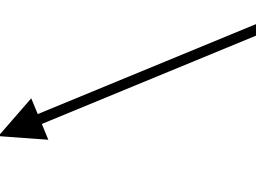
Multiclass SVM

Soft Margin SVM

Soft Margin SVM

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

slack variables > 0 iff
example is support vector



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

Soft Margin SVM

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

slack variables > 0 iff
example is support vector

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

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

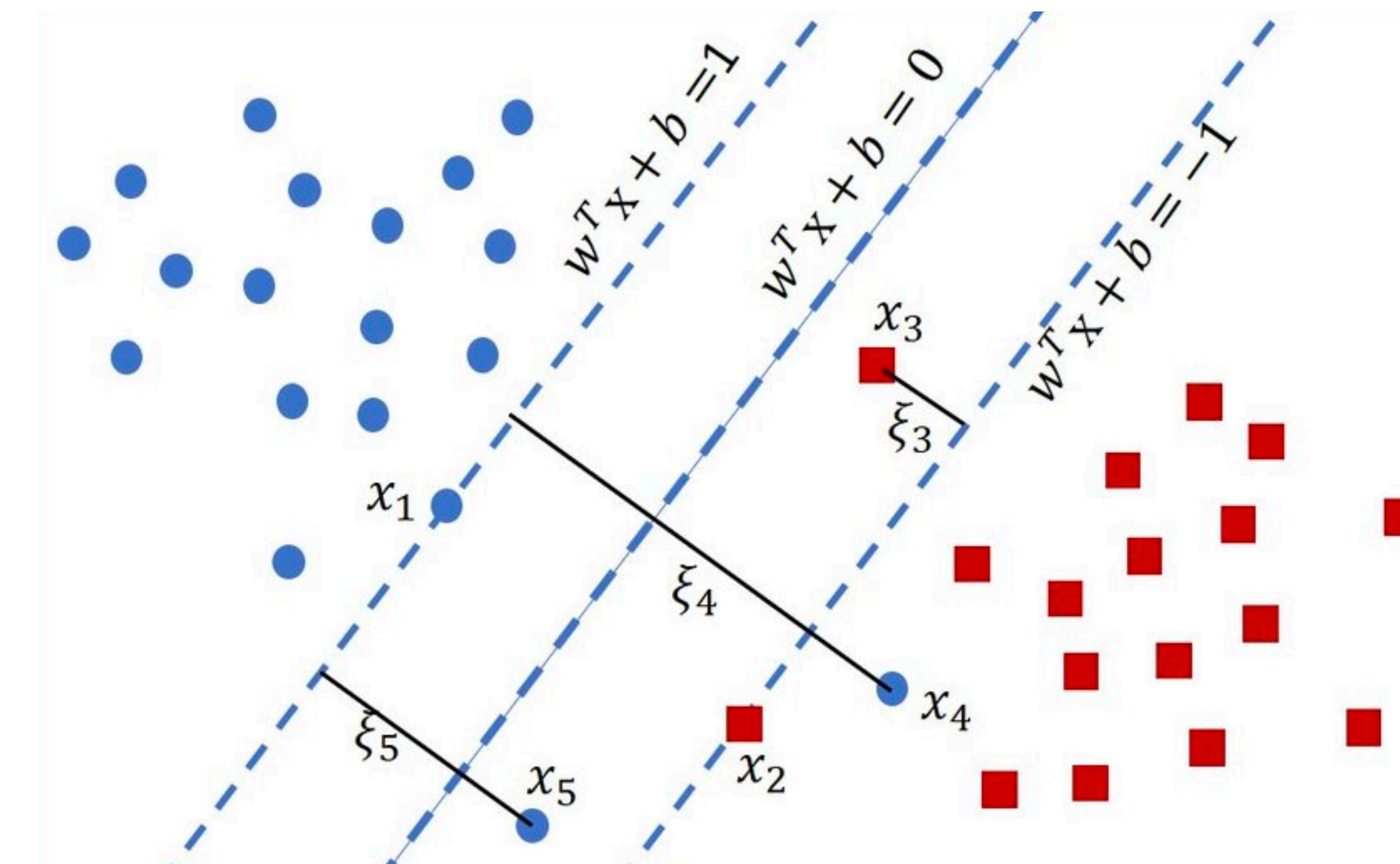


Image credit: Lang Van Tran

Multiclass SVM

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

slack variables > 0 iff
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Multiclass SVM

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Correct prediction now
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Multiclass SVM

$$\begin{aligned} & \text{Minimize } \lambda \|w\|_2^2 + \sum_{j=1}^m \xi_j && \text{slack variables } > 0 \text{ iff} \\ & \text{s.t. } \forall j \quad \xi_j \geq 0 && \text{example is support vector} \\ & \quad \cancel{\forall j \quad (2y_j - 1)(w^\top x_j) \geq 1 - \xi_j} && \\ & \quad \forall j \forall y \in \mathcal{Y} \quad w^\top f(x_j, y_j^*) \geq w^\top f(x_j, y) + \ell(y, y_j^*) - \xi_j && \end{aligned}$$

Correct prediction now
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Score comparison
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Multiclass SVM

$$\begin{aligned} \text{Minimize } & \lambda \|w\|_2^2 + \sum_{j=1}^m \xi_j && \text{slack variables } > 0 \text{ iff} \\ & \text{s.t. } \forall j \quad \xi_j \geq 0 && \text{example is support vector} \\ & \cancel{\forall j \quad (2y_j - 1)(w^\top x_j) \geq 1 - \xi_j} && \\ & \forall j \forall y \in \mathcal{Y} \quad w^\top f(x_j, y_j^*) \geq w^\top f(x_j, y) + \ell(y, y_j^*) - \xi_j && \end{aligned}$$

Correct prediction now
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The 1 that was here is
replaced by a loss
function

Training (loss-augmented)

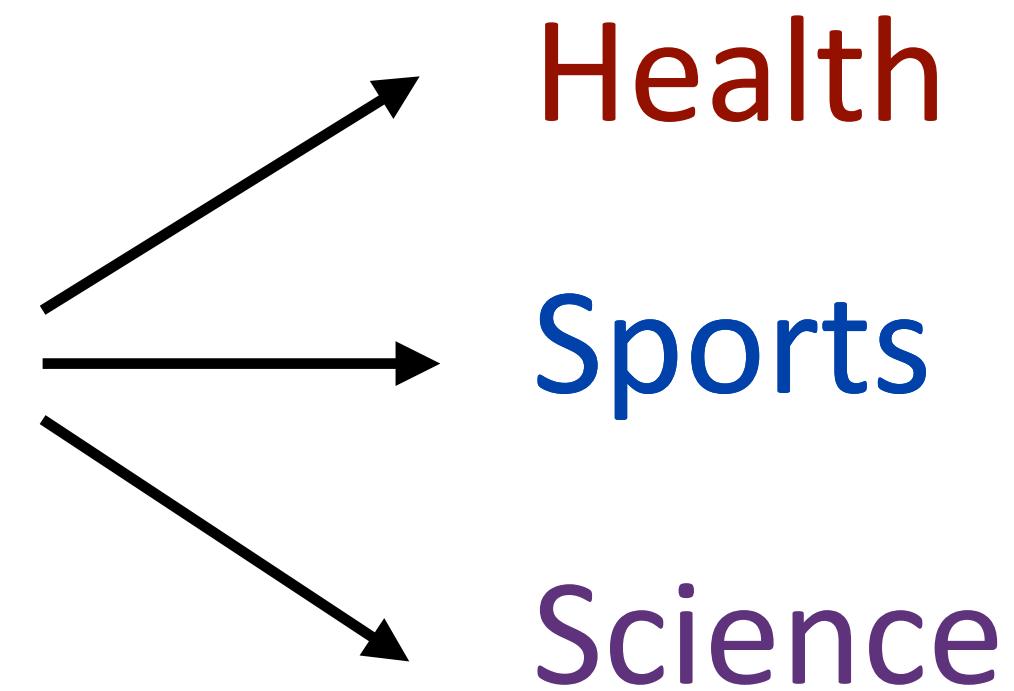
Training (loss-augmented)

- ▶ Are all decisions equally costly?

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too many drug trials, too few patients

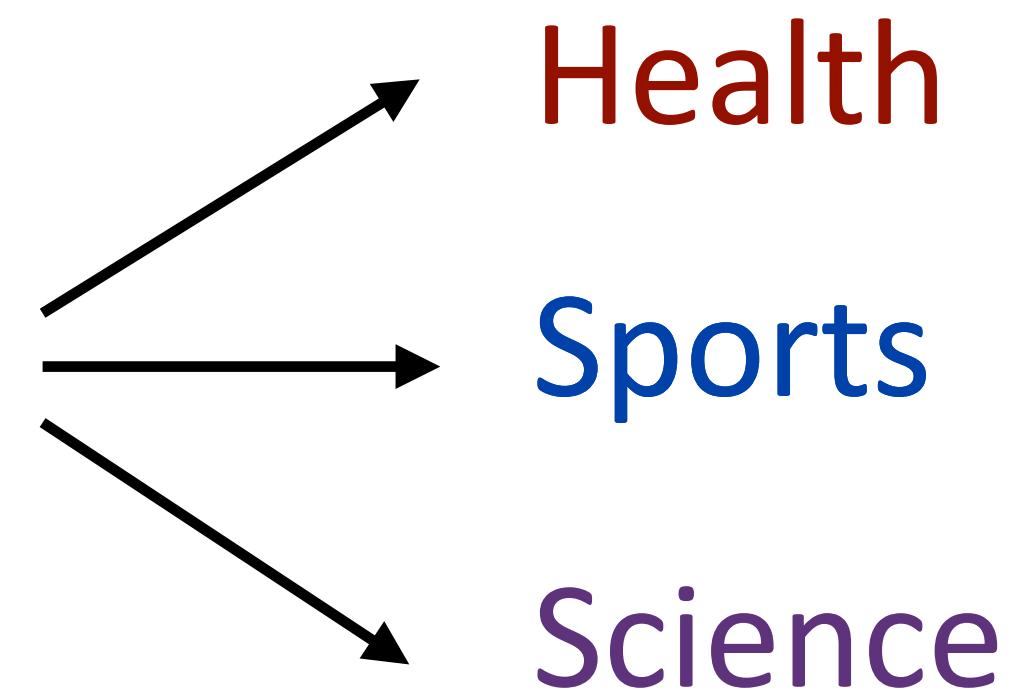


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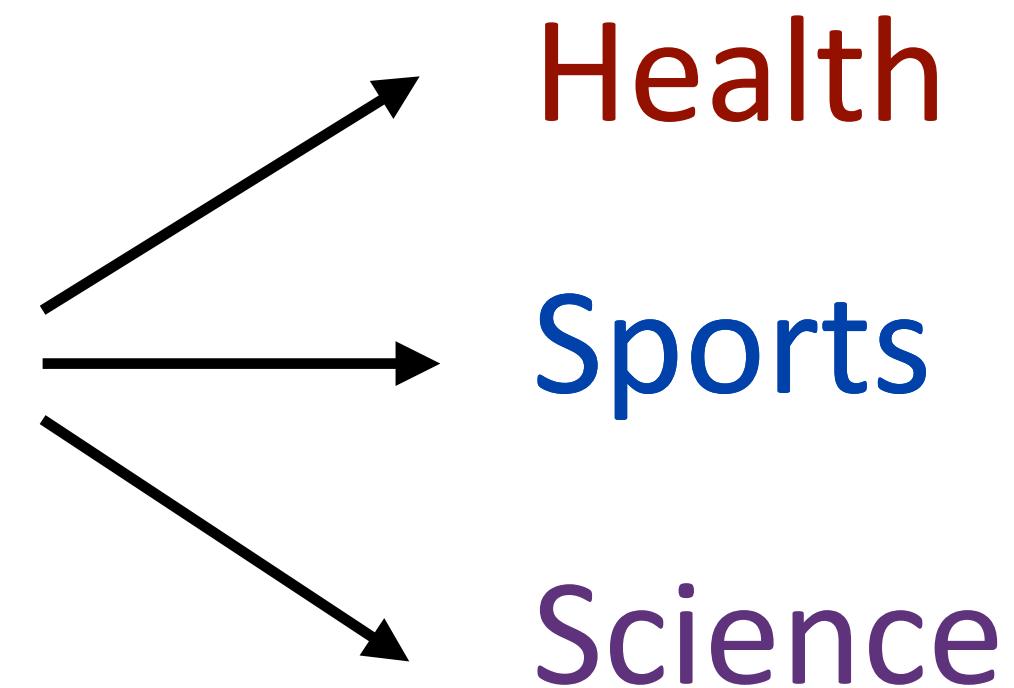
Predicted **Sports**: bad error



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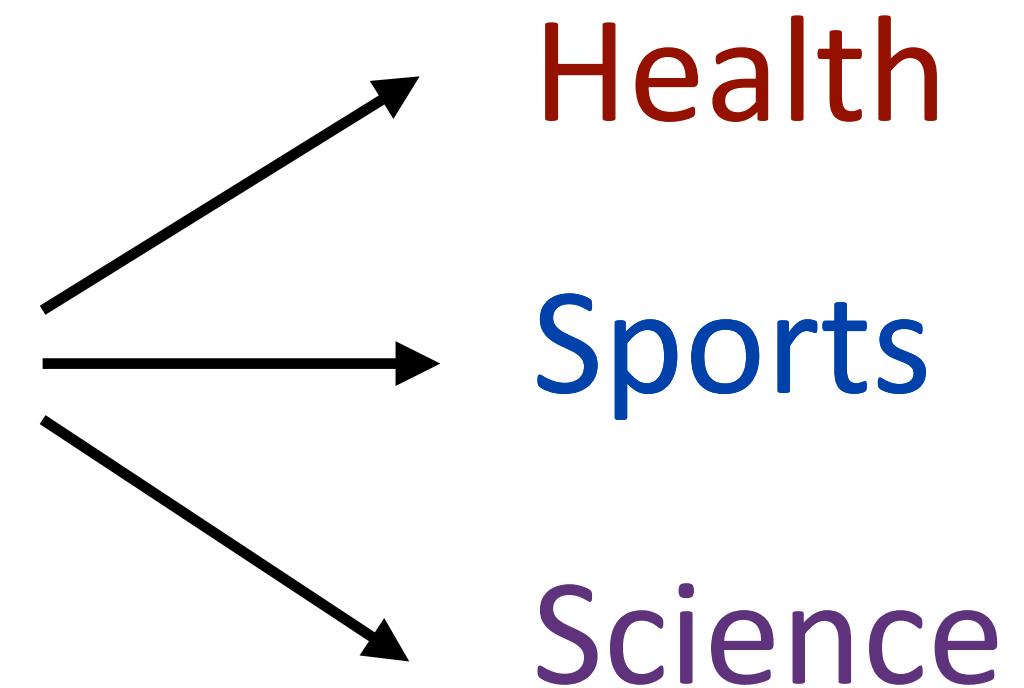
Predicted **Sports**: bad error

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Predicted **Sports**: bad error

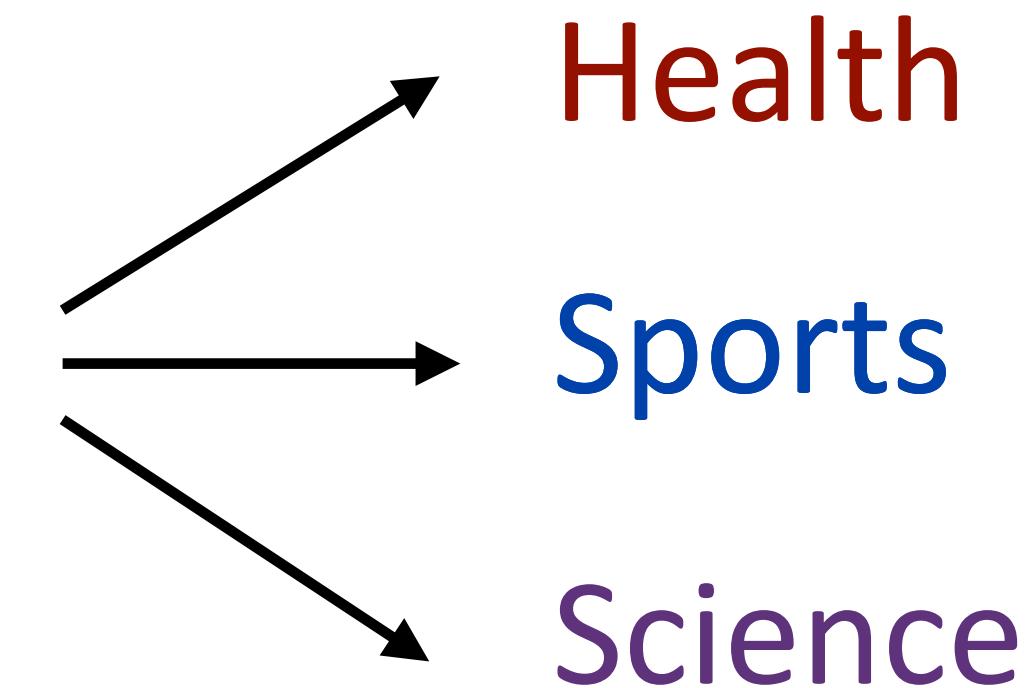
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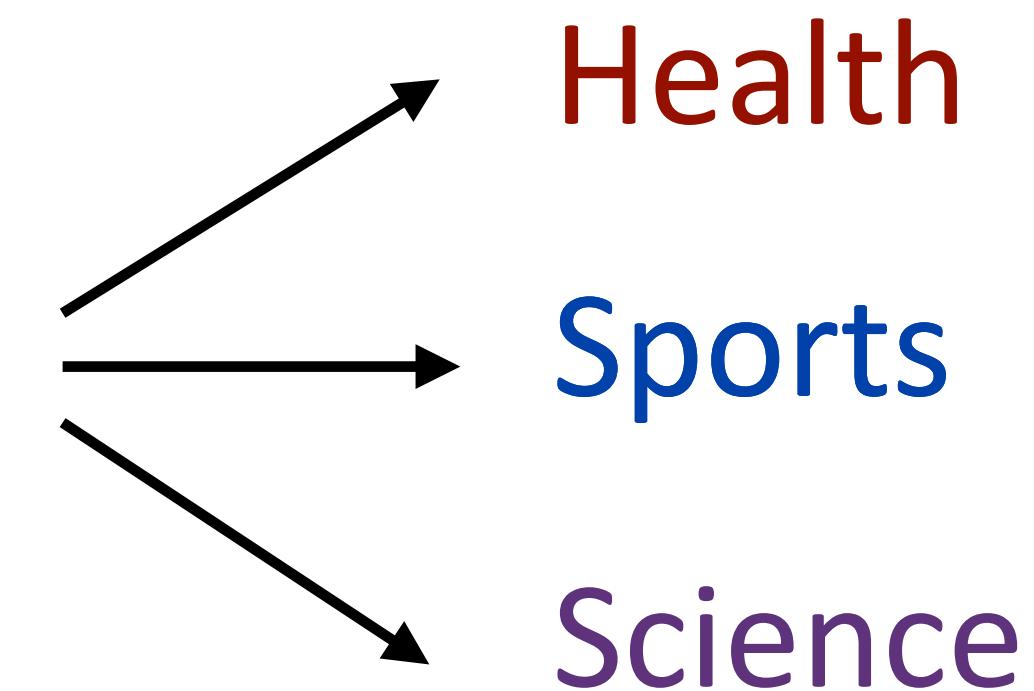
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$$\ell(\text{Sports}, \text{Health}) = 3$$

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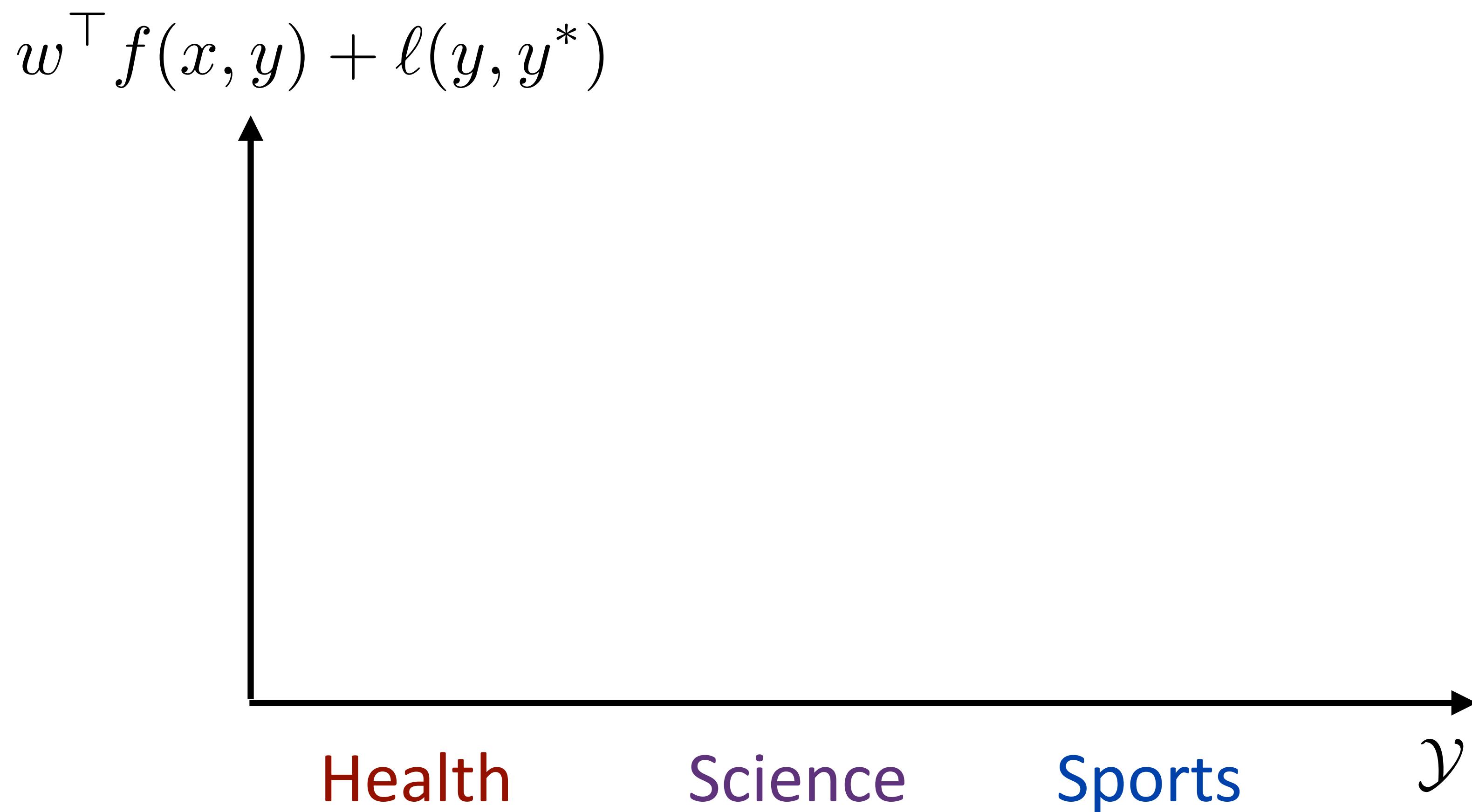
$$\ell(\text{Science}, \text{Health}) = 1$$

Multiclass SVM

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

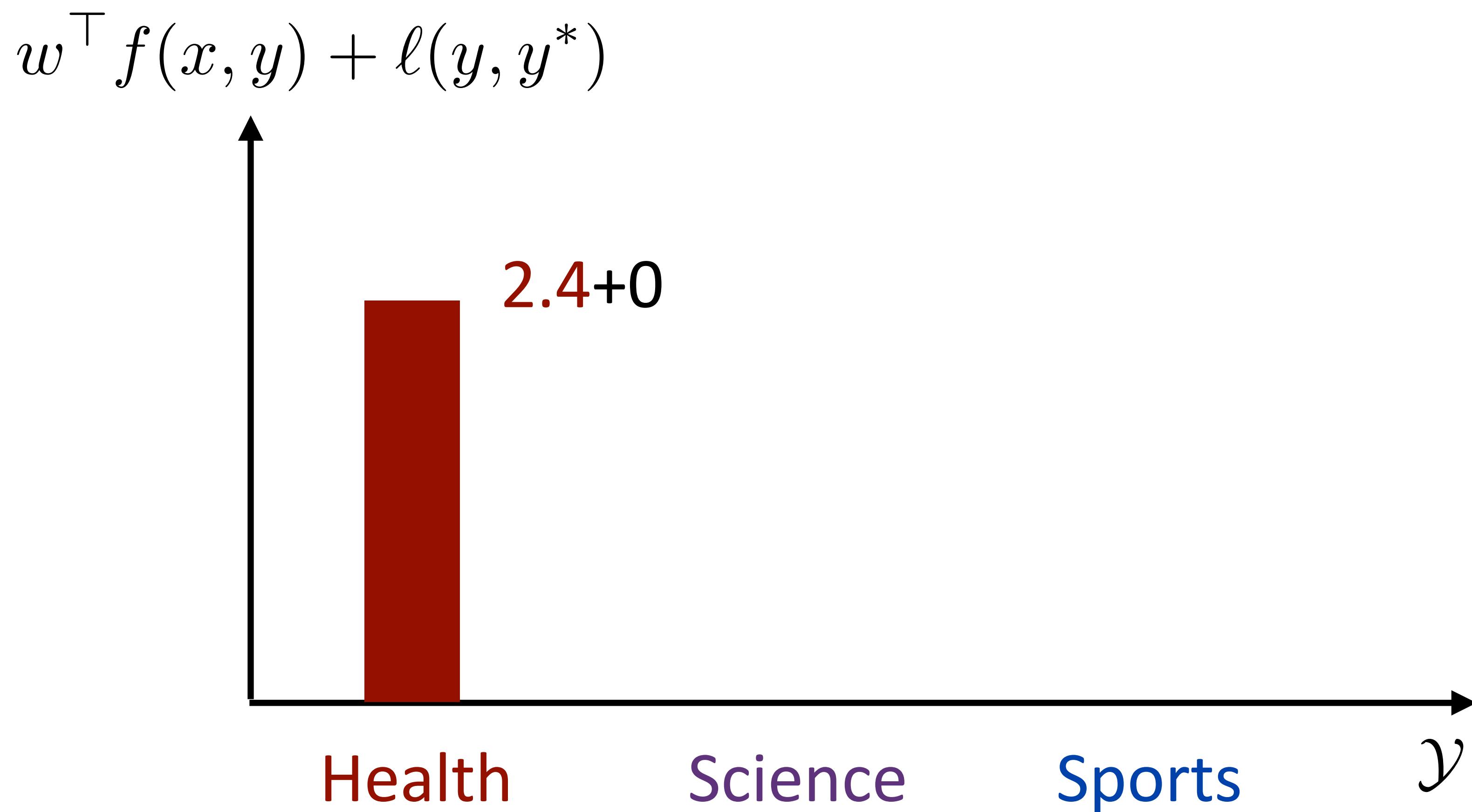
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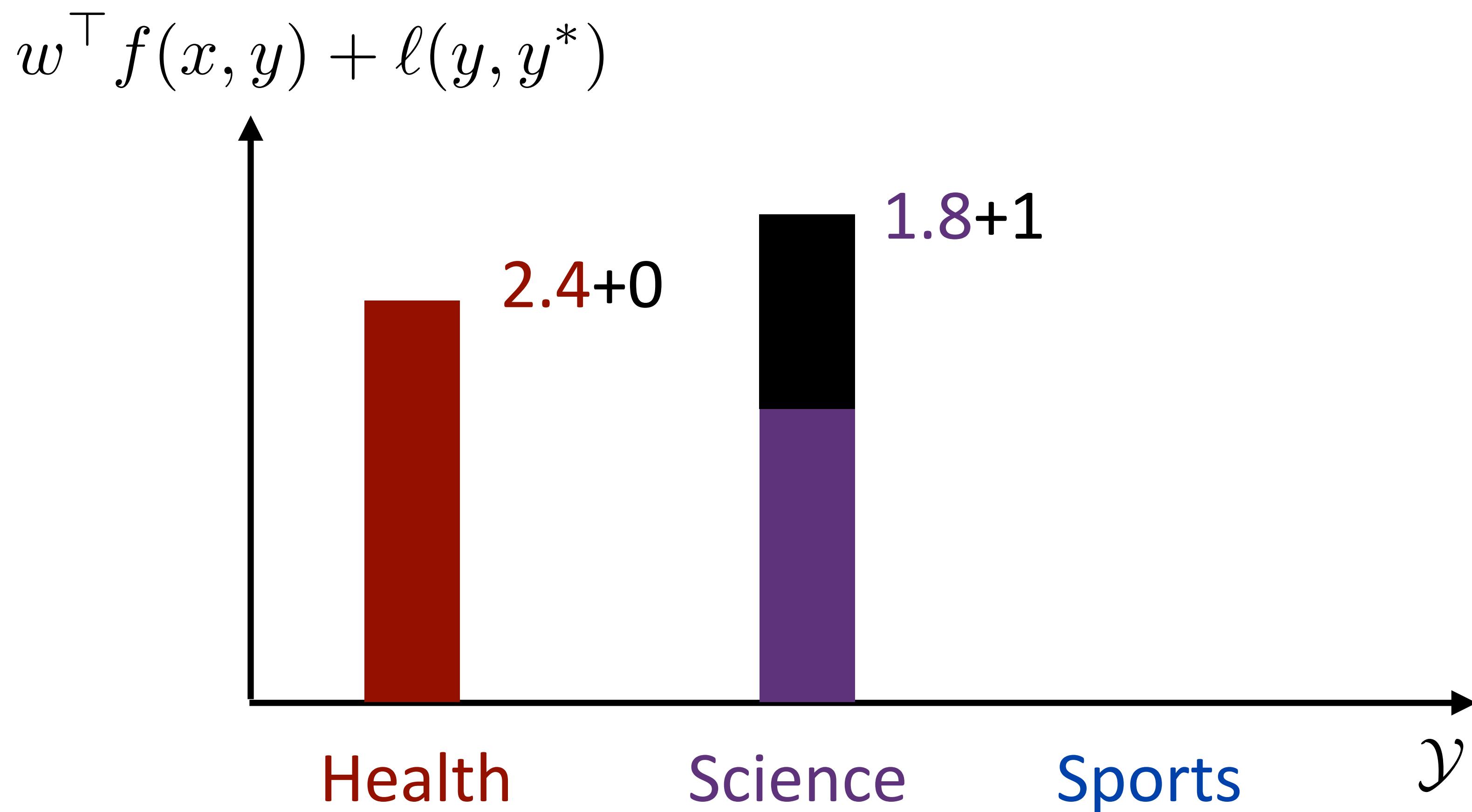
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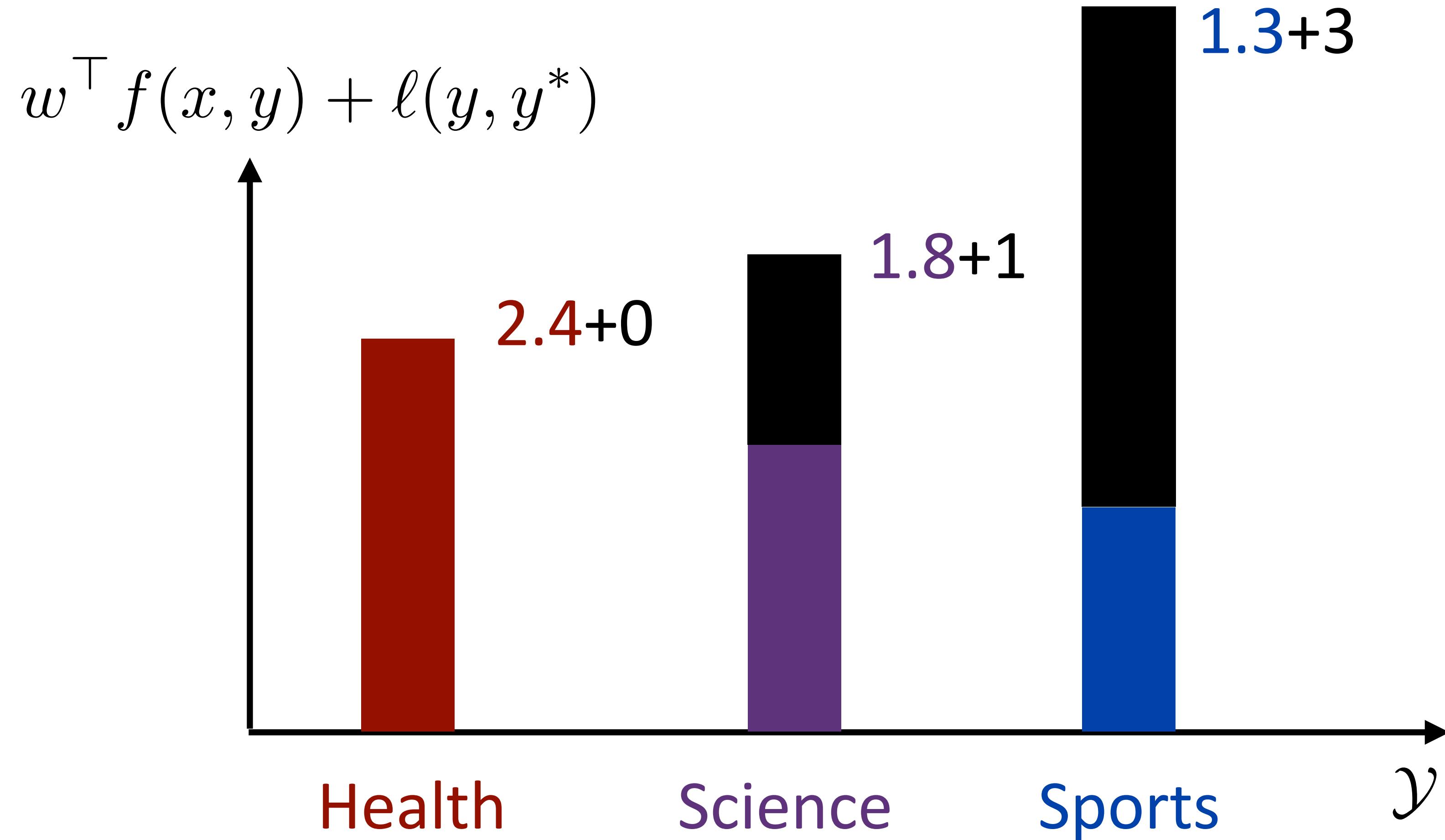
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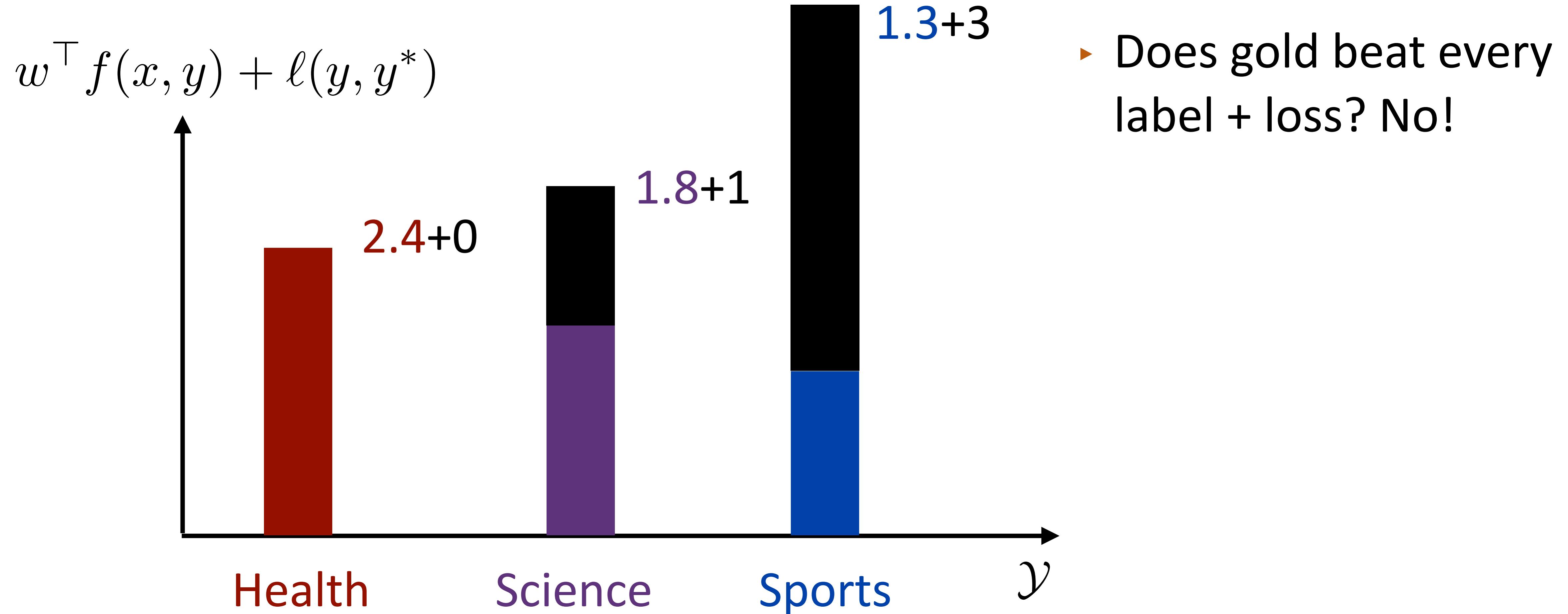
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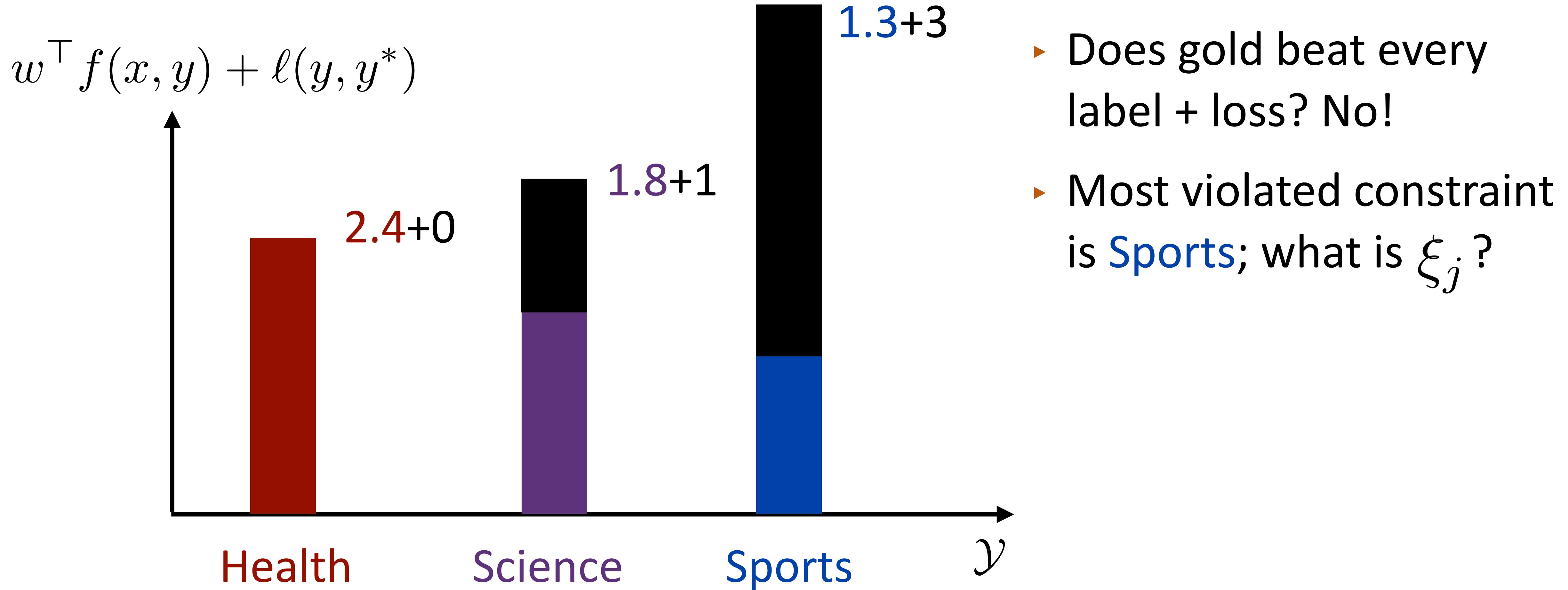
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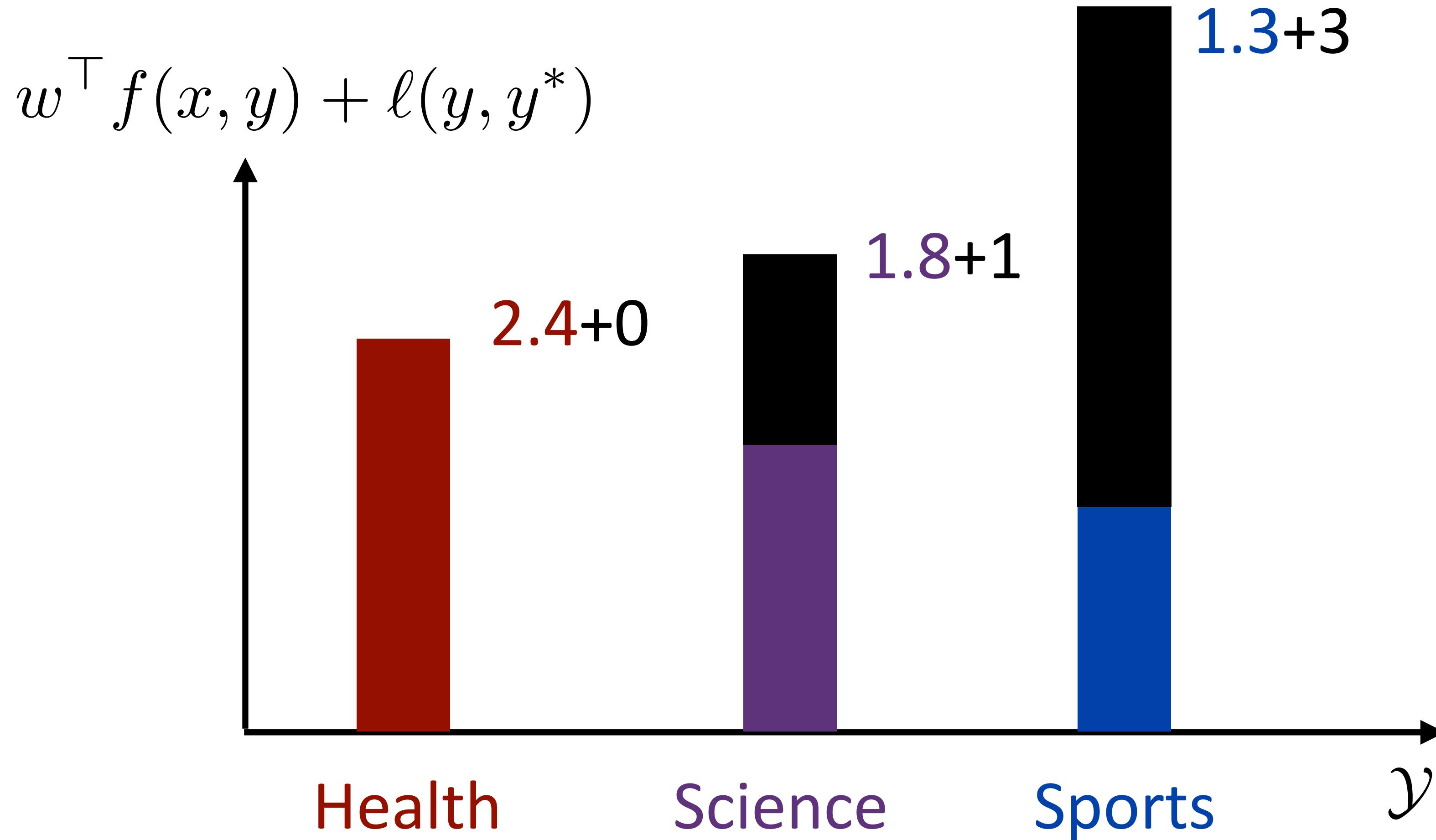
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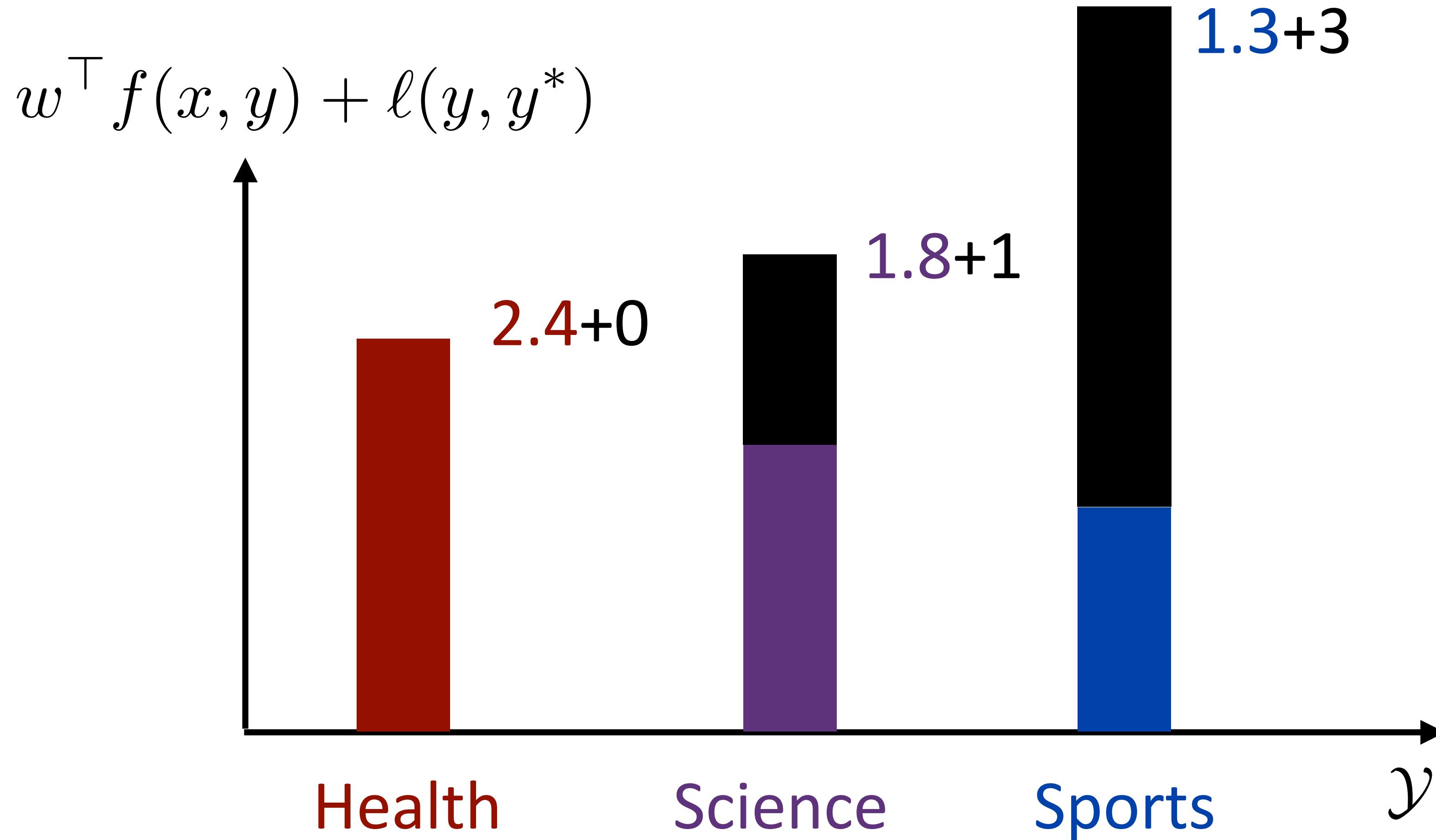
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- ▶ Does gold beat every label + loss? No!
- ▶ Most violated constraint is **Sports**; what is ξ_j ?
- ▶ $\xi_j = 4.3 - 2.4 = 1.9$

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- ▶ Most violated constraint is **Sports**; what is ξ_j ?
- ▶ $\xi_j = 4.3 - 2.4 = 1.9$
- ▶ Perceptron would make no update here

Multiclass SVM

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

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

Computing the Subgradient

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

$$\text{s.t. } \forall j \quad \xi_j \geq 0$$

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

Putting it Together

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

$$\text{s.t. } \forall j \quad \xi_j \geq 0$$

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Putting it Together

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

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- ▶ SVM: max over y s to compute gradient. LR: need to sum over y s

Optimization

Recap

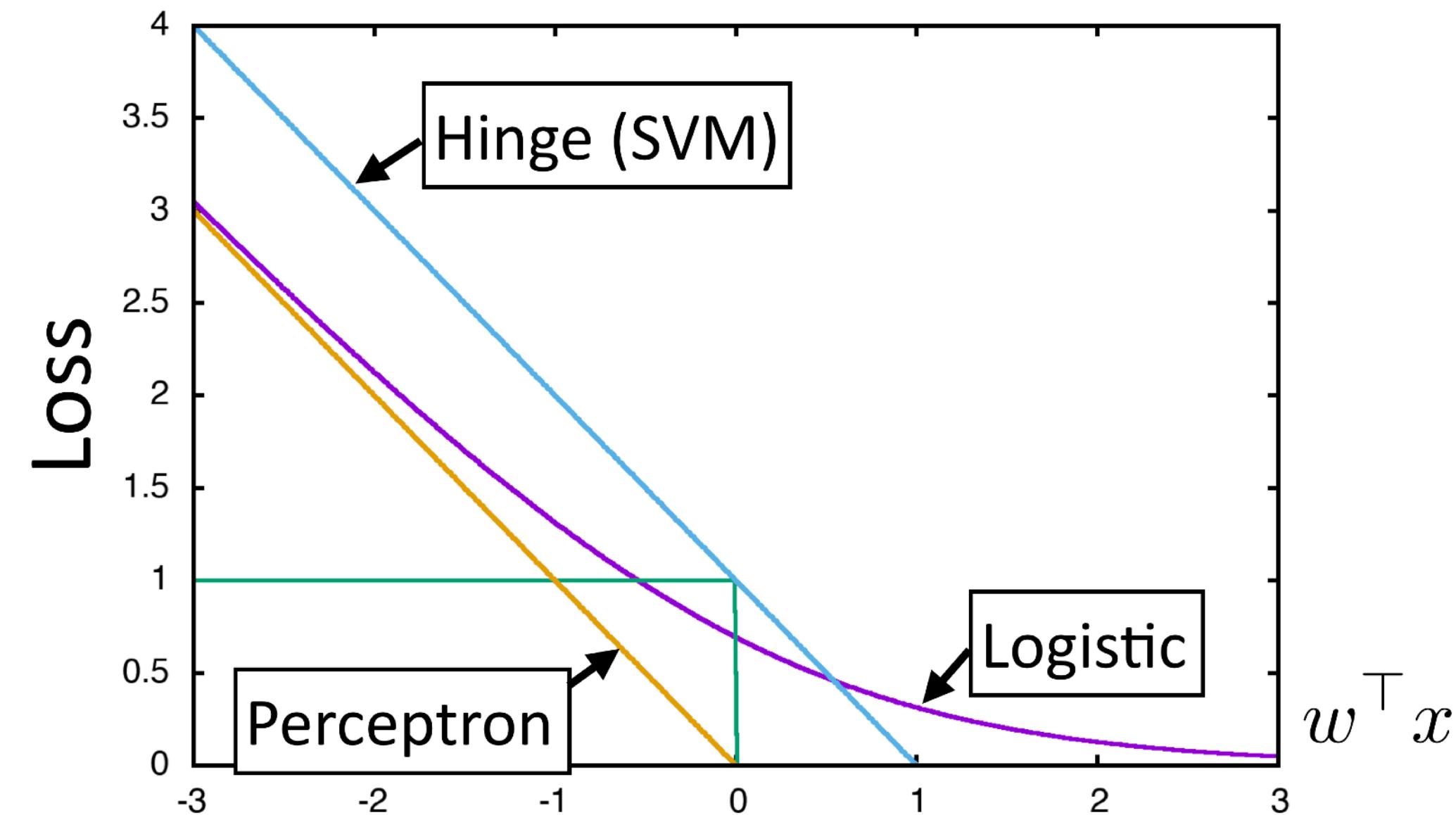
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Recap

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Recap

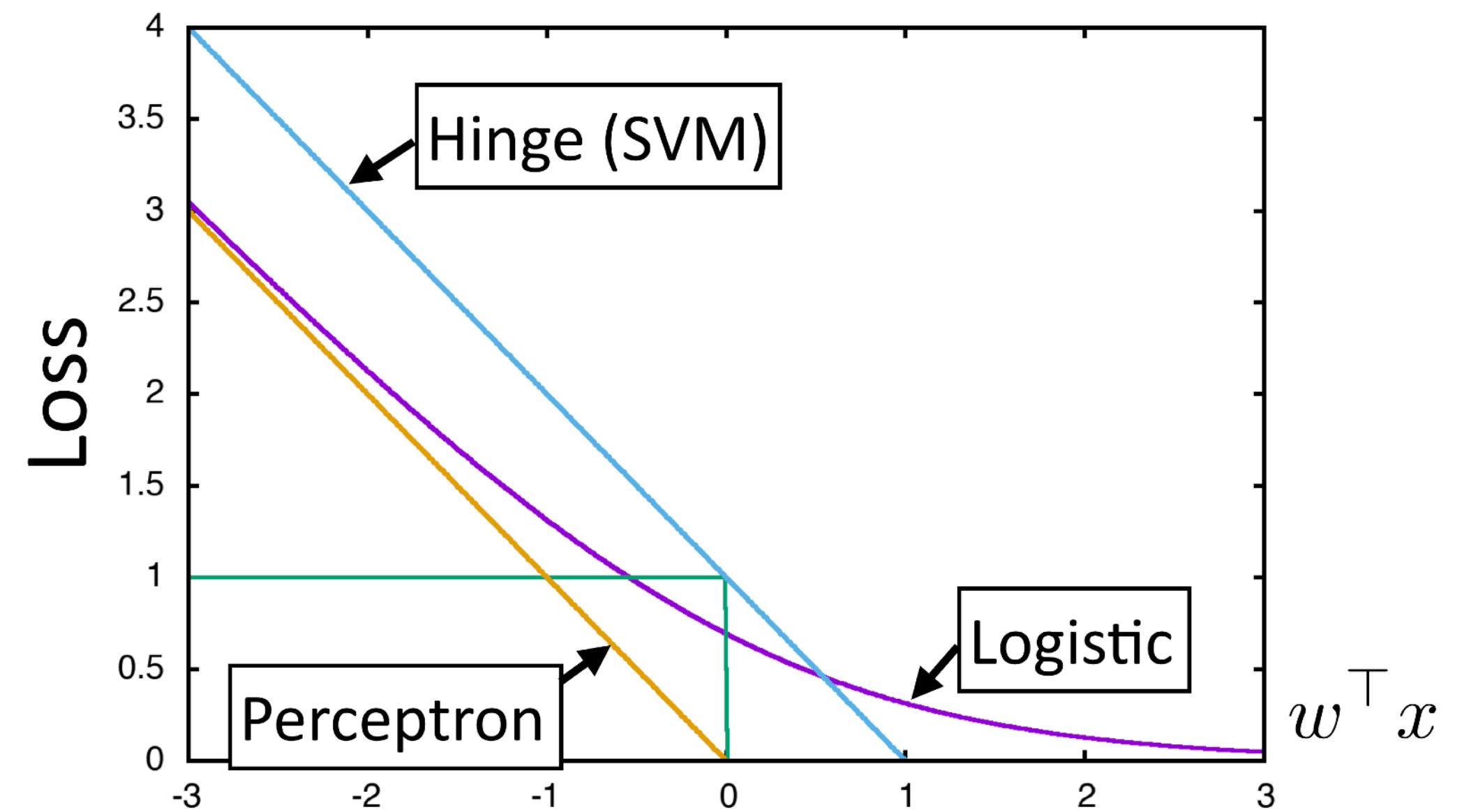
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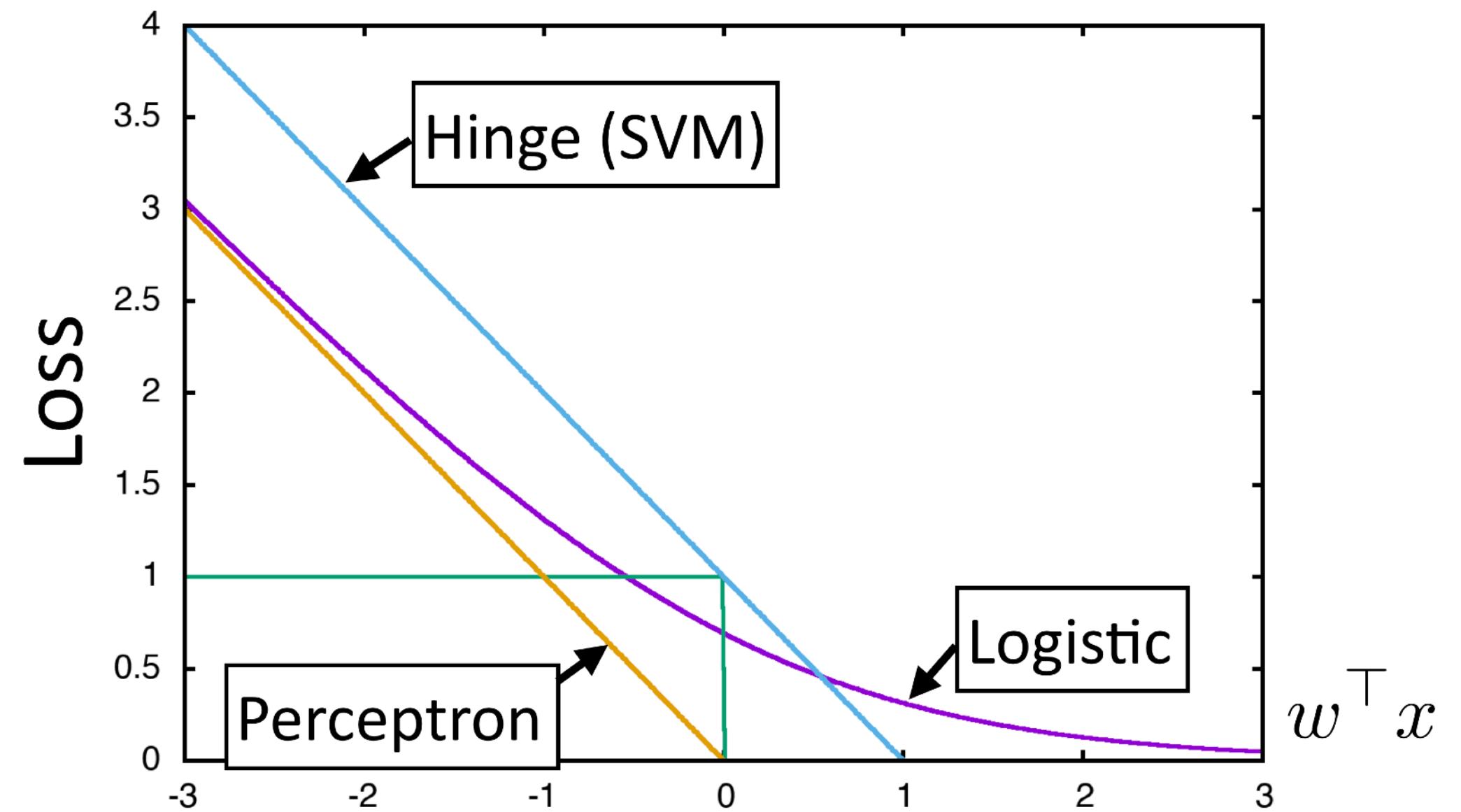


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Recap

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

Optimization

Optimization

- ▶ Stochastic gradient *ascent*

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

Optimization

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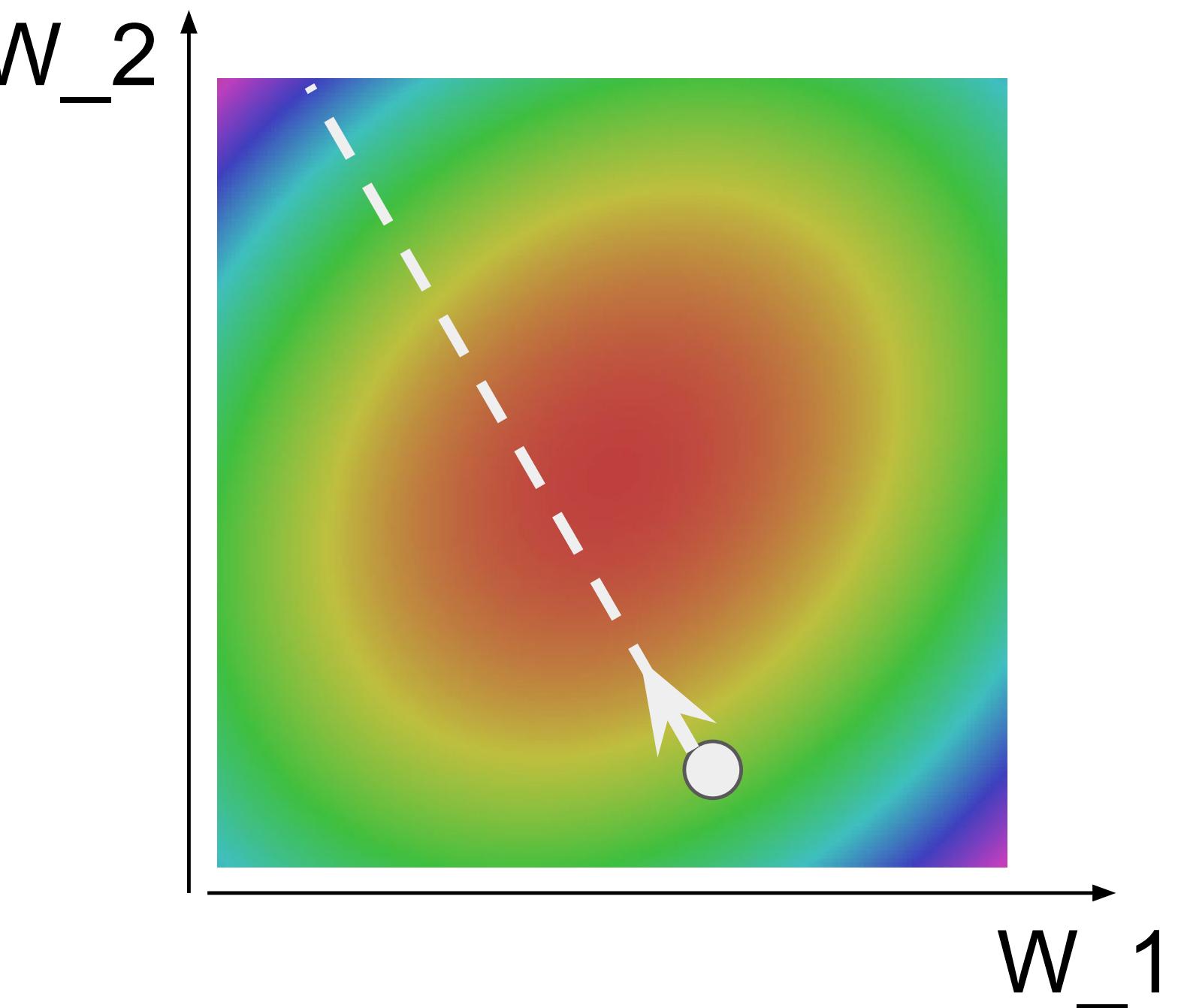
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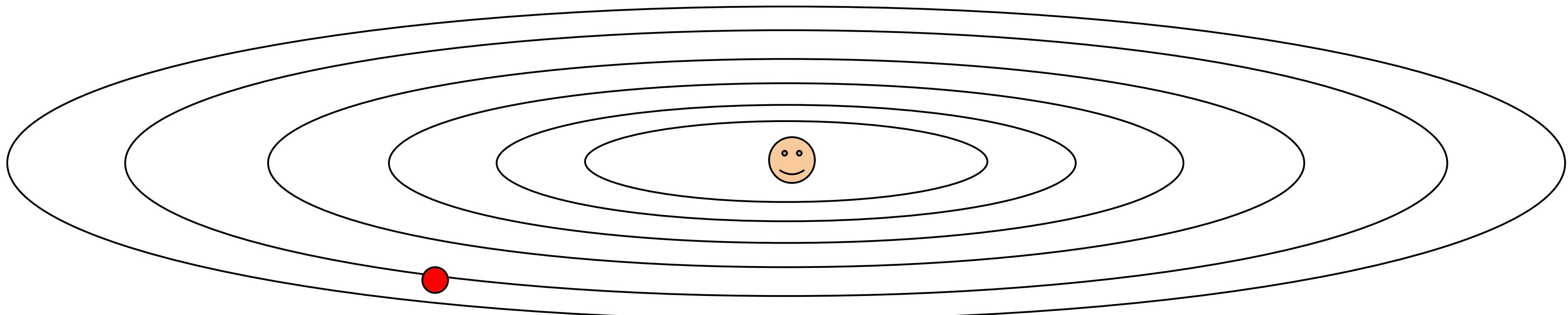
```
# Vanilla Gradient Descent

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



Optimization

- ▶ Stochastic gradient *ascent*
- ▶ Very simple to code up
- ▶ What if loss changes quickly in one direction and slowly in another direction?

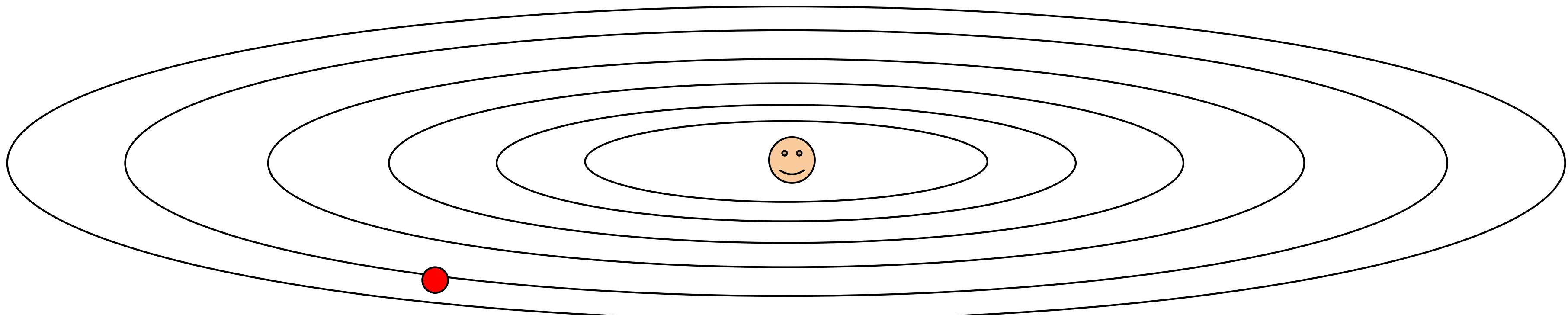


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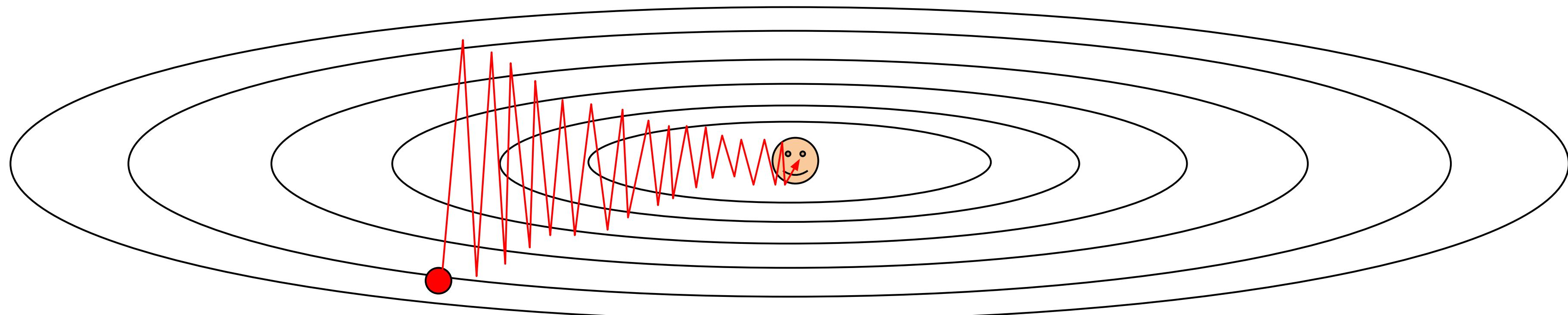
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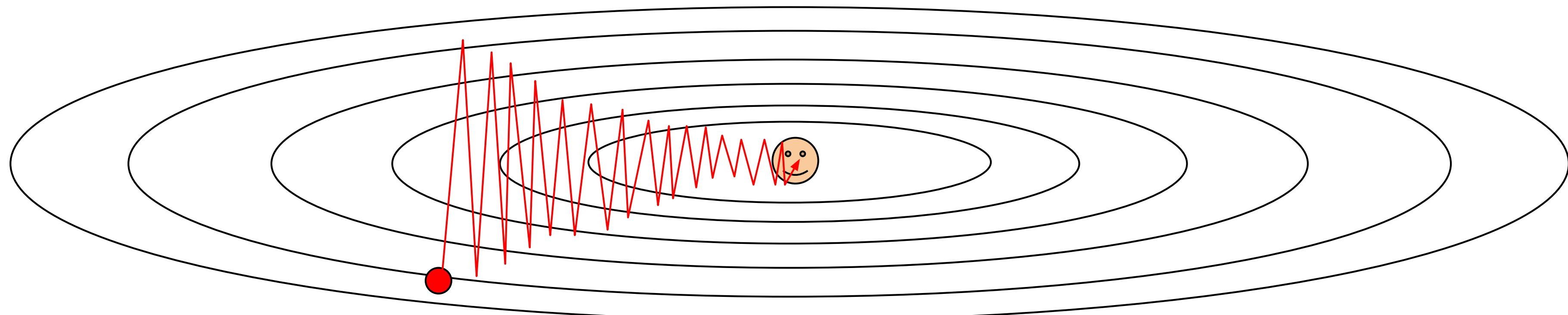


Optimization

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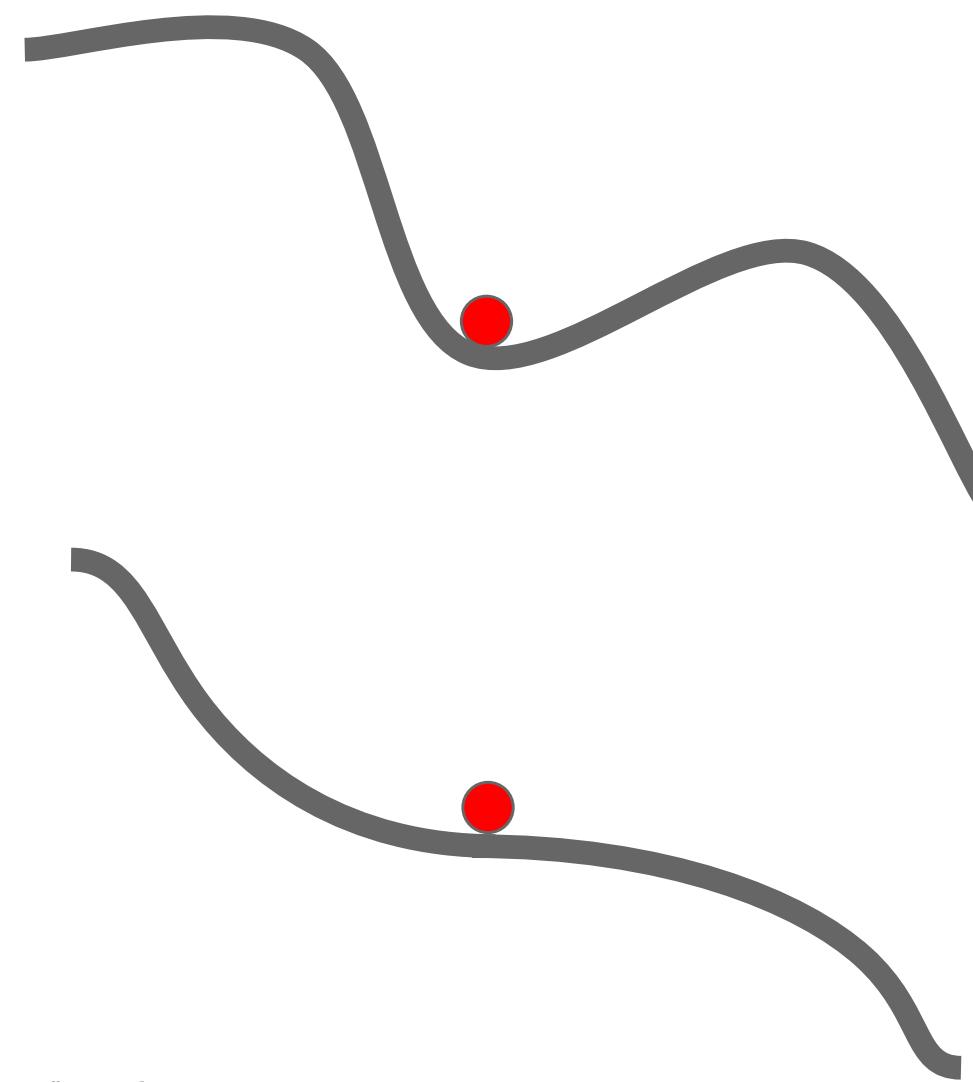
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Optimization

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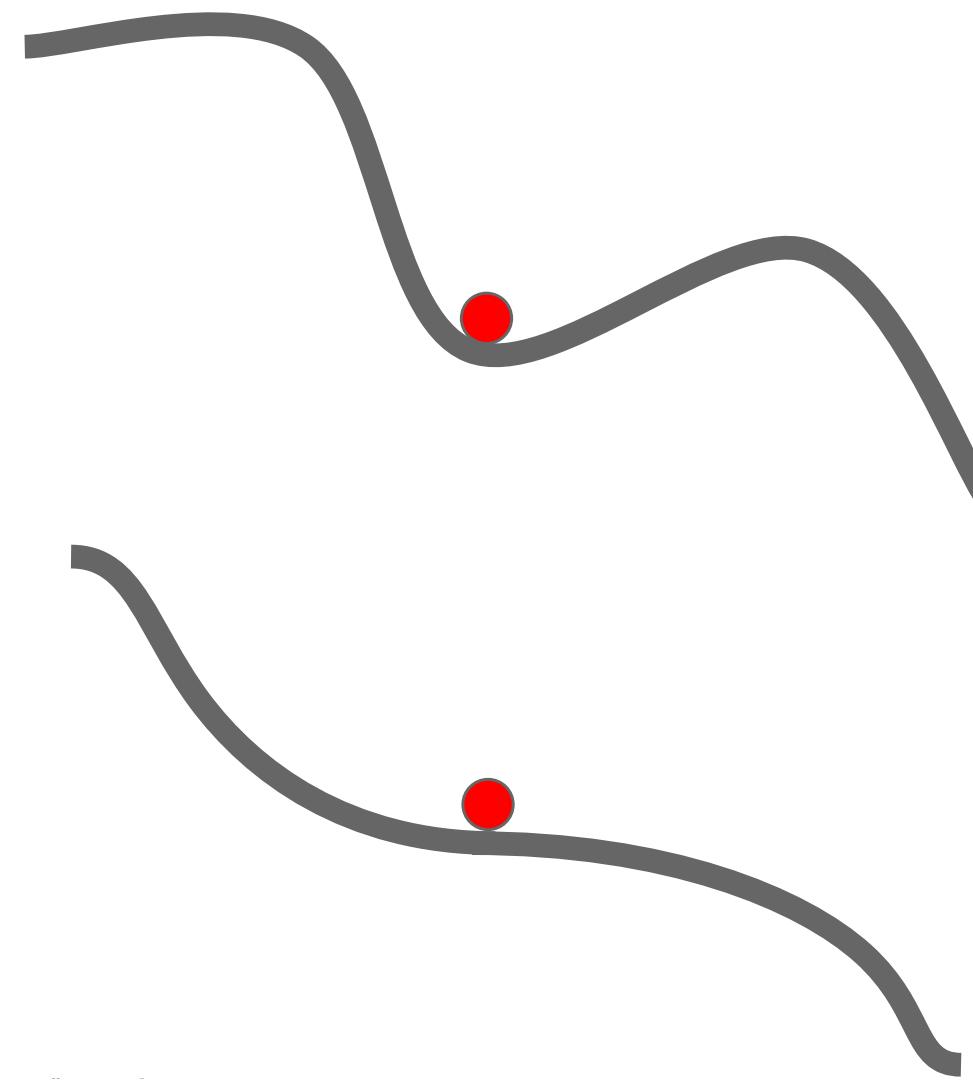
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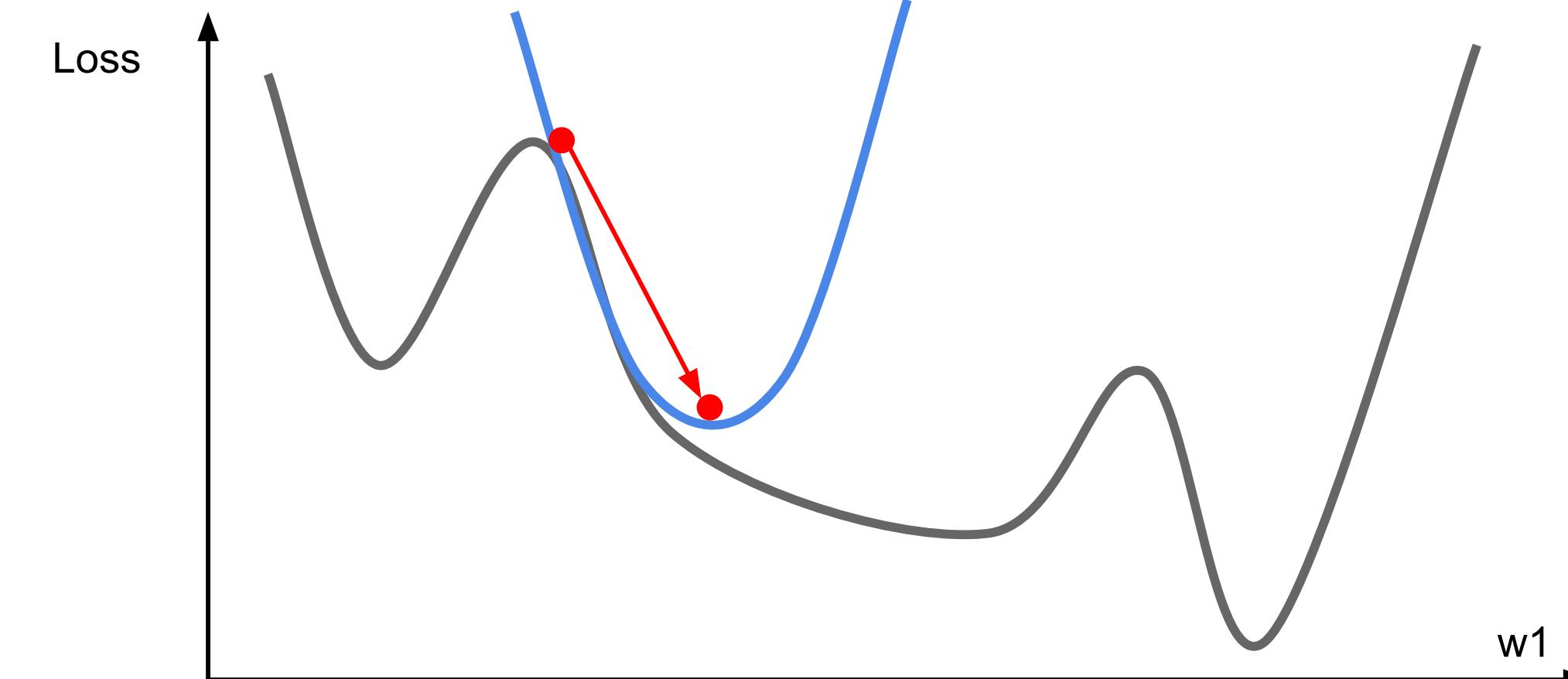
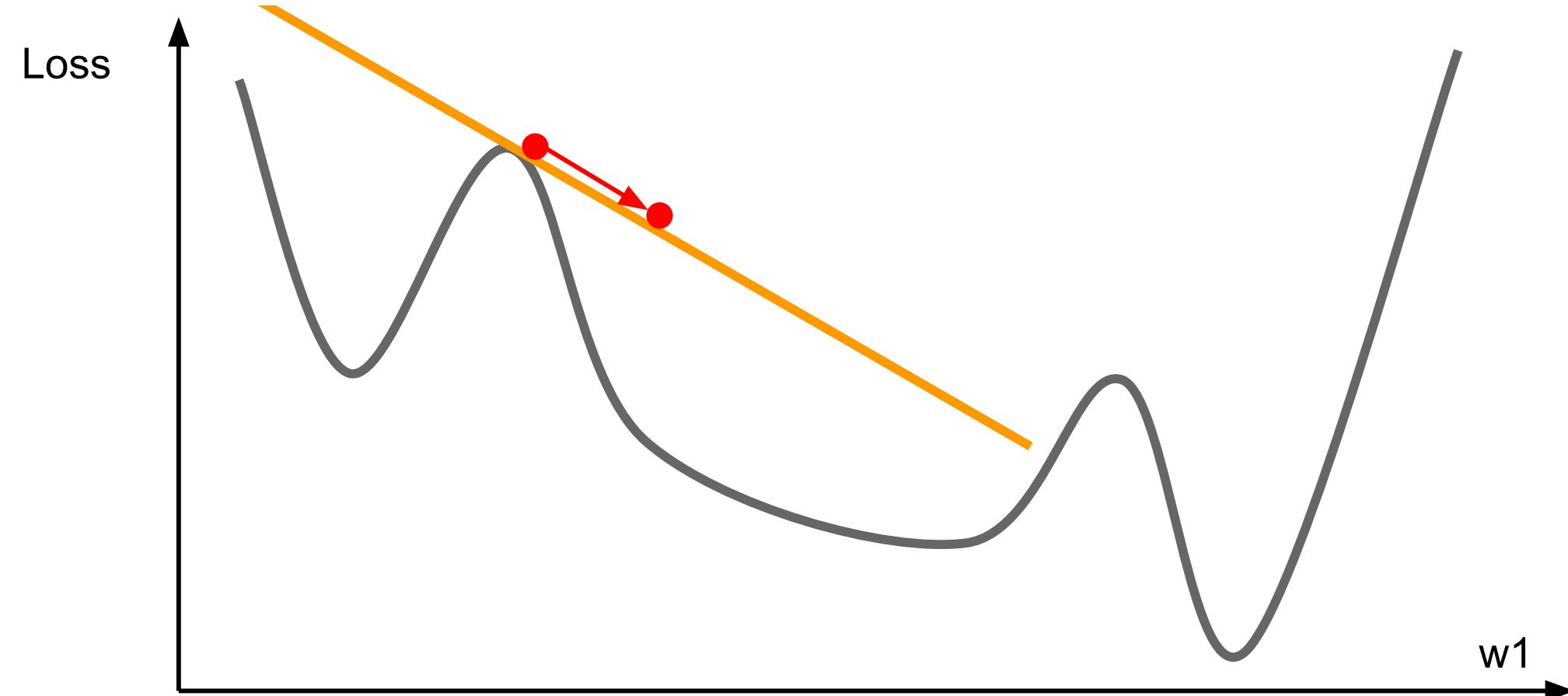


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- ▶ Quasi-Newton methods: L-BFGS, etc. approximate inverse Hessian

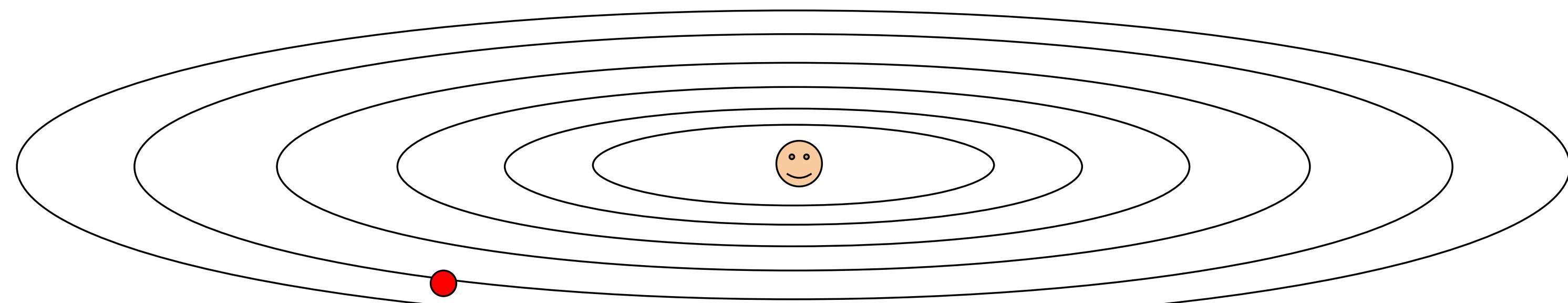
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- ▶ Optimized for problems with sparse features
- ▶ Per-parameter learning rate: smaller updates are made to parameters that get updated frequently

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



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- ▶ Other techniques for optimizing deep models — more later!

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- ▶ ...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