

# Multiclass Classification

Alan Ritter

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

# This Lecture

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

# Multiclass Fundamentals

# Text Classification

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## 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

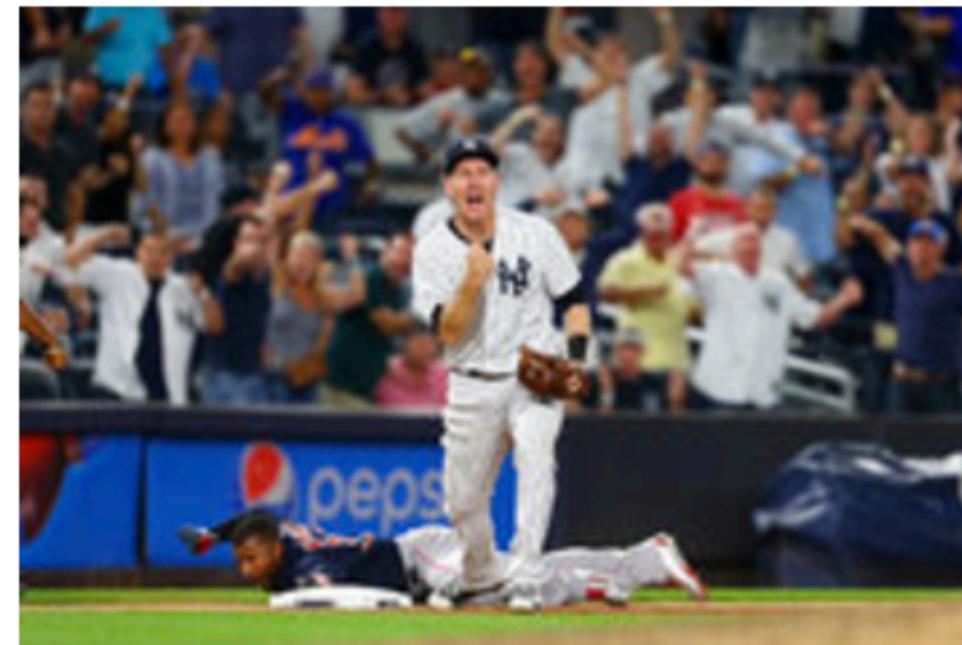
## Yankees and Mets Are on Opposite Tracks This Subway Series

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

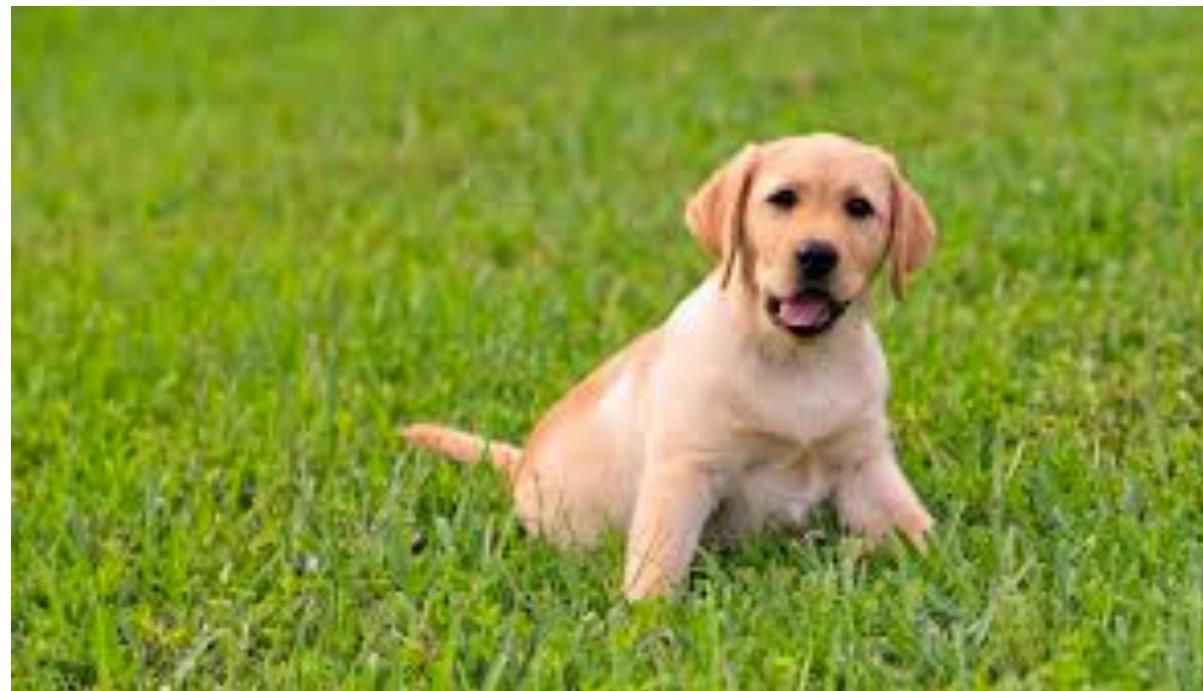


→ Sports

~20 classes

# Image Classification

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→ Dog



→ Car

- ▶ Thousands of classes (ImageNet)

# Entity Linking

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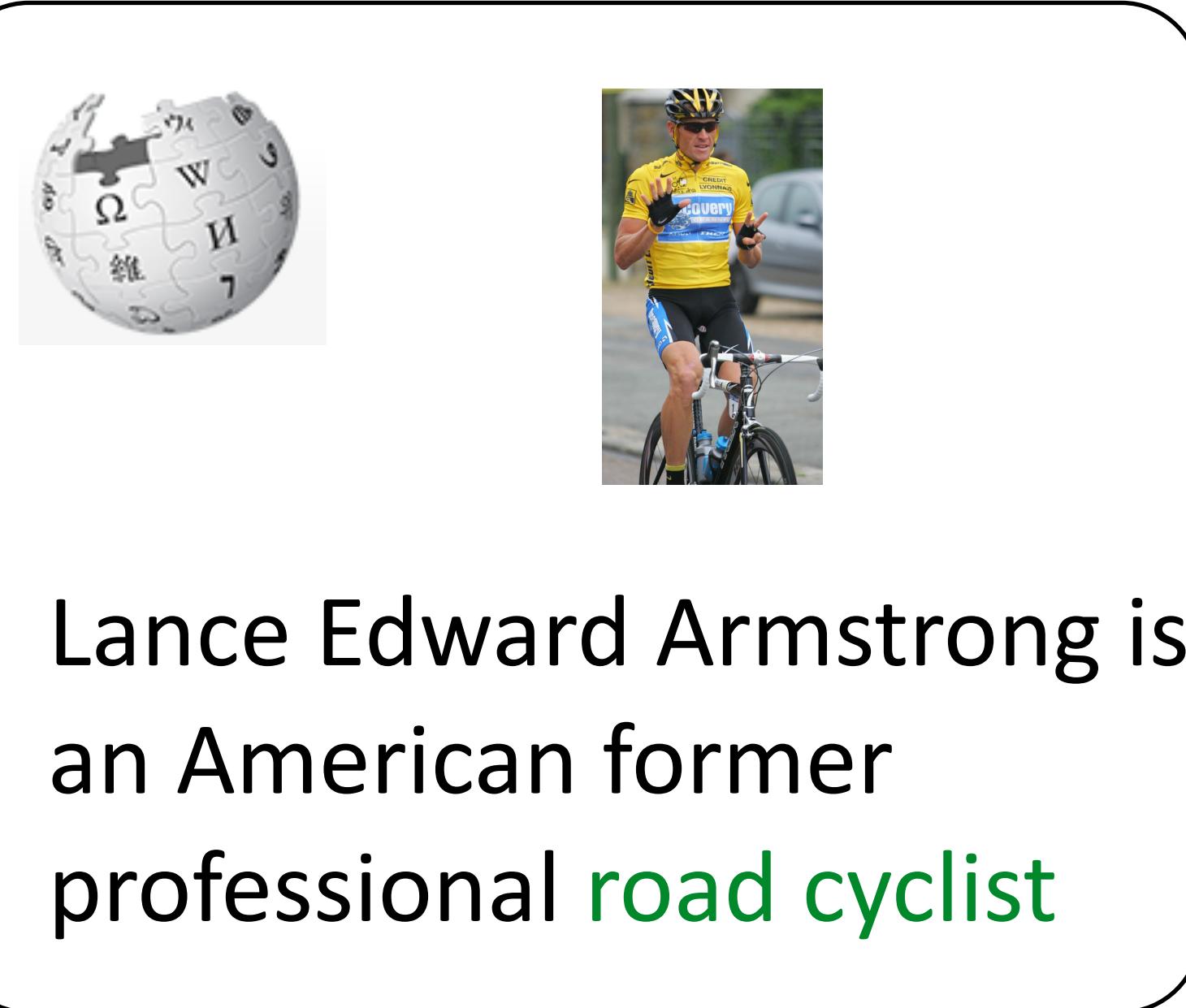
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Although he originally won the event, the United States Anti-Doping Agency announced in August 2012 that they had disqualified Armstrong from his seven consecutive Tour de France wins from 1999–2005.

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Armstrong County is a county in Pennsylvania...

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# 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)

# Reading Comprehension

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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?

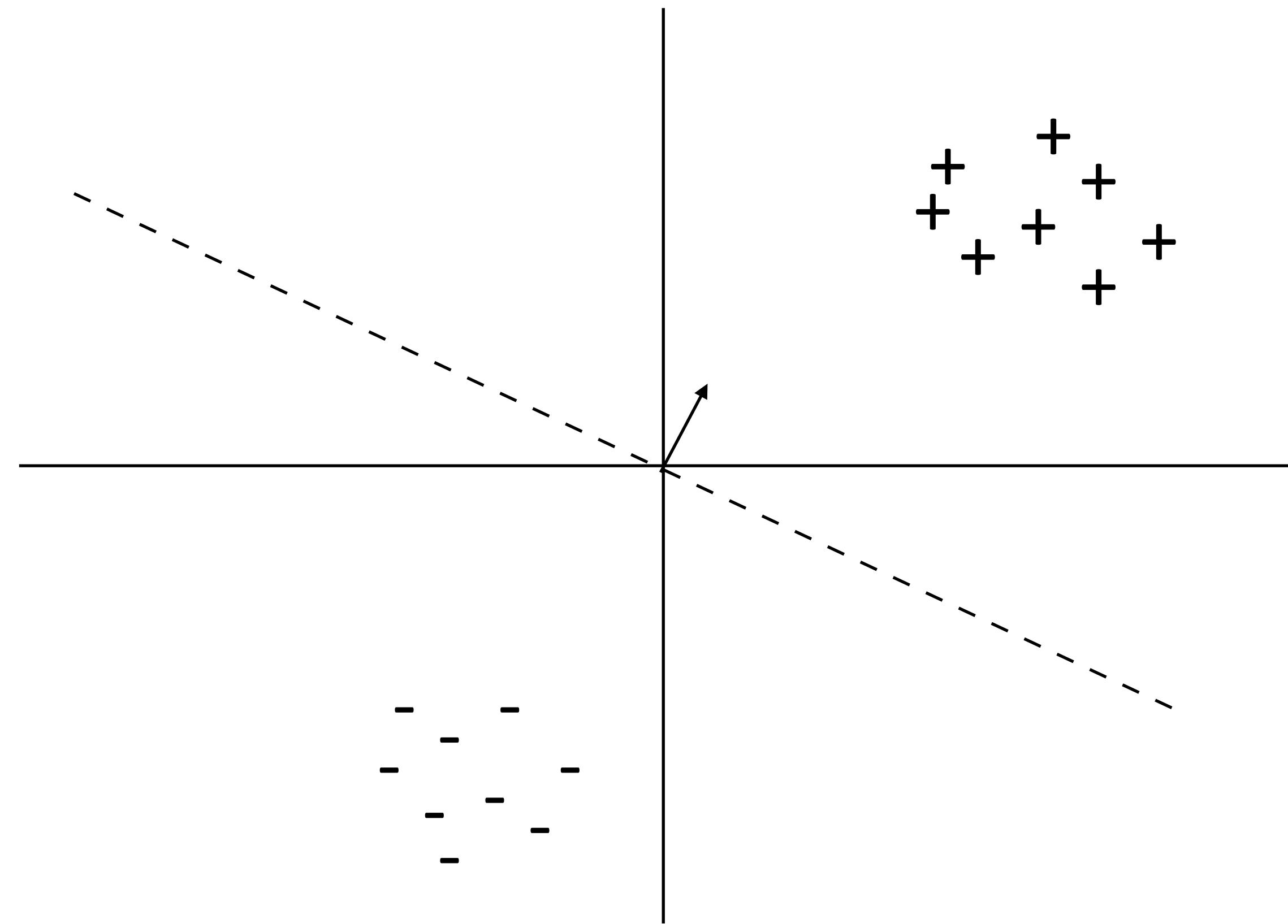
- A) his deck
- B) his freezer
- C) a fast food restaurant
- D) his room

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

# Binary Classification

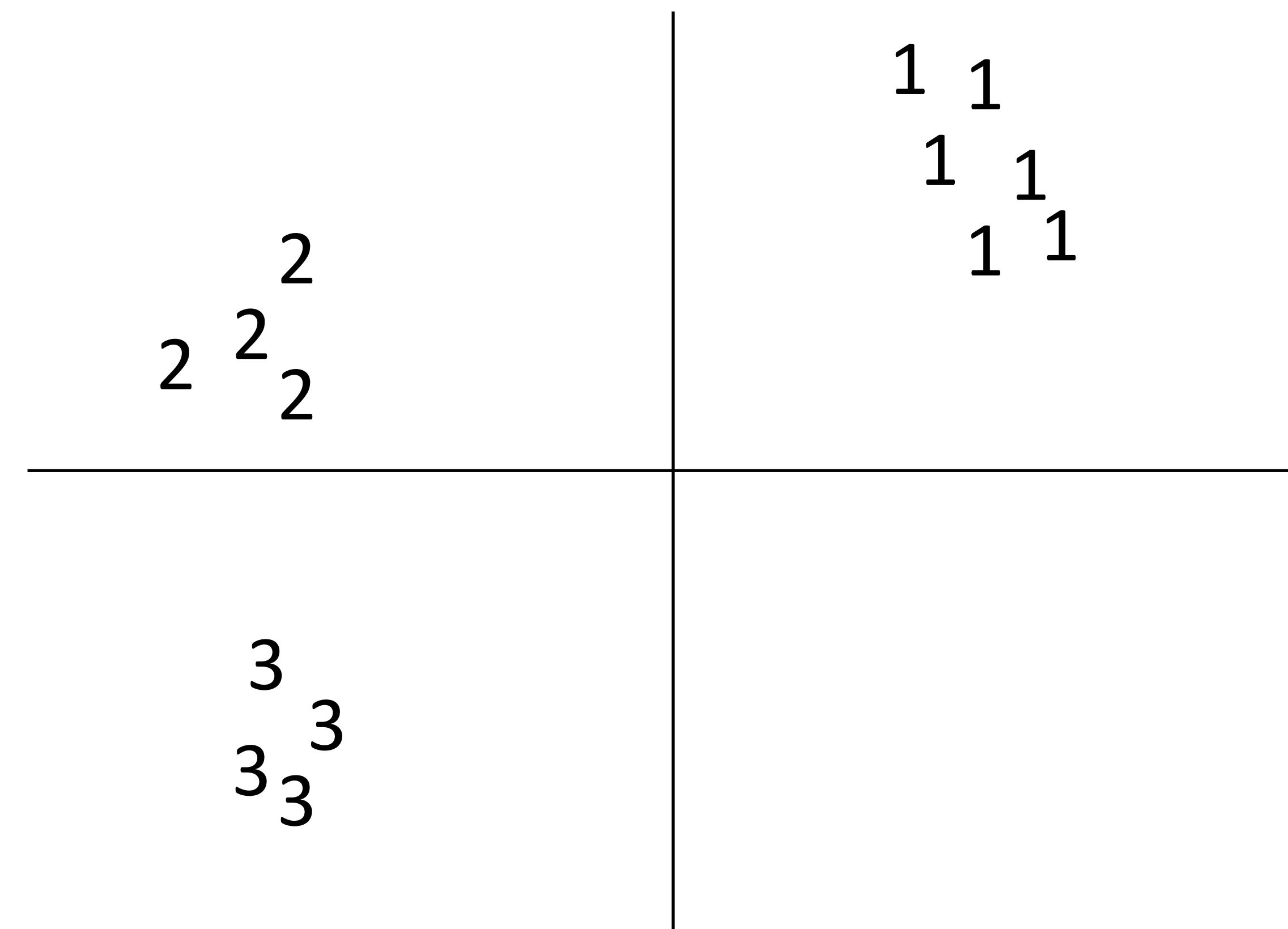
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- ▶ Binary classification: one weight vector defines positive and negative classes



# Multiclass Classification

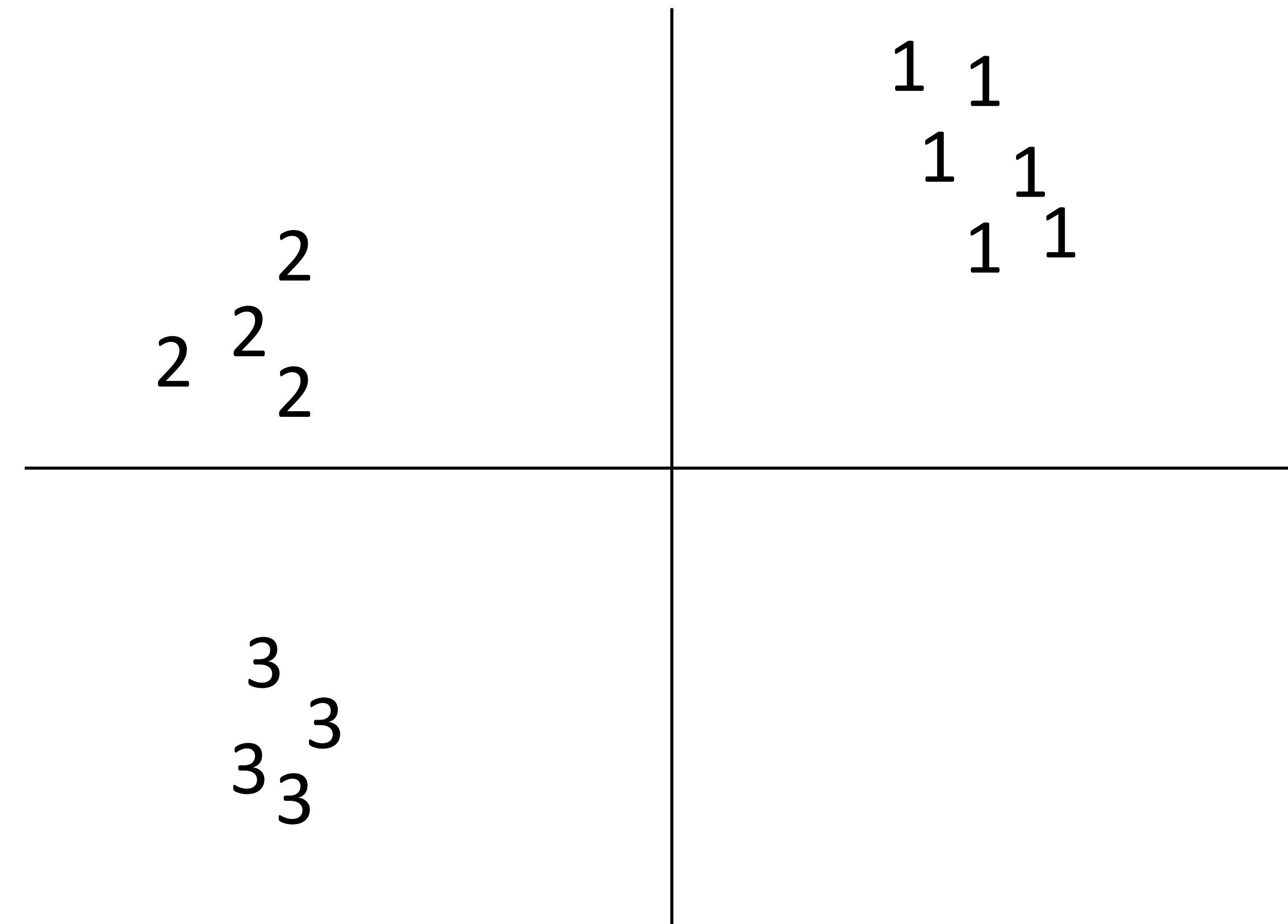
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# Multiclass Classification

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- ▶ Can we just use binary classifiers here?



# Multiclass Classification

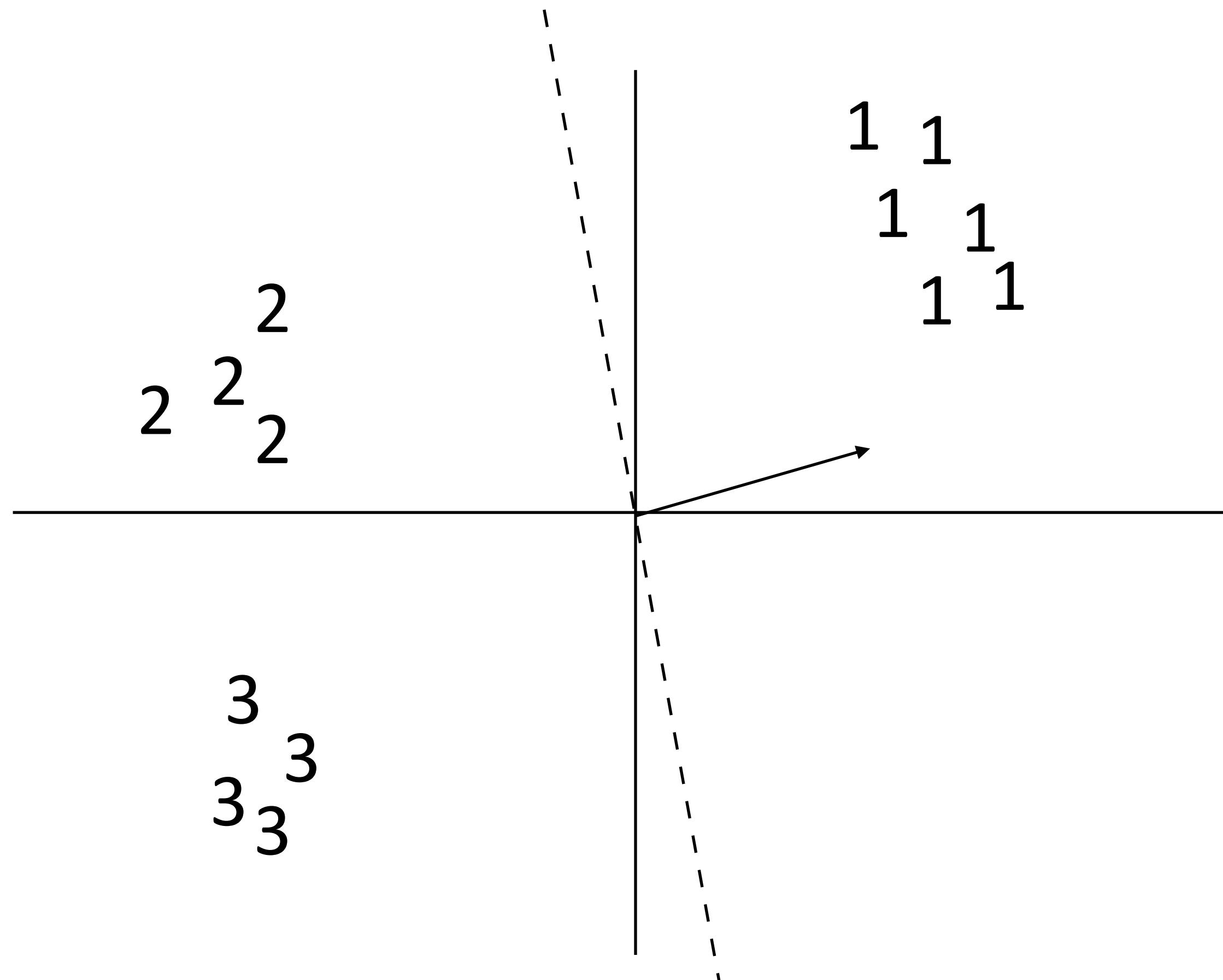
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- ▶ One-vs-all: train  $k$  classifiers, one to distinguish each class from all the rest

# Multiclass Classification

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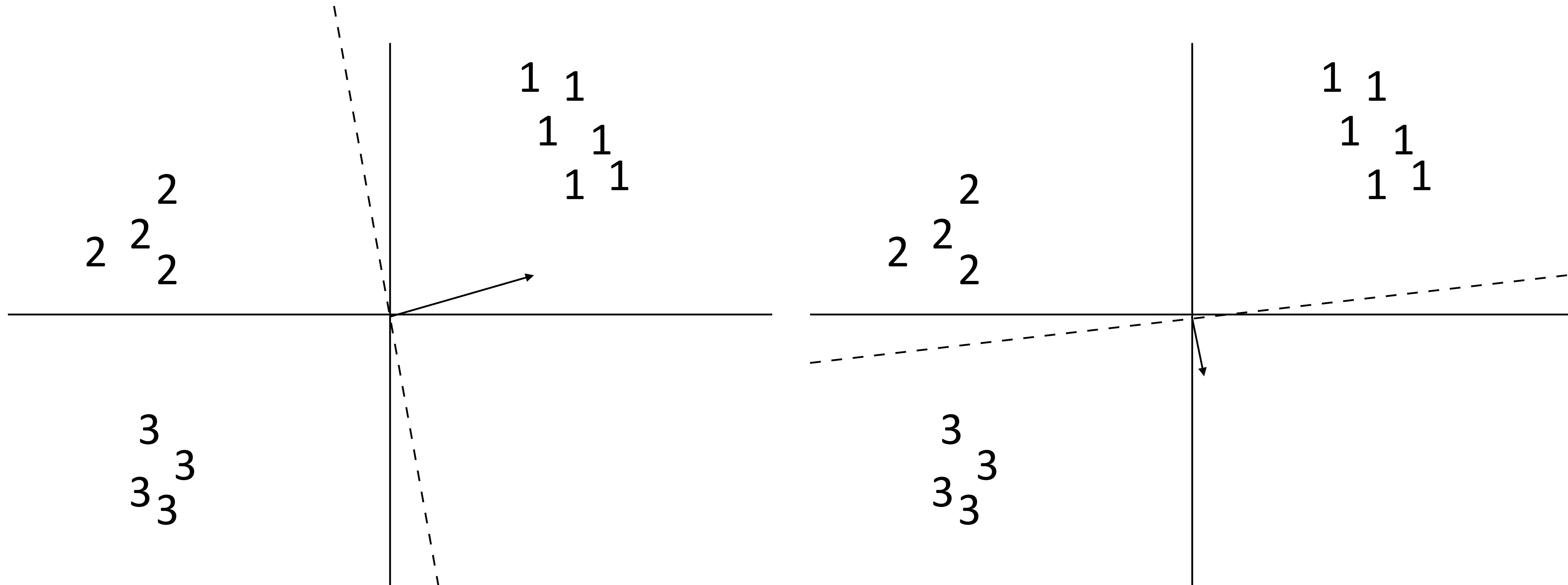
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# Multiclass Classification

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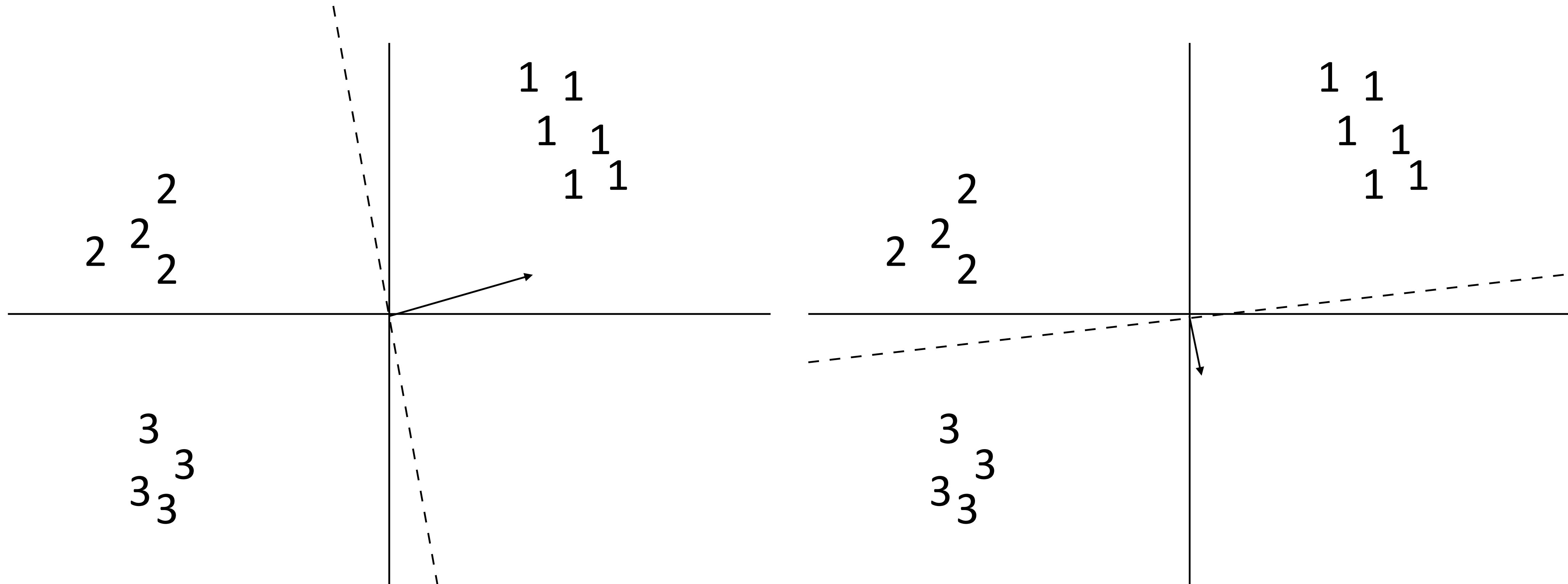
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# Multiclass Classification

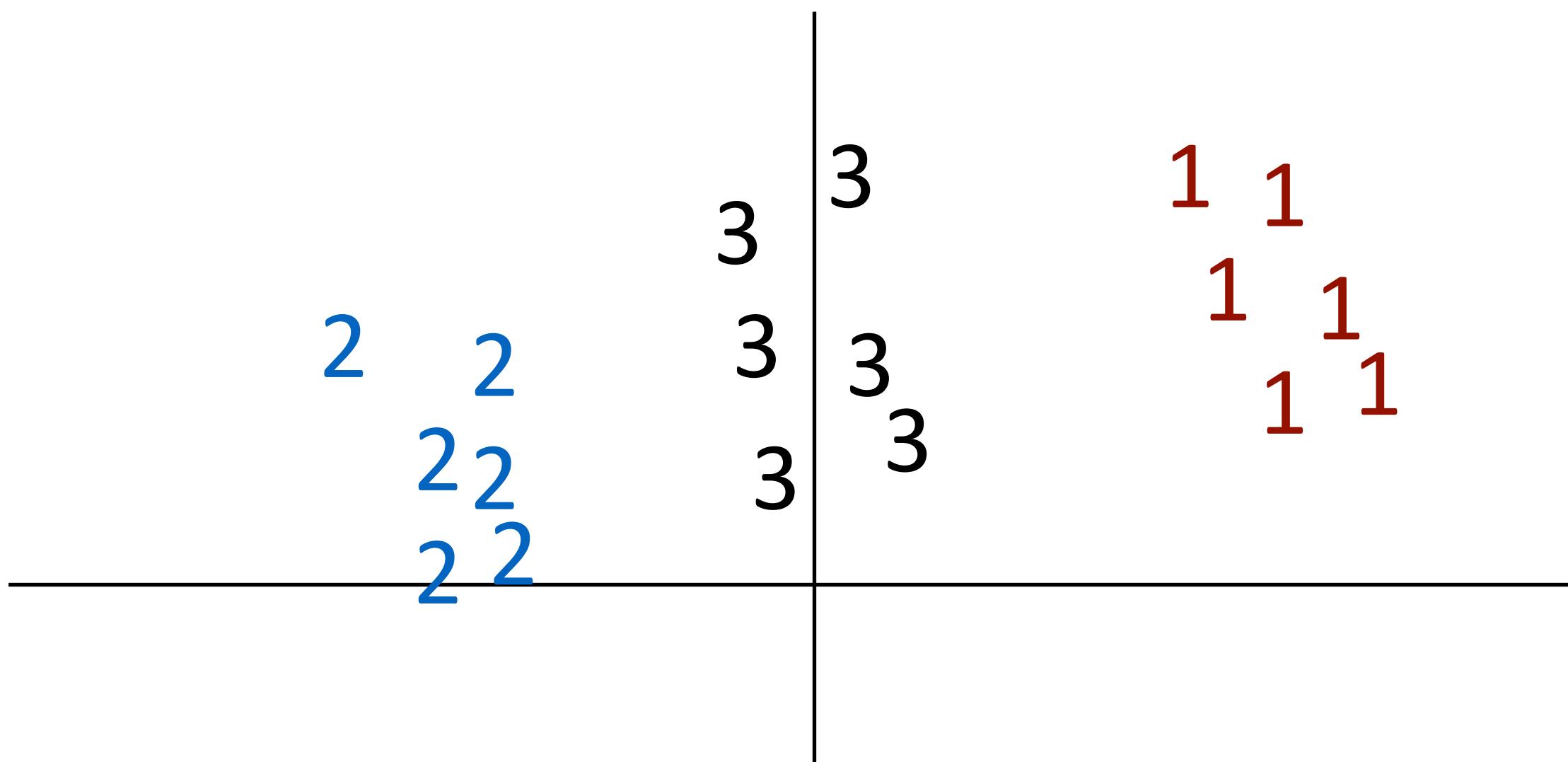
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- ▶ One-vs-all: train  $k$  classifiers, one to distinguish each class from all the rest
- ▶ How do we reconcile multiple positive predictions? Highest score?



# Multiclass Classification

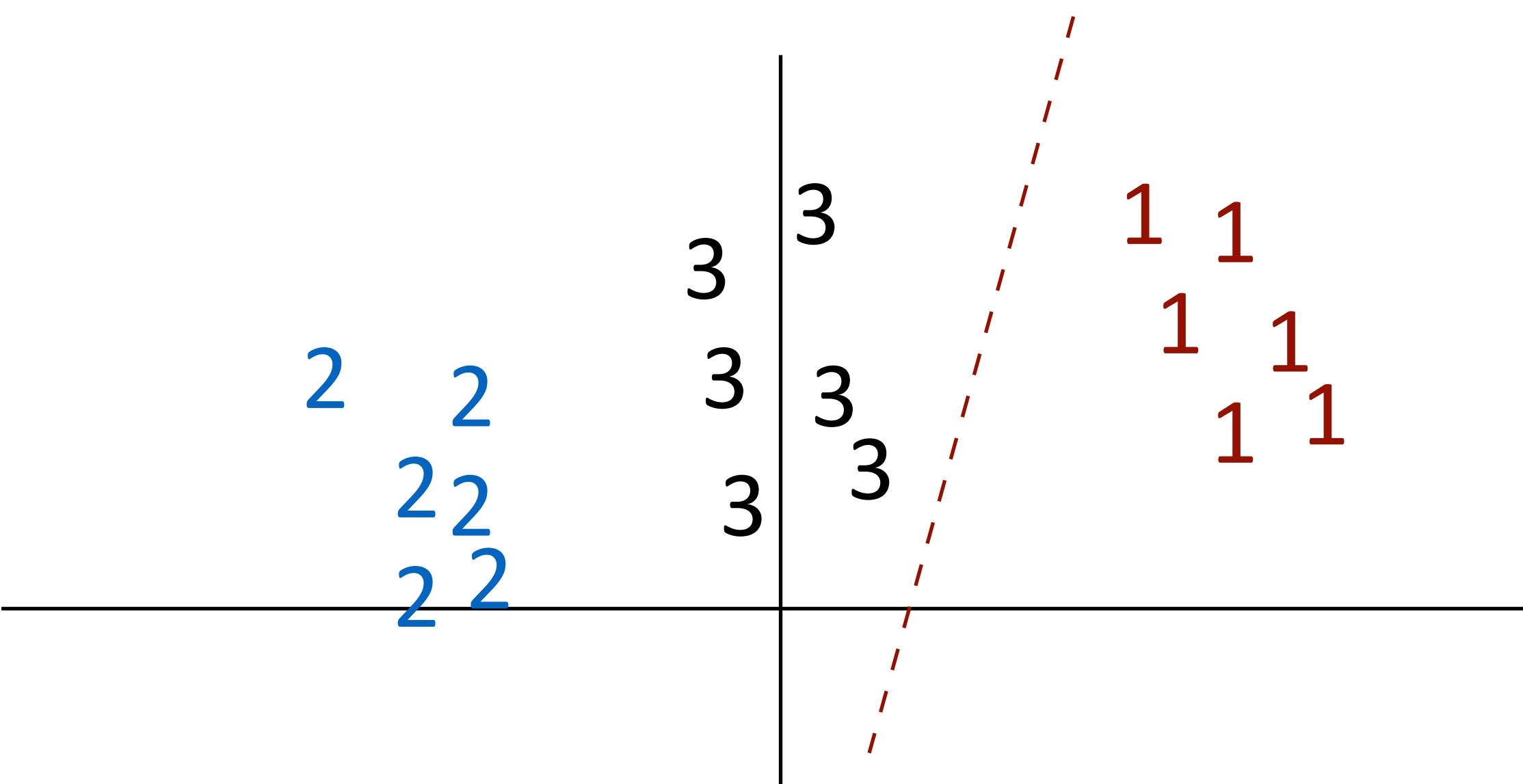
- ▶ Not all classes may even be separable using this approach



# Multiclass Classification

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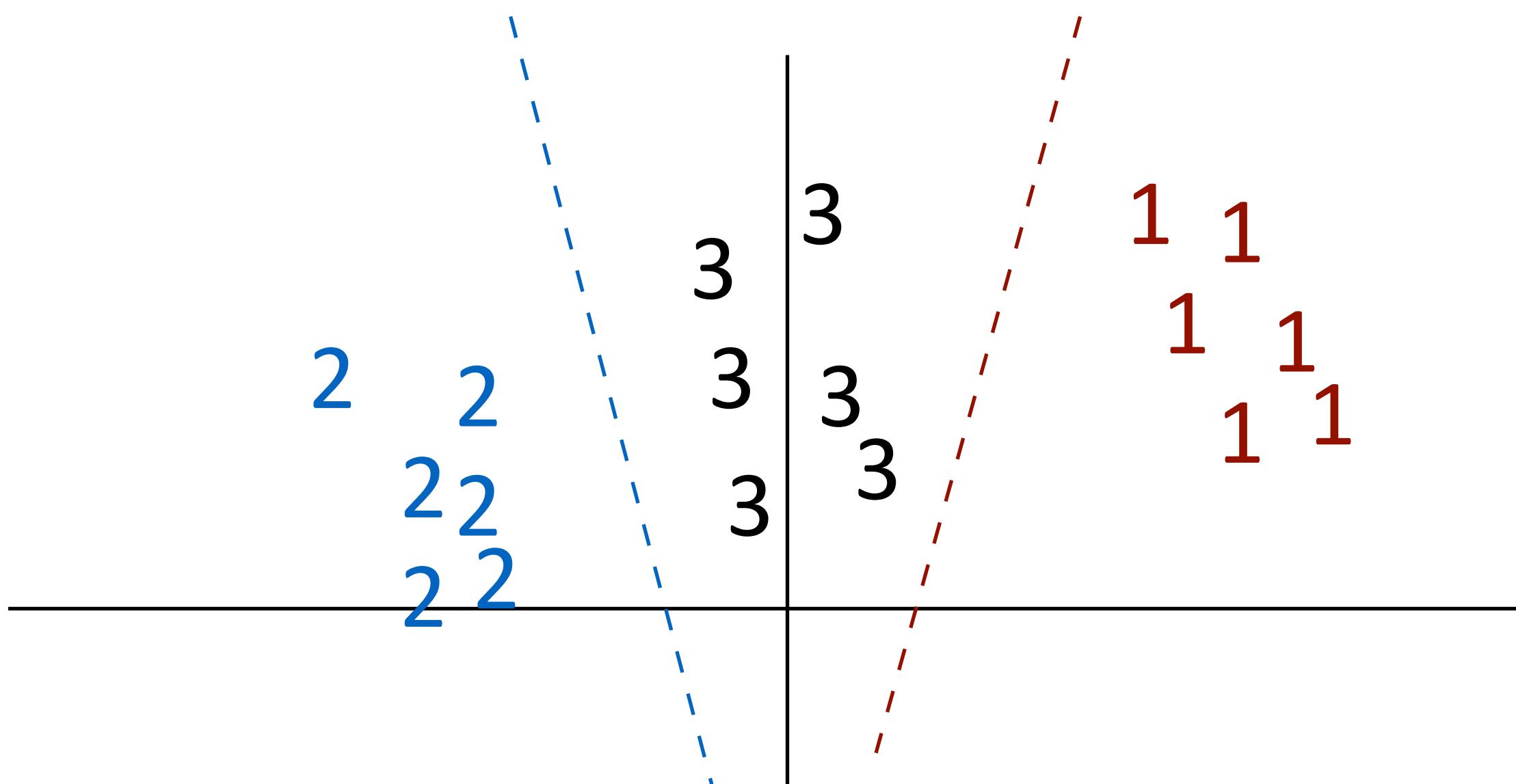
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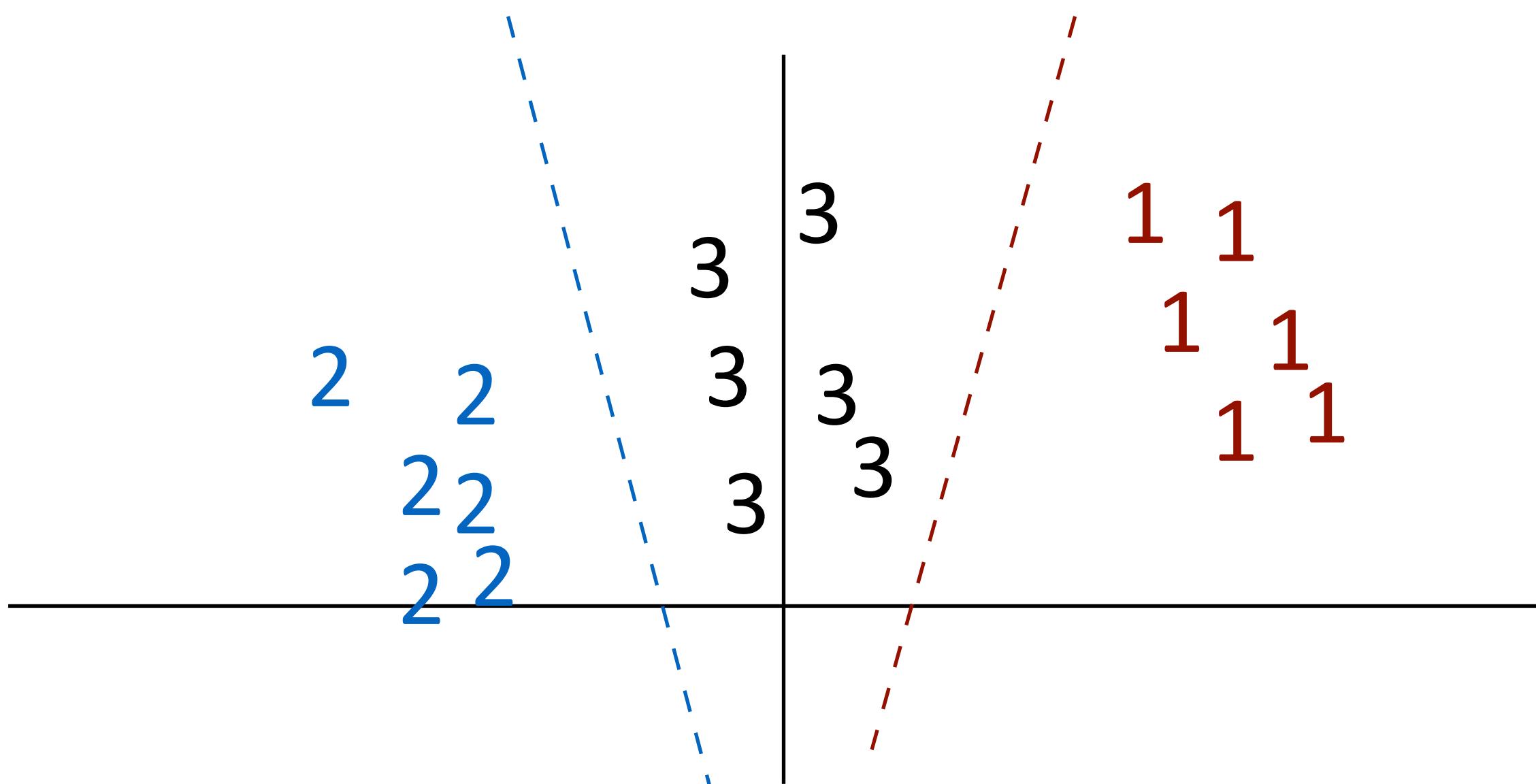
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# Multiclass Classification

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- ▶ 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

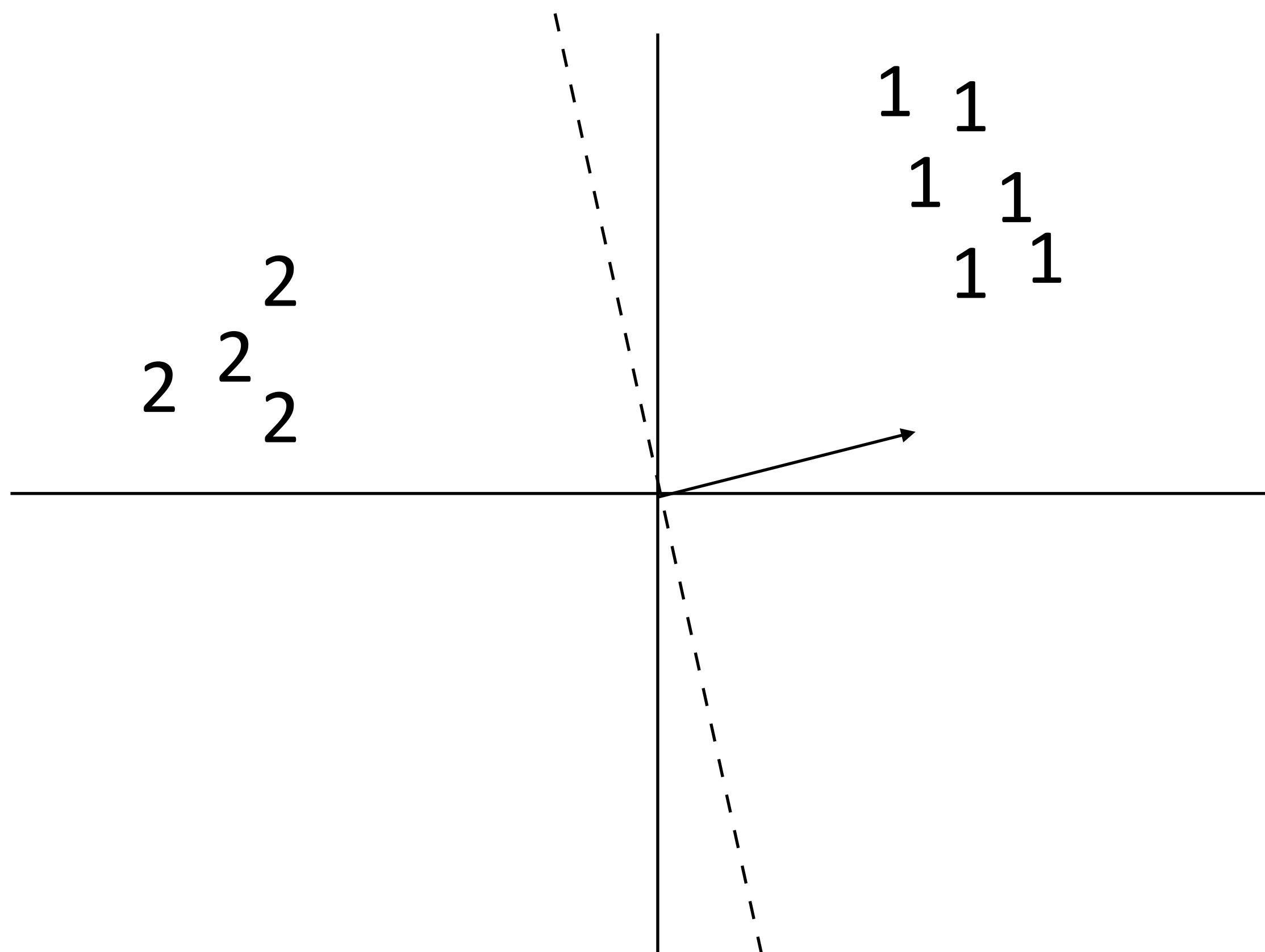
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- ▶ All-vs-all: train  $n(n-1)/2$  classifiers to differentiate each pair of classes

# Multiclass Classification

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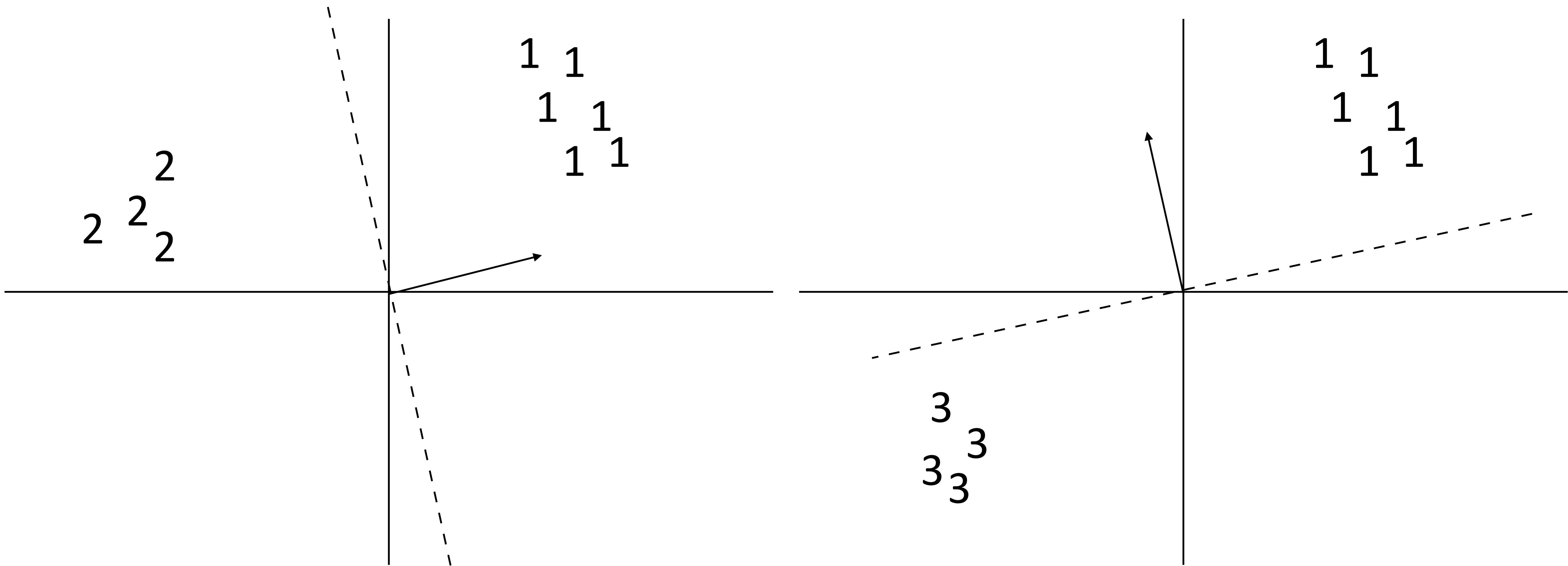
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# Multiclass Classification

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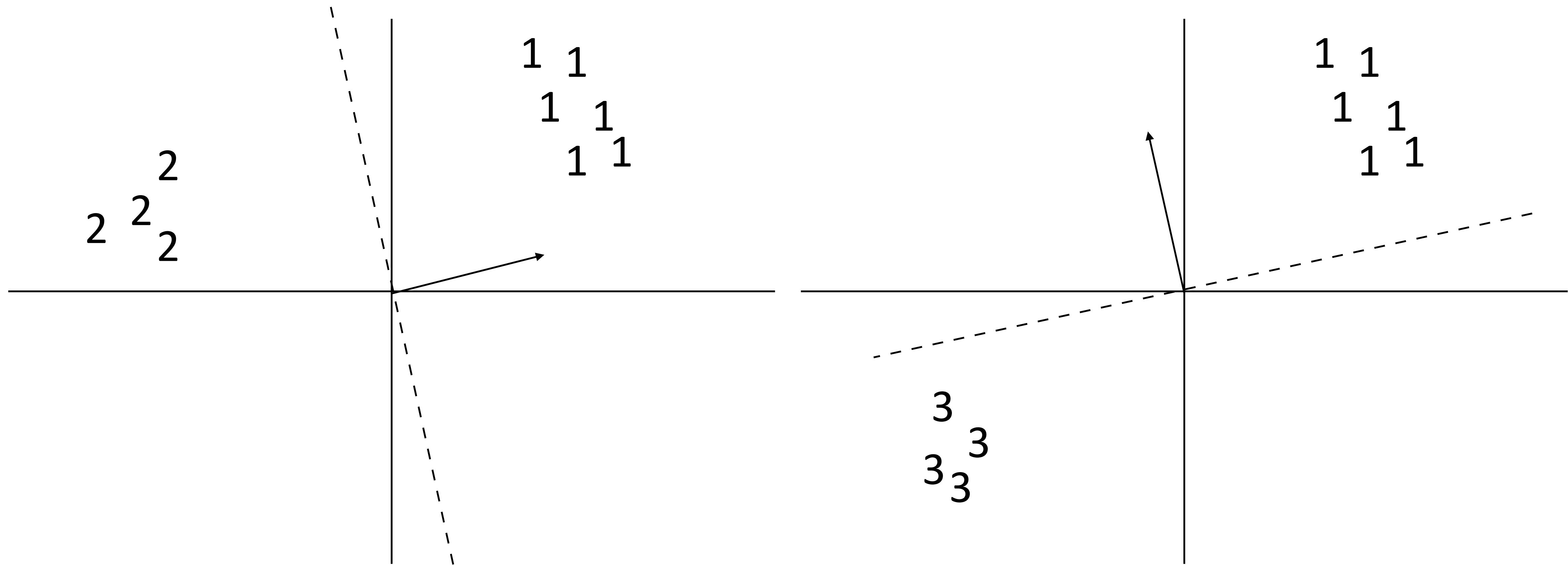
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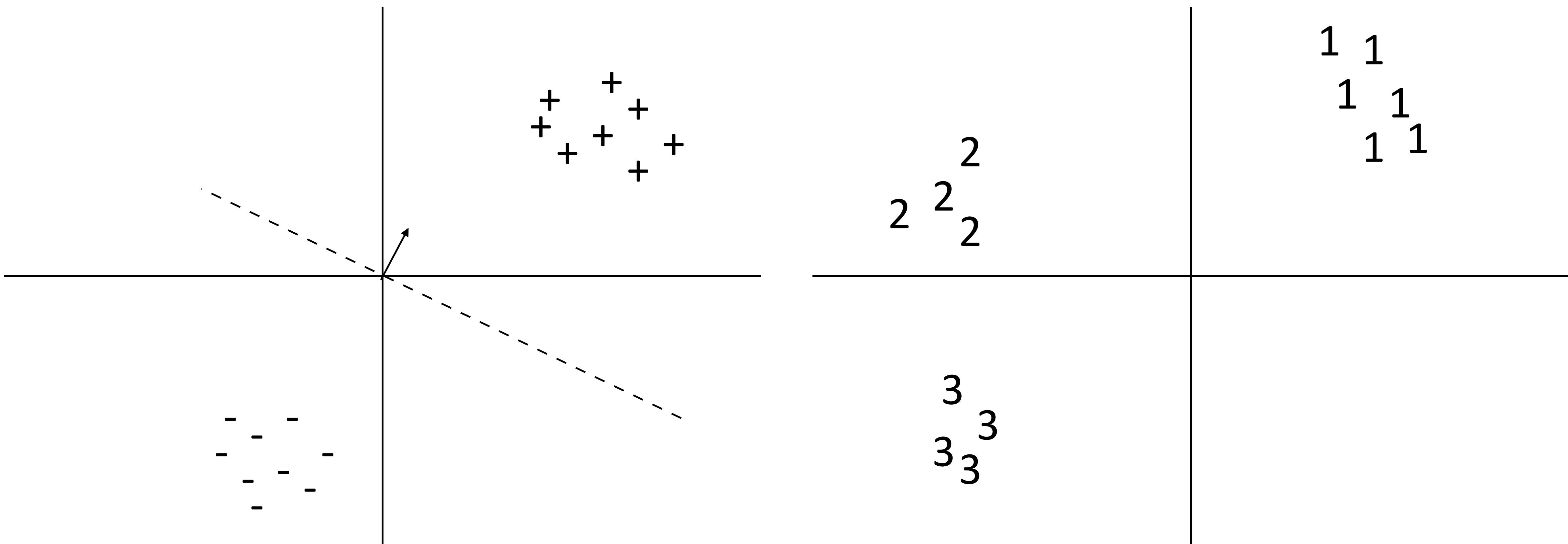
- ▶ All-vs-all: train  $n(n-1)/2$  classifiers to differentiate each pair of classes
- ▶ Again, how to reconcile?



# Multiclass Classification

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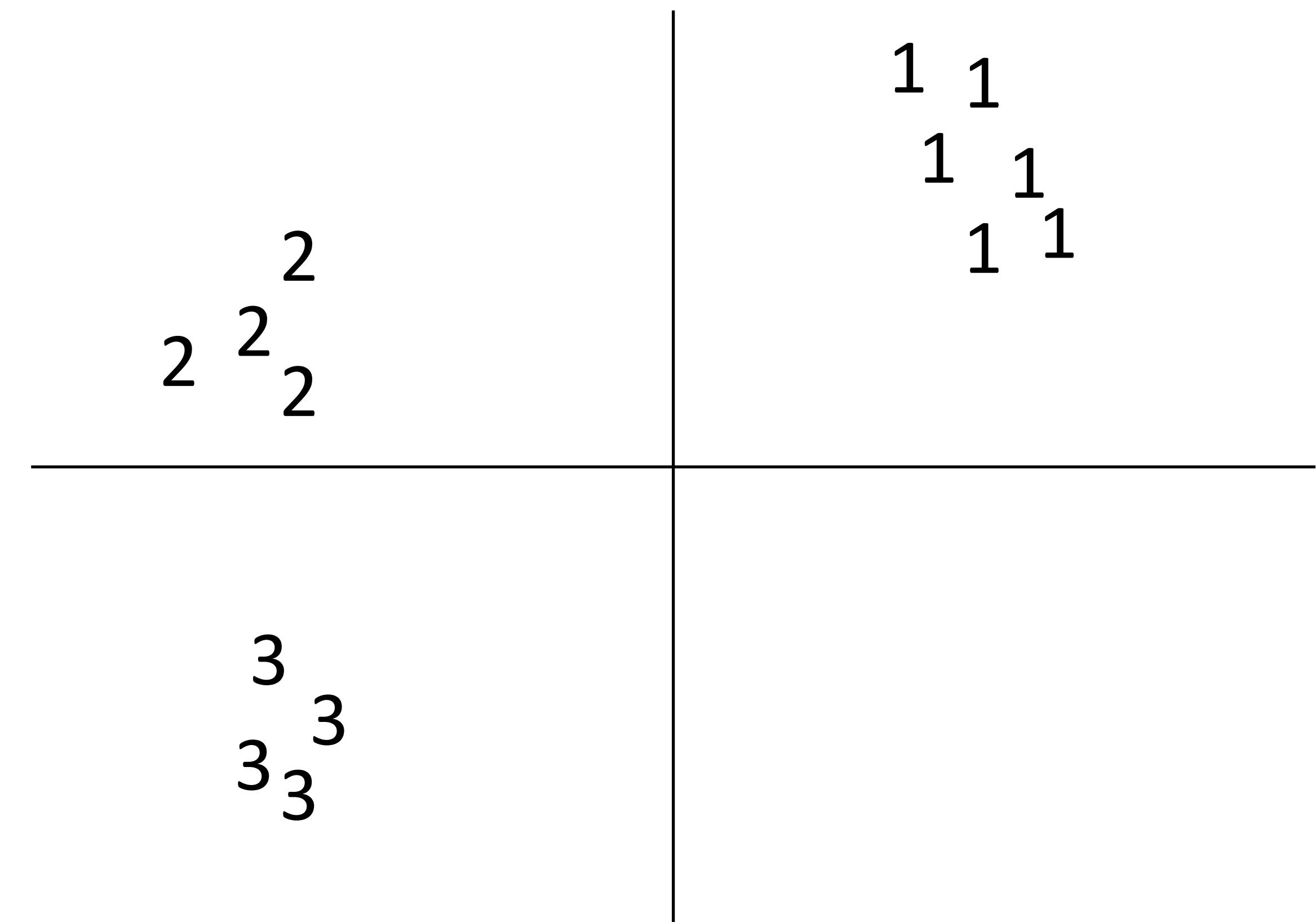
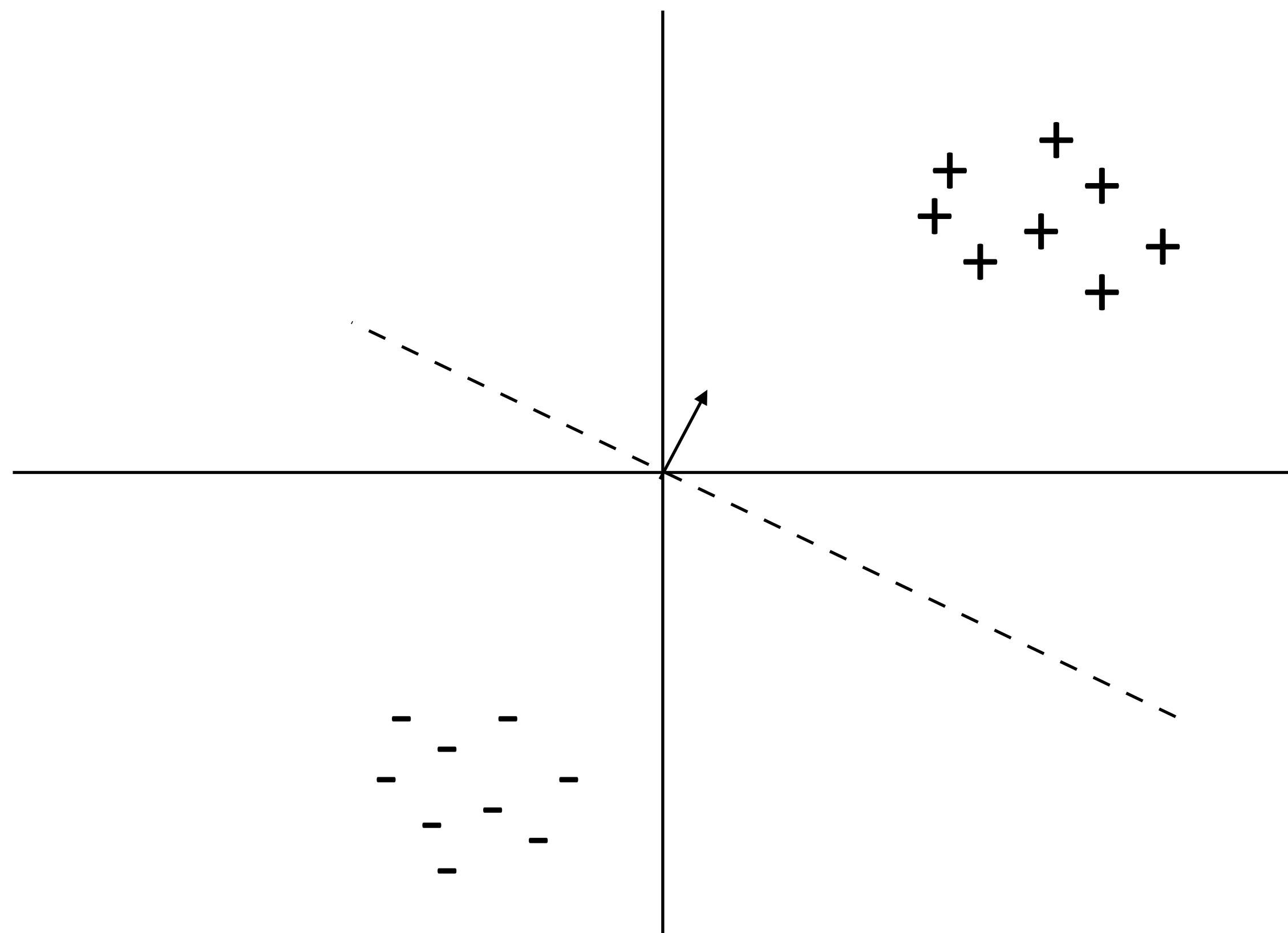
- ▶ Binary classification: one weight vector defines both classes



# Multiclass Classification

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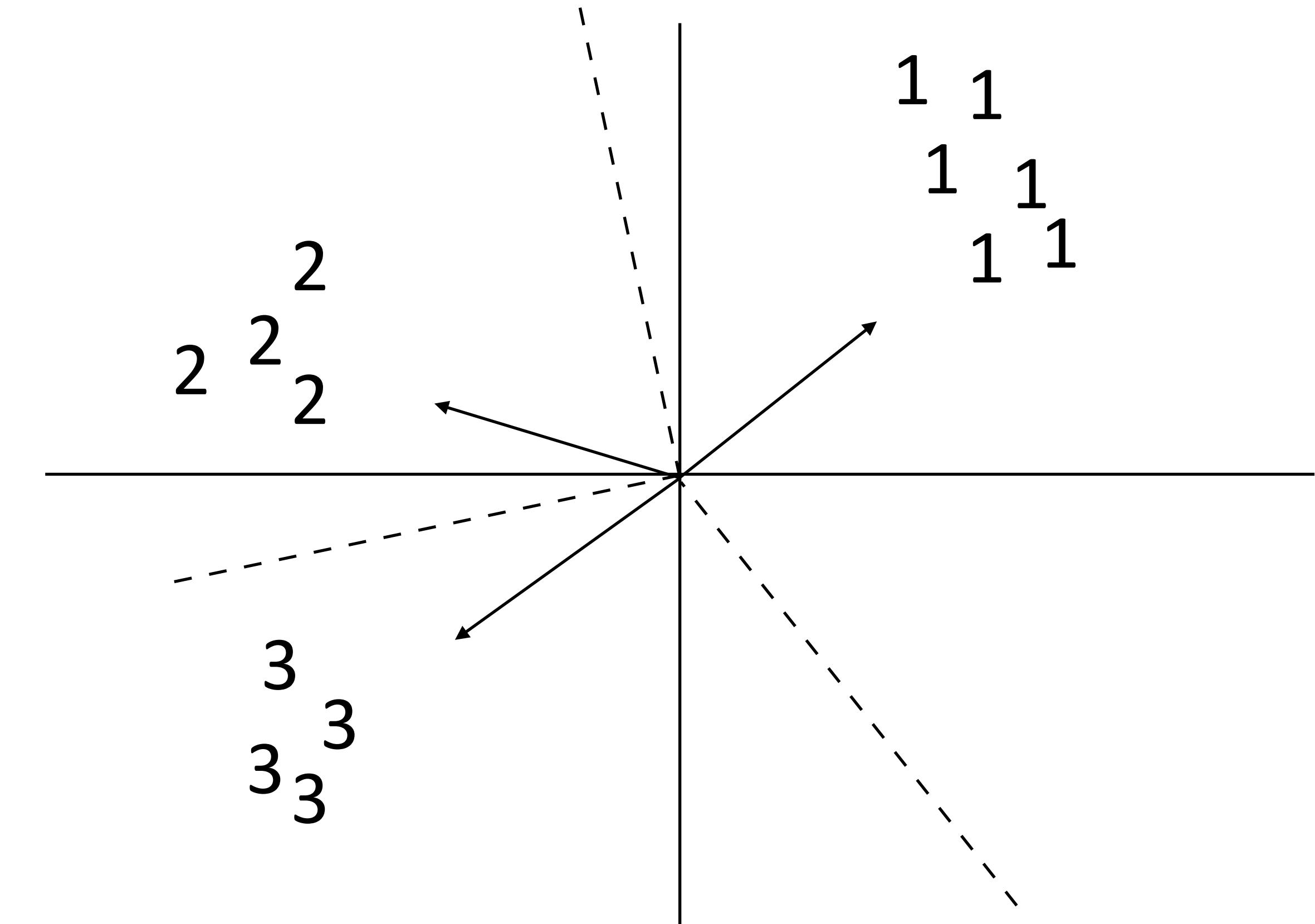
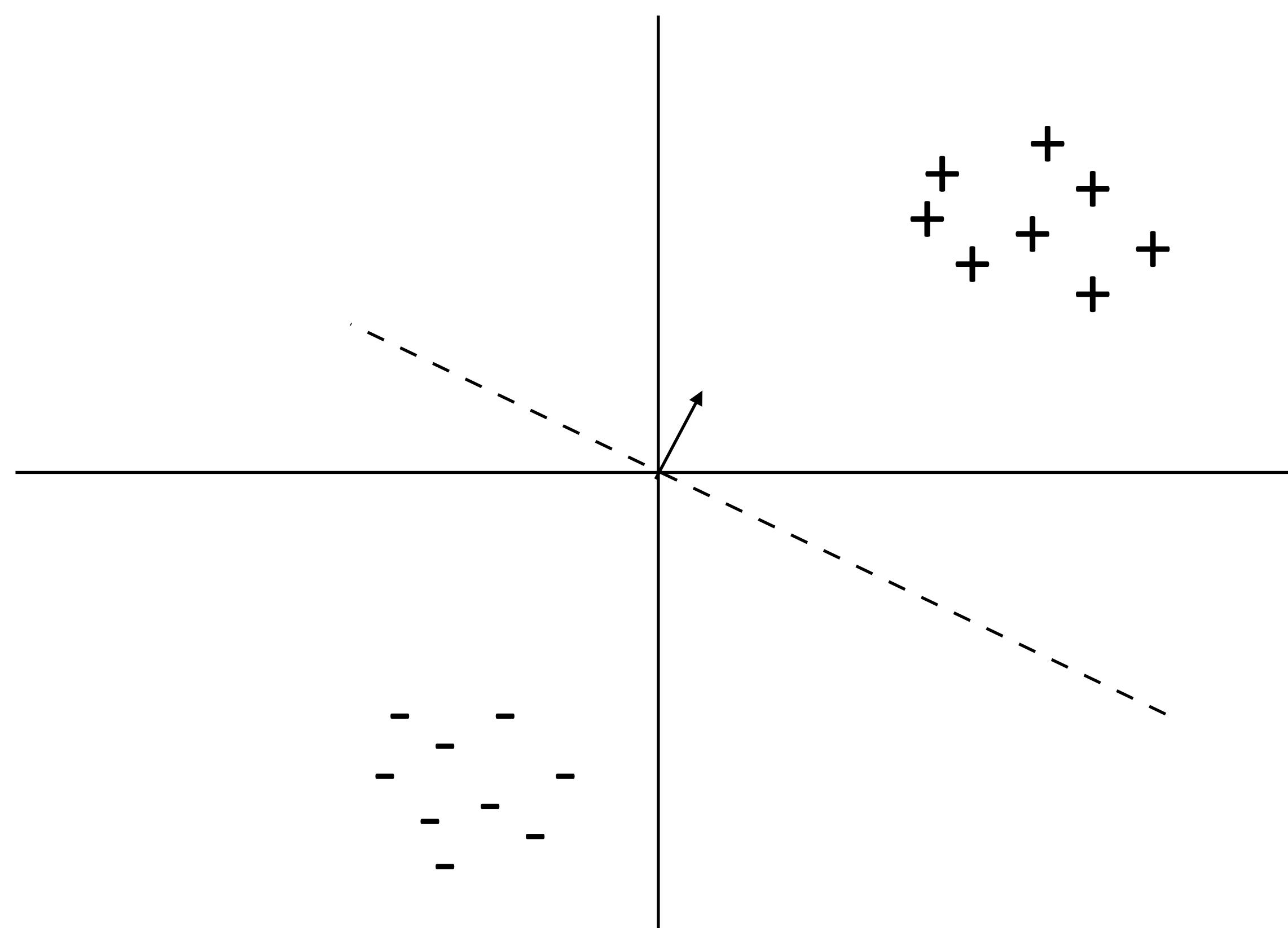
- ▶ Binary classification: one weight vector defines both classes
- ▶ Multiclass classification: different weights and/or features per class



# Multiclass Classification

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



# Multiclass Classification

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# Multiclass Classification

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- ▶ Formally: instead of two labels, we have an output space  $\gamma$  containing a number of possible classes
  - ▶ Same machinery that we'll use later for exponentially large output spaces, including sequences and trees

# Multiclass Classification

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- ▶ Formally: instead of two labels, we have an output space  $\mathcal{Y}$  containing a number of possible classes
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- ▶ Decision rule:  $\operatorname{argmax}_{y \in \mathcal{Y}} w^\top f(x, y)$

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  - ▶ Multiple feature vectors, one weight vector

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  - ▶ Multiple feature vectors, one weight vector
  - ▶ Can also have one weight vector per class:  $\operatorname{argmax}_{y \in \mathcal{Y}} w_y^\top f(x)$

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  - ▶ Multiple feature vectors, one weight vector
  - ▶ 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

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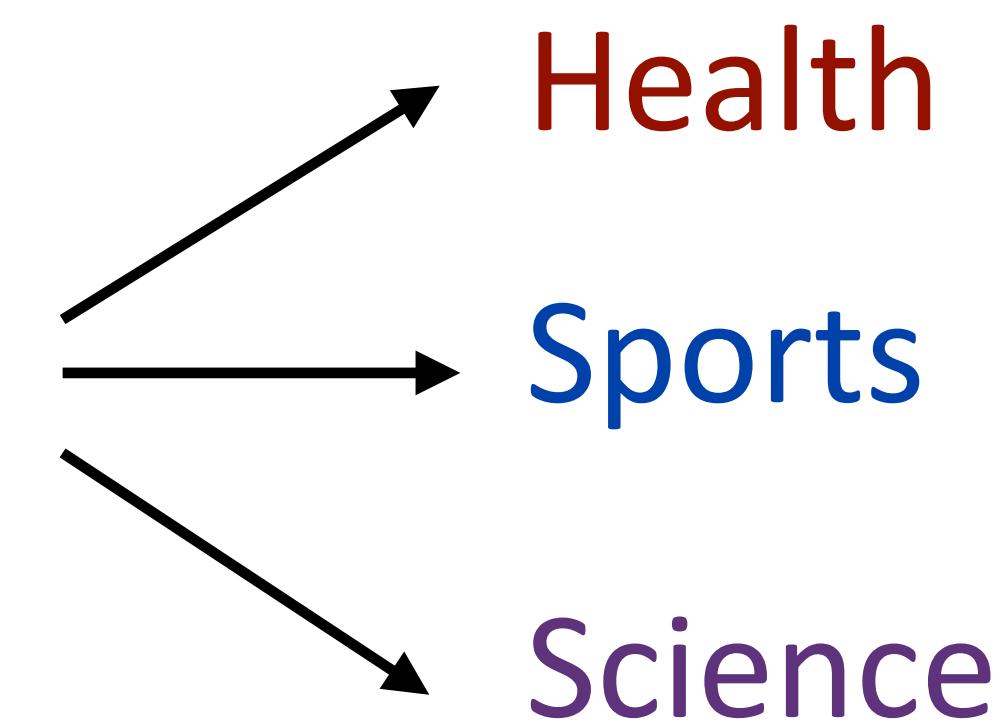
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# Block Feature Vectors

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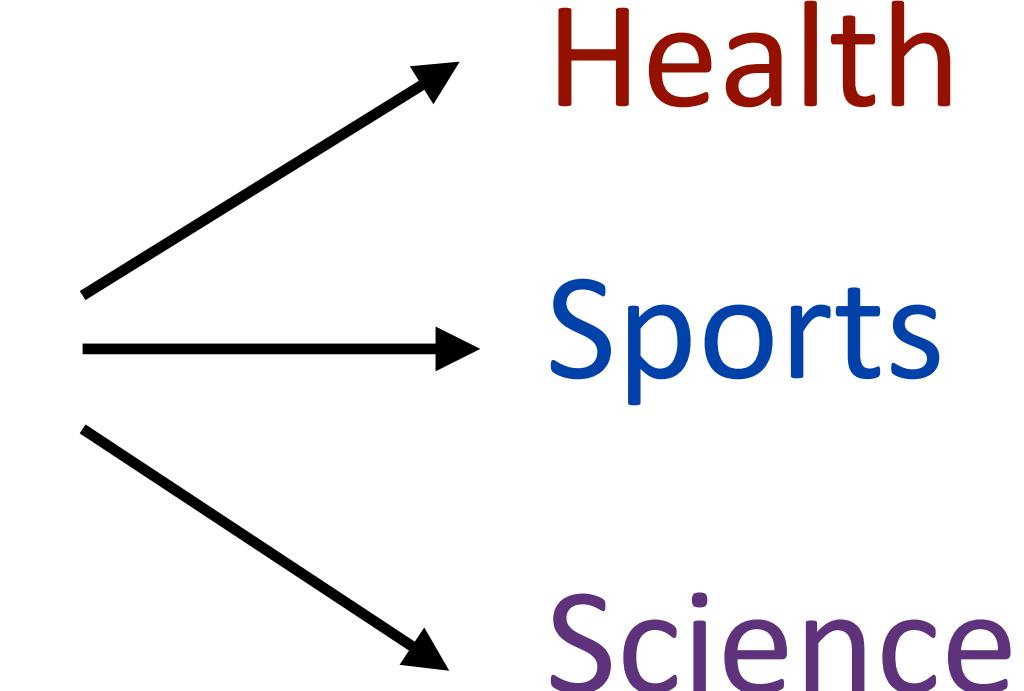
- ▶ Decision rule:  $\operatorname{argmax}_{y \in \mathcal{Y}} w^\top f(x, y)$

*too many drug trials, too few patients*



# Block Feature Vectors

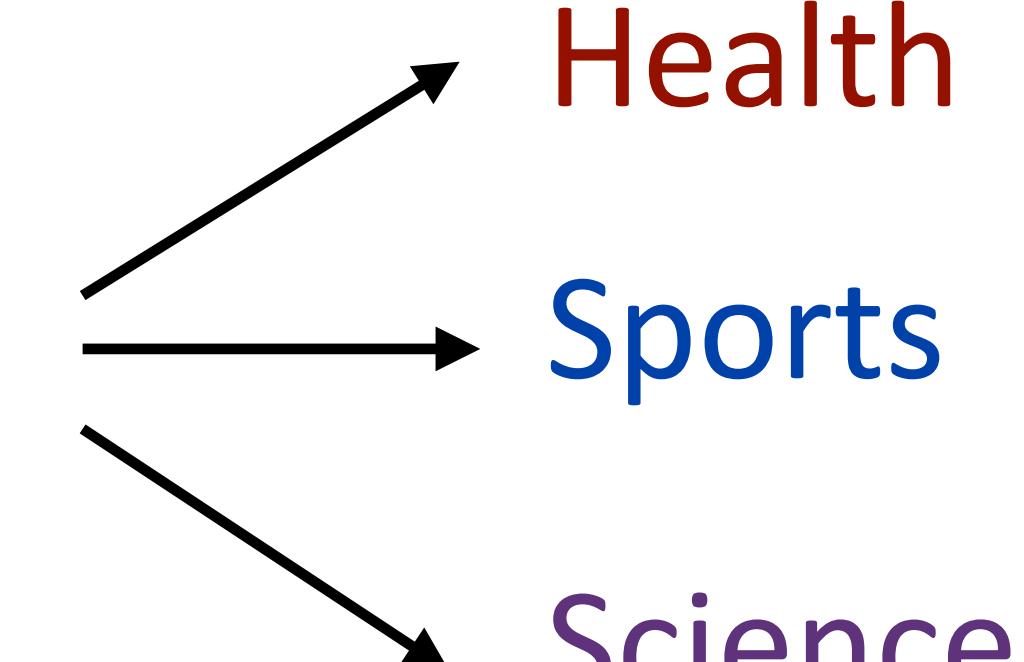
---

- ▶ Decision rule:  $\operatorname{argmax}_{y \in \mathcal{Y}} w^\top f(x, y)$   
*too many drug trials, too few patients*

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

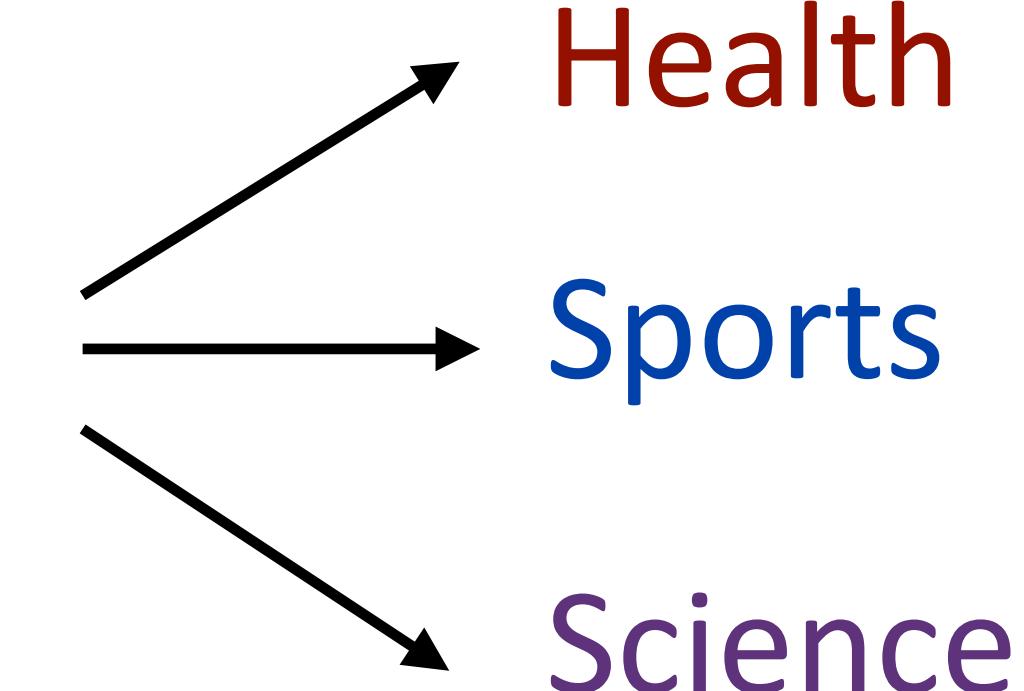
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- ▶ Decision rule:  $\operatorname{argmax}_{y \in \mathcal{Y}} w^\top f(x, y)$   
*too many drug trials, too few patients*
- ▶ Base feature function:  
 $f(x) = I[\text{contains } drug], I[\text{contains } patients], I[\text{contains } baseball]$

# Block Feature Vectors

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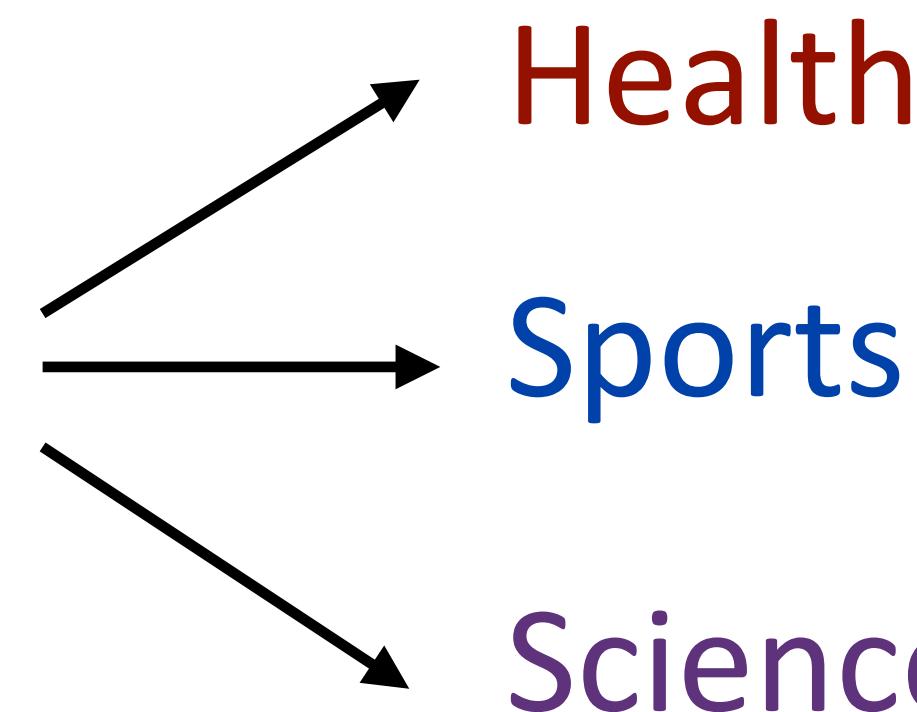
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*too many drug trials, too few patients*



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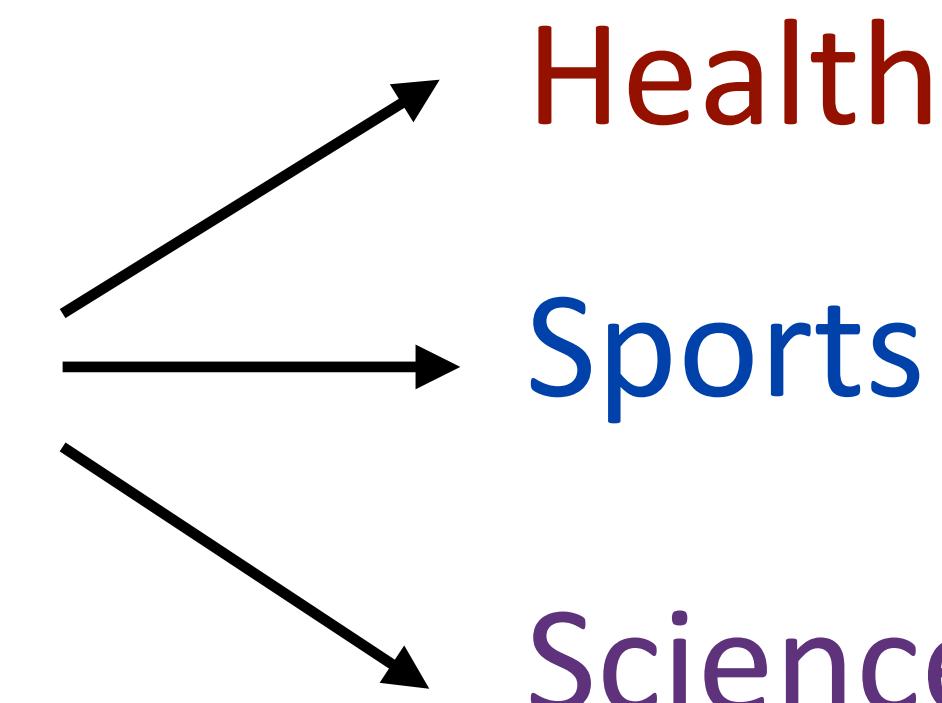
$$f(x) = I[\text{contains } drug], I[\text{contains } patients], I[\text{contains } baseball] = [1, 1, 0]$$

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

# Block Feature Vectors

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- ▶ Decision rule:  $\operatorname{argmax}_{y \in \mathcal{Y}} w^\top f(x, y)$   
*too many drug trials, too few patients*



- ▶ Base feature function:

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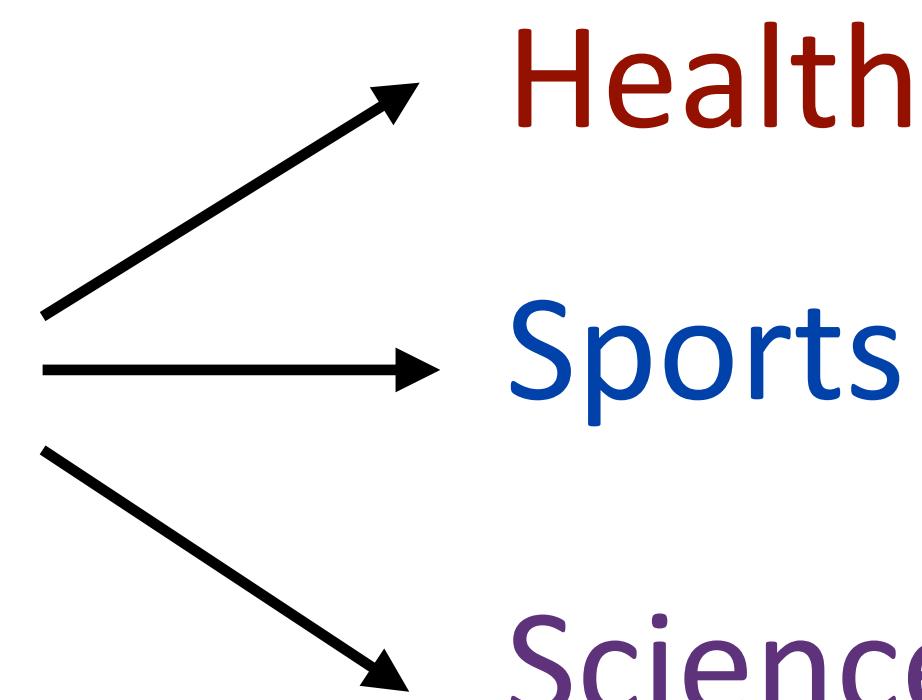
$$f(x, y = \text{Health}) = [1, 1, 0, 0, 0, 0, 0, 0, 0]$$

# Block Feature Vectors

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*too many drug trials, too few patients*



- Base feature function:

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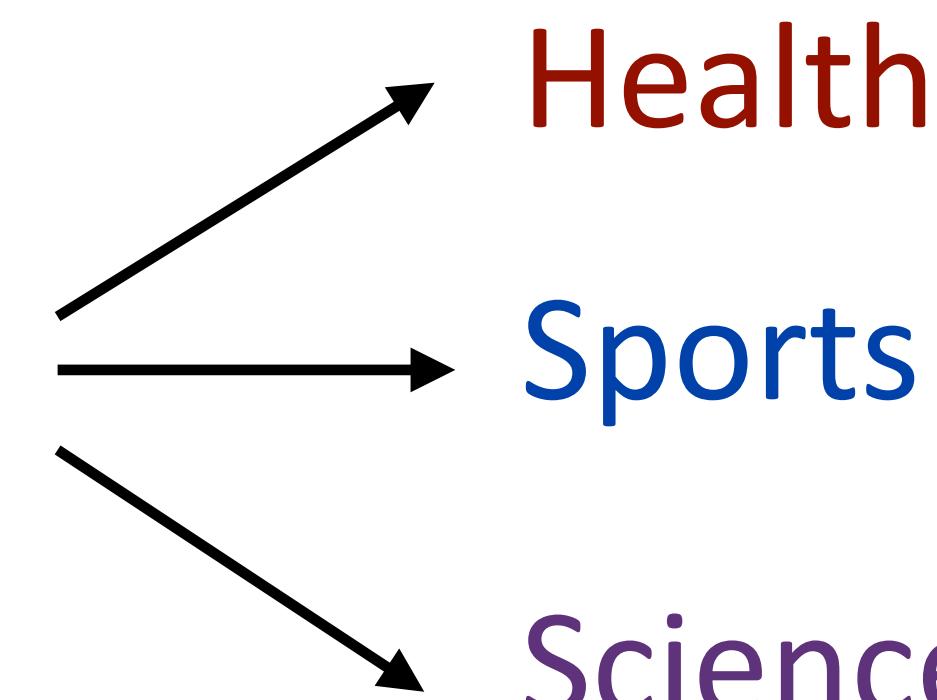
feature vector blocks for each label

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

# Block Feature Vectors

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

*too many drug trials, too few patients*



- Base feature function:

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feature vector blocks for each label

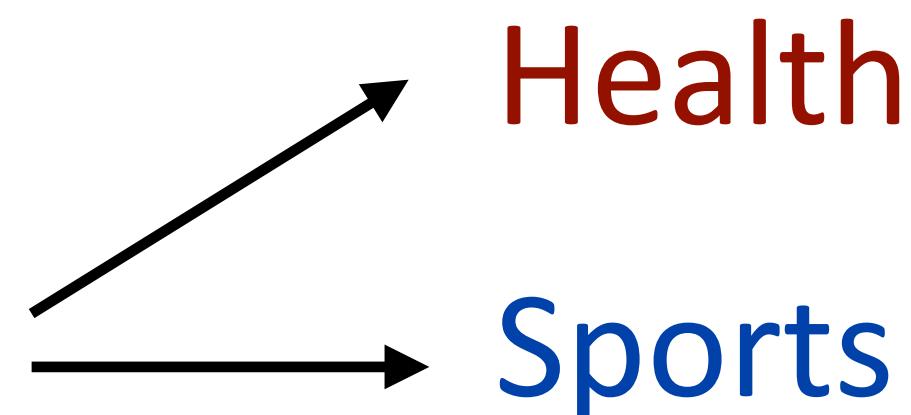
$$f(x, y = \text{Health}) = [1, 1, 0, 0, 0, 0]$$

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

# Block Feature Vectors

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

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- Base feature function:

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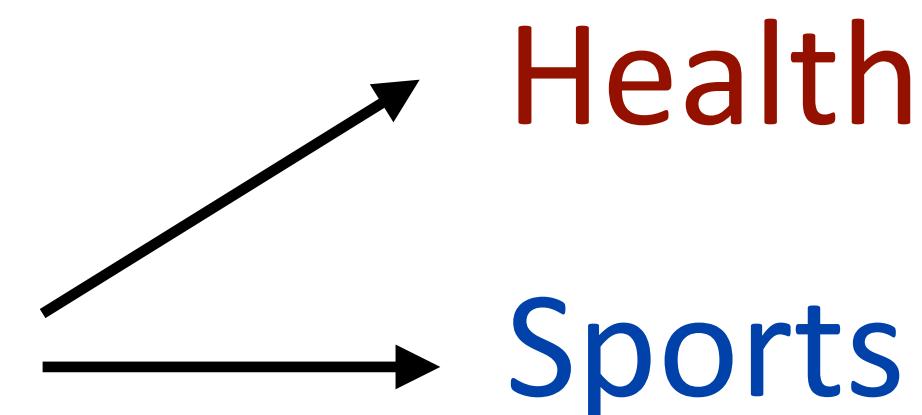
$$f(x, y = \text{Health}) = [1, 1, 0, 0, 0, 0] \quad I[\text{contains } drug \text{ & label} = \text{Health}]$$

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# Block Feature Vectors

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- Base feature function:

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feature vector blocks for each label

$$f(x, y = \text{Health}) = [1, 1, 0, 0, 0, 0] \quad I[\text{contains } drug \text{ & label} = \text{Health}]$$

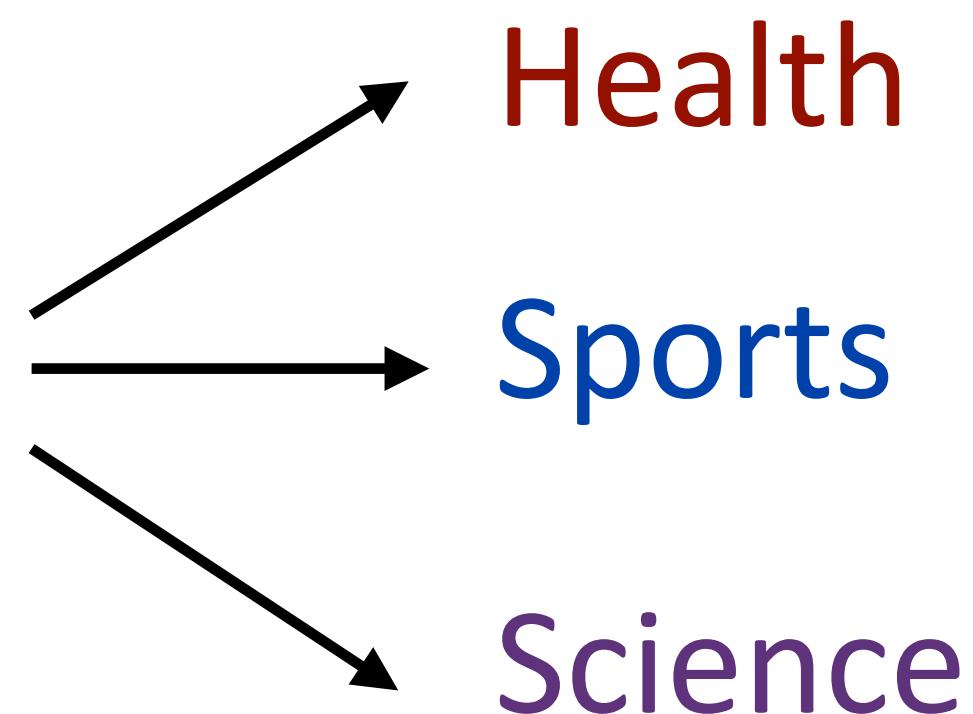
$$f(x, y = \text{Sports}) = [0, 0, 0, 1, 1, 0, 0, 0]$$

- Equivalent to having three weight vectors in this case

# Making Decisions

---

*too many drug trials, too few patients*



$$f(x) = \mathbf{I}[\text{contains } drug], \mathbf{I}[\text{contains } patients], \mathbf{I}[\text{contains } baseball]$$

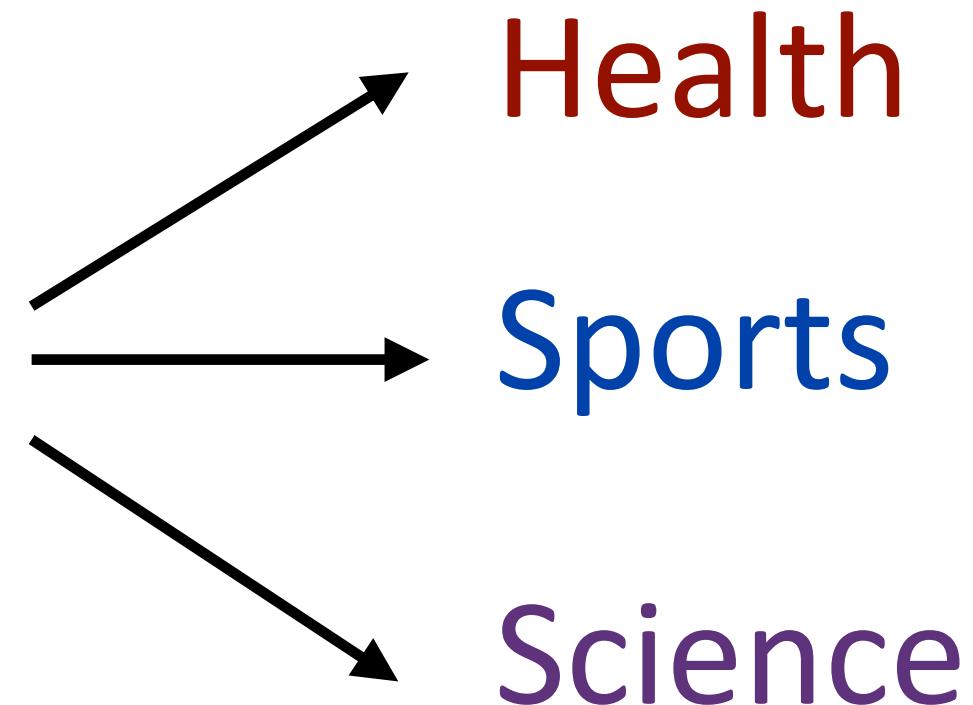
$$f(x, y = \text{Health}) = [1, 1, 0, 0, 0, 0, 0]$$

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

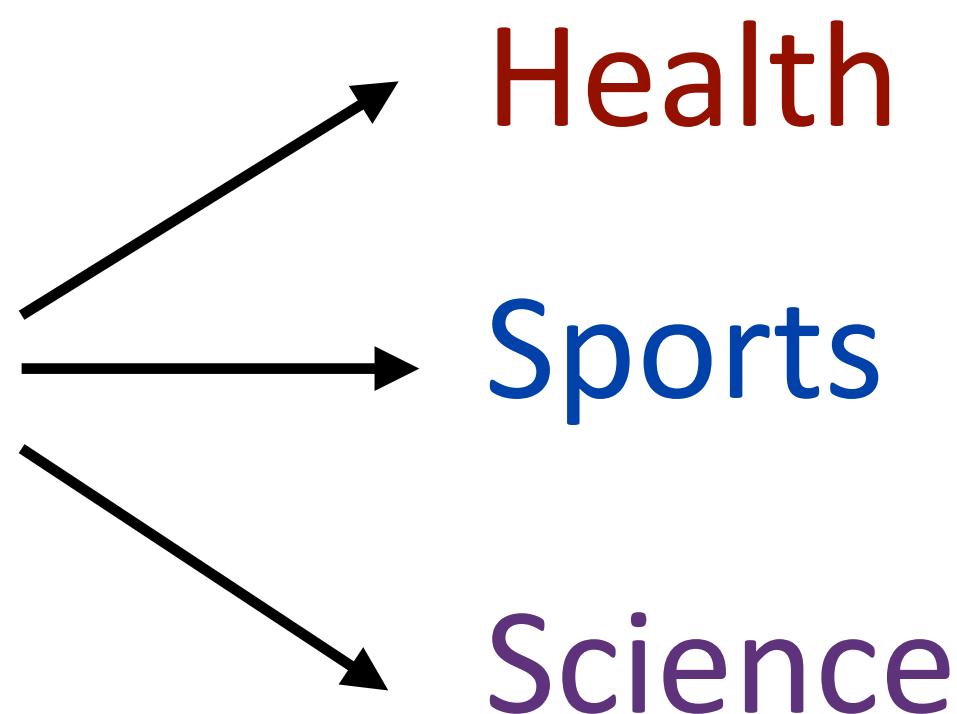
$$f(x, y = \text{Sports}) = [0, 0, 0, 1, 1, 0, 0, 0]$$

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

# Making Decisions

---

*too many drug trials, too few patients*



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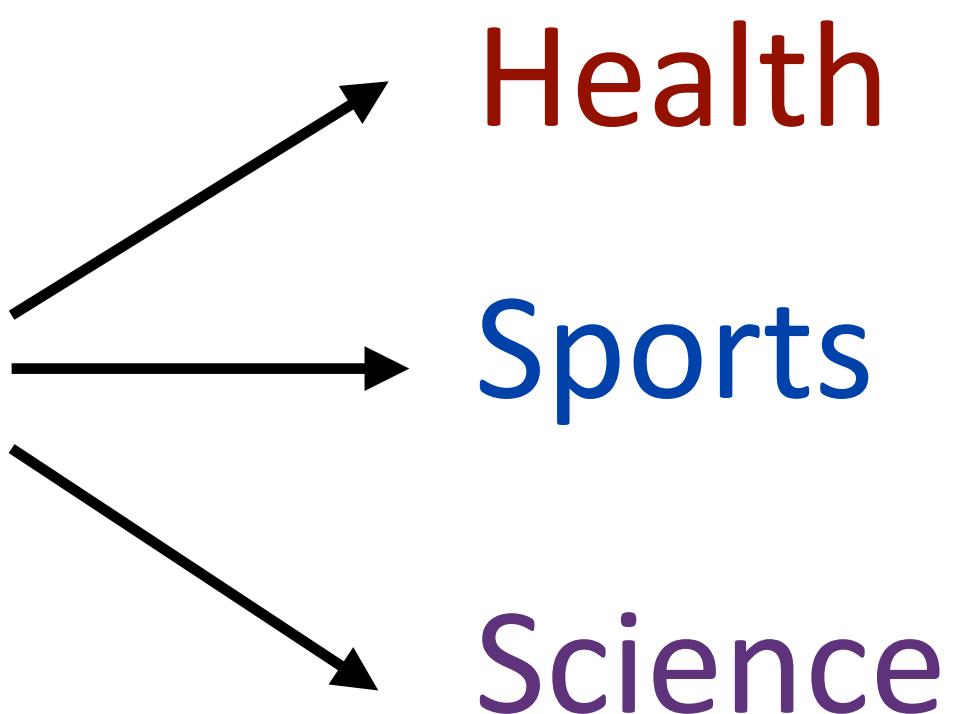
“word drug in Science article” = +1.1

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

# Making Decisions

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*too many drug trials, too few patients*



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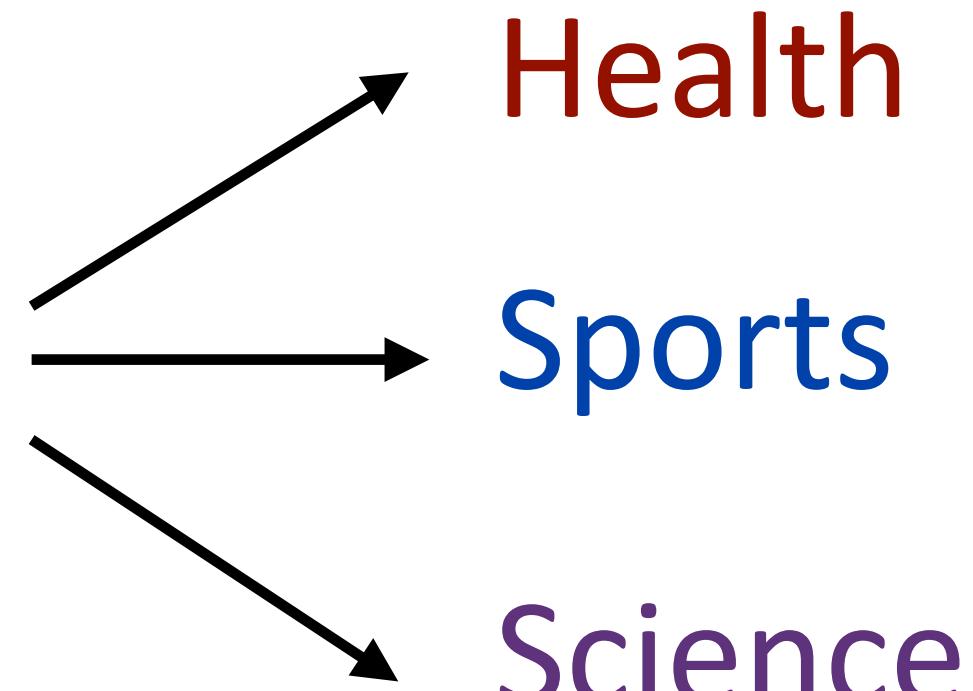
$$w = [+2.1, +2.3, -5, -2.1, -3.8, 0, +1.1, -1.7, -1.3]$$

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

# Making Decisions

---

*too many drug trials, too few patients*



Health  
Sports  
Science

$$f(x) = \mathbf{I}[\text{contains } drug], \mathbf{I}[\text{contains } patients], \mathbf{I}[\text{contains } baseball]$$

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

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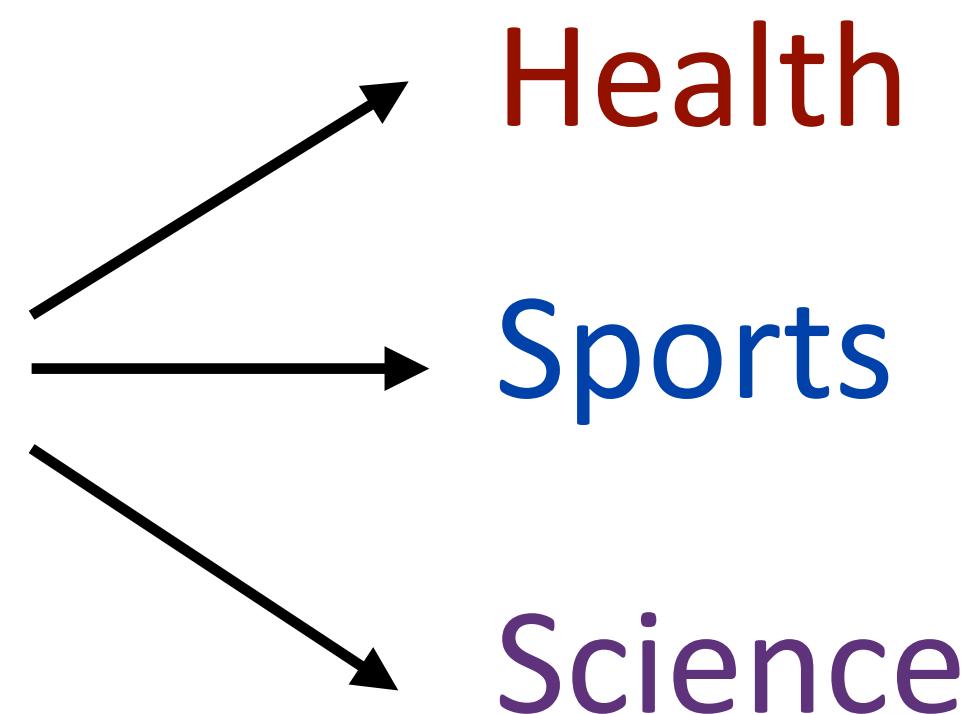
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$$w = [+2.1, +2.3, -5, -2.1, -3.8, 0, +1.1, -1.7, -1.3]$$

$$w^\top f(x, y) = \begin{array}{lll} \text{Health: +4.4} & \text{Sports: -5.9} & \text{Science: -0.6} \end{array}$$

# Making Decisions

*too many drug trials, too few patients*



$$f(x) = \mathbf{I}[\text{contains } drug], \mathbf{I}[\text{contains } patients], \mathbf{I}[\text{contains } baseball]$$

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$$w^\top f(x, y) = \begin{array}{lll} \text{Health: } +4.4 & \text{Sports: } -5.9 & \text{Science: } -0.6 \end{array}$$

↑ argmax

# Another example: POS tagging

---

*blocks*

# Another example: POS tagging

---

*the router blocks the packets*

# Another example: POS tagging

---

*the router blocks the packets*

NNS  
VBZ  
NN  
DT  
...

# Another example: POS tagging

---

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

*the router blocks the packets*

NNS  
VBZ  
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DT  
...

# Another example: POS tagging

---

- ▶ Classify *blocks* as one of 36 POS tags
- ▶ Example x: sentence with a word (in this case, *blocks*) highlighted

*the router blocks the packets*

NNS  
VBZ  
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...

# Another example: POS tagging

---

- ▶ Classify *blocks* as one of 36 POS tags
- ▶ Example x: sentence with a word (in this case, *blocks*) highlighted
- ▶ Extract features with respect to this word:

*the router* **'blocks'** *the packets*

NNS  
VBZ  
NN  
DT  
...

# Another example: POS tagging

---

- ▶ Classify *blocks* as one of 36 POS tags
- ▶ Example  $x$ : sentence with a word (in this case, *blocks*) highlighted
- ▶ Extract features with respect to this word:

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

*the router* *'blocks'* *the packets*

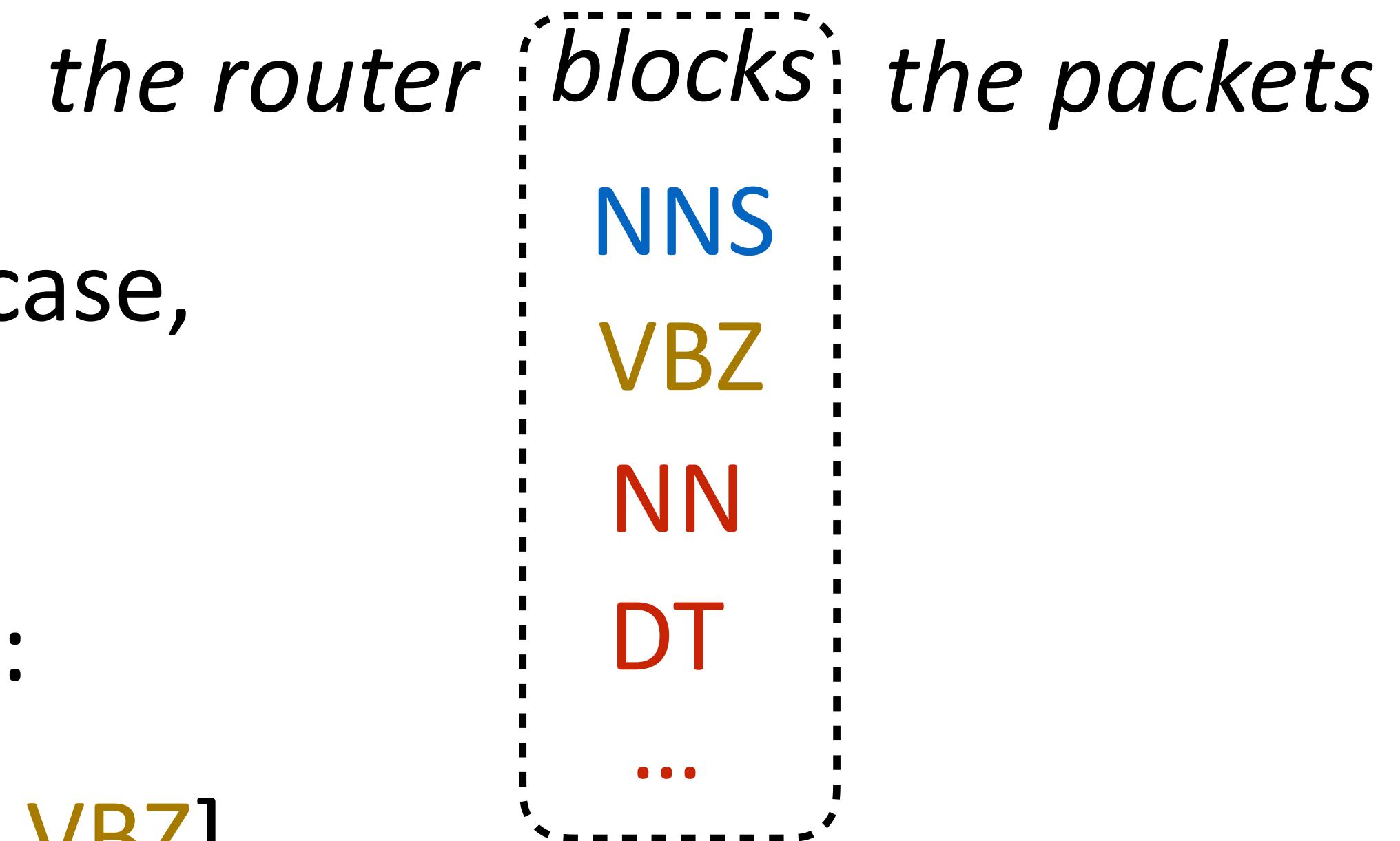
NNS
VBZ
NN
DT
...

# Another example: POS tagging

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

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

- ▶ Extract features with respect to this word:

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


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:

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

# 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:

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

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

# Multiclass Logistic Regression

---

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# Multiclass Logistic Regression

---

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

Softmax  
function

↑  
sum over output  
space to normalize

# Multiclass Logistic Regression

---

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Softmax  
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sum over output  
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Why? Interpret raw classifier scores as **probabilities**

# Multiclass Logistic Regression

---

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Softmax  
function

sum over output  
space to normalize

*too many drug trials,  
too few patients*

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

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Softmax  
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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

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

# Multiclass Logistic Regression

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

Softmax  
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probabilities  
must be  $\geq 0$

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

$\exp$

6.05  
22.2  
0.55  
unnormalized  
probabilities

# 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

*too many drug trials,  
too few patients*

**Health: +2.2**

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

probabilities  
must be  $\geq 0$

6.05  
22.2  
0.55  
unnormalized  
probabilities

Softmax  
function

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

probabilities  
must sum to 1

0.21  
0.77  
0.02  
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

*too many drug trials,  
too few patients*

**Health: +2.2**

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

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

Softmax  
function

probabilities  
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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  
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**Health: +2.2**

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

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

Softmax  
function

probabilities  
must be  $\geq 0$

probabilities  
must sum to 1

unnormalized  
probabilities

probabilities

$\exp$

normalize

compare

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

correct (gold)  
probabilities

# Multiclass Logistic Regression

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

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

probabilities  
must be  $\geq 0$

6.05  
22.2  
0.55

unnormalized  
probabilities

probabilities  
must sum to 1

0.21  
0.77  
0.02

probabilities

1.00  
0.00  
0.00  
correct (gold)  
probabilities

$\exp$

normalize

$\log(0.21) = -1.56$

compare

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

# 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

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

# 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

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

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

# 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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gold feature value

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

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

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

# Training

---

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

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

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

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

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

gradient:

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

# 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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$$f(x, y = \text{Health}) = [1, 1, 0, 0, 0, 0, 0, 0] \quad P_w(y|x) = [0.21, 0.77, 0.02]$$

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

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

# 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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$$f(x, y = \text{Health}) = [1, 1, 0, 0, 0, 0, 0, 0] \quad P_w(y|x) = [0.21, 0.77, 0.02]$$

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$$\begin{aligned} \text{gradient: } & [1, 1, 0, 0, 0, 0, 0, 0] - 0.21 [1, 1, 0, 0, 0, 0, 0, 0] \\ & - 0.77 [0, 0, 0, 1, 1, 0, 0, 0] - 0.02 [0, 0, 0, 0, 0, 0, 1, 1, 0] \end{aligned}$$

# 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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$$f(x, y = \text{Health}) = [1, 1, 0, 0, 0, 0, 0, 0] \quad P_w(y|x) = [0.21, 0.77, 0.02]$$

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$$\begin{aligned} \text{gradient: } & [1, 1, 0, 0, 0, 0, 0, 0] - 0.21 [1, 1, 0, 0, 0, 0, 0, 0] \\ & - 0.77 [0, 0, 0, 1, 1, 0, 0, 0] - 0.02 [0, 0, 0, 0, 0, 0, 1, 1, 0] \\ & = [0.79, 0.79, 0, -0.77, -0.77, 0, -0.02, -0.02, 0] \end{aligned}$$

# 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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$$f(x, y = \text{Health}) = [1, 1, 0, 0, 0, 0, 0, 0] \quad P_w(y|x) = [0.21, 0.77, 0.02]$$

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update  $w^\top$ :

# Training

---

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

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

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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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$$f(x, y = \text{Health}) = [1, 1, 0, 0, 0, 0, 0, 0] \quad P_w(y|x) = [0.21, 0.77, 0.02]$$

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

$$\begin{aligned} \text{gradient: } & [1, 1, 0, 0, 0, 0, 0, 0] - 0.21 [1, 1, 0, 0, 0, 0, 0, 0] \\ & - 0.77 [0, 0, 0, 1, 1, 0, 0, 0] - 0.02 [0, 0, 0, 0, 0, 0, 1, 1] \\ & = [0.79, 0.79, 0, -0.77, -0.77, 0, -0.02, -0.02, 0] \end{aligned}$$

update  $w^\top$ :

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

# 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*  $y^* = \text{Health}$

$$f(x, y = \text{Health}) = [1, 1, 0, 0, 0, 0, 0, 0] \quad P_w(y|x) = [0.21, 0.77, 0.02]$$

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

$$\begin{aligned} \text{gradient: } & [1, 1, 0, 0, 0, 0, 0, 0] - 0.21 [1, 1, 0, 0, 0, 0, 0, 0] \\ & - 0.77 [0, 0, 0, 1, 1, 0, 0, 0] - 0.02 [0, 0, 0, 0, 0, 0, 1, 1, 0] \\ & = [0.79, 0.79, 0, -0.77, -0.77, 0, -0.02, -0.02, 0] \end{aligned}$$

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

---

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

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

$$f(x, y = \text{Health}) = [1, 1, 0, 0, 0, 0, 0, 0] \quad P_w(y|x) = [0.21, 0.77, 0.02]$$

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

$$\begin{aligned} \text{gradient: } & [1, 1, 0, 0, 0, 0, 0, 0] - 0.21 [1, 1, 0, 0, 0, 0, 0, 0] \\ & - 0.77 [0, 0, 0, 1, 1, 0, 0, 0] - 0.02 [0, 0, 0, 0, 0, 0, 1, 1, 0] \\ & = [0.79, 0.79, 0, -0.77, -0.77, 0, -0.02, -0.02, 0] \end{aligned}$$

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

---

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

# Logistic Regression: Summary

---

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

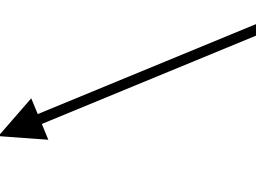
---

# 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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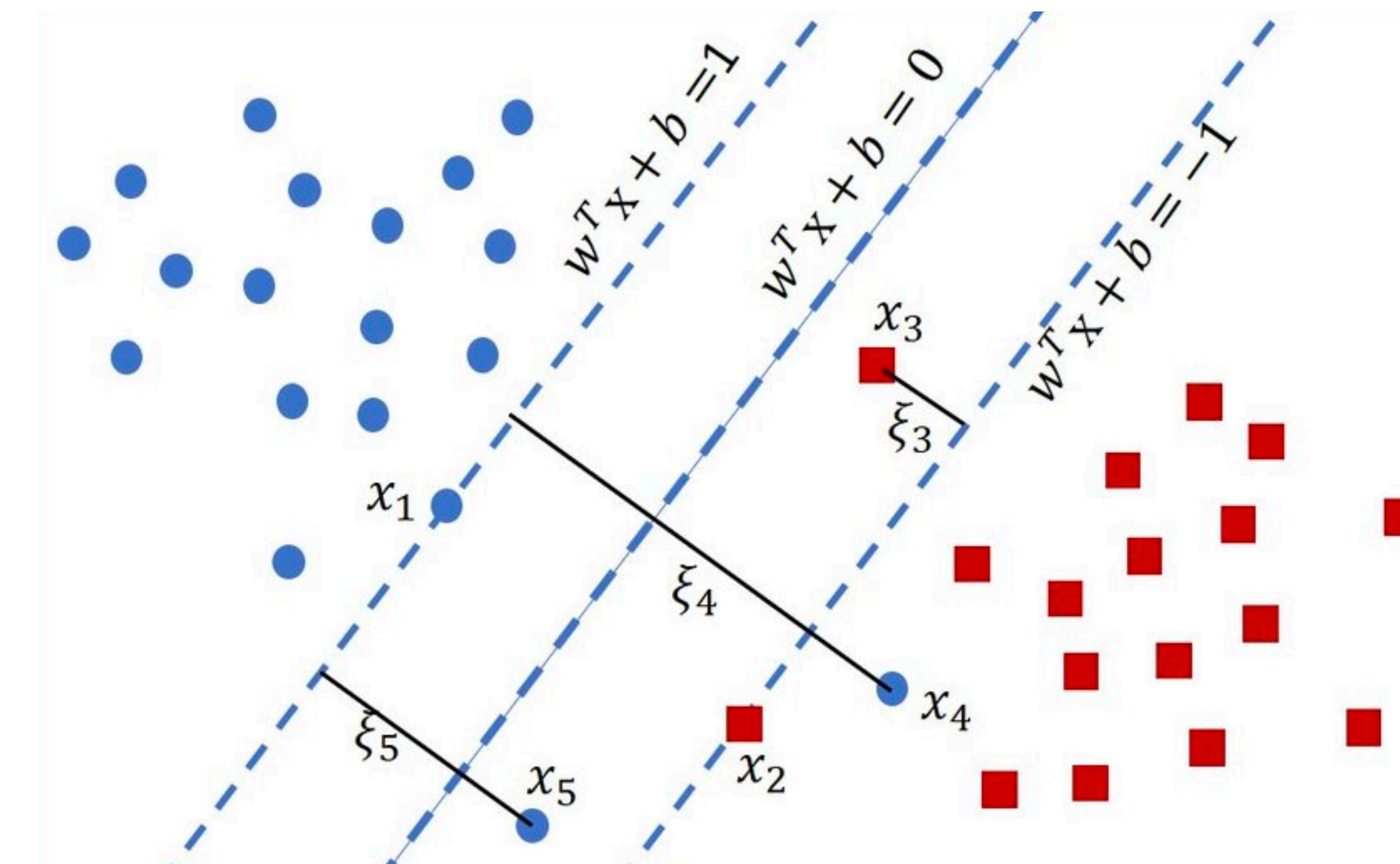


Image credit: Lang Van Tran

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

# Training (loss-augmented)

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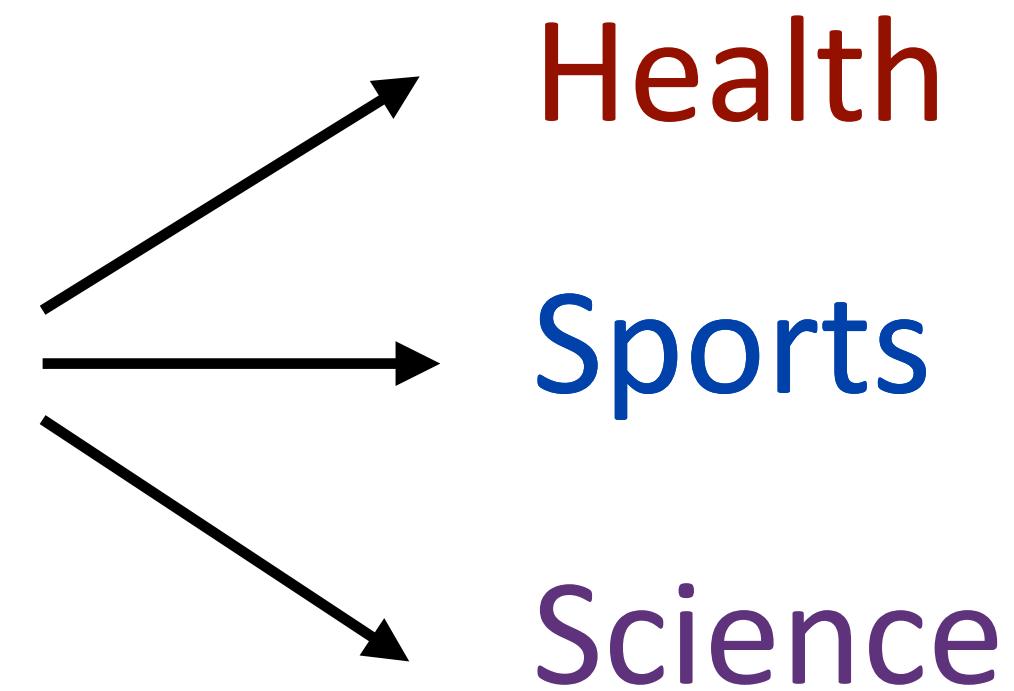
- ▶ Are all decisions equally costly?

# Training (loss-augmented)

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- ▶ Are all decisions equally costly?

*too many drug trials, too few patients*



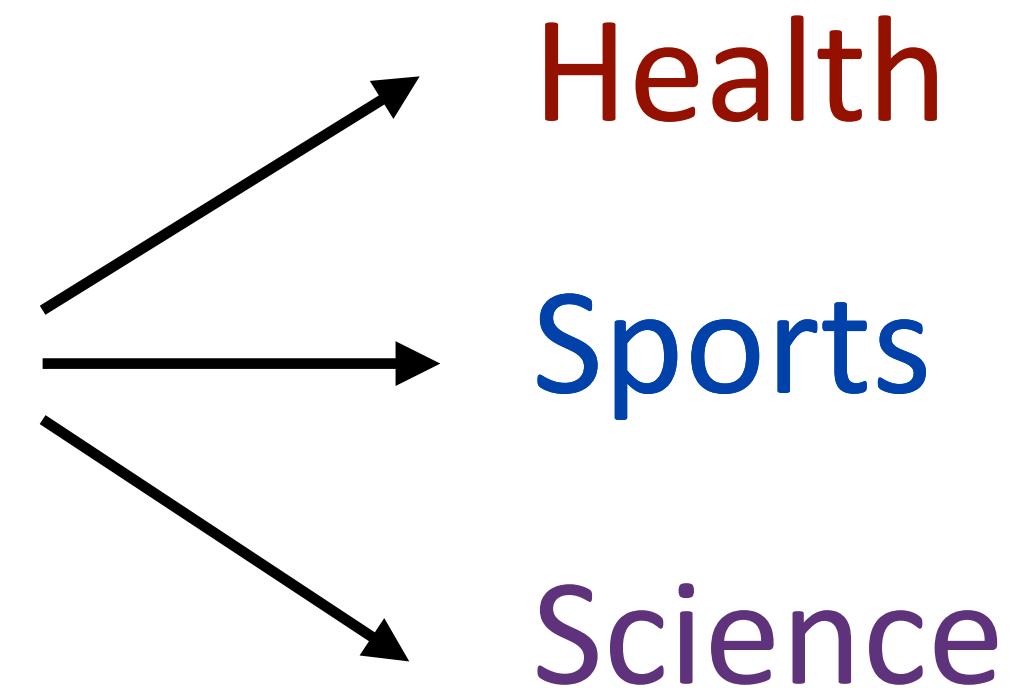
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Predicted **Sports**: bad error

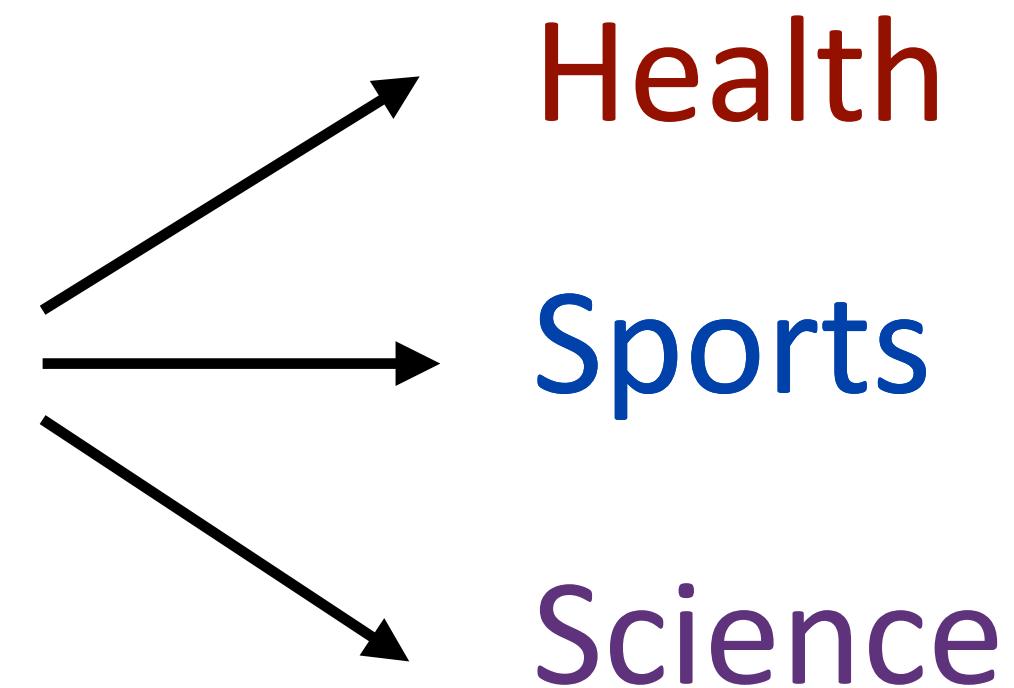


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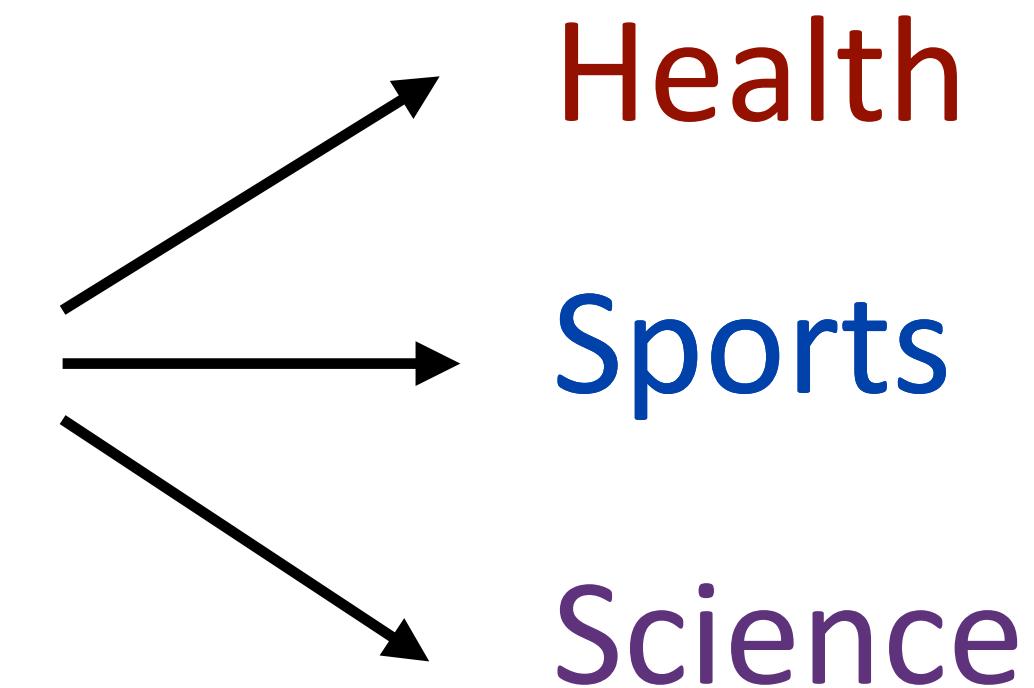
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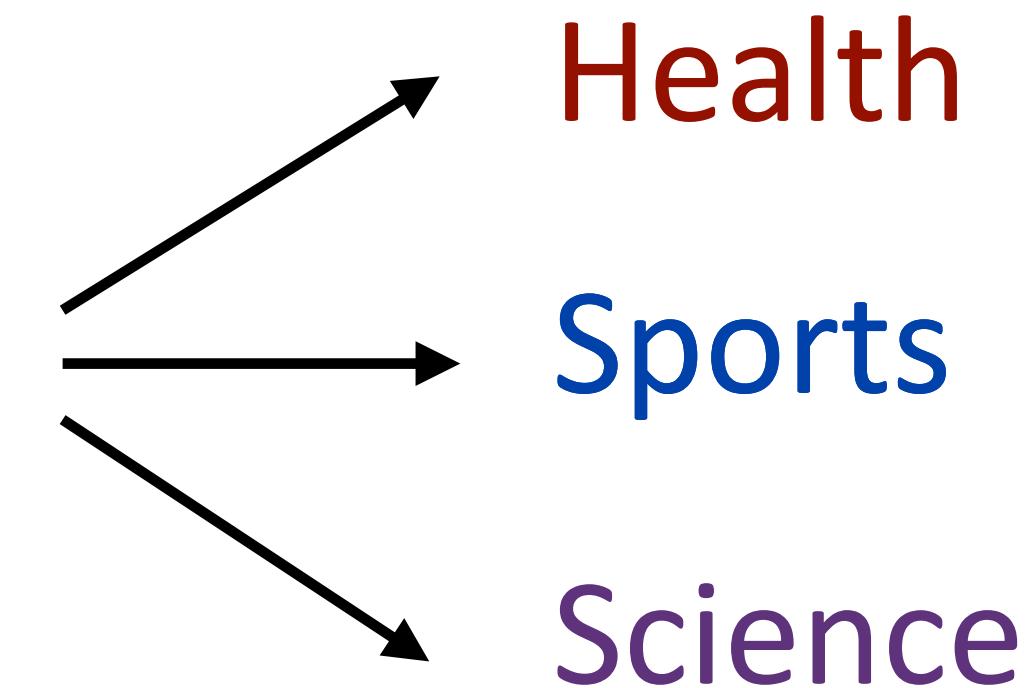
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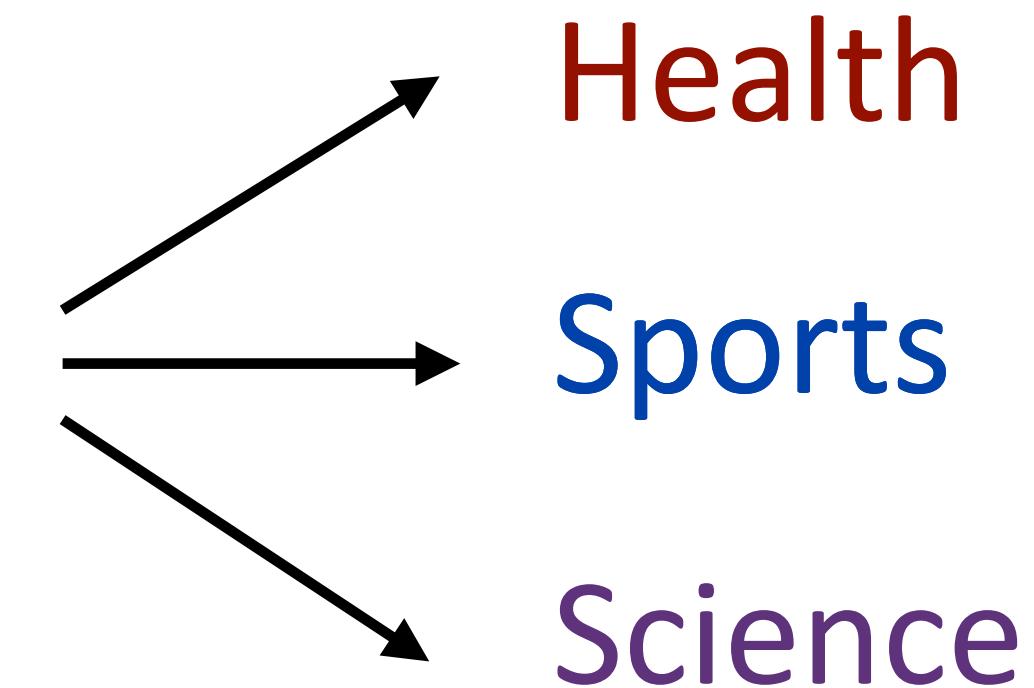
$$\ell(\text{Sports}, \text{Health}) = 3$$

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

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

# Multiclass SVM

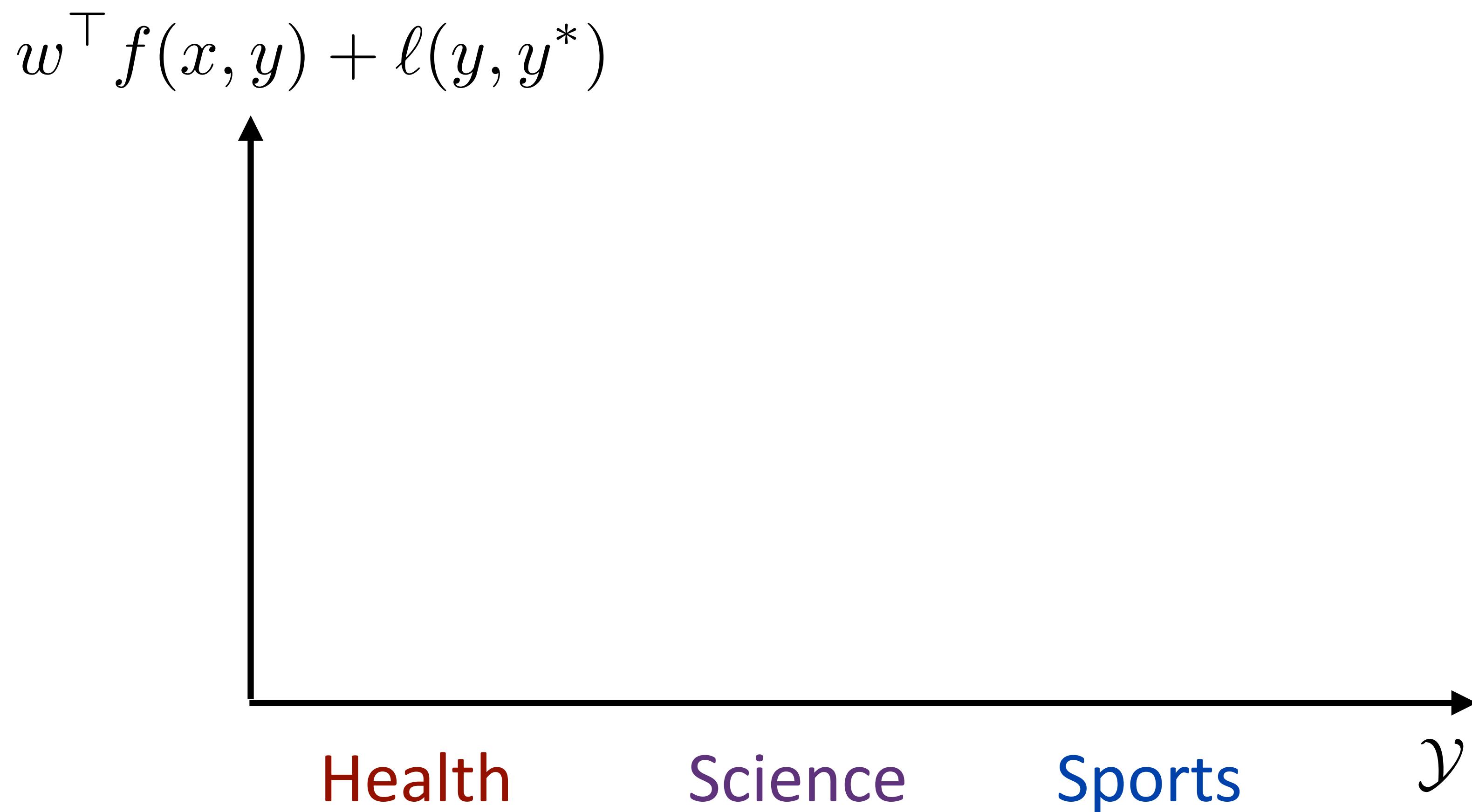
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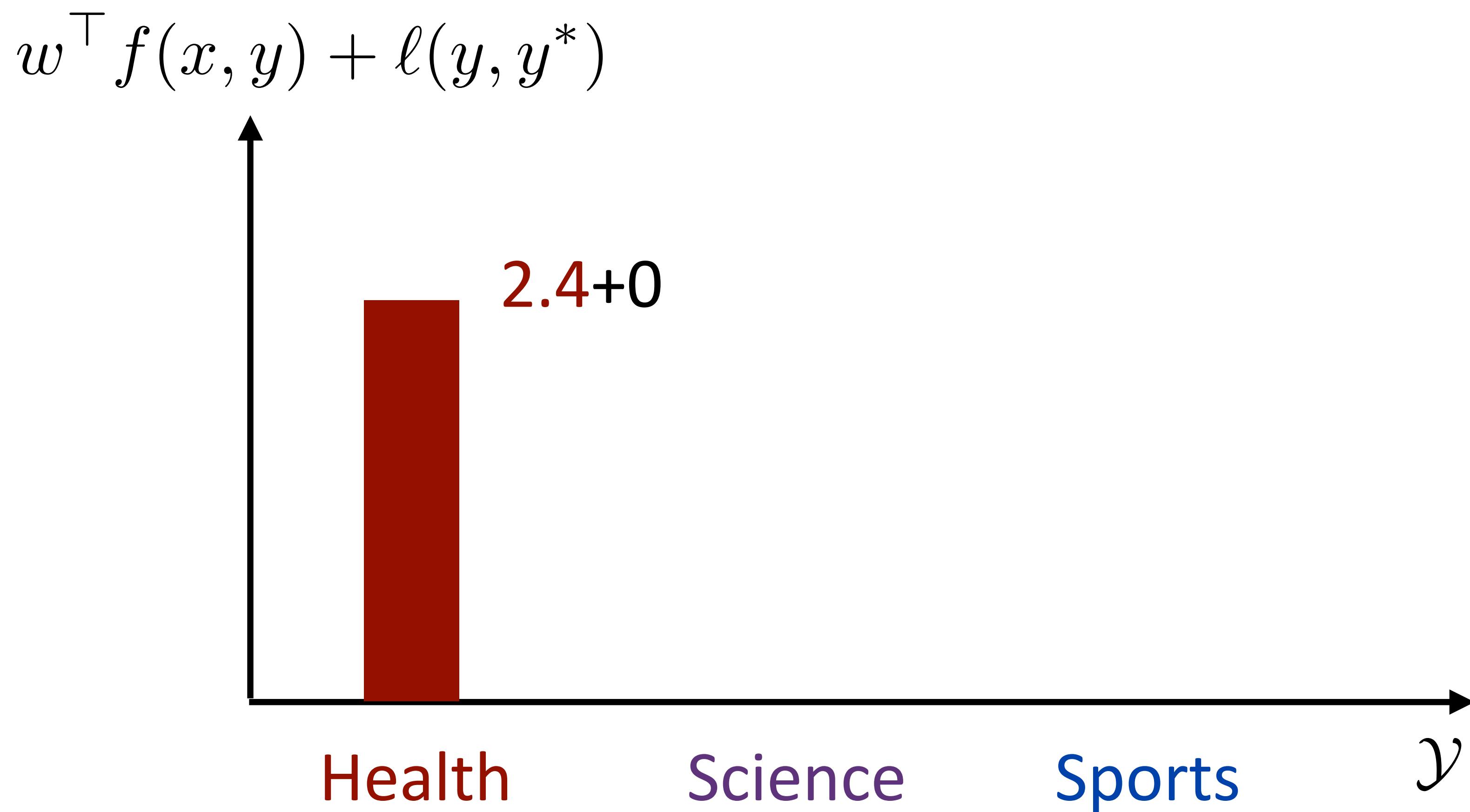
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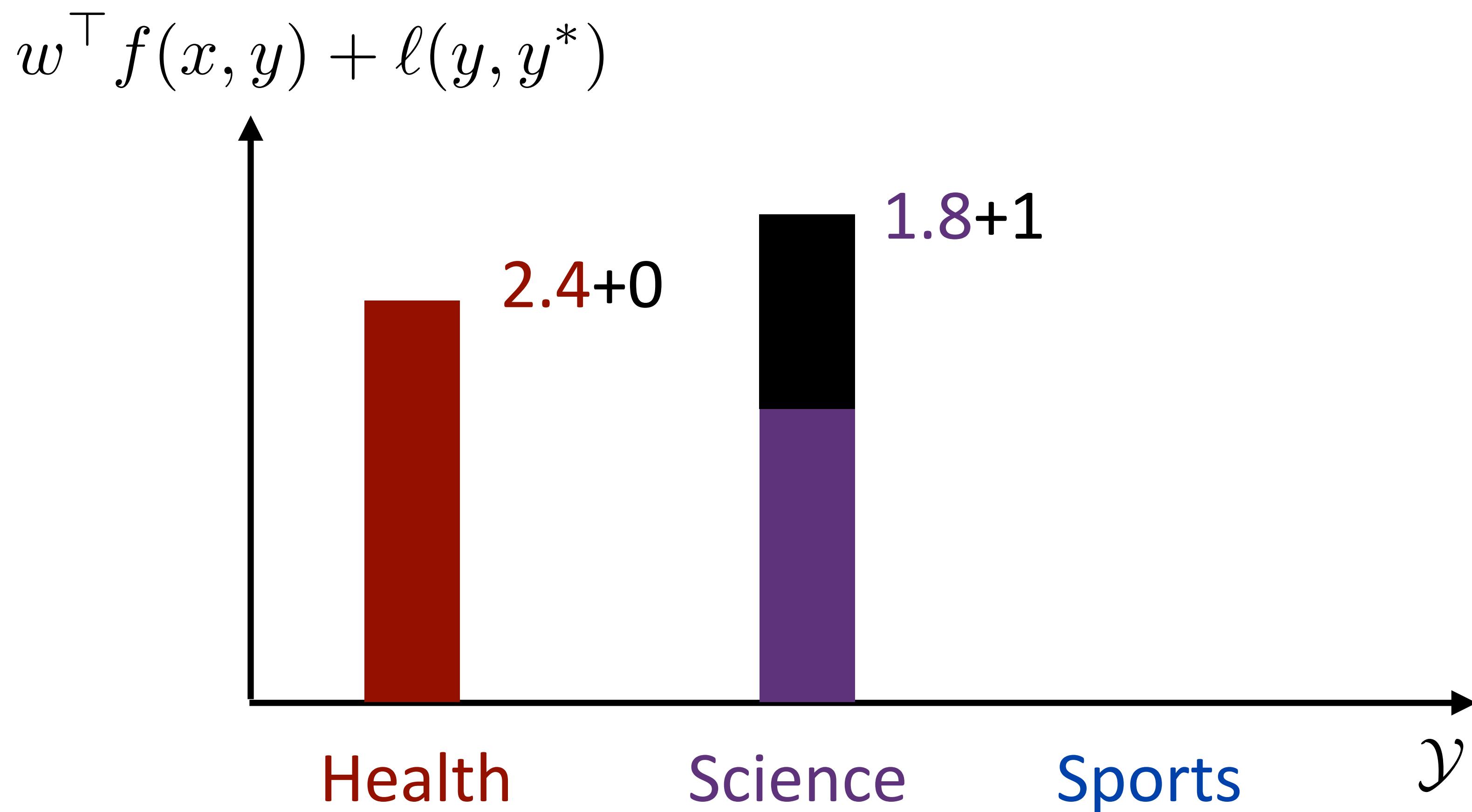
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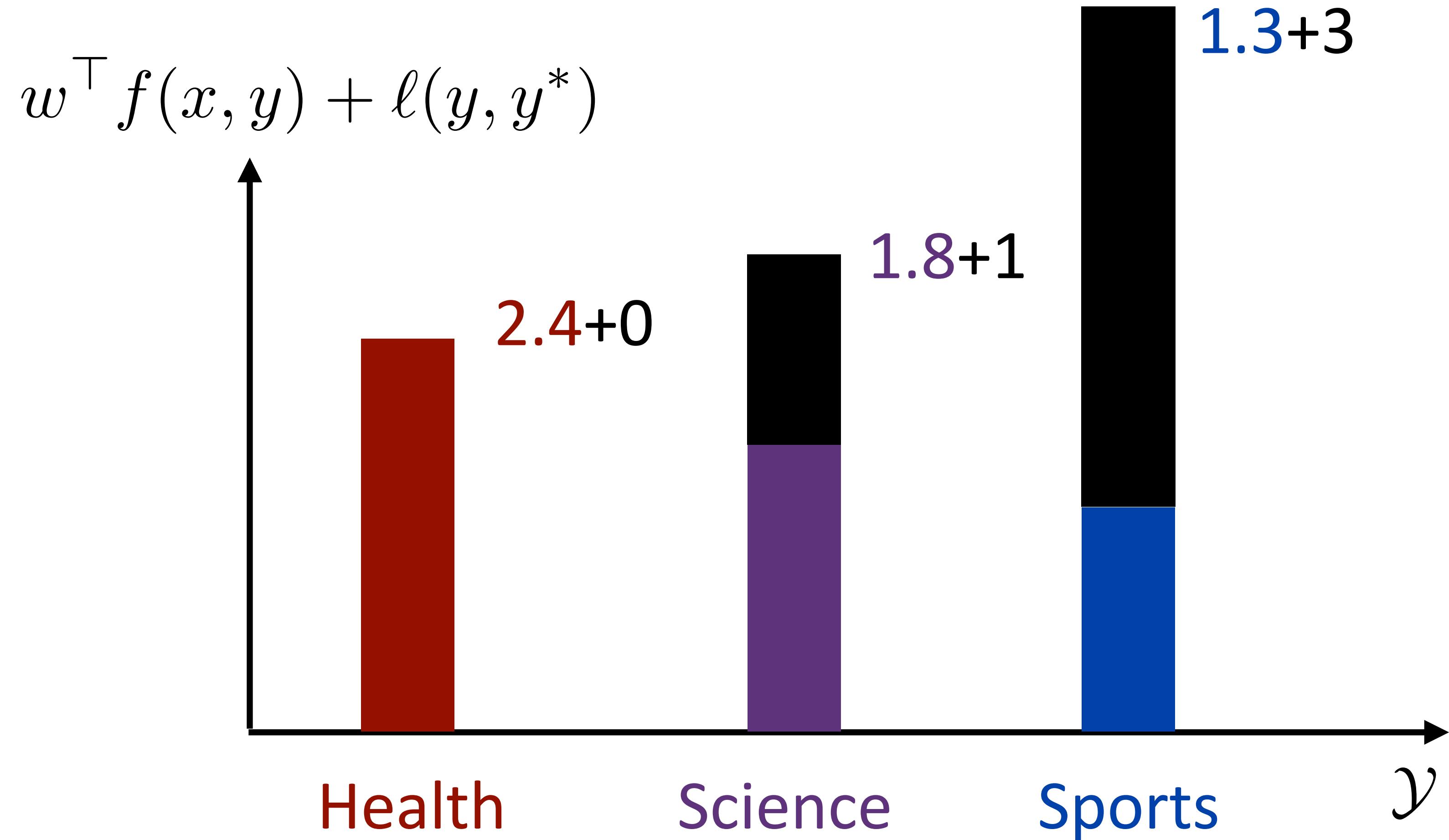
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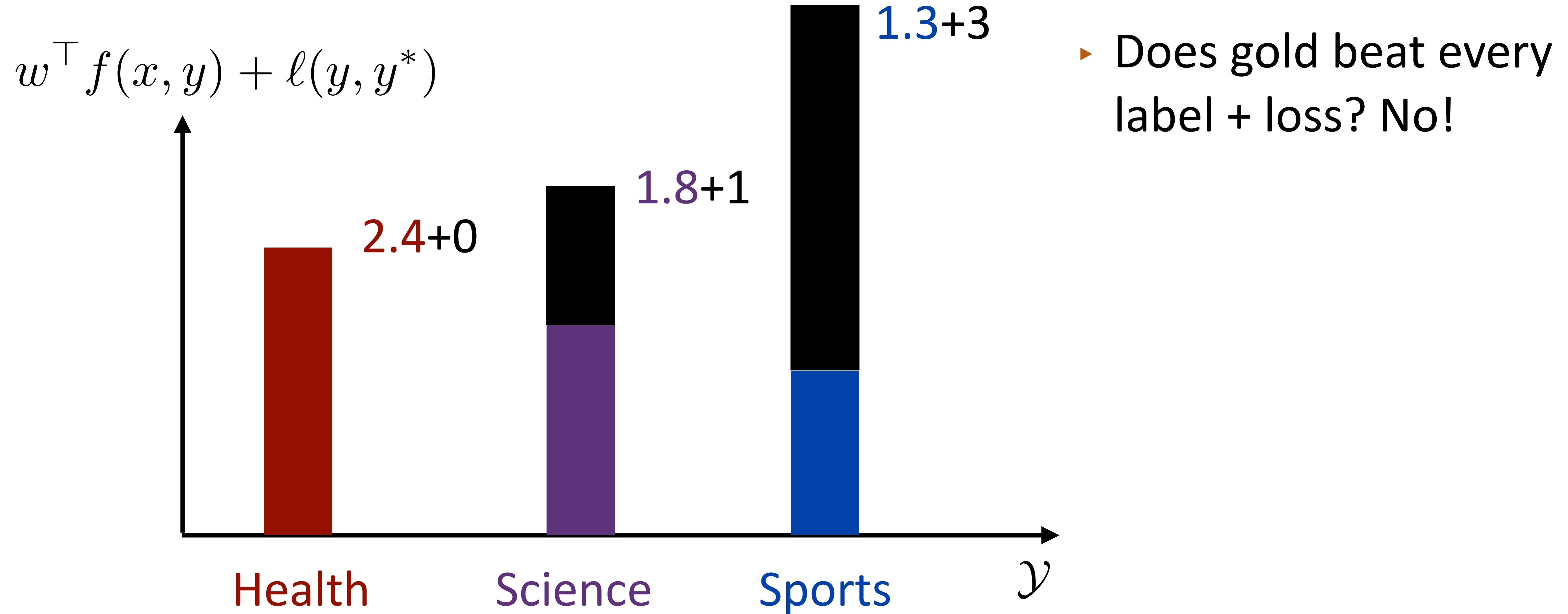
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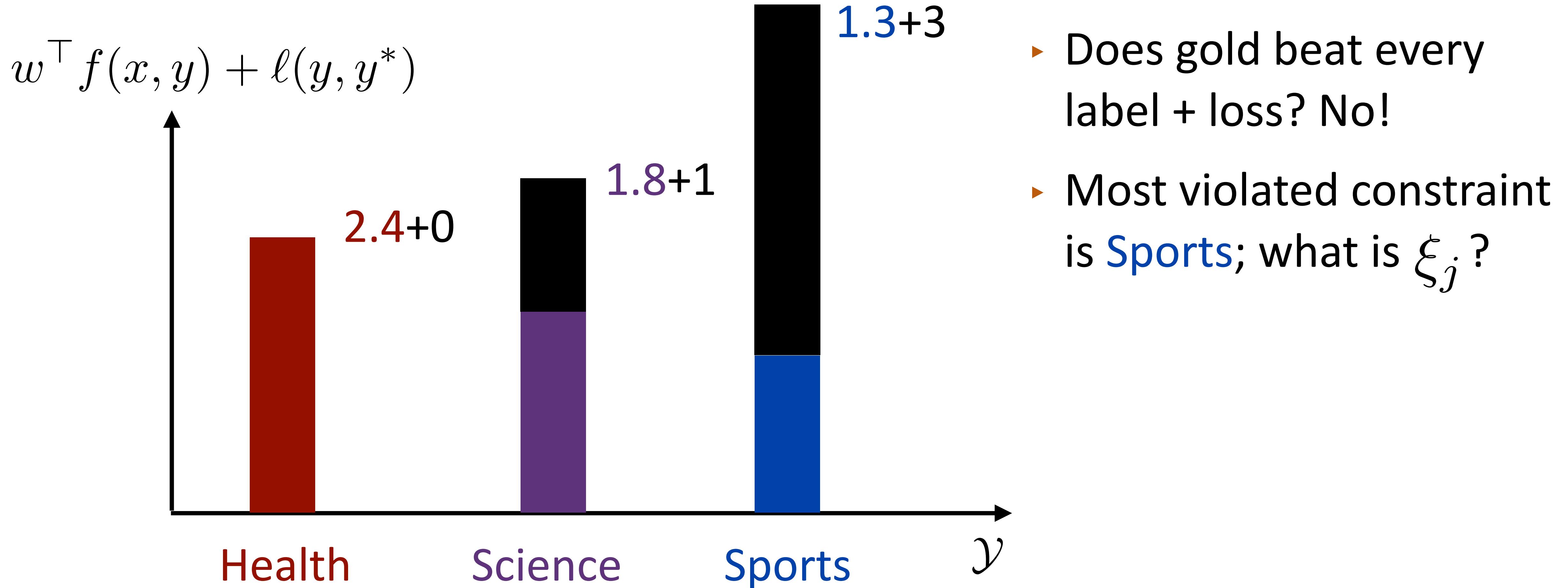
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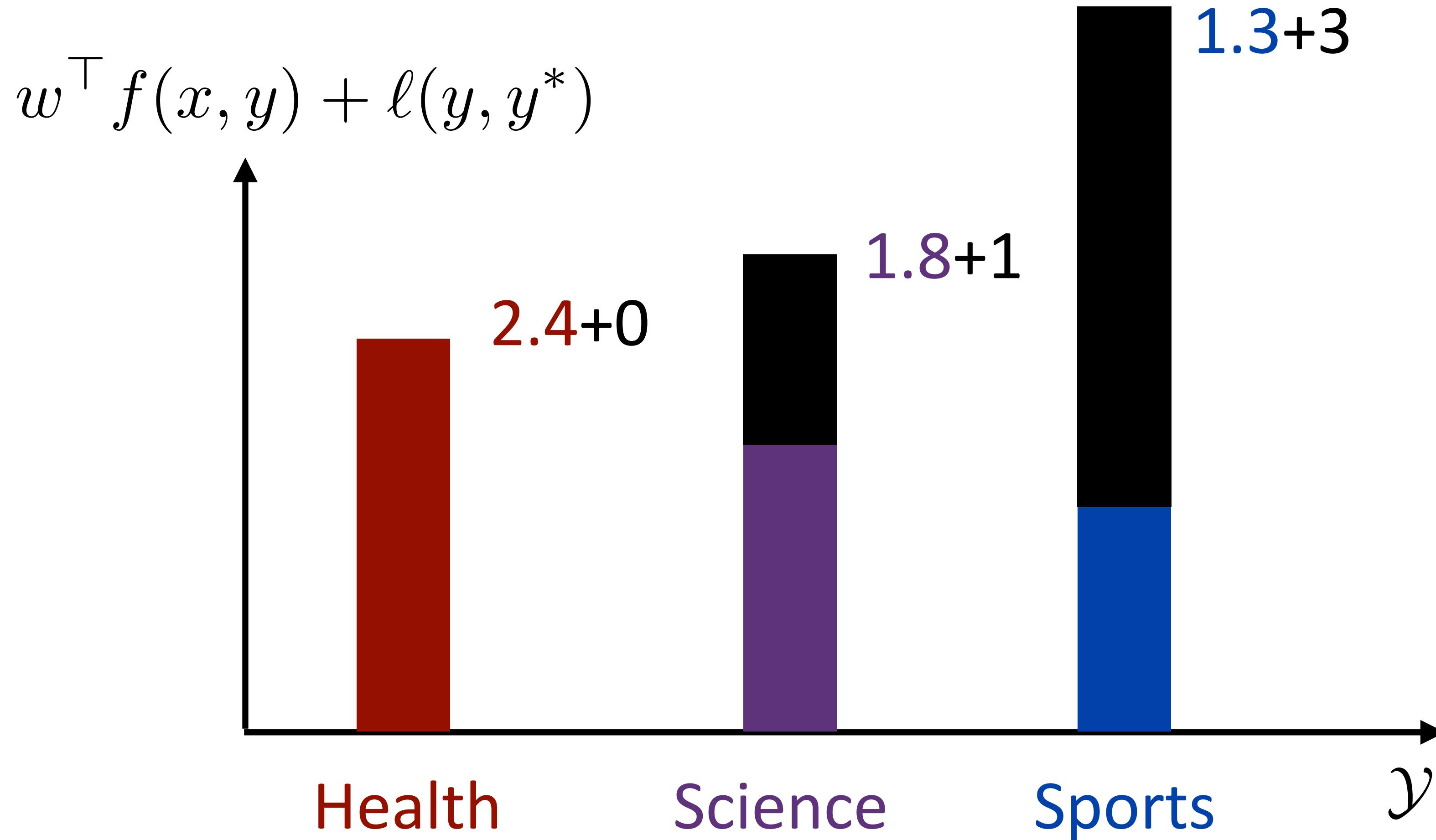
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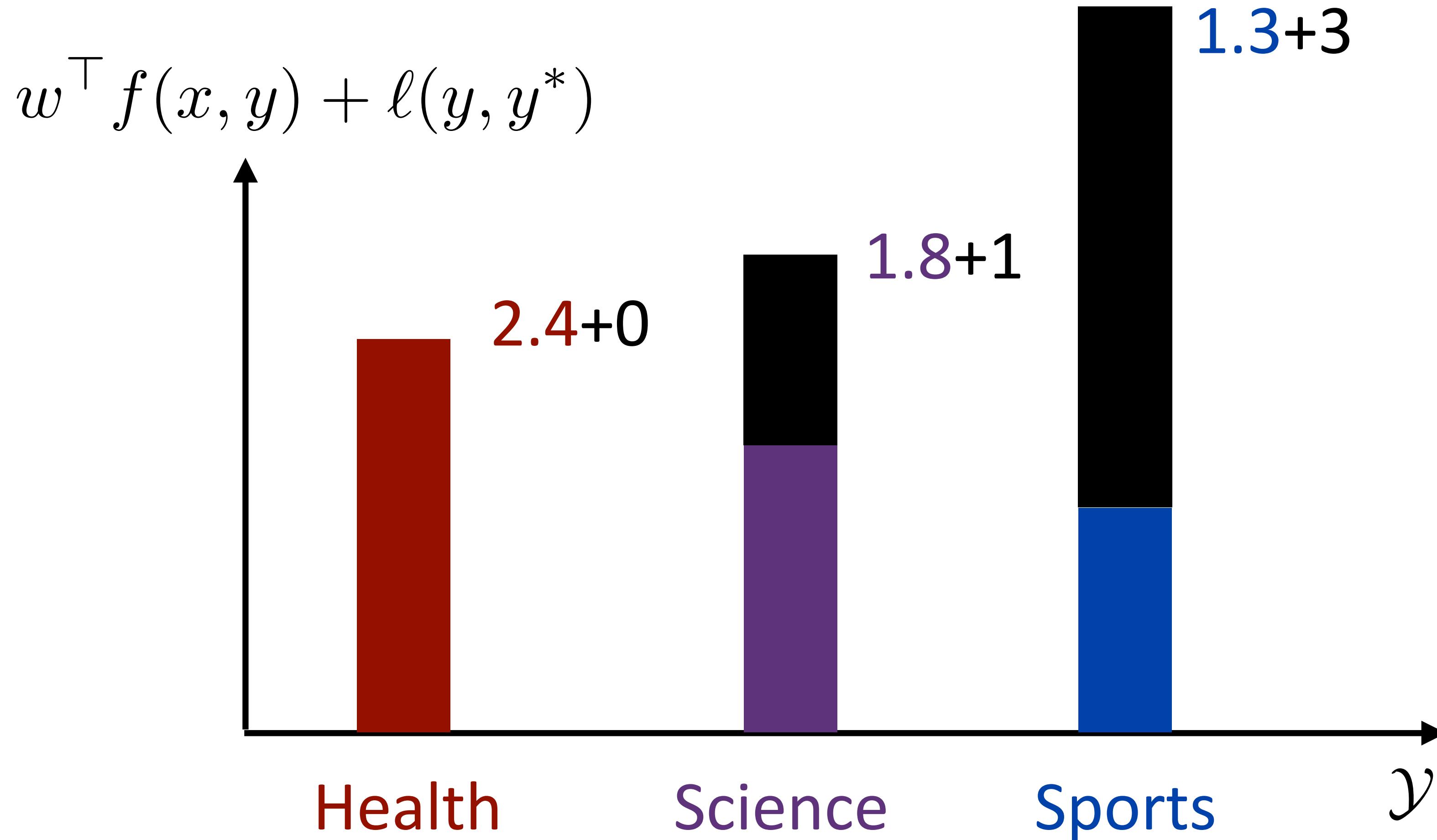
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- ▶ Does gold beat every label + loss? No!
- ▶ Most violated constraint is **Sports**; what is  $\xi_j$ ?
- ▶  $\xi_j = 4.3 - 2.4 = 1.9$

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- ▶  $\xi_j = 4.3 - 2.4 = 1.9$
- ▶ Perceptron would make no update here

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

# Computing the Subgradient

---

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

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

# Putting it Together

---

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# Putting it Together

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

# Optimization

# Recap

---

- ▶ Four elements of a machine learning method:

# Recap

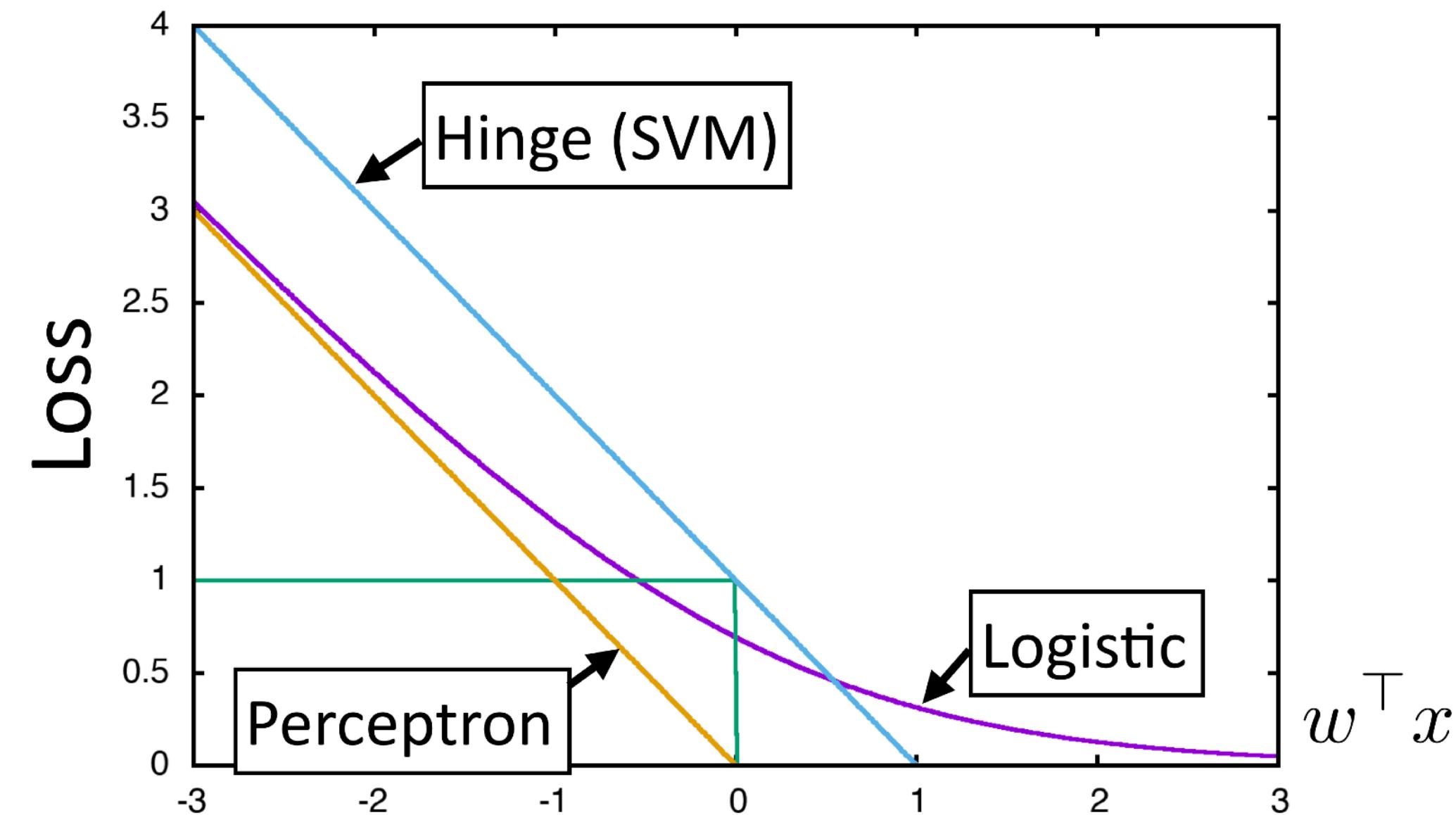
---

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

# Recap

---

- ▶ Four elements of a machine learning method:
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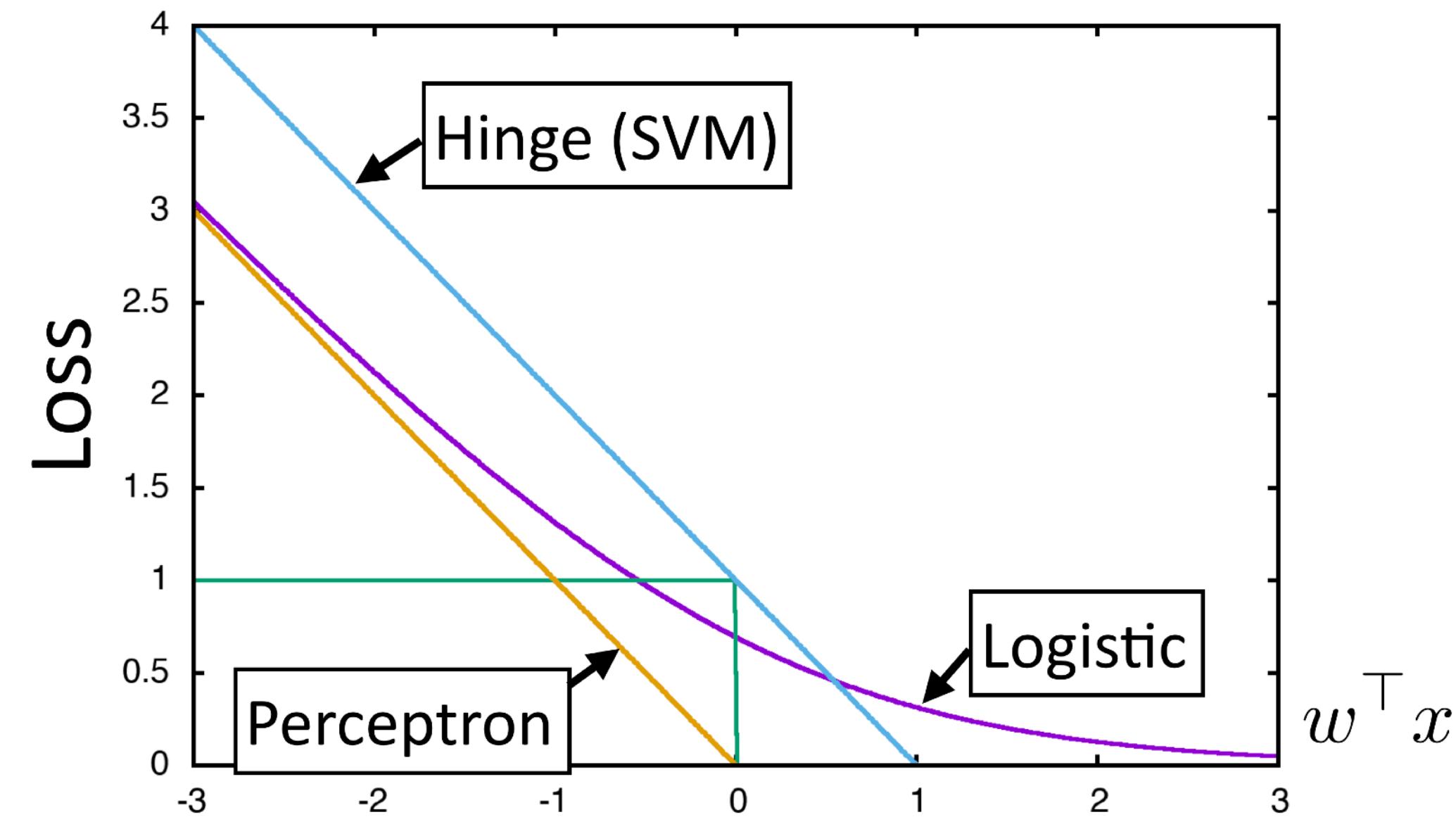


# Recap

---

- ▶ Four elements of a machine learning method:
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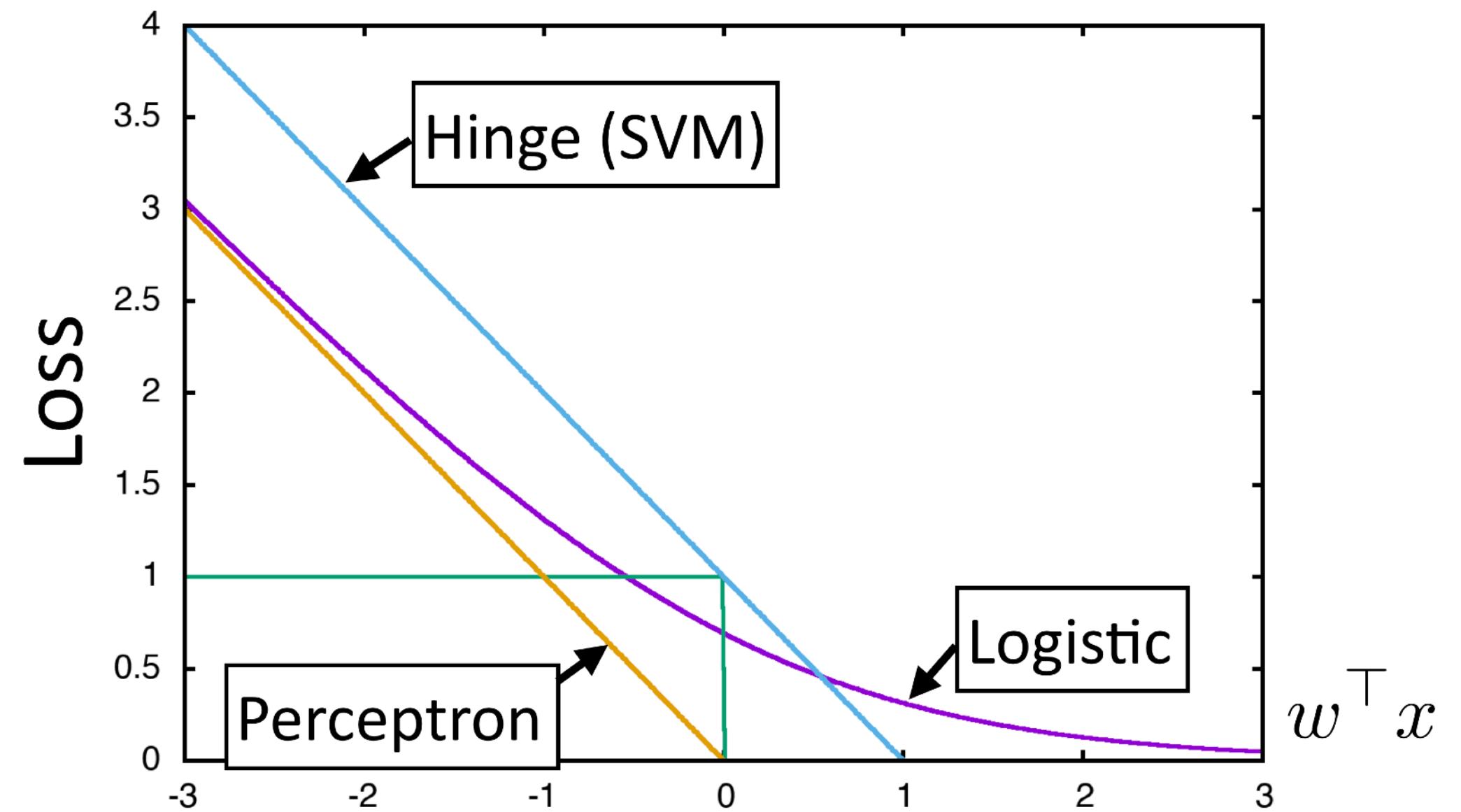
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# Recap

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- ▶ 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

---

# Optimization

---

- ▶ Stochastic gradient \*ascent\*

# Optimization

---

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

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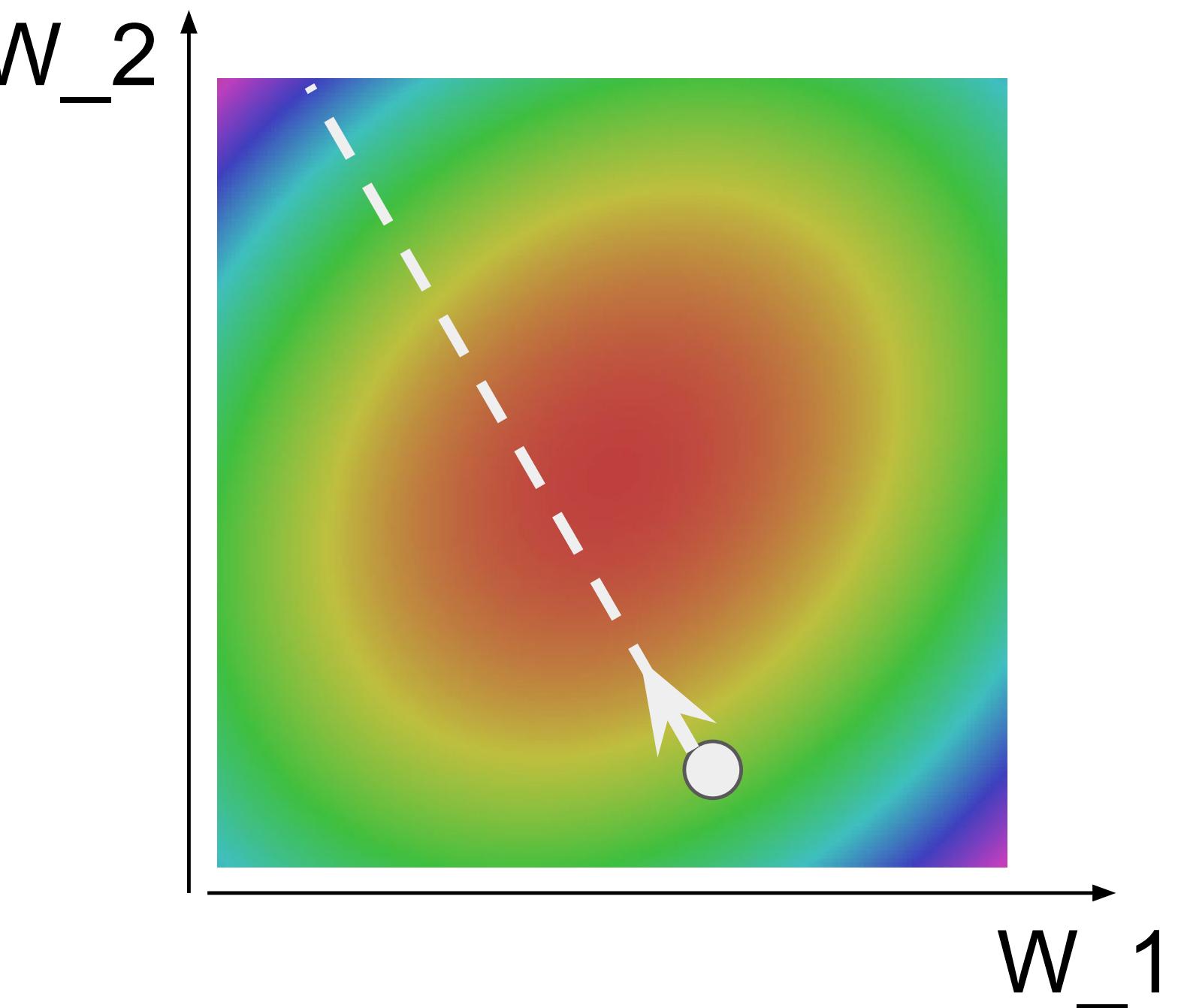
# Optimization

- ▶ Stochastic gradient \*ascent\*
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```
# Vanilla Gradient Descent

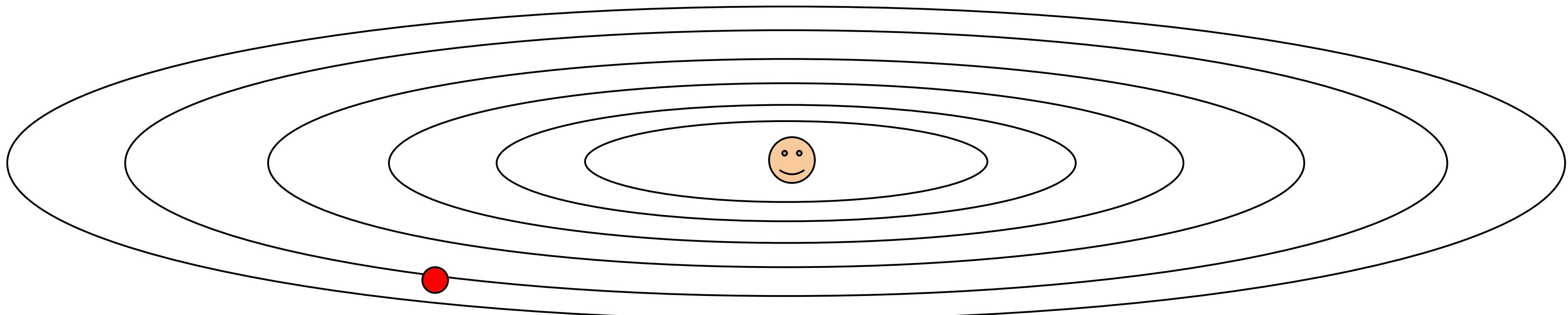
while True:
    weights_grad = evaluate_gradient(loss_fun, data, weights)
    weights += - step_size * weights_grad # perform parameter update
```



# Optimization

---

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



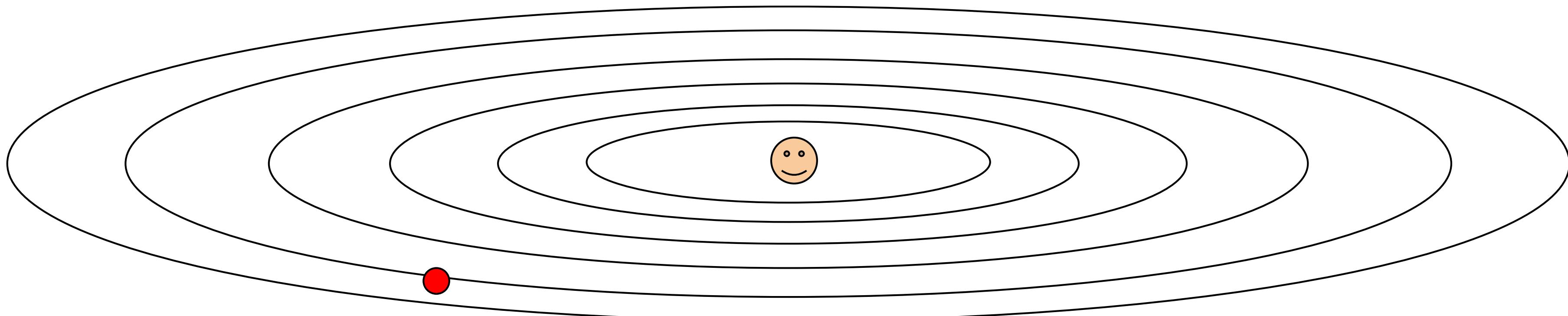
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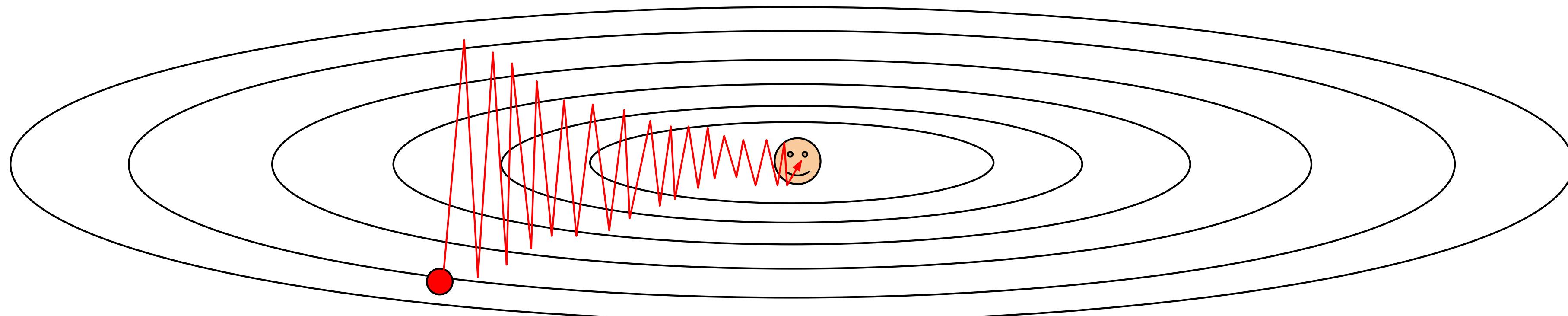
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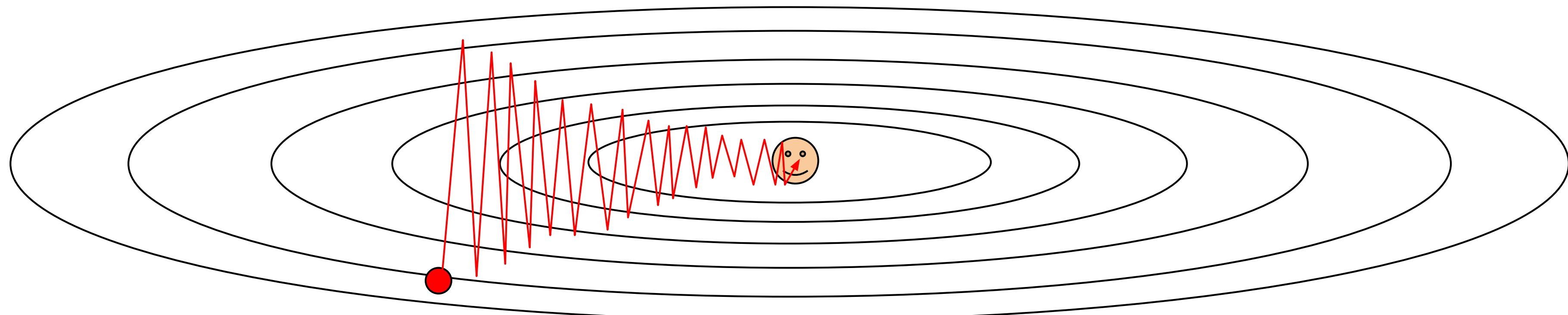
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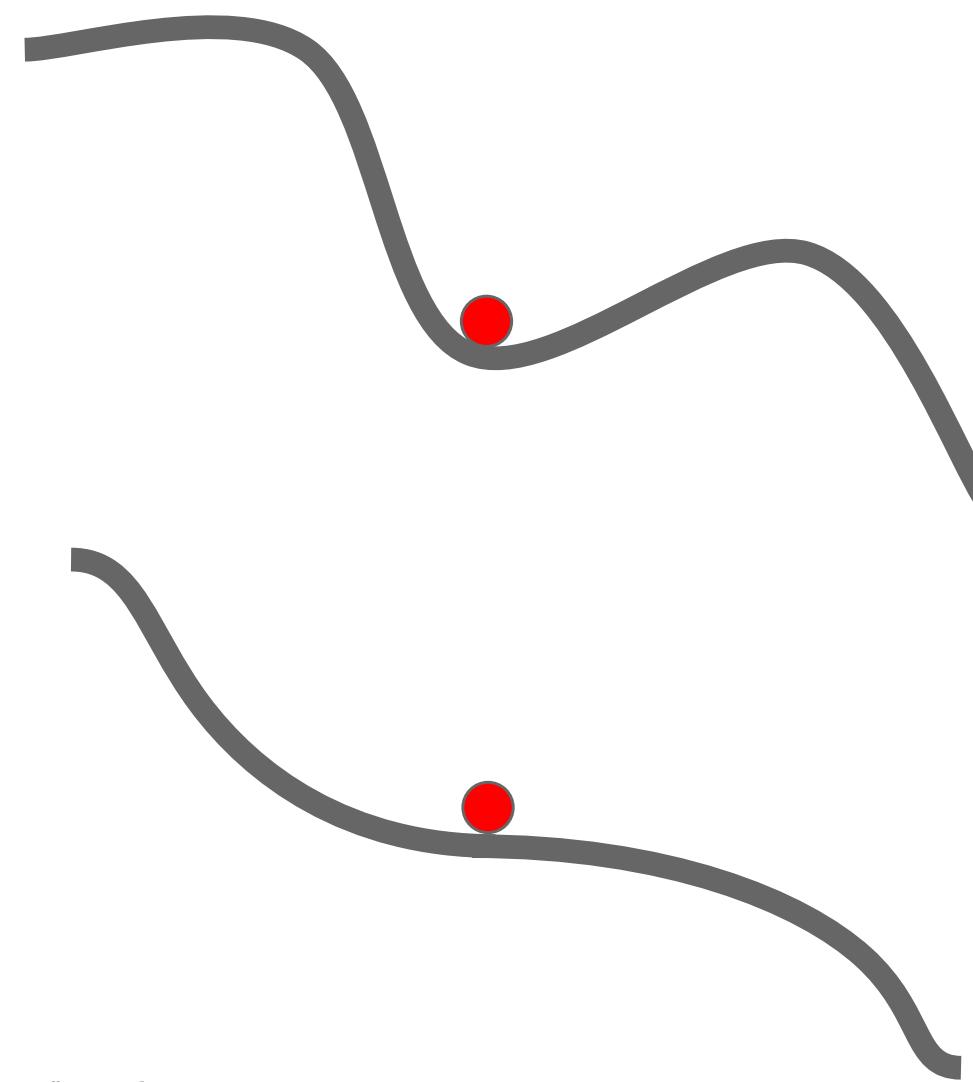
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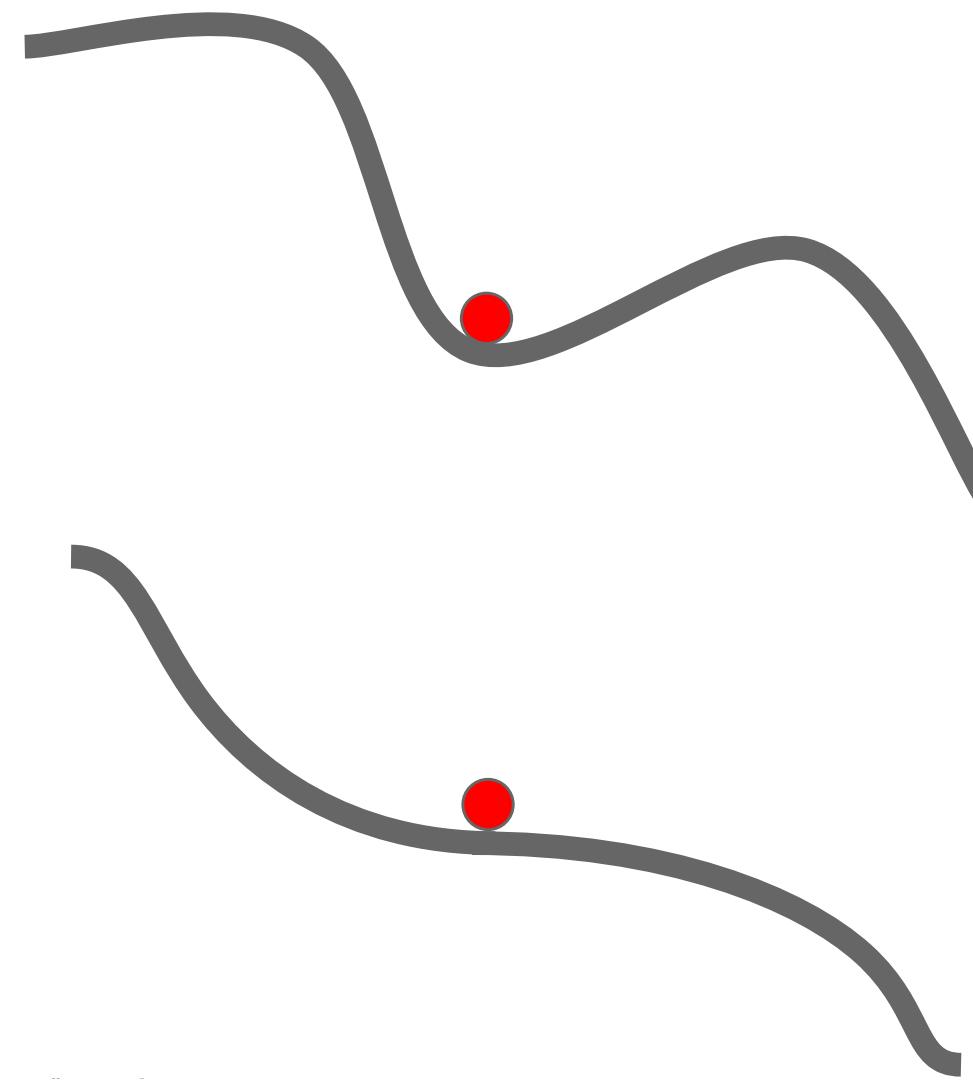
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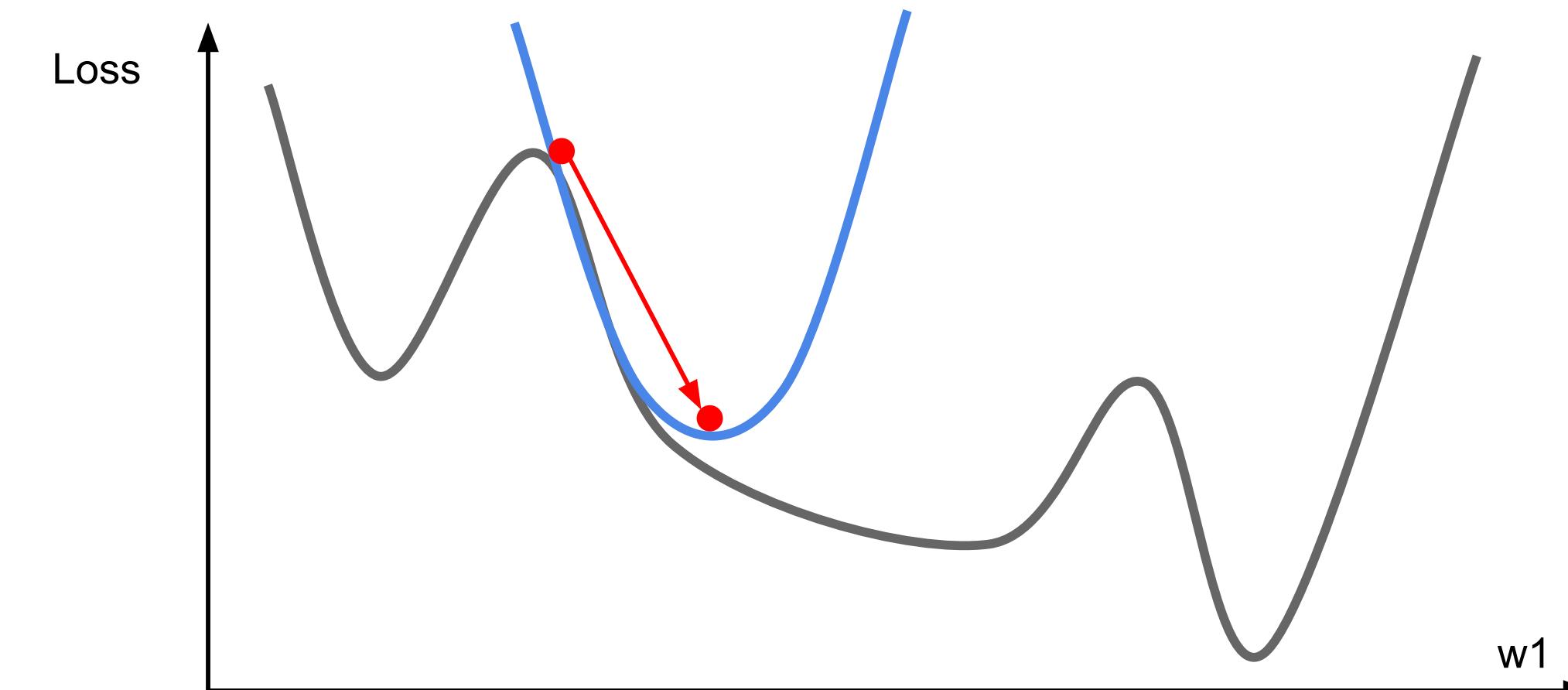
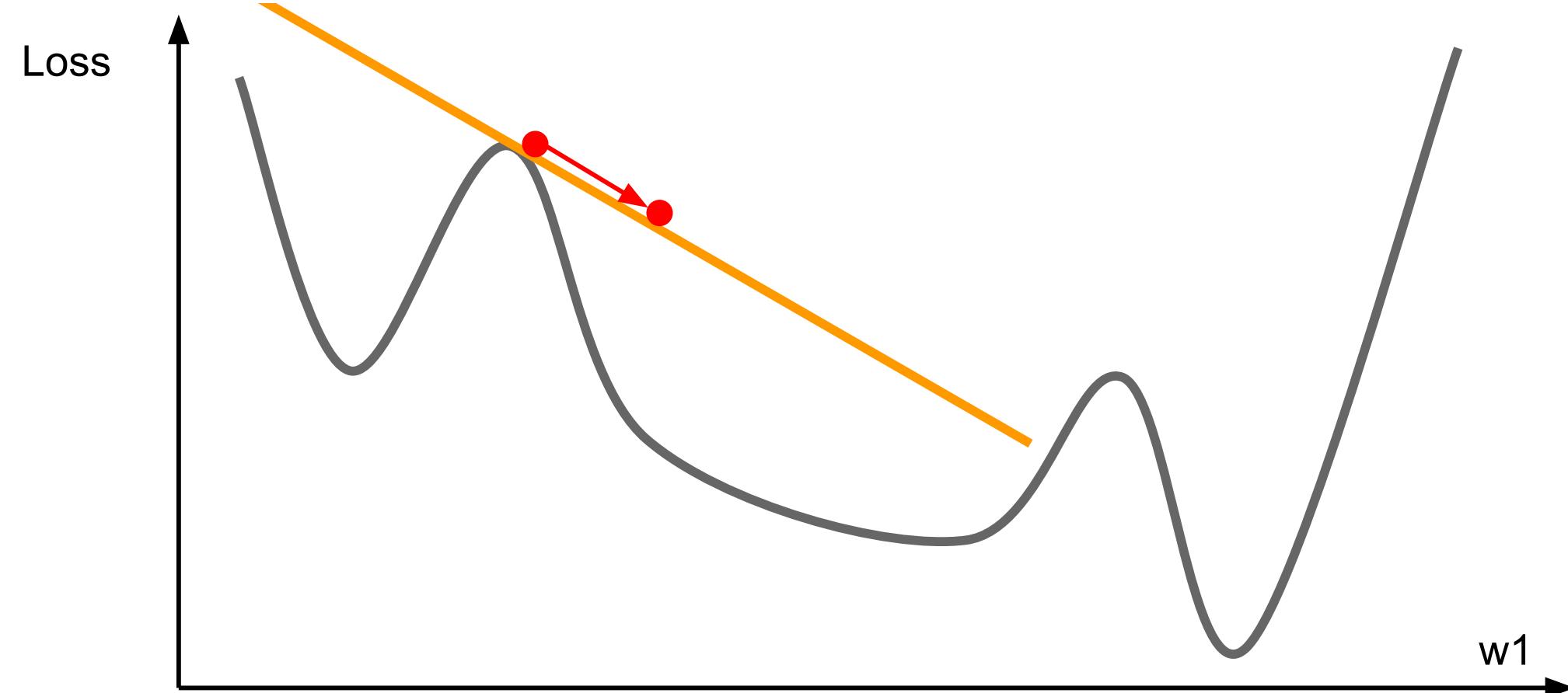
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- ▶ Quasi-Newton methods: L-BFGS, etc. approximate inverse Hessian

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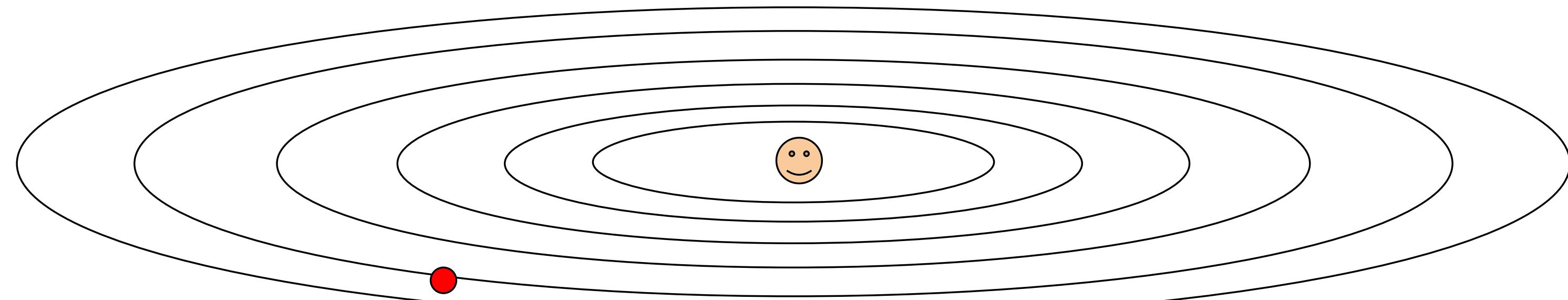
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# AdaGrad

---

- ▶ 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)
```



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

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- ▶ 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