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.

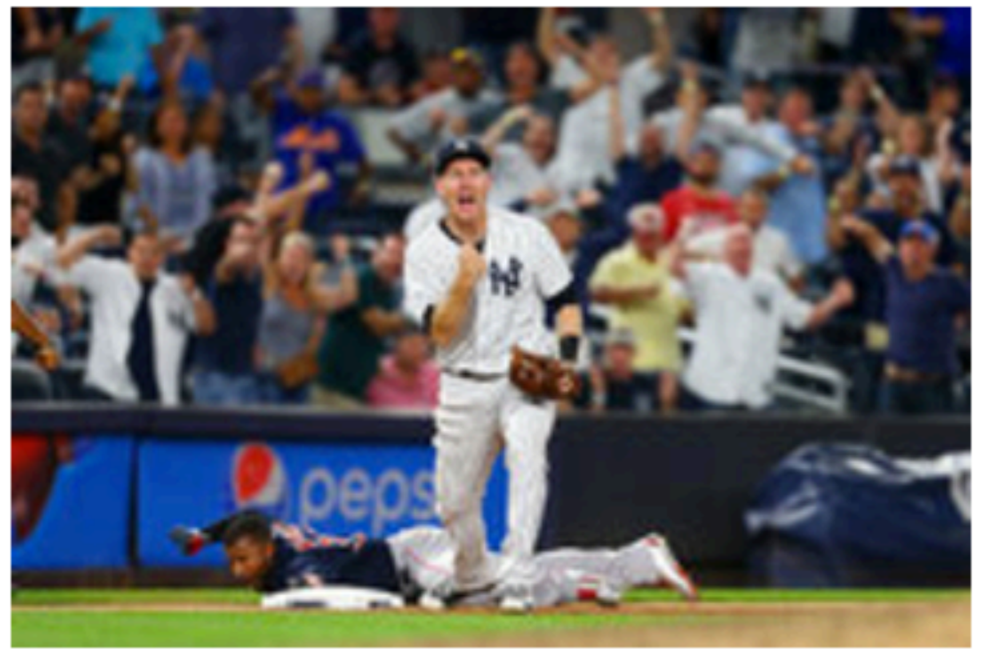
By GINA KOLATA

→ 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

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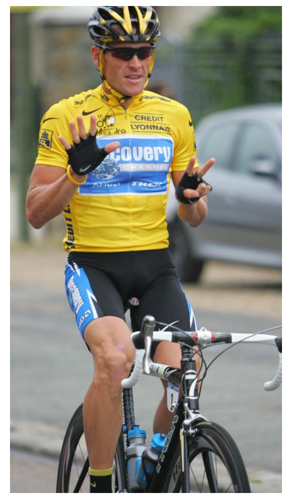

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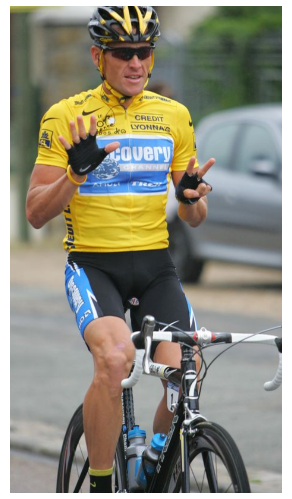

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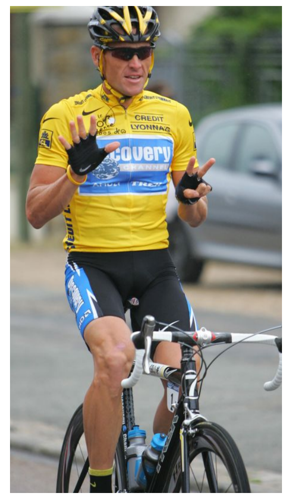

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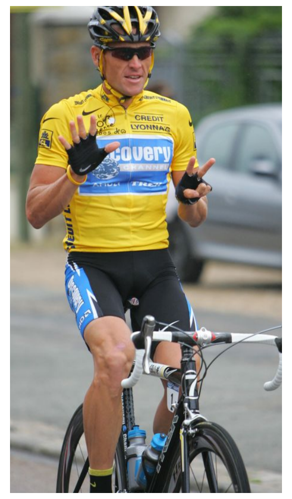

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- 4,500,000 classes (all articles in Wikipedia)

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.

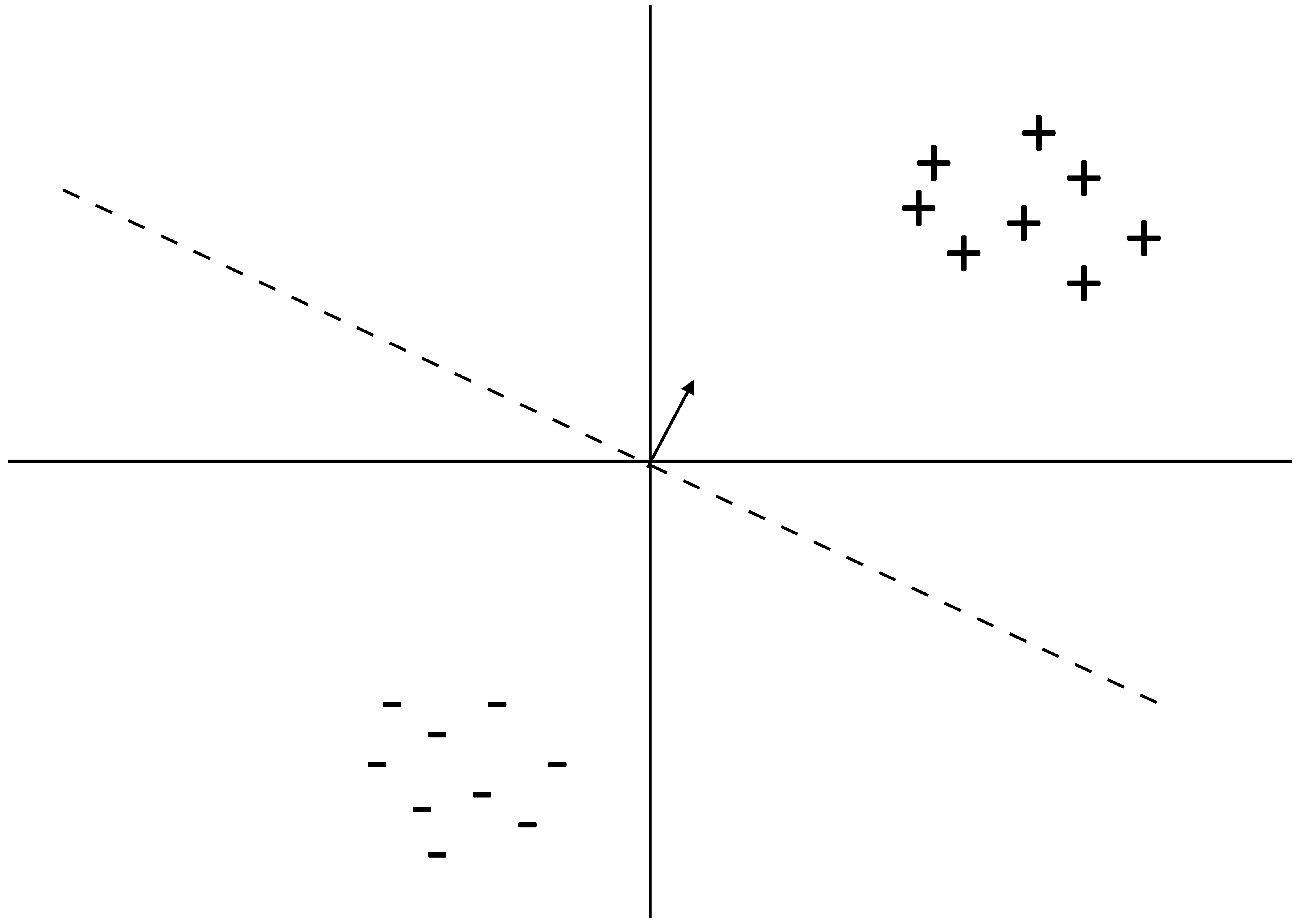
3) Where did James go after he went to the grocery store?
A) his deck
B) his freezer
C) a fast food restaurant
D) his room

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

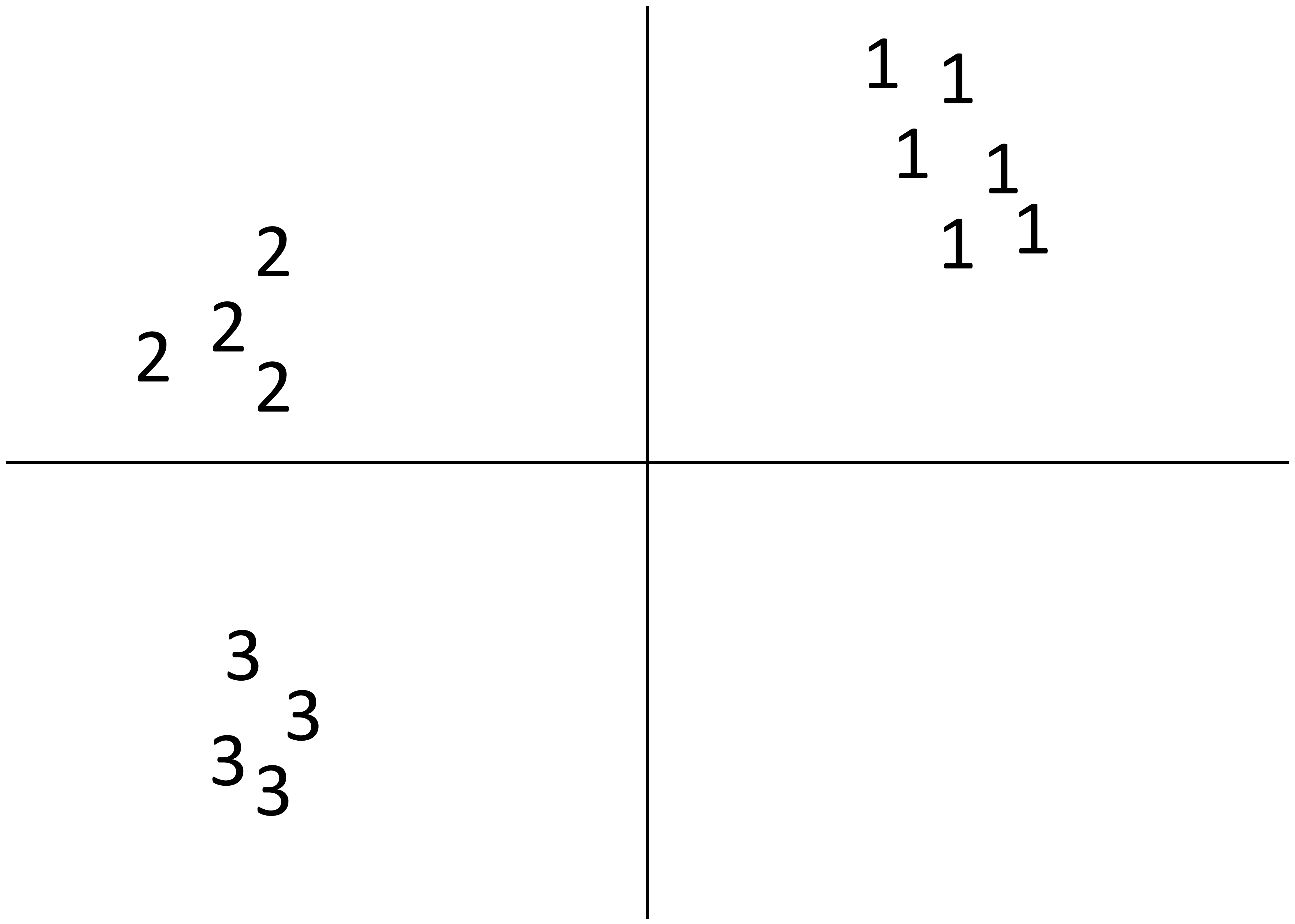
Richardson (2013)

Binary Classification

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

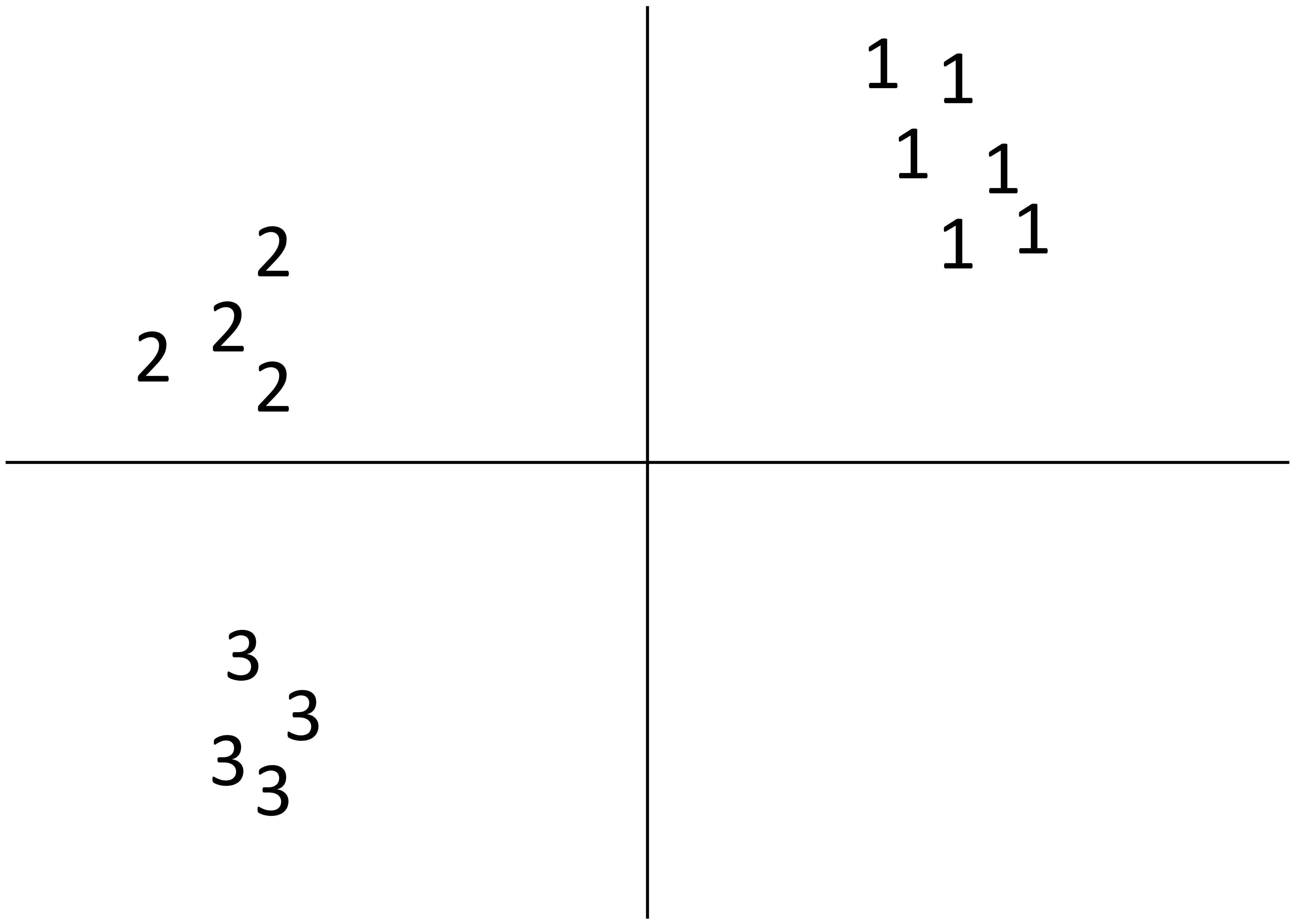


Multiclass Classification



Multiclass Classification

- Can we just use binary classifiers here?



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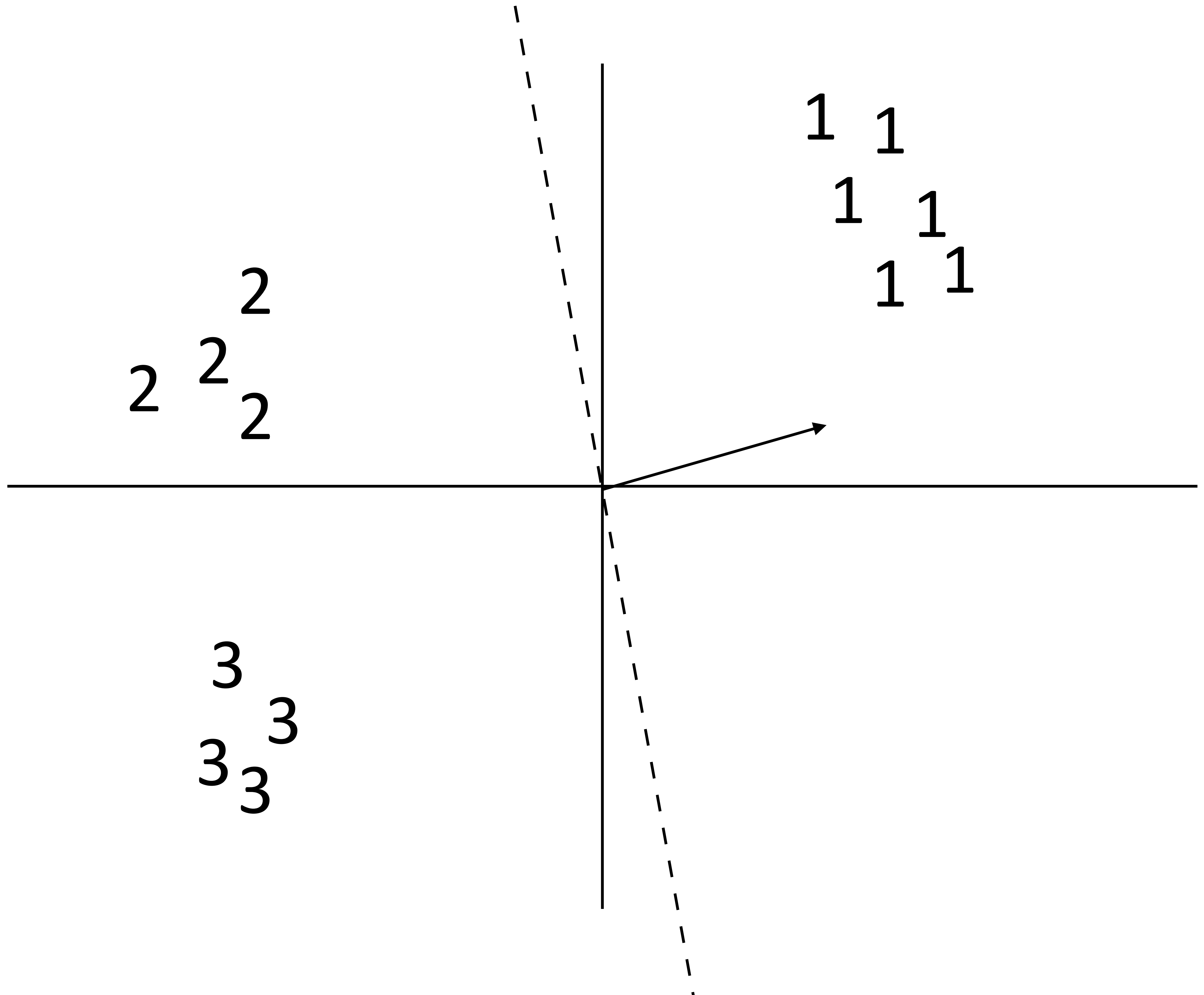

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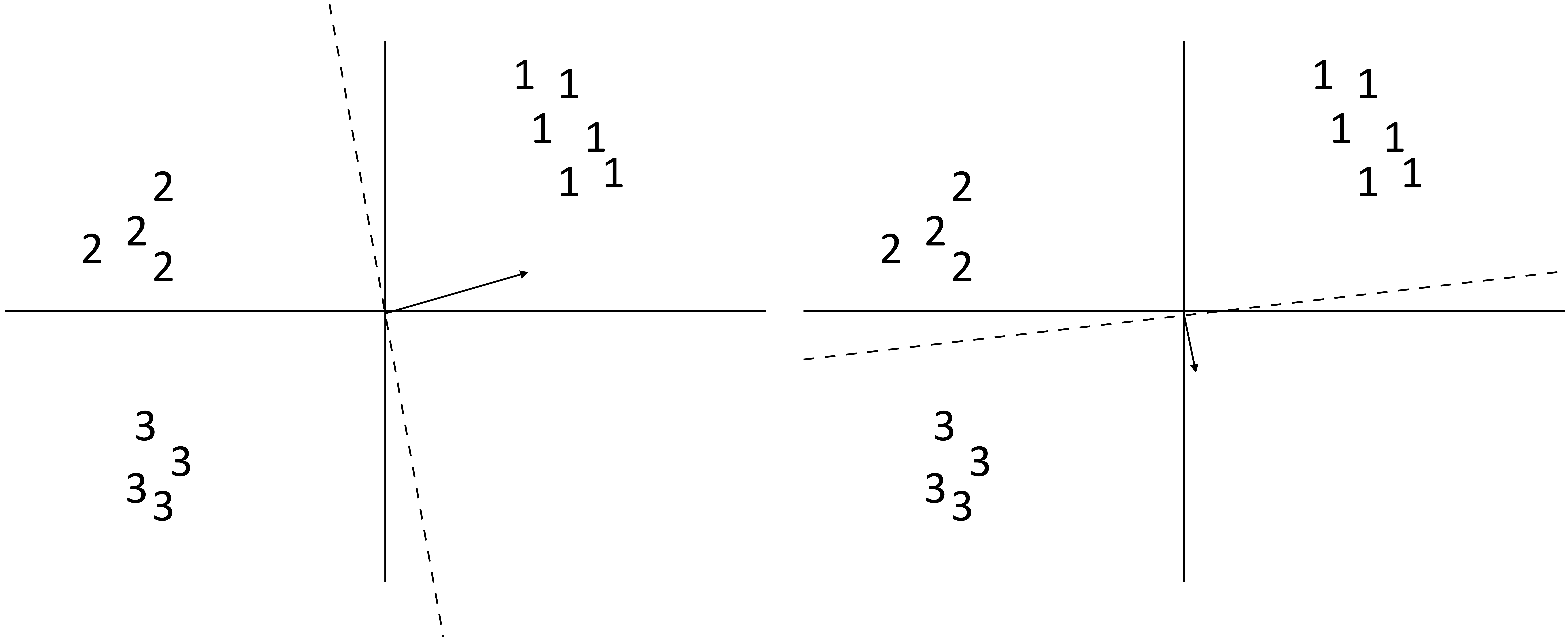
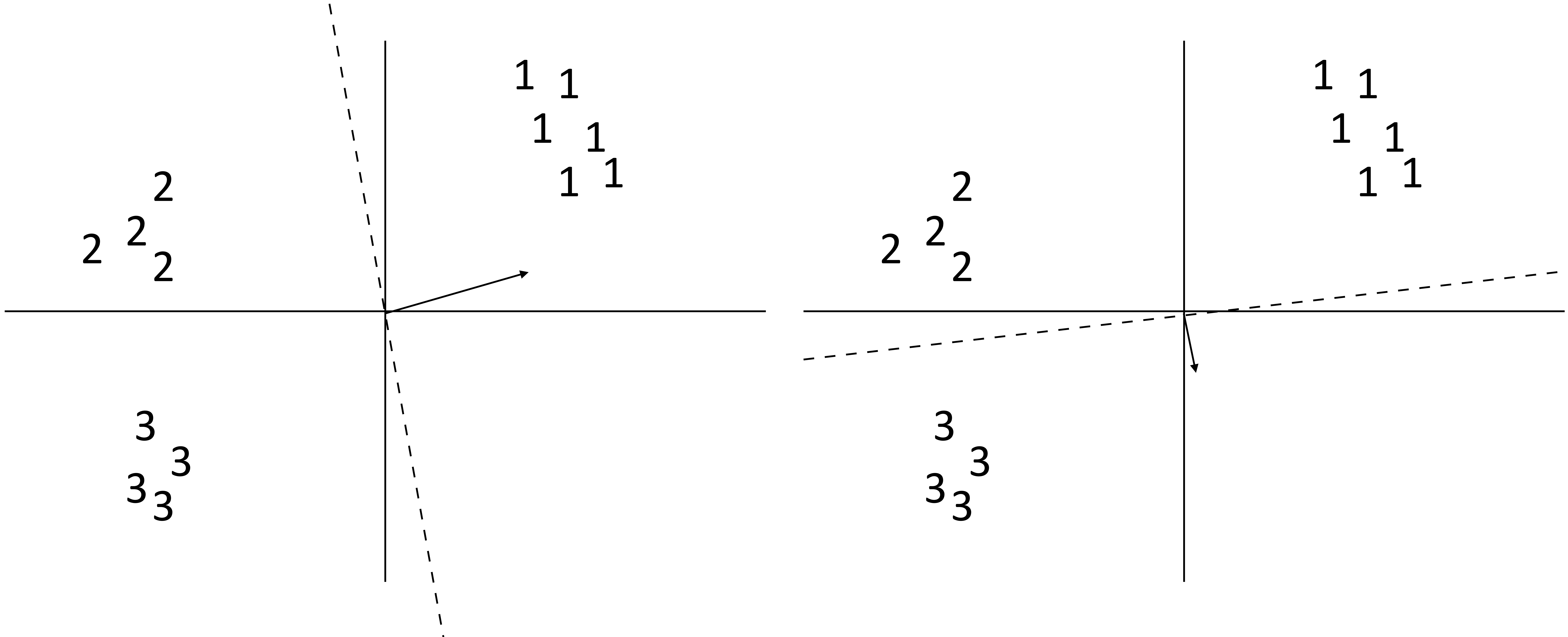


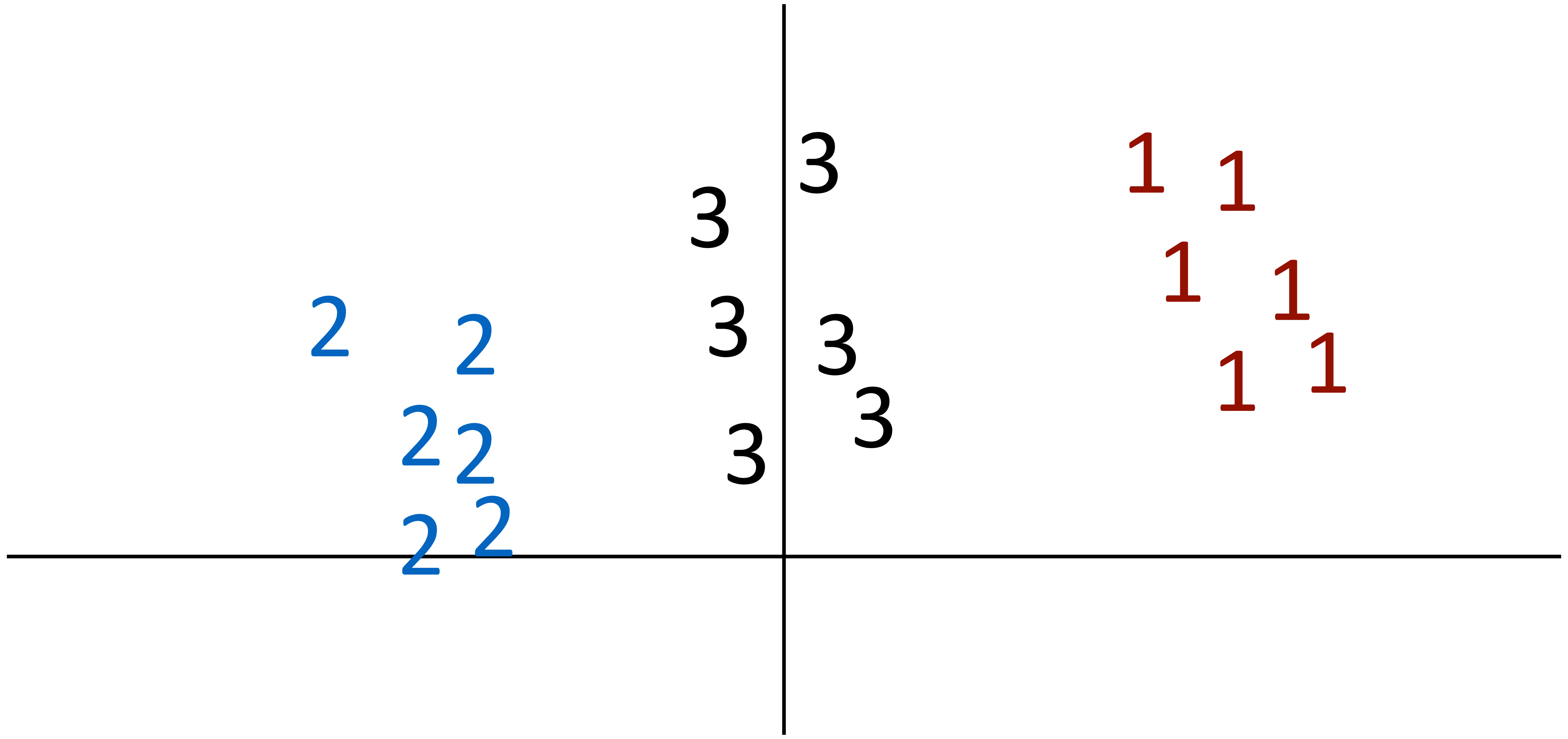
Multiclass Classification

- 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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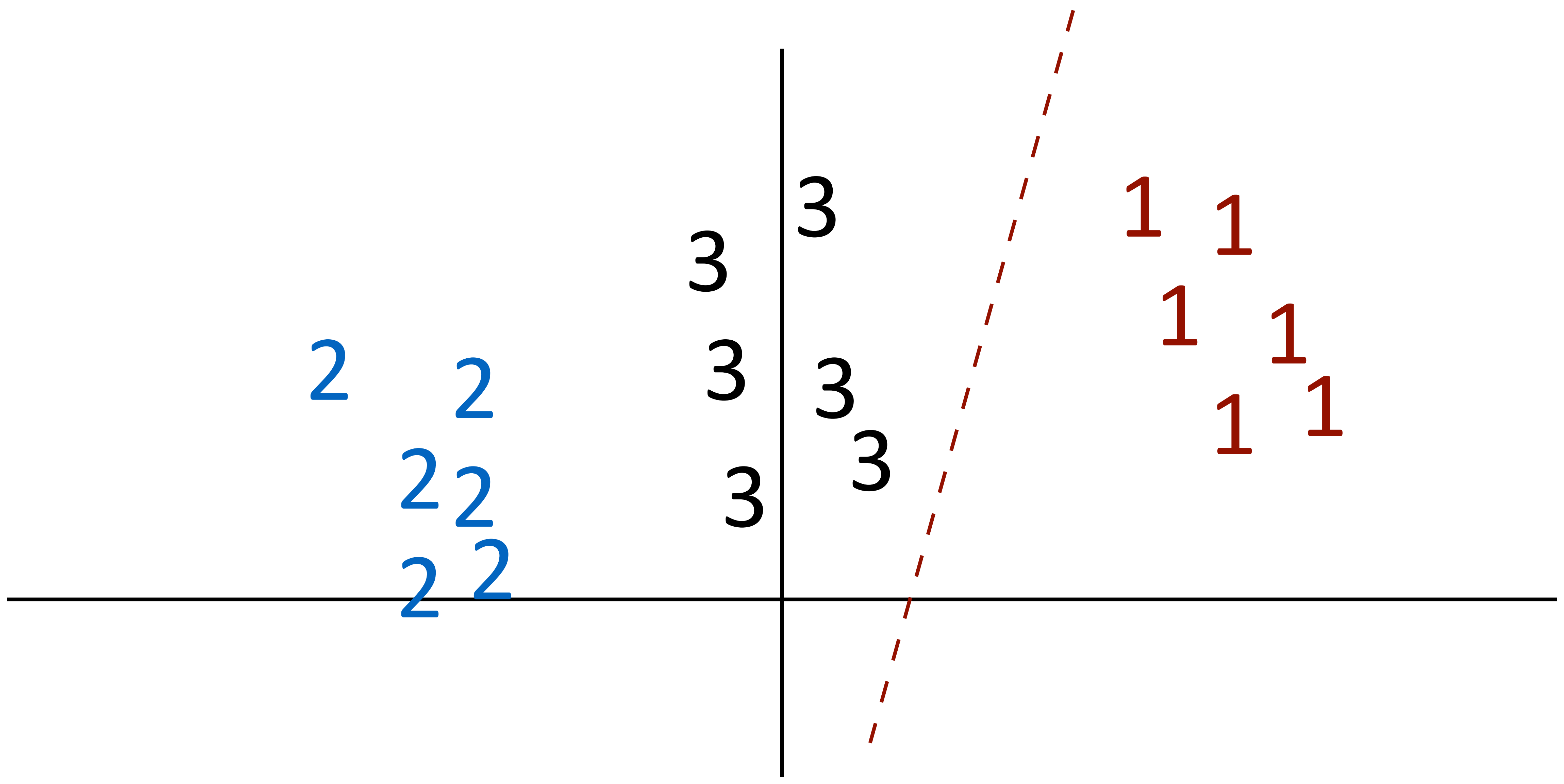

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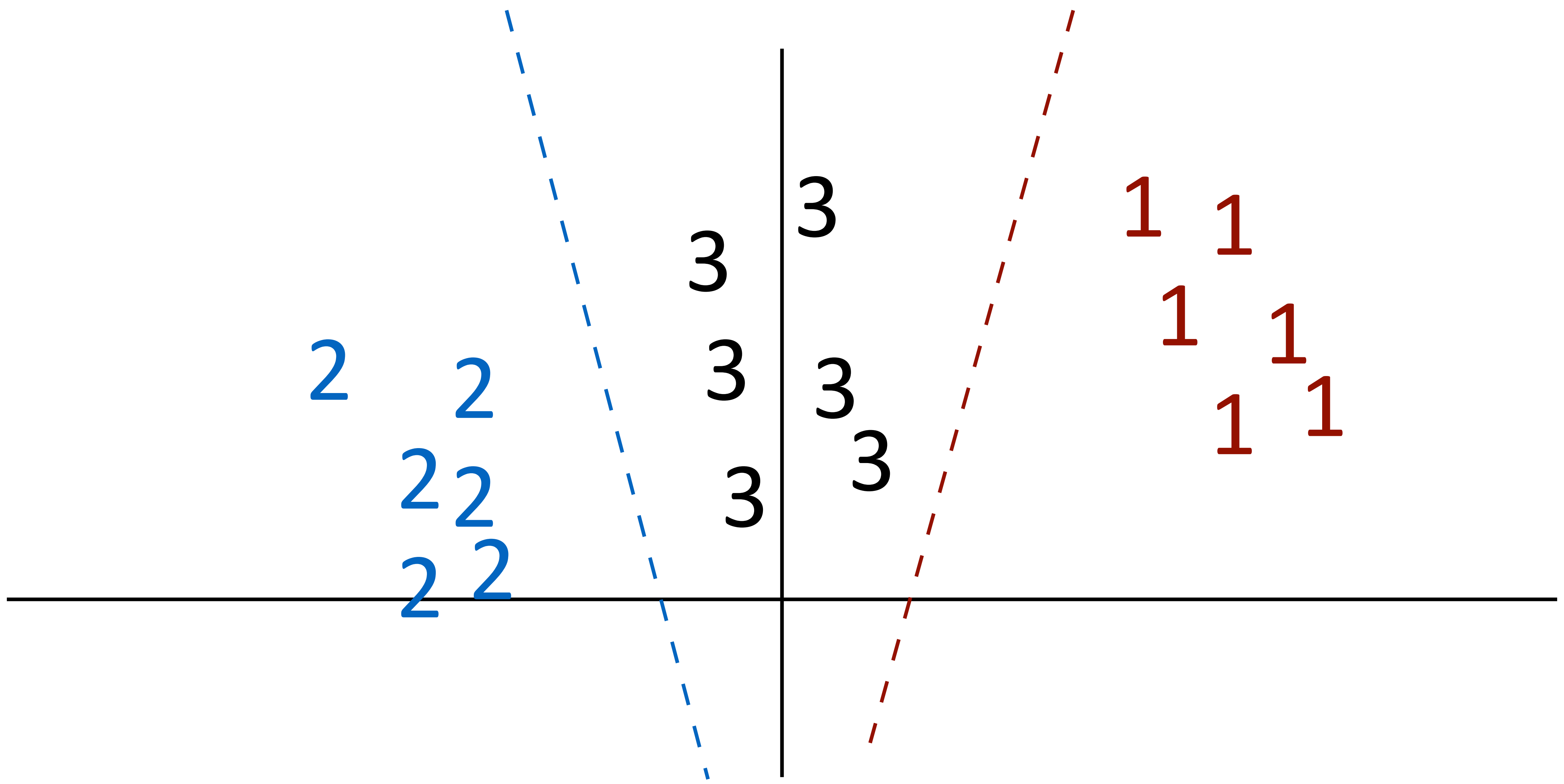

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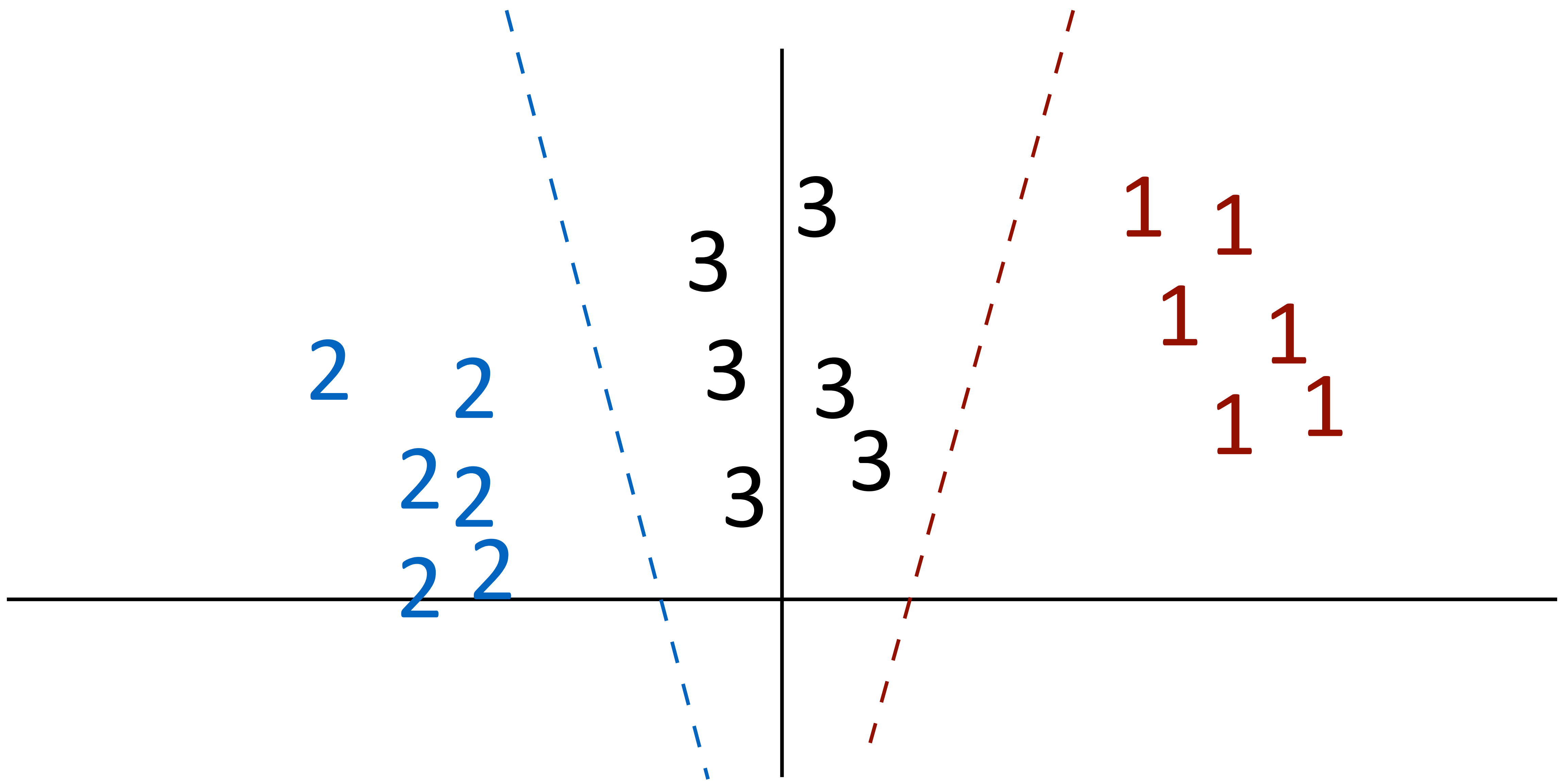

- Can separate 1 from 2+3 and 2 from 1+3 but not 3 from the others (with these features)

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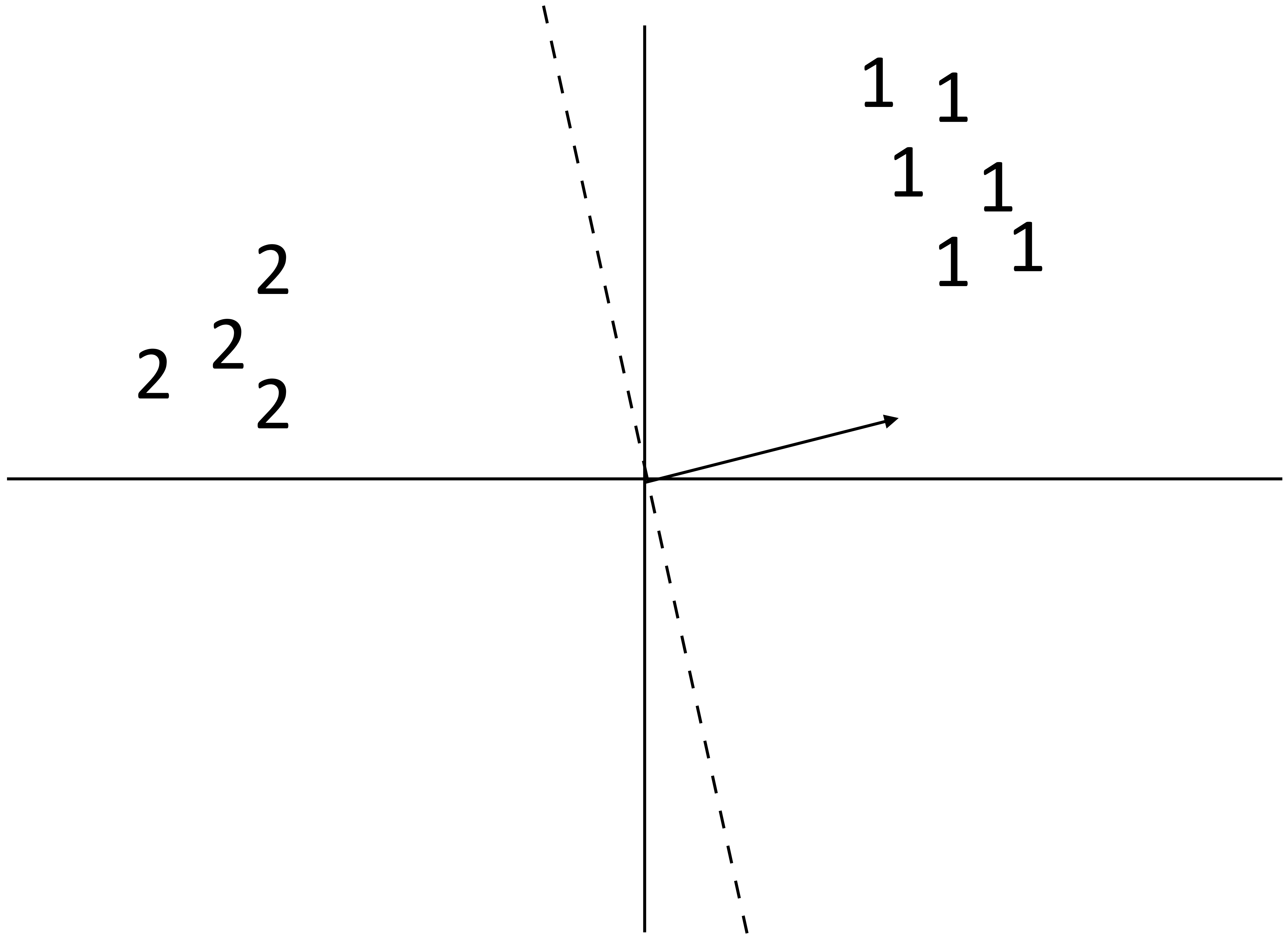

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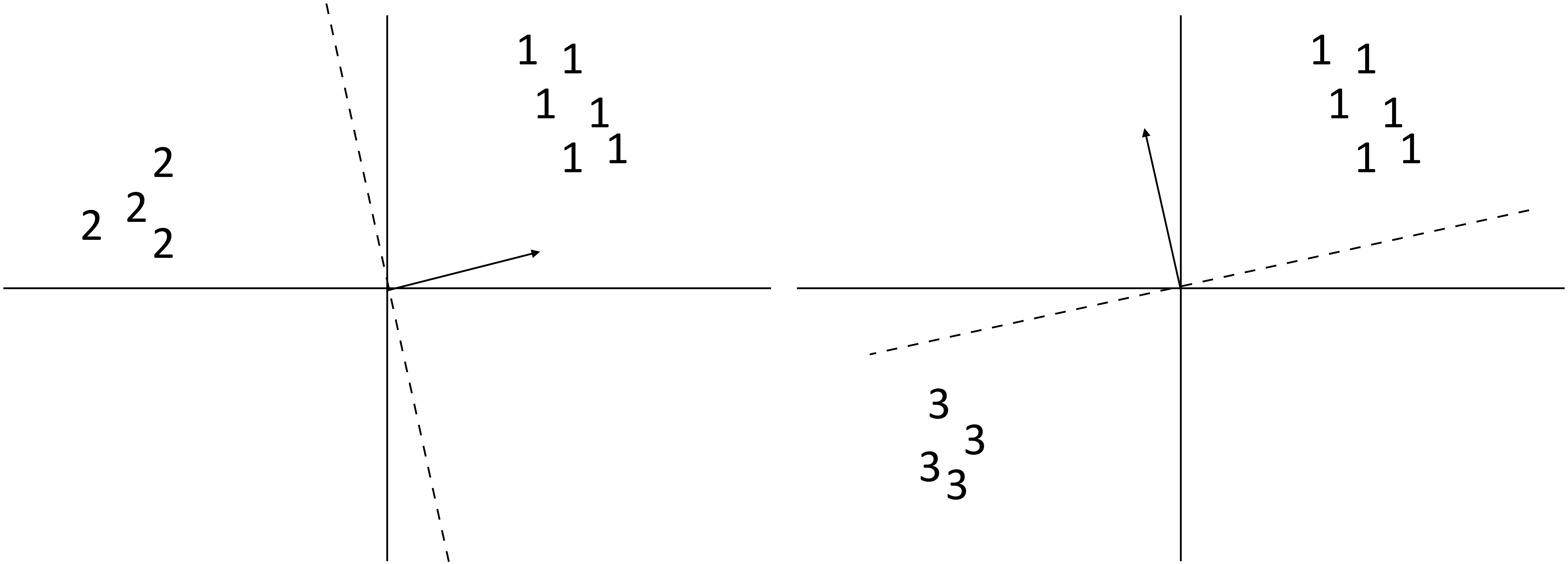
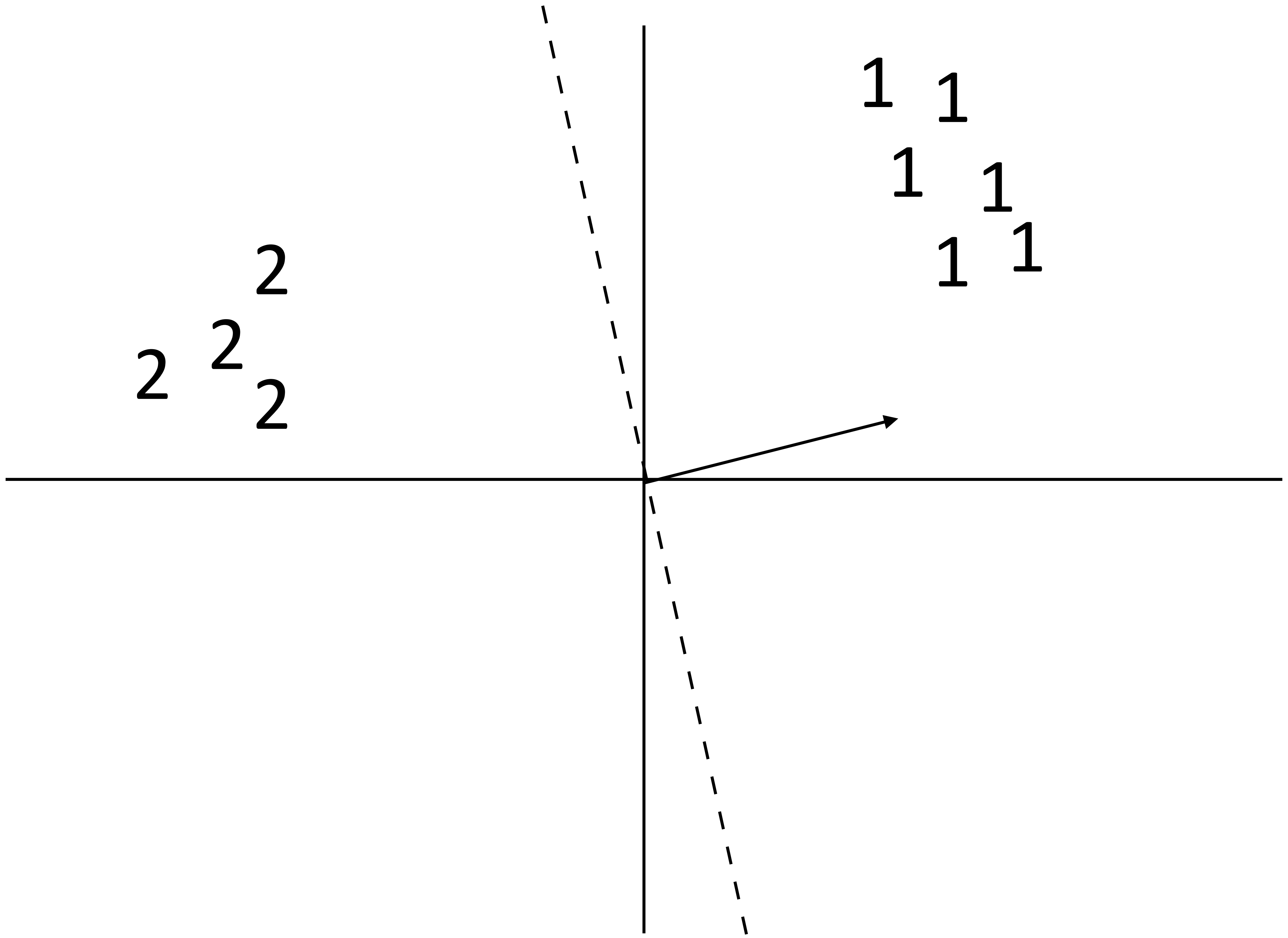
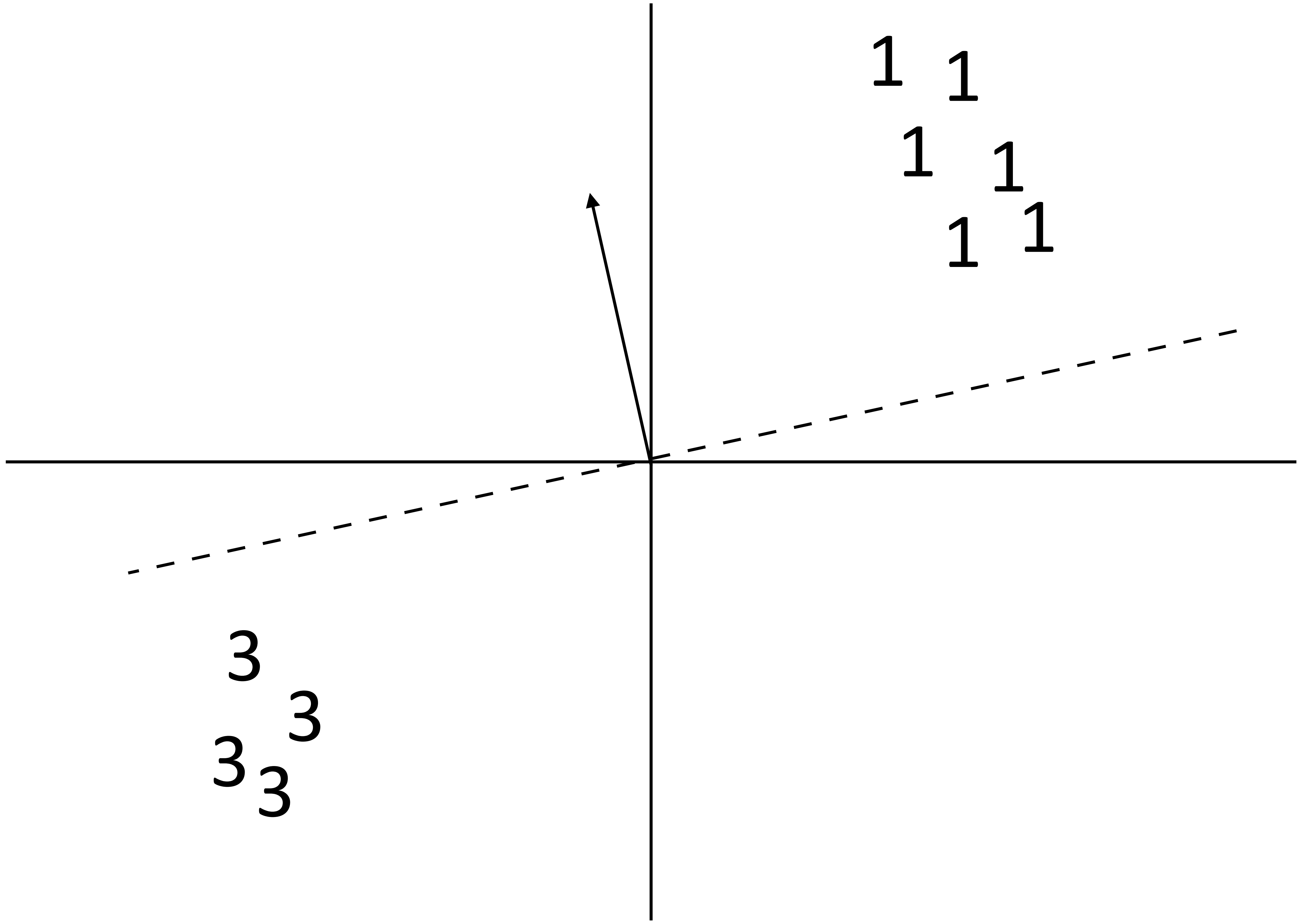


Multiclass Classification

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





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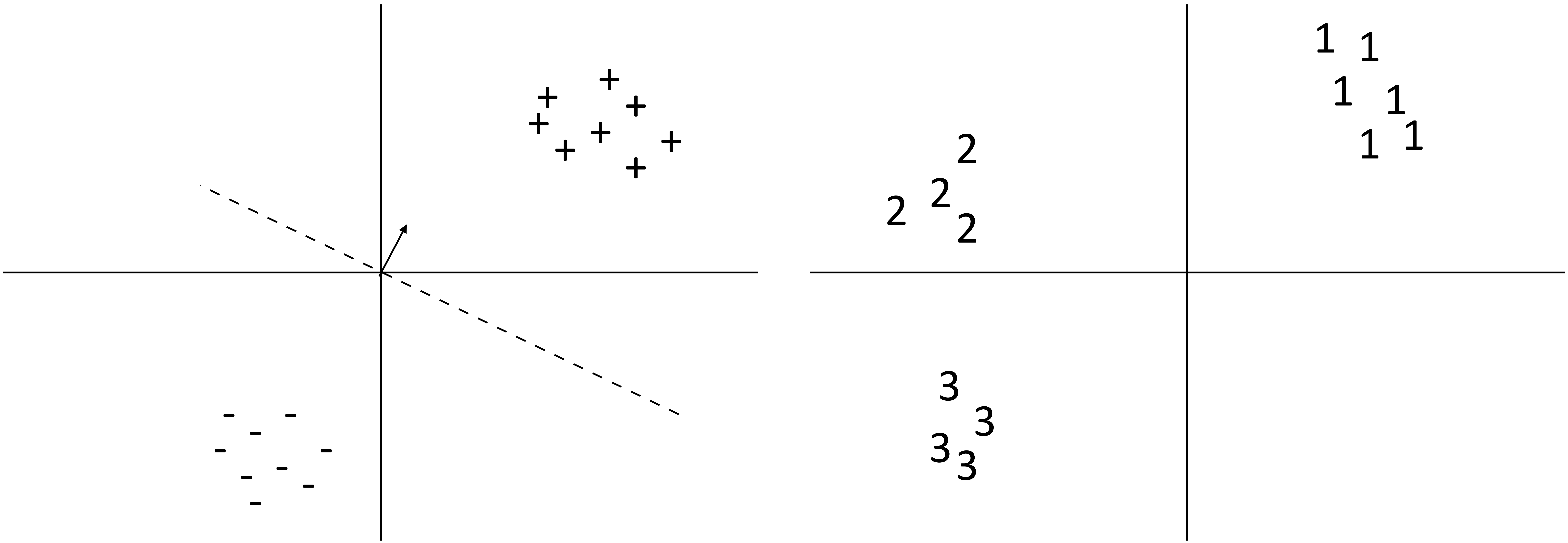
- Binary classification: one weight vector defines both classes



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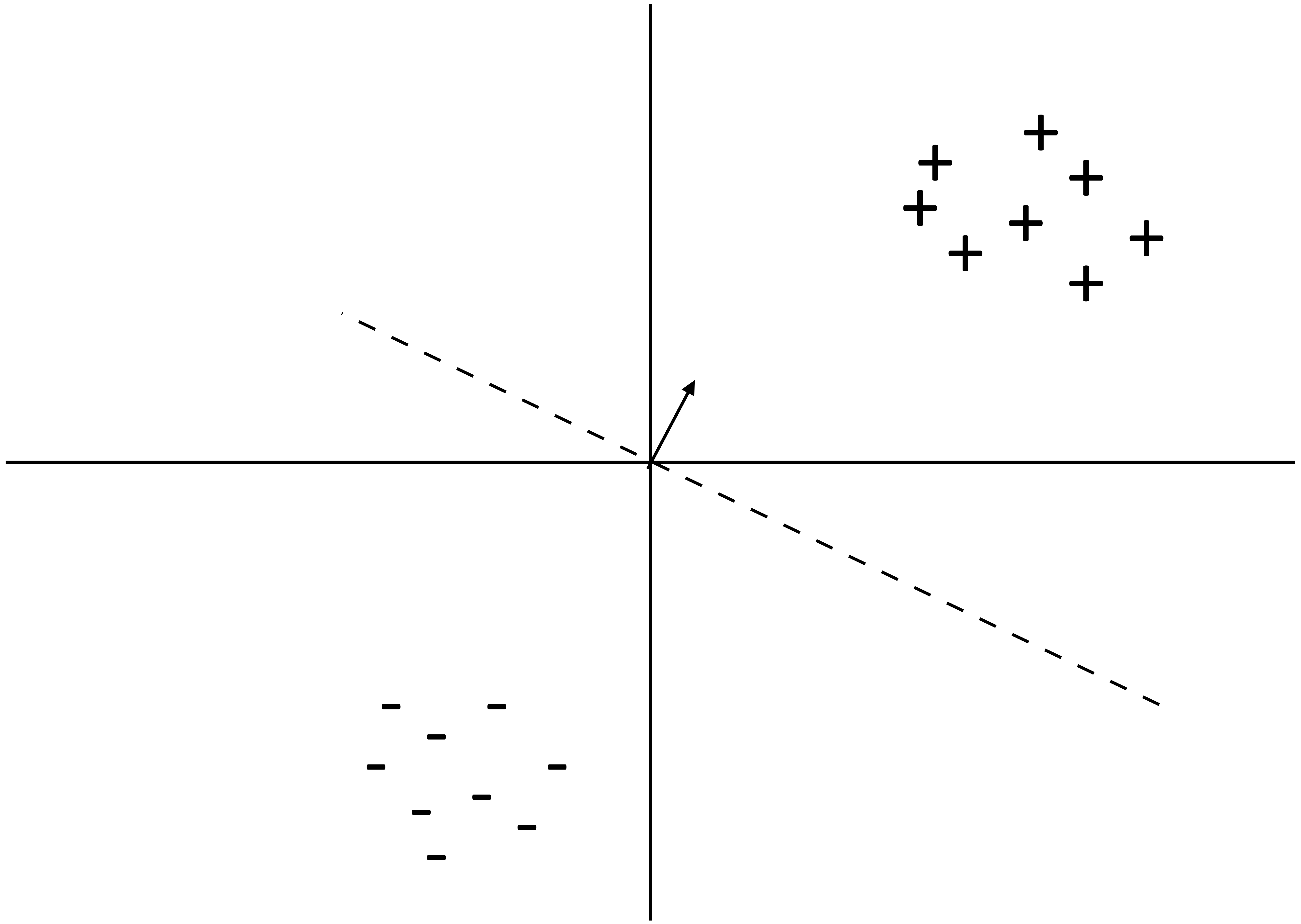
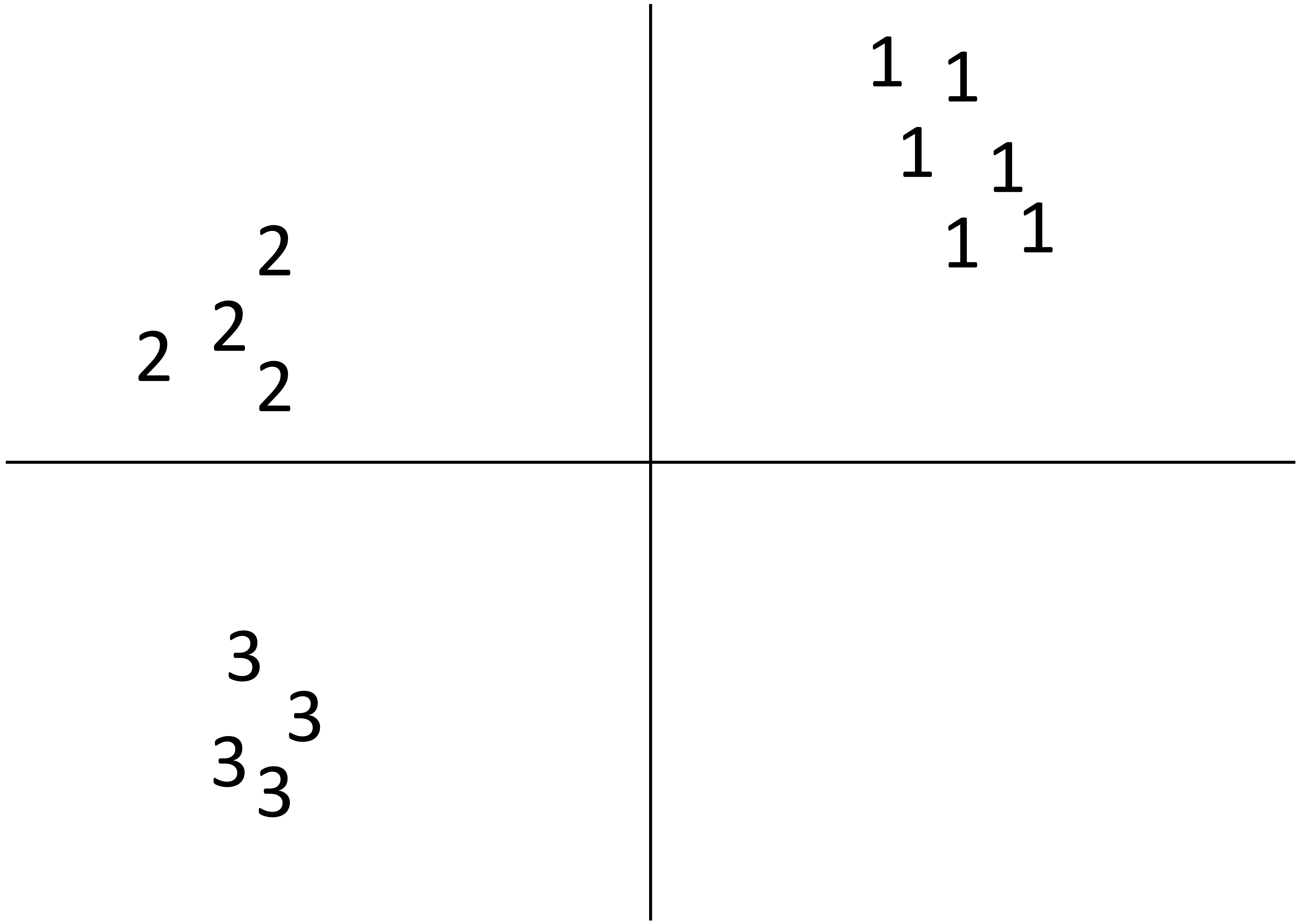


- Multiclass classification: different weights and/or features per class



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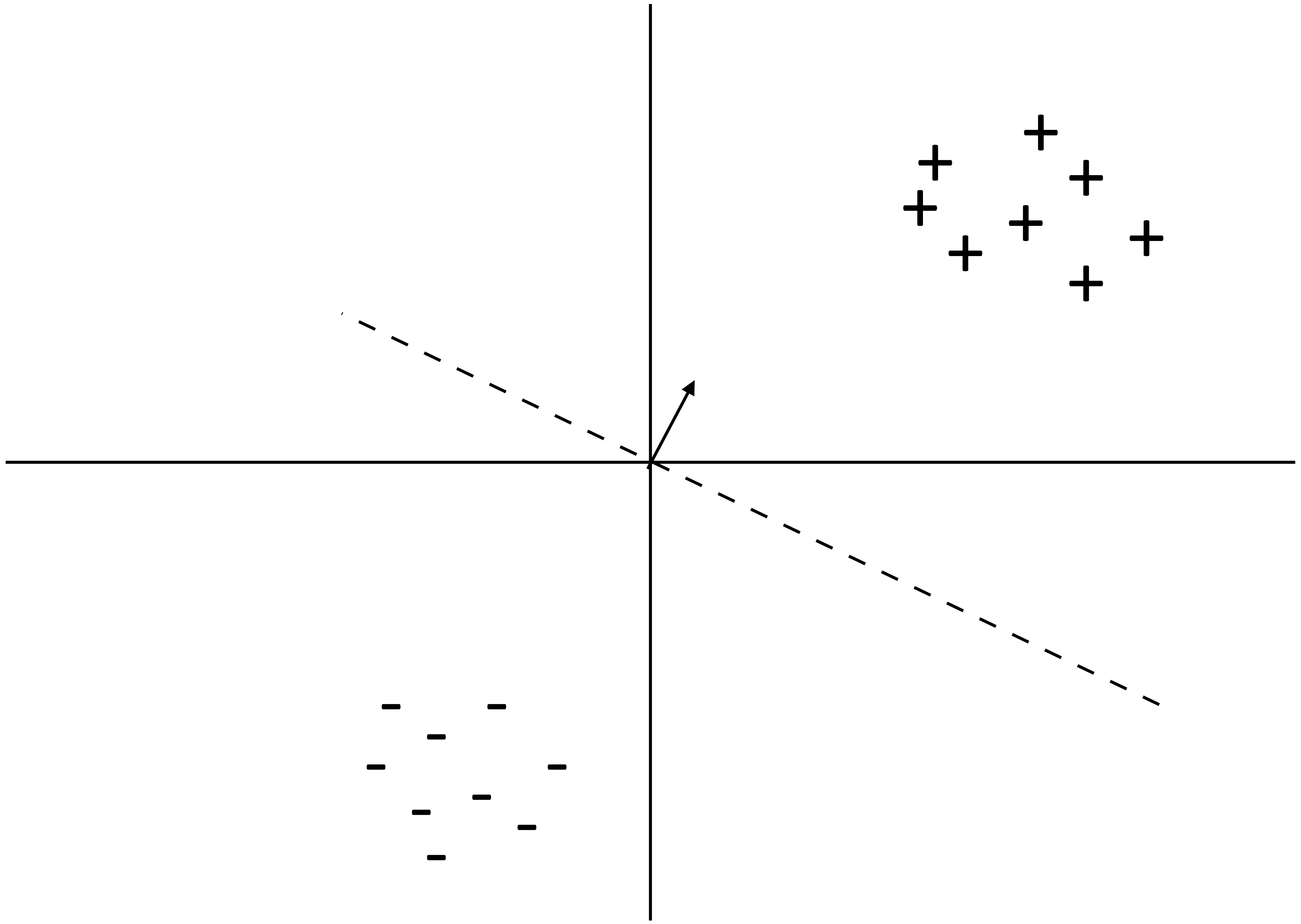

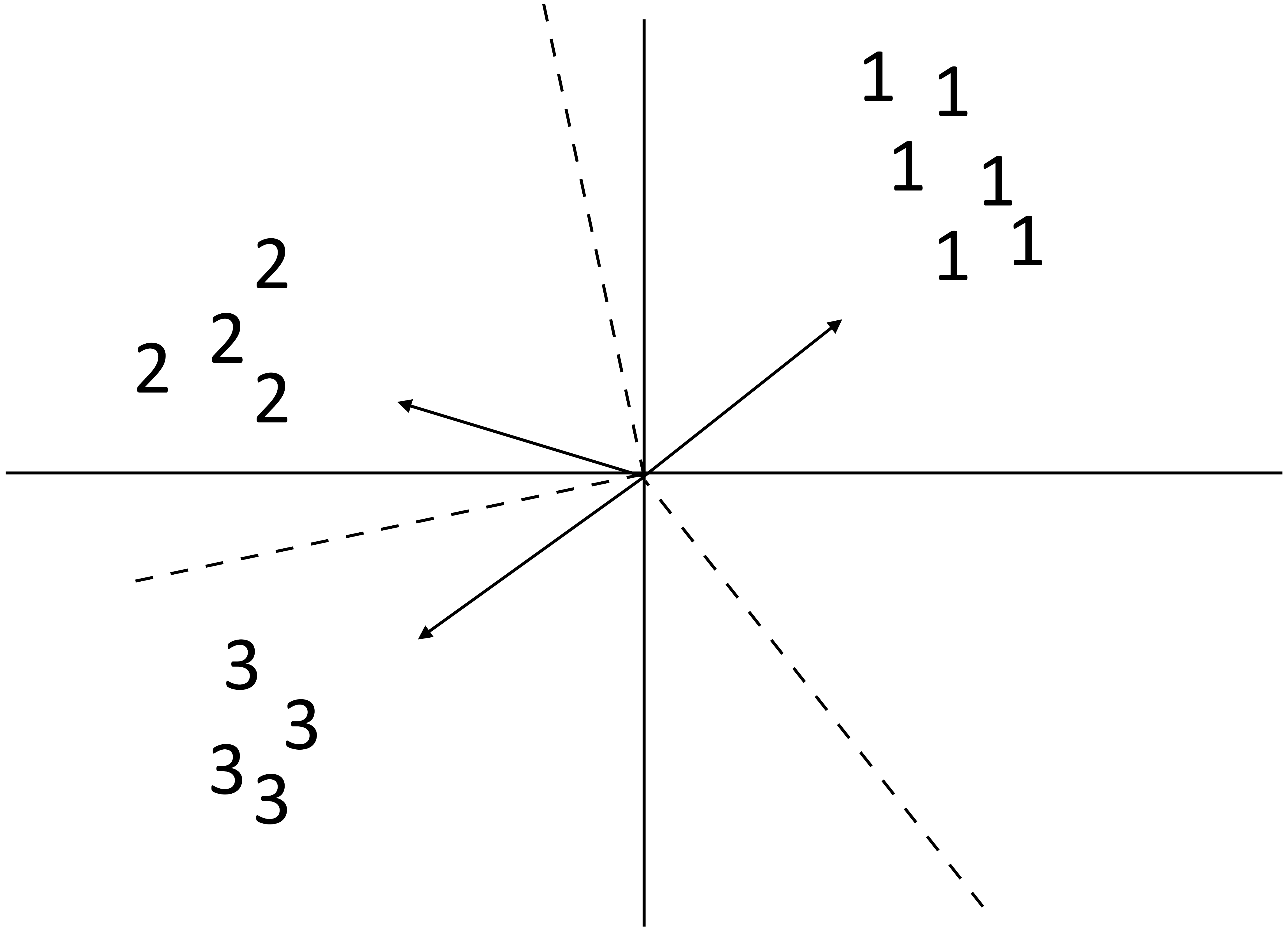

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  - The single weight vector approach will generalize to structured output spaces, whereas per-class weight vectors won't

Feature Extraction

Block Feature Vectors

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too many drug trials, too few patients

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Sports

Science

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$f(x, y =$ Health $) =$

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feature vector blocks for each label

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

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- Equivalent to having three weight vectors in this case

Making Decisions

too many drug trials, too few patients → Health

too many drug trials, too few patients → Sports

too many drug trials, too few patients → Science

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

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

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argmax

Another example: POS tagging

blocks

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the router *blocks* *the packets*

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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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- 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:

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- Example *x*: sentence with a word (in this case, *blocks*) highlighted
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$f(x, y=\text{VBZ}) = $ I[curr_word=*blocks* & tag = VBZ],
I[prev_word=*router* & tag = VBZ]
I[next_word=*the* & tag = VBZ]
I[curr_suffix=*s* & tag = VBZ]

Another example: POS tagging

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

Multiclass Logistic Regression

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

sum over output
space to normalize

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- Compare to binary:

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

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

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

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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

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

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

too many drug trials, too few patients

probabilities must be >= 0

$w^\top f(x,y)$	exp	unnormalized probabilities
Health: +2.2	$\longrightarrow$	6.05
Sports: +3.1	$\longrightarrow$	22.2
Science: -0.6	$\longrightarrow$	0.55

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

$\xrightarrow{\text{exp}}$

probabilities must be >= 0

6.05

22.2

0.55

unnormalized probabilities

$\xrightarrow{\text{normalize}}$

probabilities must sum to 1

0.21

0.77

0.02

probabilities

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Softmax function

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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 (probabilities)	correct (gold) probabilities
Health: +2.2	exp $\longrightarrow$	6.05	normalize $\longrightarrow$	0.21	1.00
Sports: +3.1		22.2		0.77	0.00
Science: -0.6		0.55		0.02	0.00

Multiclass Logistic Regression

Softmax function

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sum over output space to normalize

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$w^\top f(x,y)$		unnormalized probabilities (probabilities must be >= 0)		probabilities (probabilities must sum to 1)		correct (gold) probabilities
Health: +2.2	exp →	6.05	normalize →	0.21	← compare →	1.00
Sports: +3.1		22.2		0.77		0.00
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$$\mathcal{L}(x_j, y_j^*) = \log P(y_j^*|x_j)$$

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Health: +2.2		6.05		0.21	$\log(0.21) = -1.56$	1.00
Sports: +3.1		22.2		0.77		0.00
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$$\mathcal{L}(x_j, y_j^*) = \log P(y_j^*|x_j)$$

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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

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

sum over output space to normalize

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

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

Training

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

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

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gold feature value

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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]

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

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gradient:

Training

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$P_w(y|x)$ = [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]

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

update $w^\top$:

Training

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— 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]

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]

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

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

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]

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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gradient: [1, 1, 0, 0, 0, 0, 0, 0, 0] — 0.21 [1, 1, 0, 0, 0, 0, 0, 0, 0]
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= [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]

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]

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$P_w(y|x)$ = [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]

Logistic Regression: Summary

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

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: $\mathrm{argmax}_y P_w(y|x)$

Logistic Regression: Summary

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

- Inference: $\text{argmax}_y P_w(y|x)$

- Learning: gradient ascent on the discriminative log-likelihood

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

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

Multiclass SVM

Soft Margin SVM

Soft Margin SVM

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

slack variables > 0 iff
example is support vector

Soft Margin SVM

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

slack variables > 0 iff
example is support vector

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

Soft Margin SVM

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

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

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

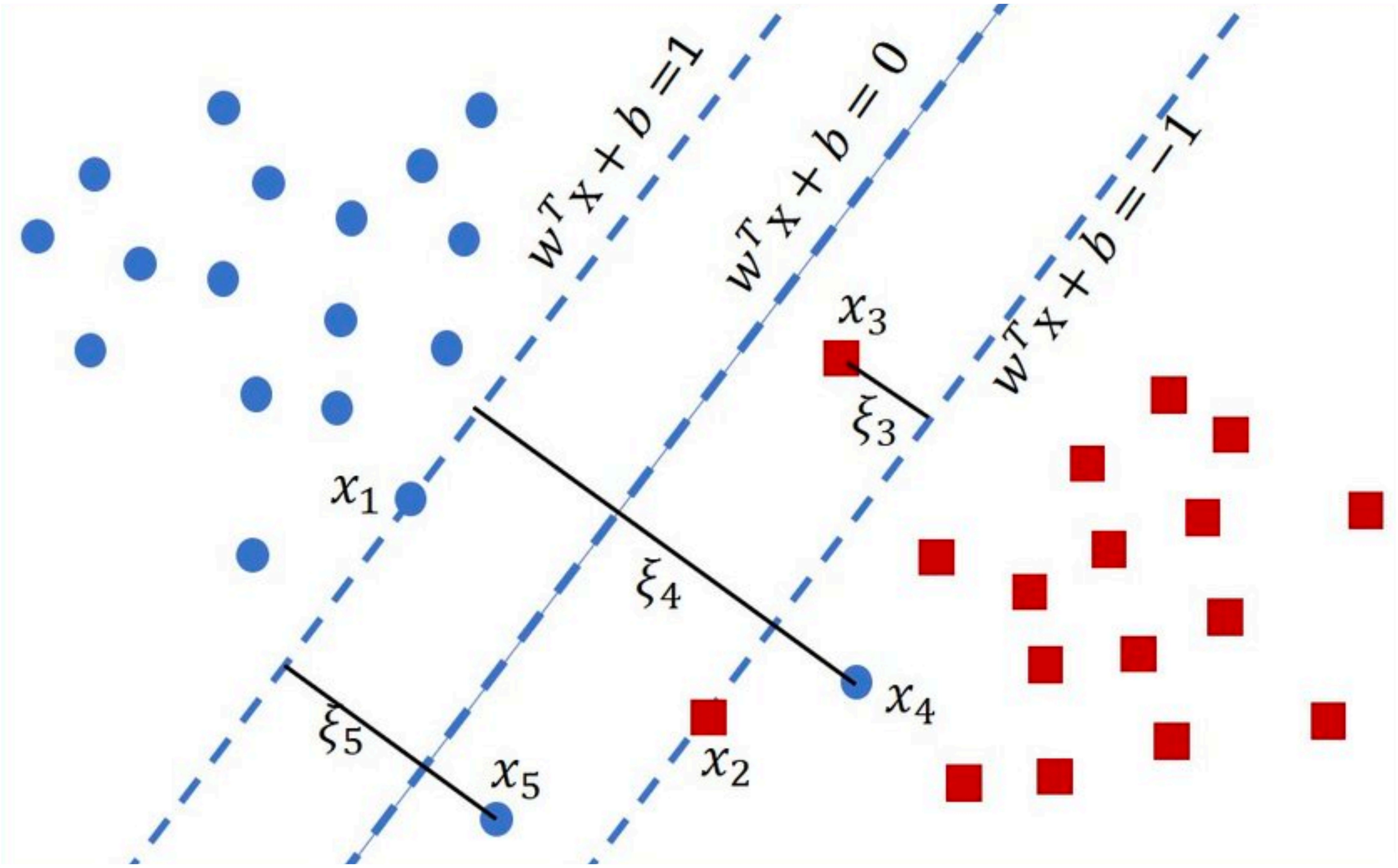

Image credit: Lang Van Tran

Multiclass SVM

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

slack variables > 0 iff example is support vector

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

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Multiclass SVM

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

slack variables > 0 iff example is support vector

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slack variables > 0 iff example is support vector

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

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

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

Multiclass SVM

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

slack variables > 0 iff example is support vector

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

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

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

Correct prediction now has to beat every other class

Multiclass SVM

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

slack variables > 0 iff example is support vector

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

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

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

Correct prediction now has to beat every other class

Score comparison is more explicit now

Multiclass SVM

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

slack variables > 0 iff example is support vector

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

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

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

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)

Training (loss-augmented)

- Are all decisions equally costly?

Training (loss-augmented)

- Are all decisions equally costly?

too many drug trials, too few patients

Health

Sports

Science

Training (loss-augmented)

- Are all decisions equally costly?

too many drug trials, too few patients

Health

Sports

Science

Predicted Sports: bad error

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

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 $\ell(y, y^*)$

Training (loss-augmented)

- Are all decisions equally costly?

too many drug trials, too few patients $\rightarrow$ Health / Sports / Science

Predicted Sports: bad error

Predicted Science: not so bad

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

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

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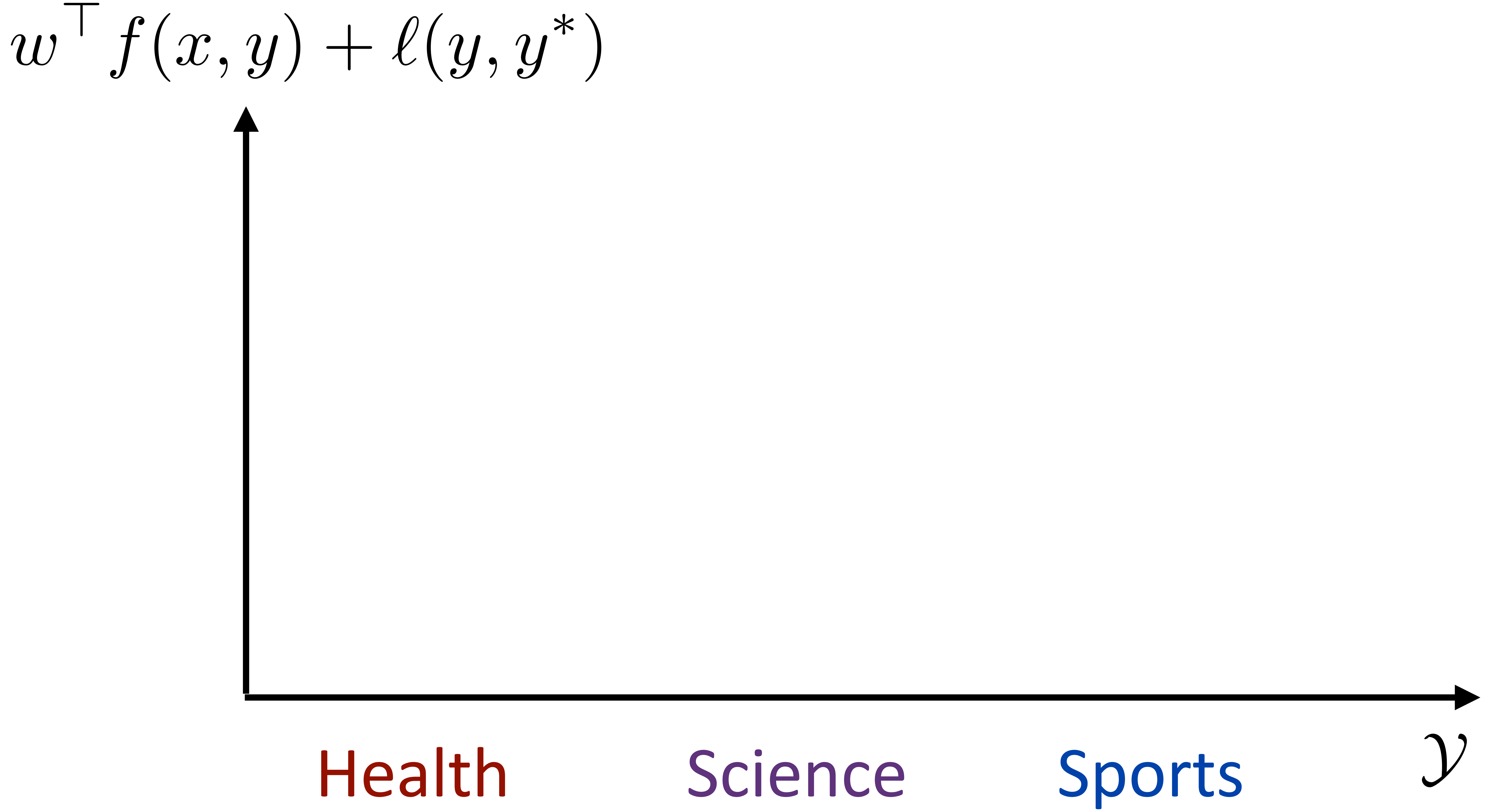

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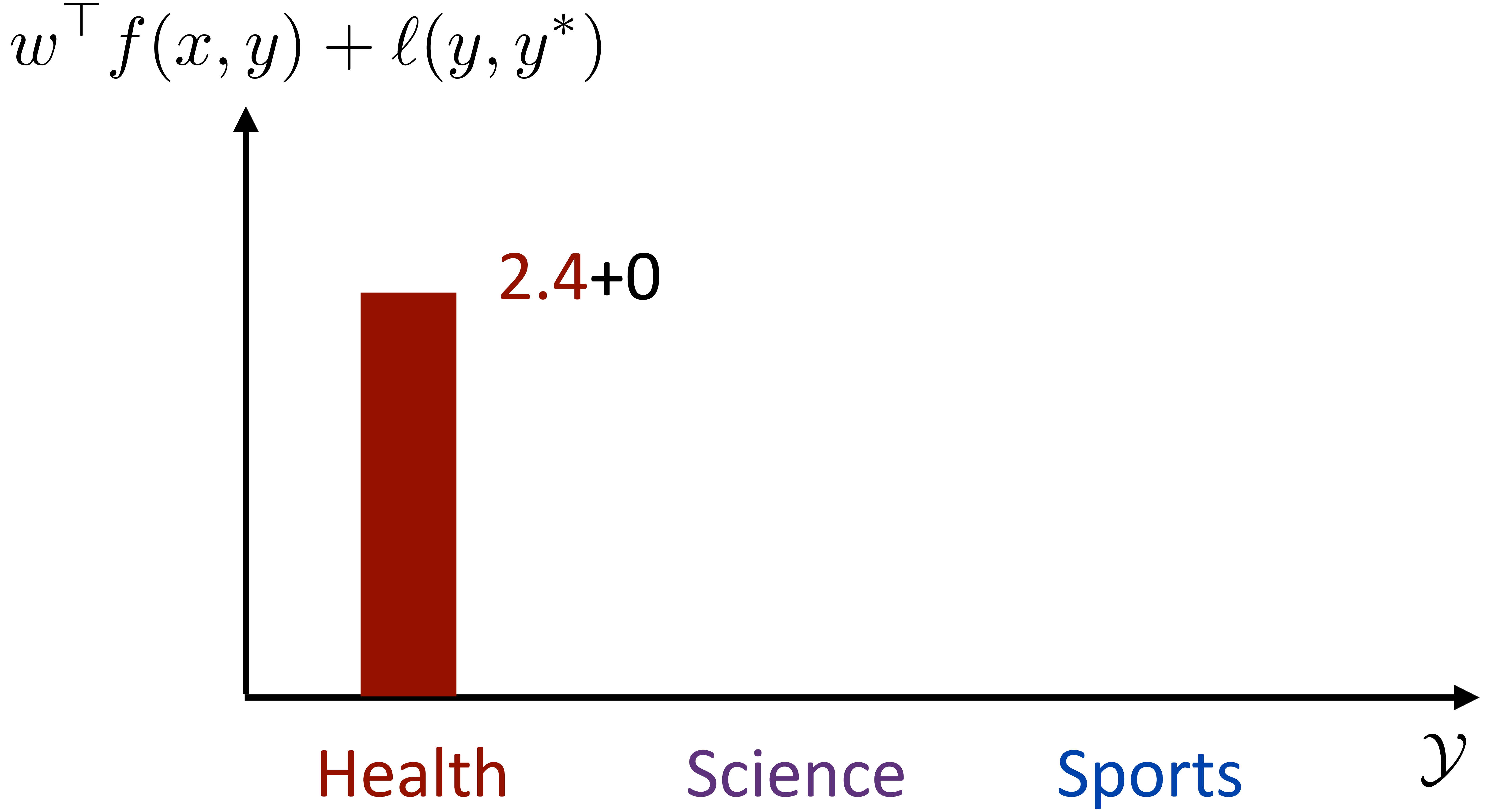

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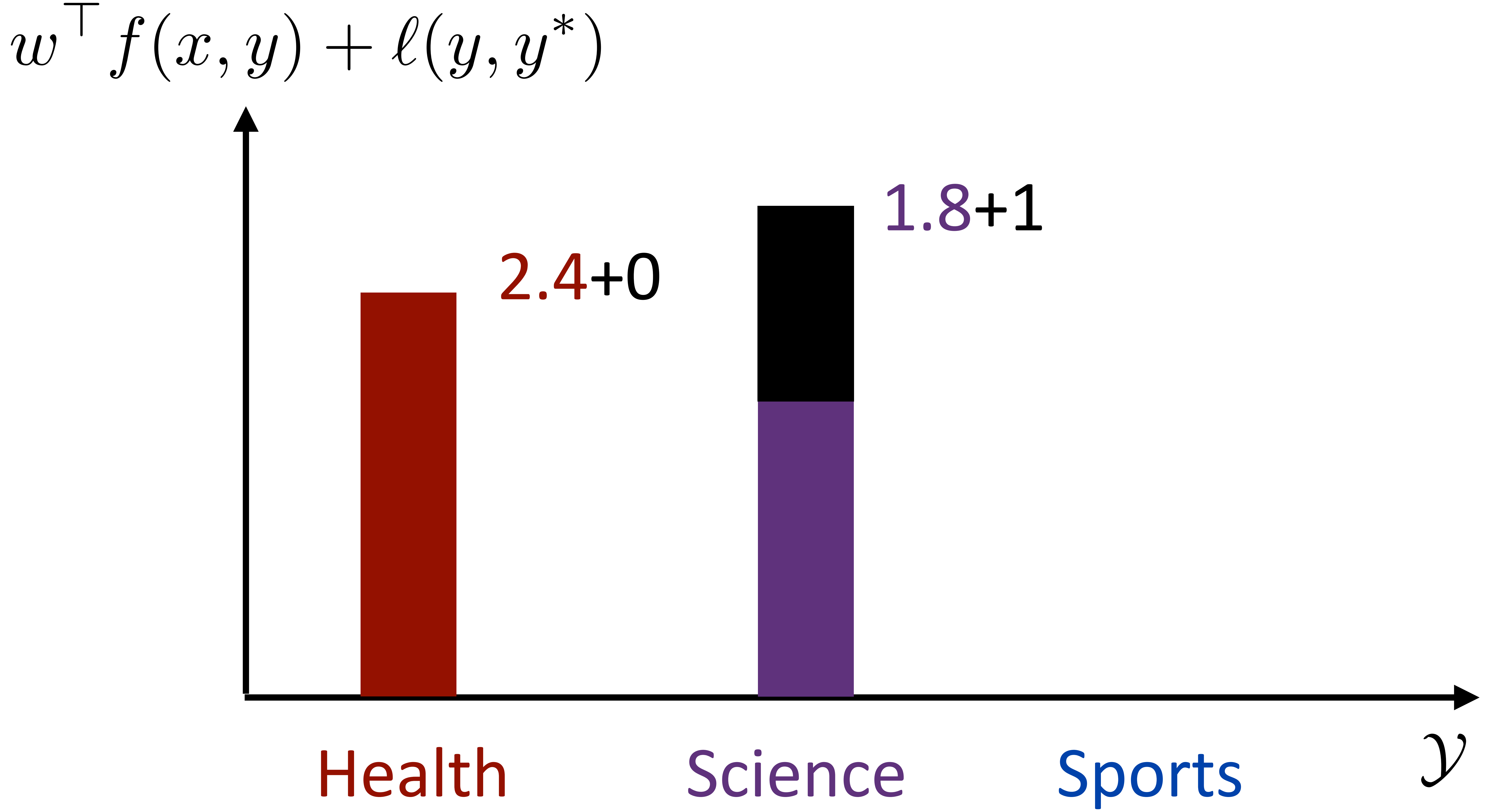

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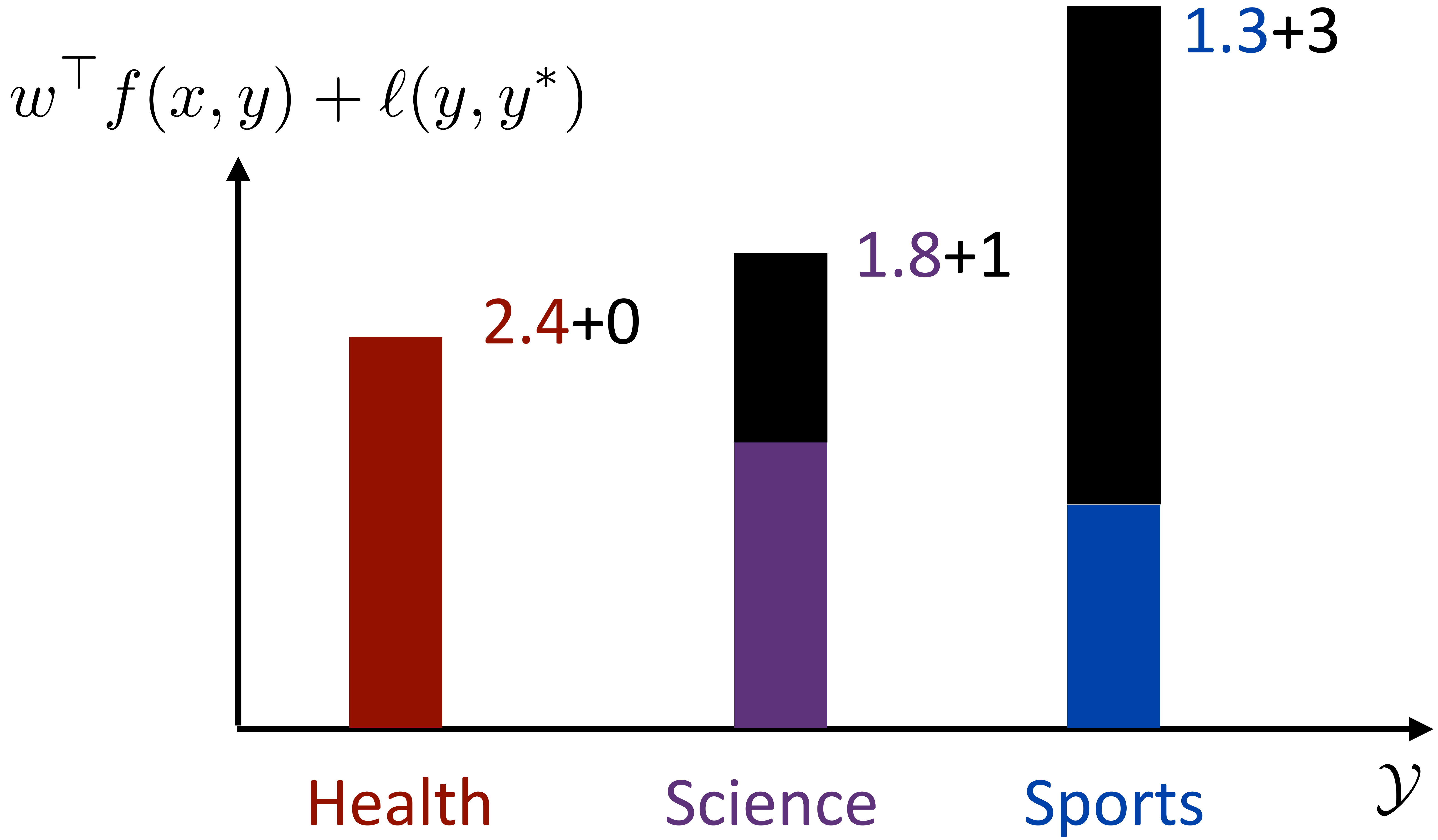

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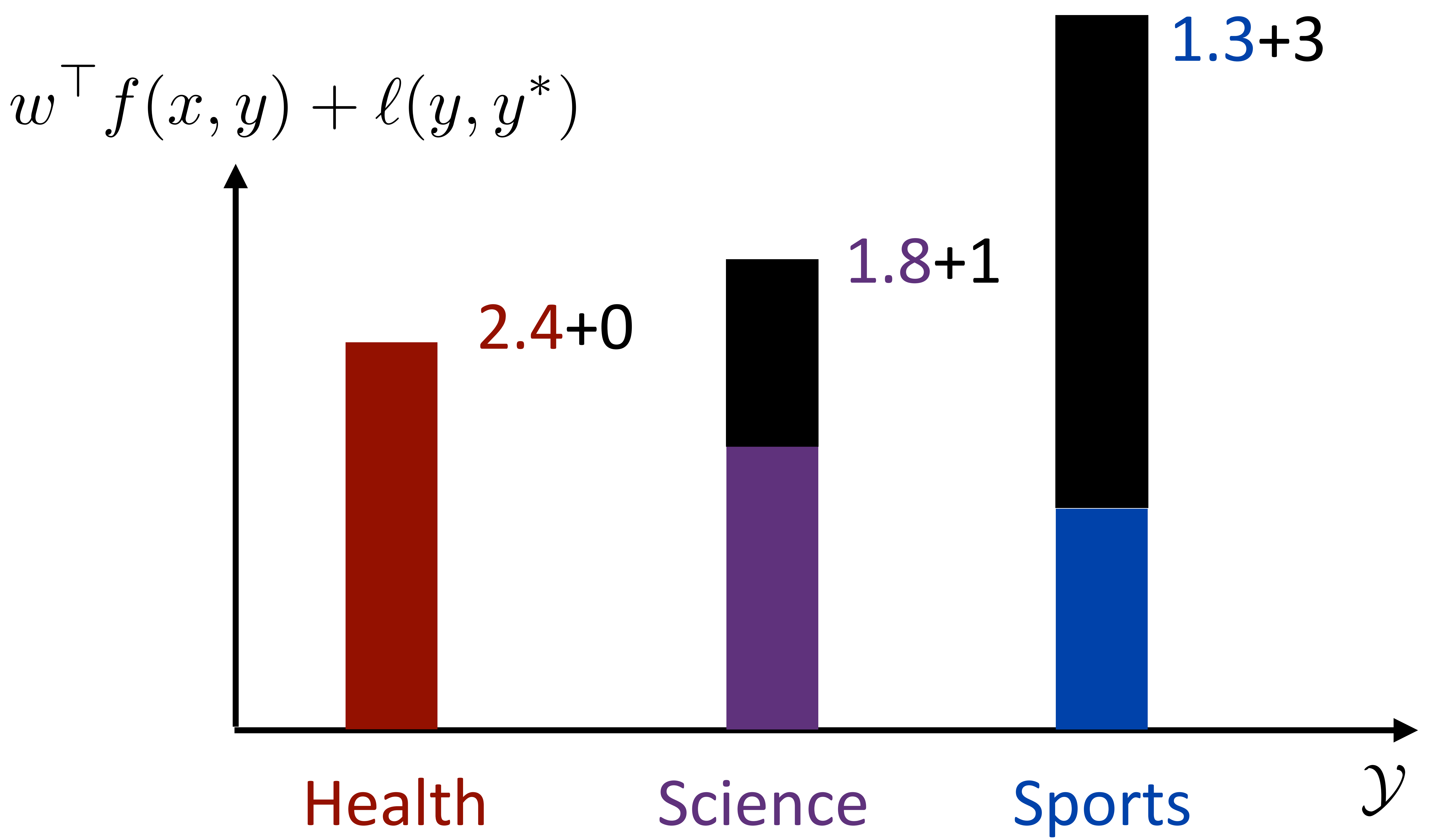

- Does gold beat every label + loss? No!

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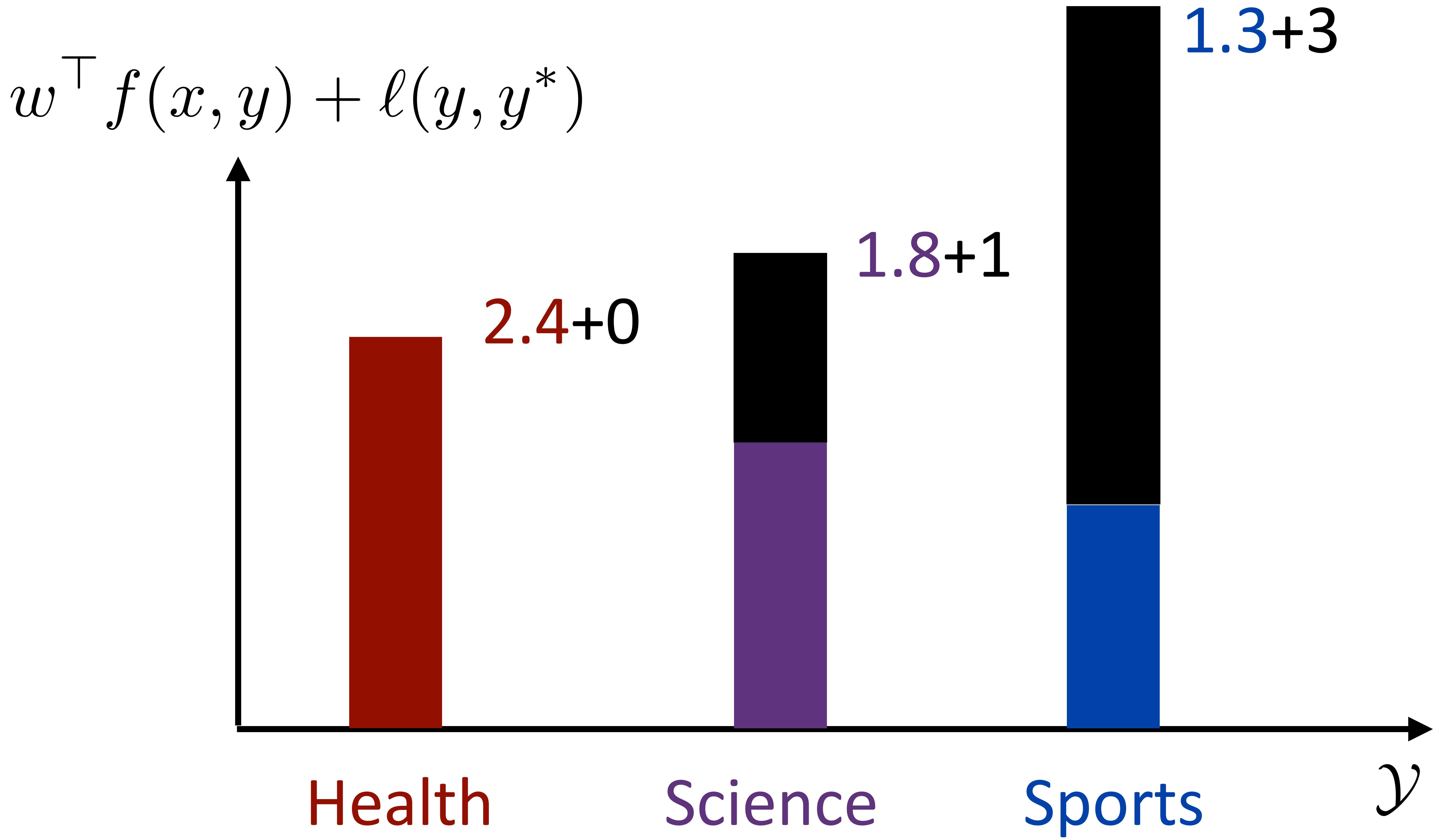

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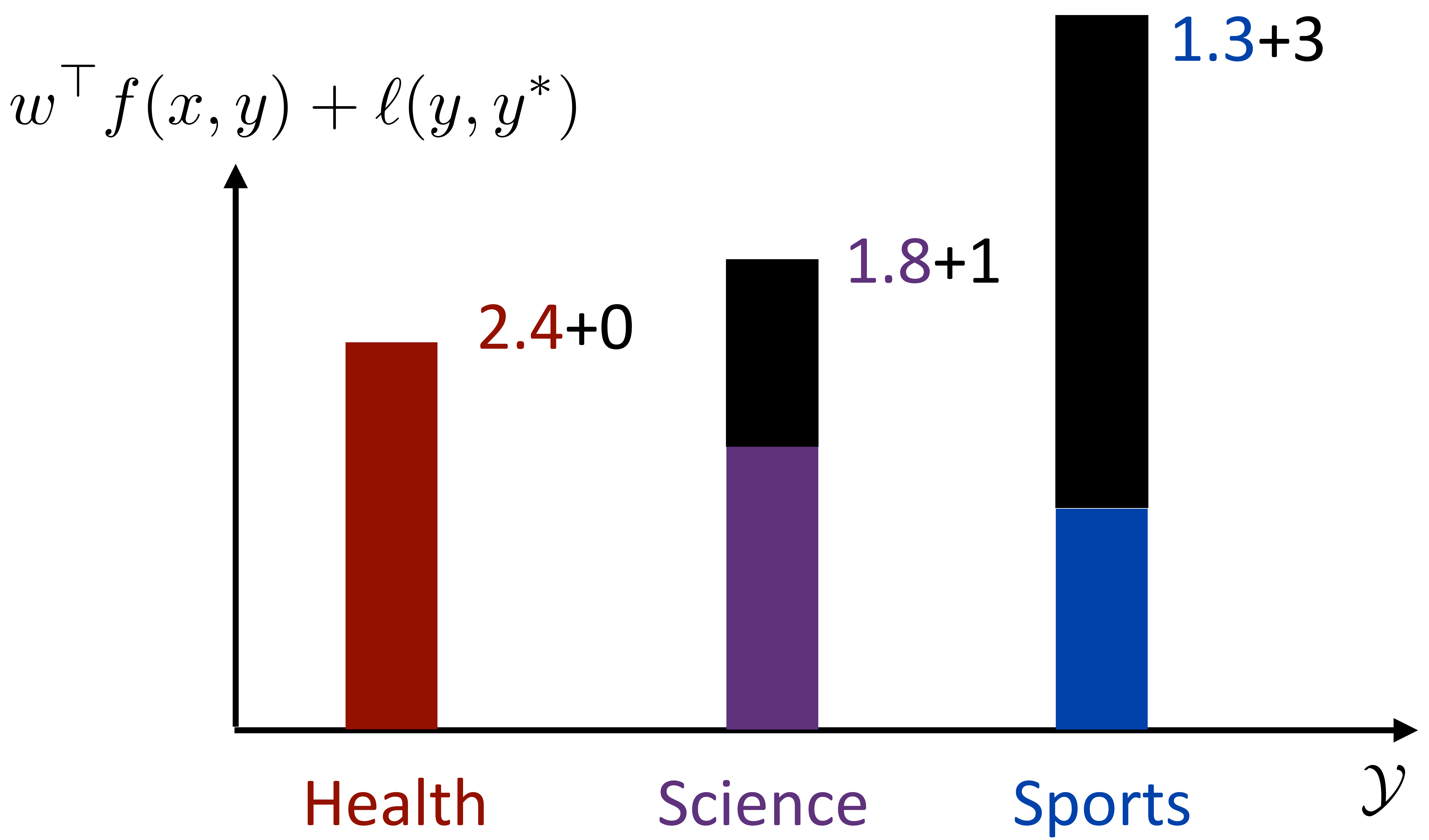

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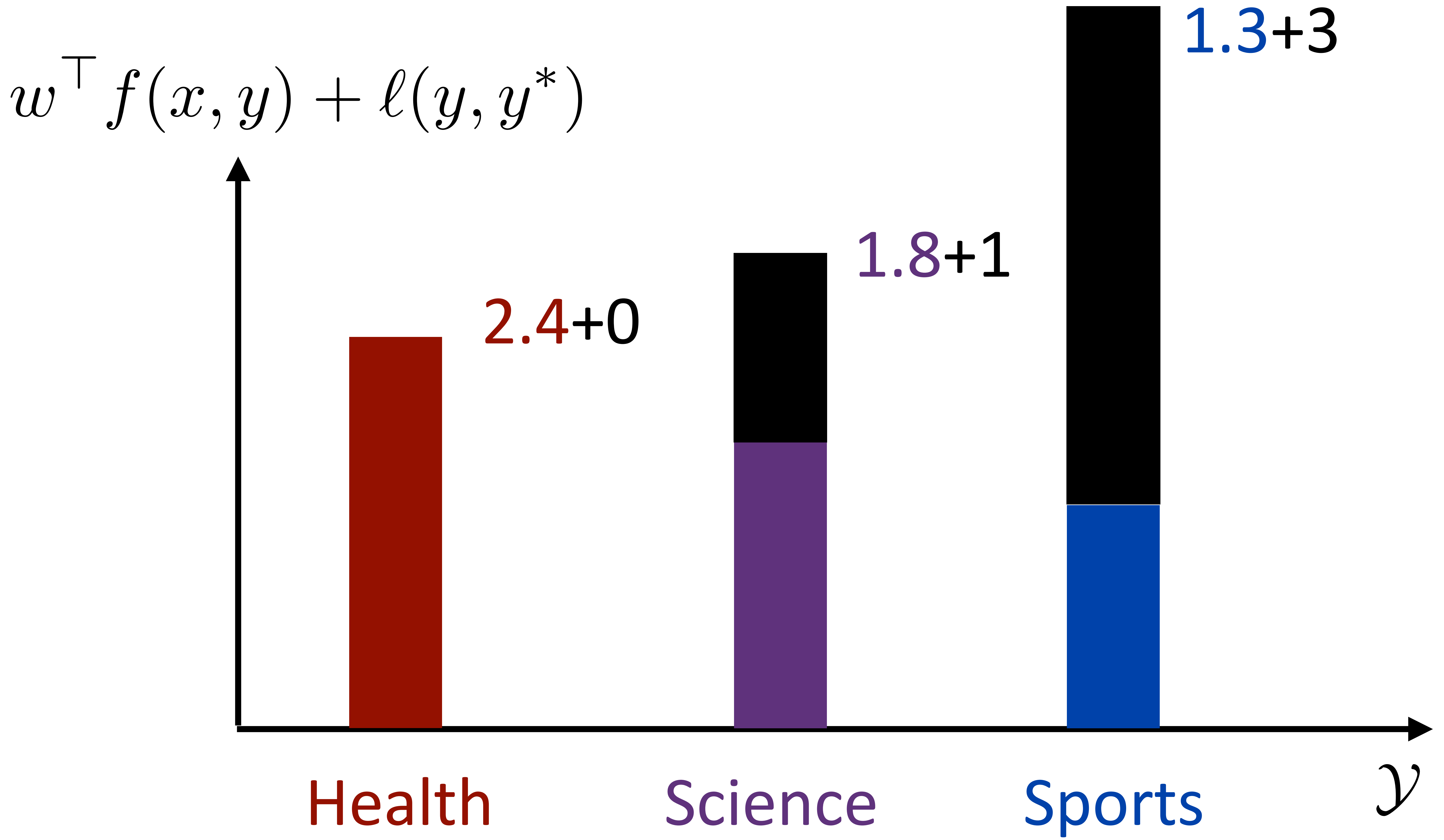

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Minimize $\lambda\|w\|_2^2 + \sum_{j=1}^{m} \xi_j$

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

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

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- SVM: max over ys to compute gradient. LR: need to sum over ys

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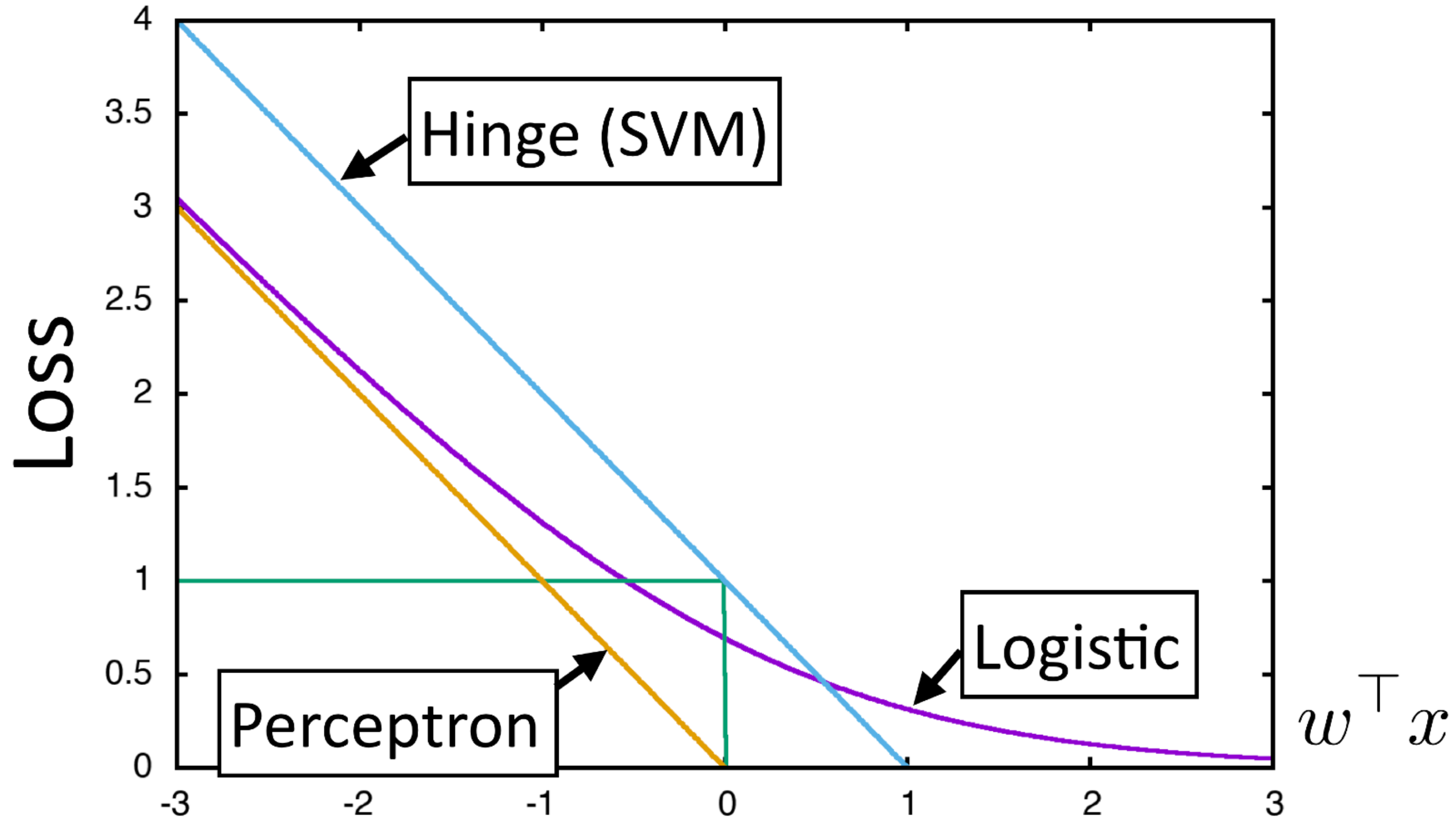

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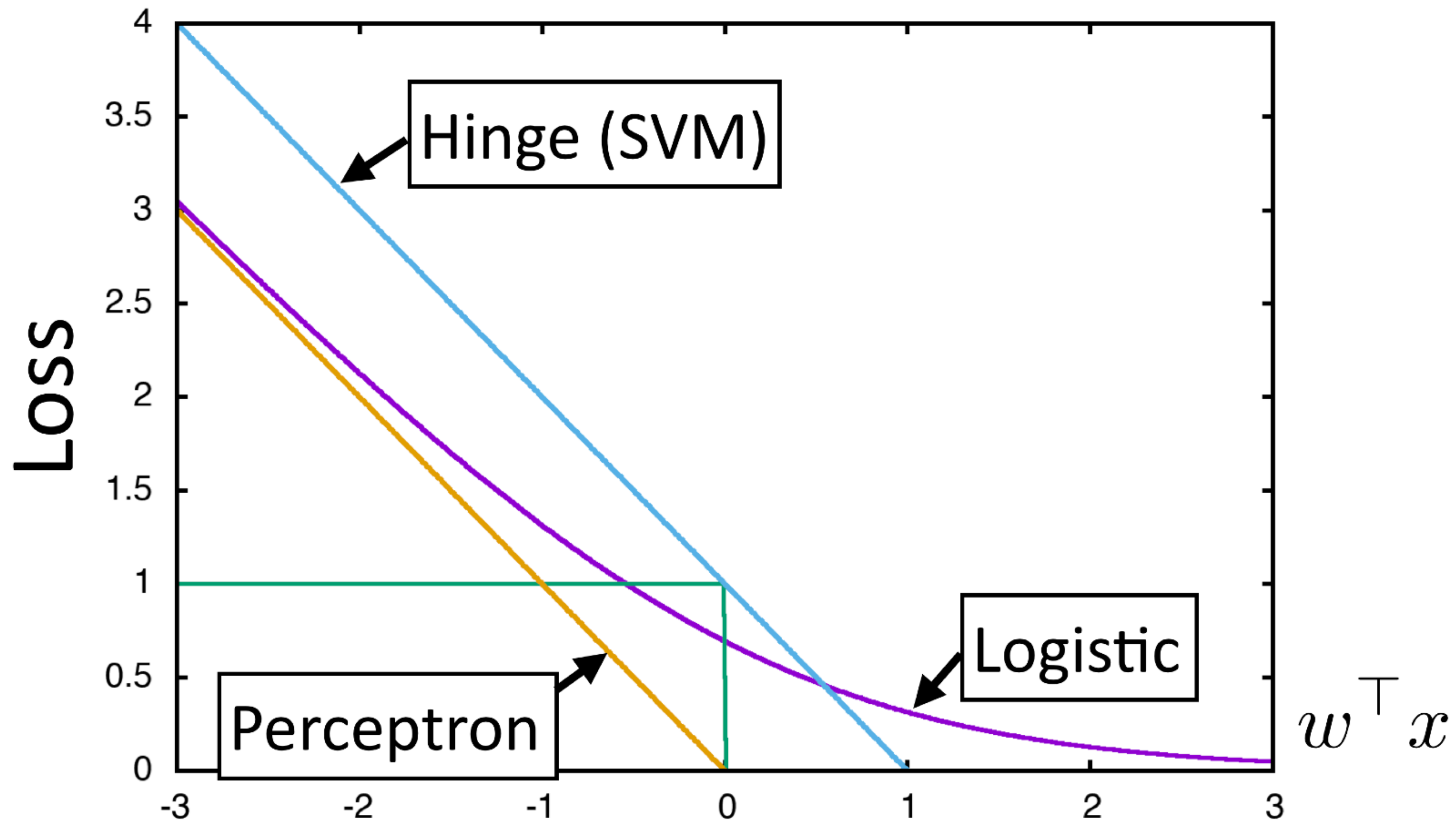

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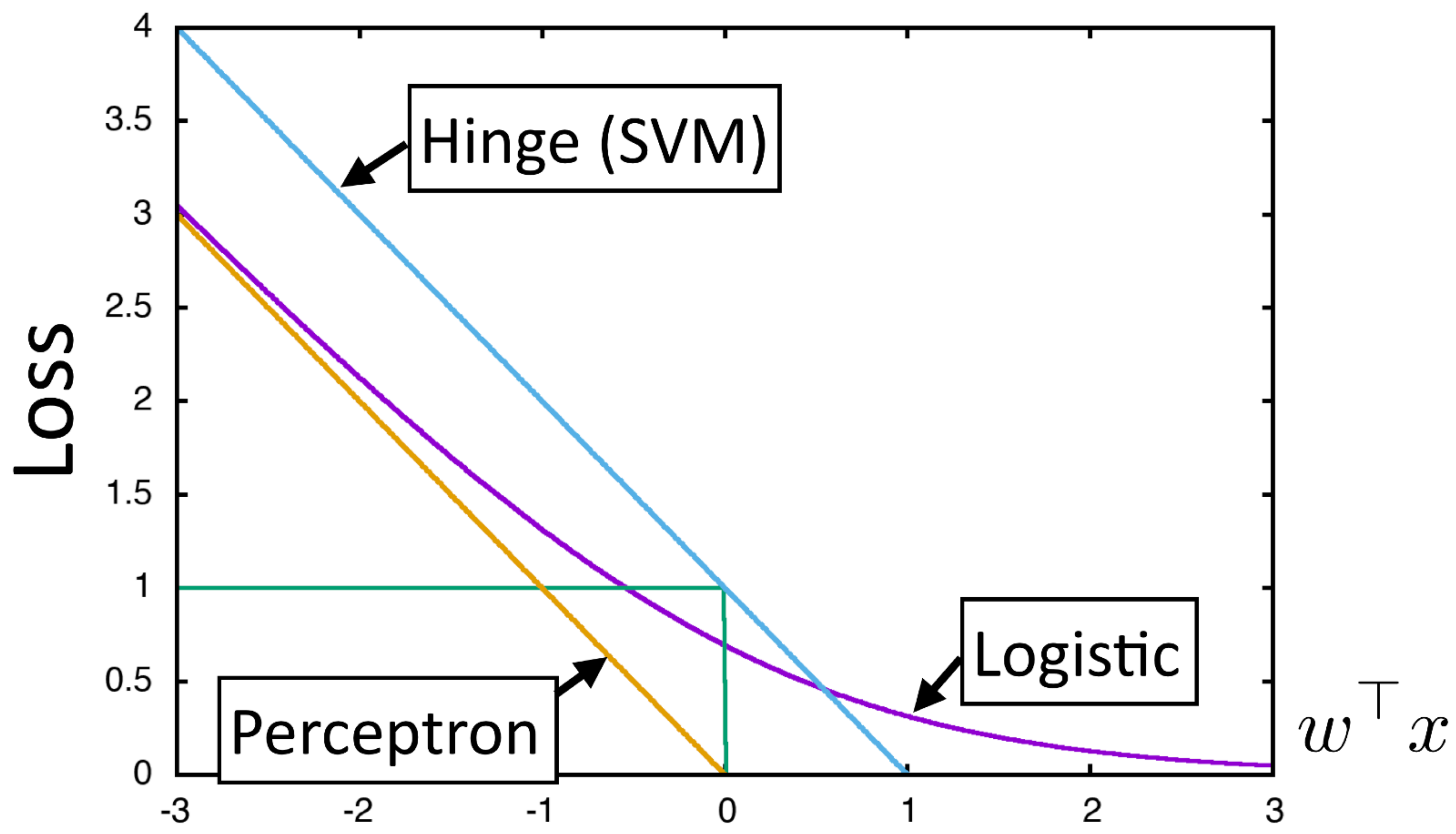

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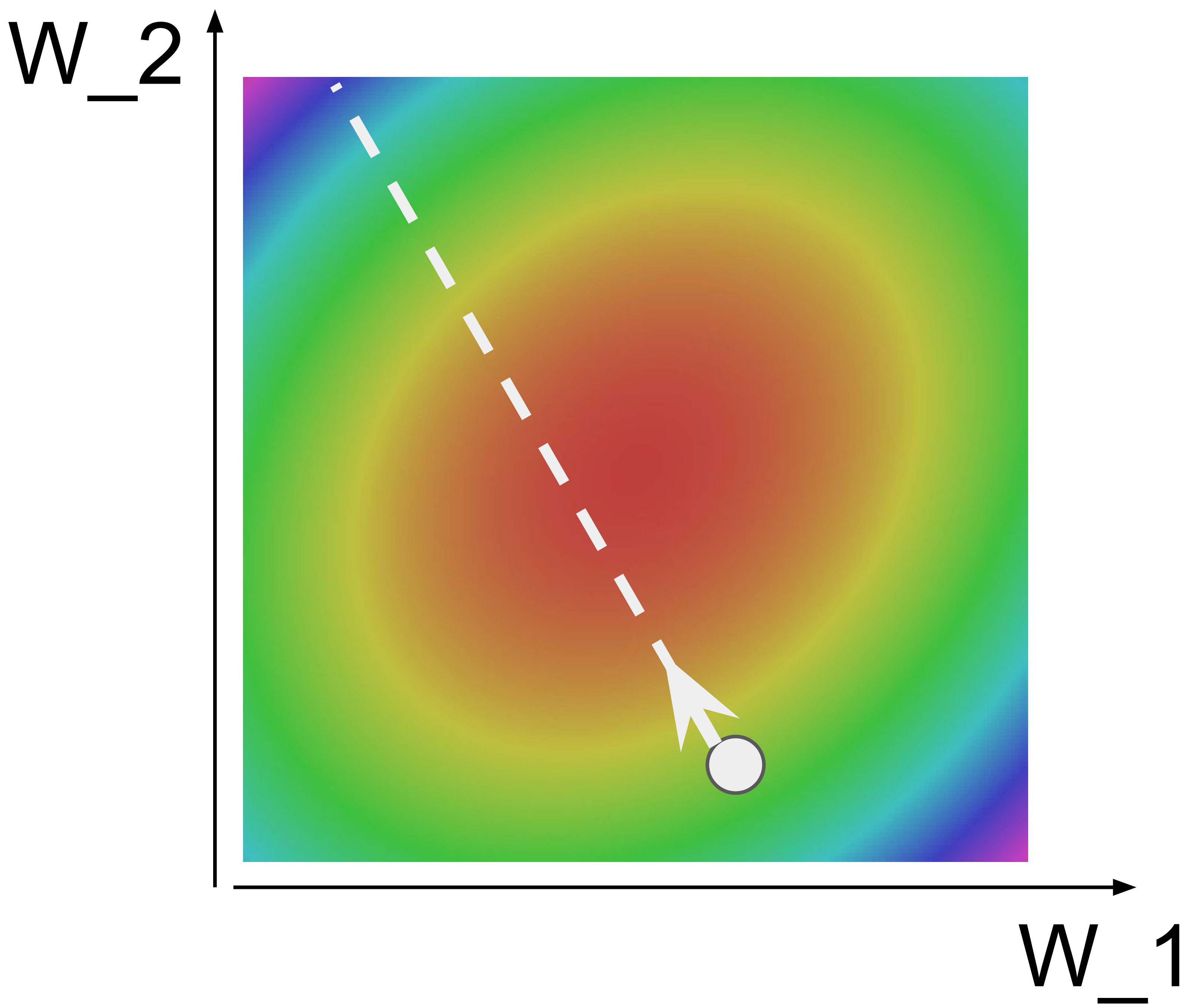
```
# Vanilla Gradient Descent

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



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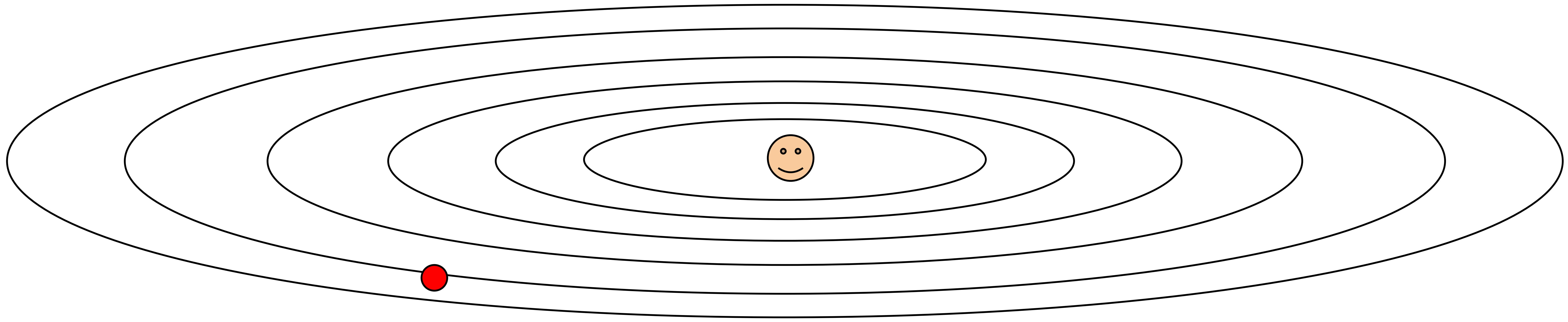

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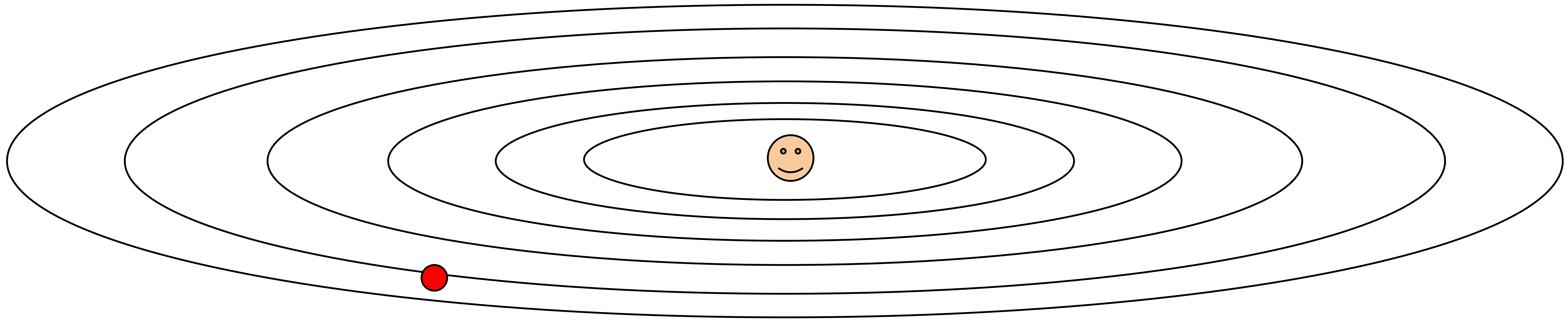

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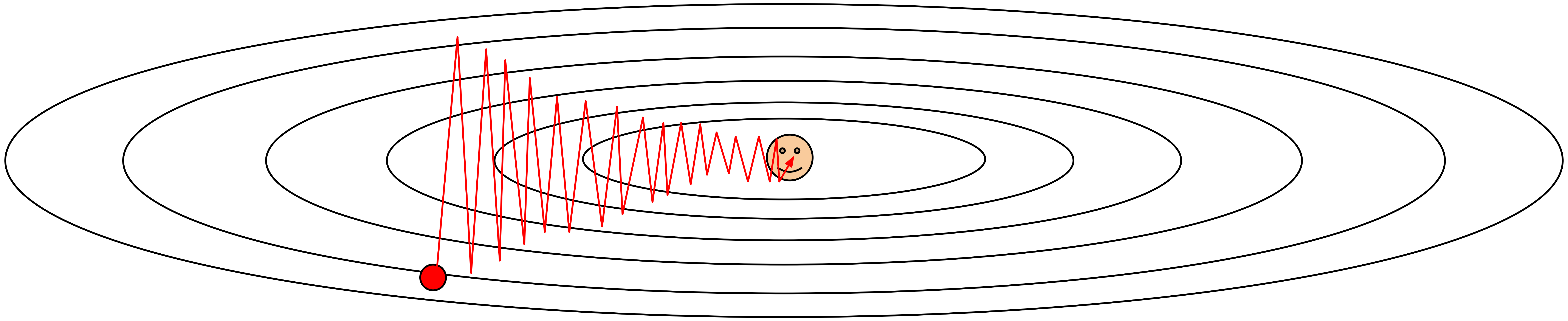

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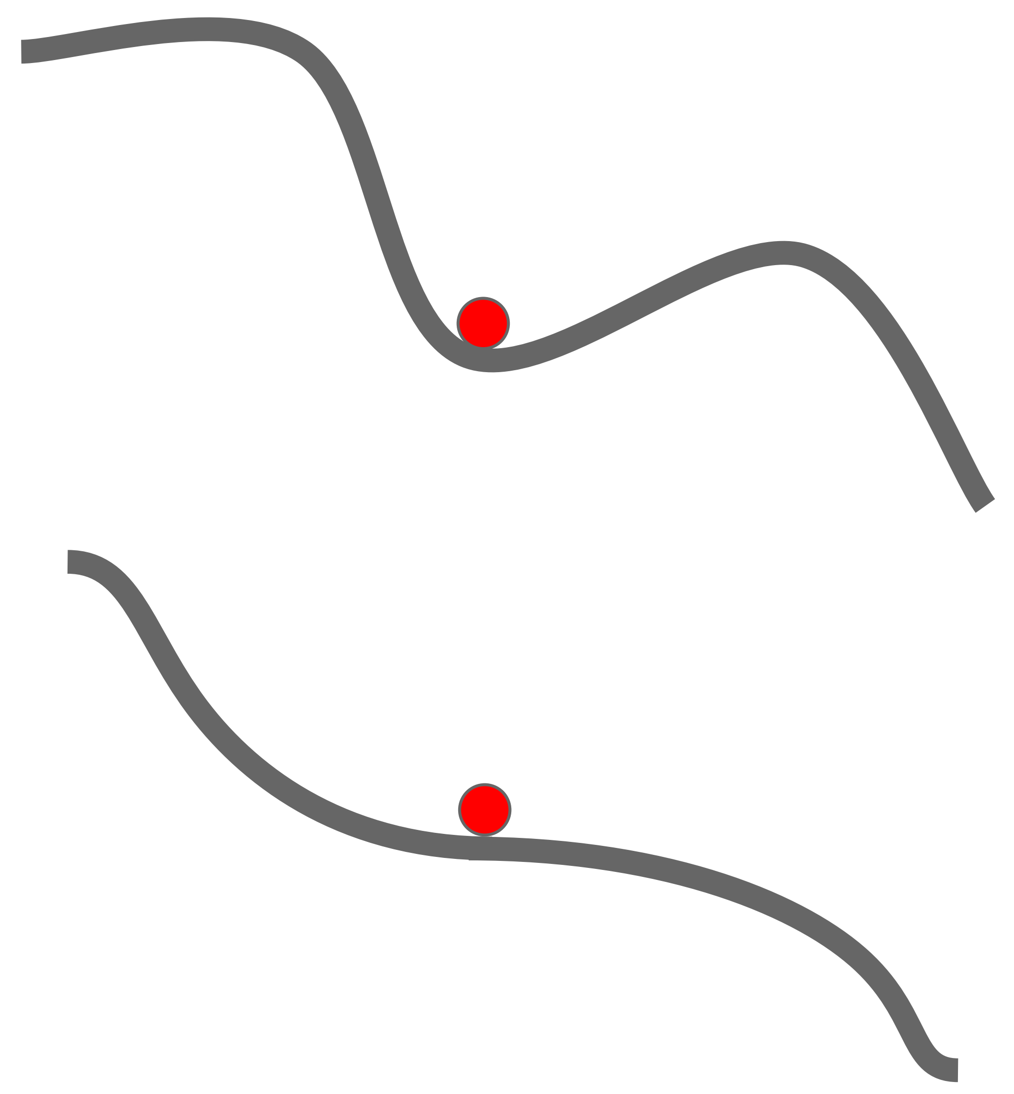

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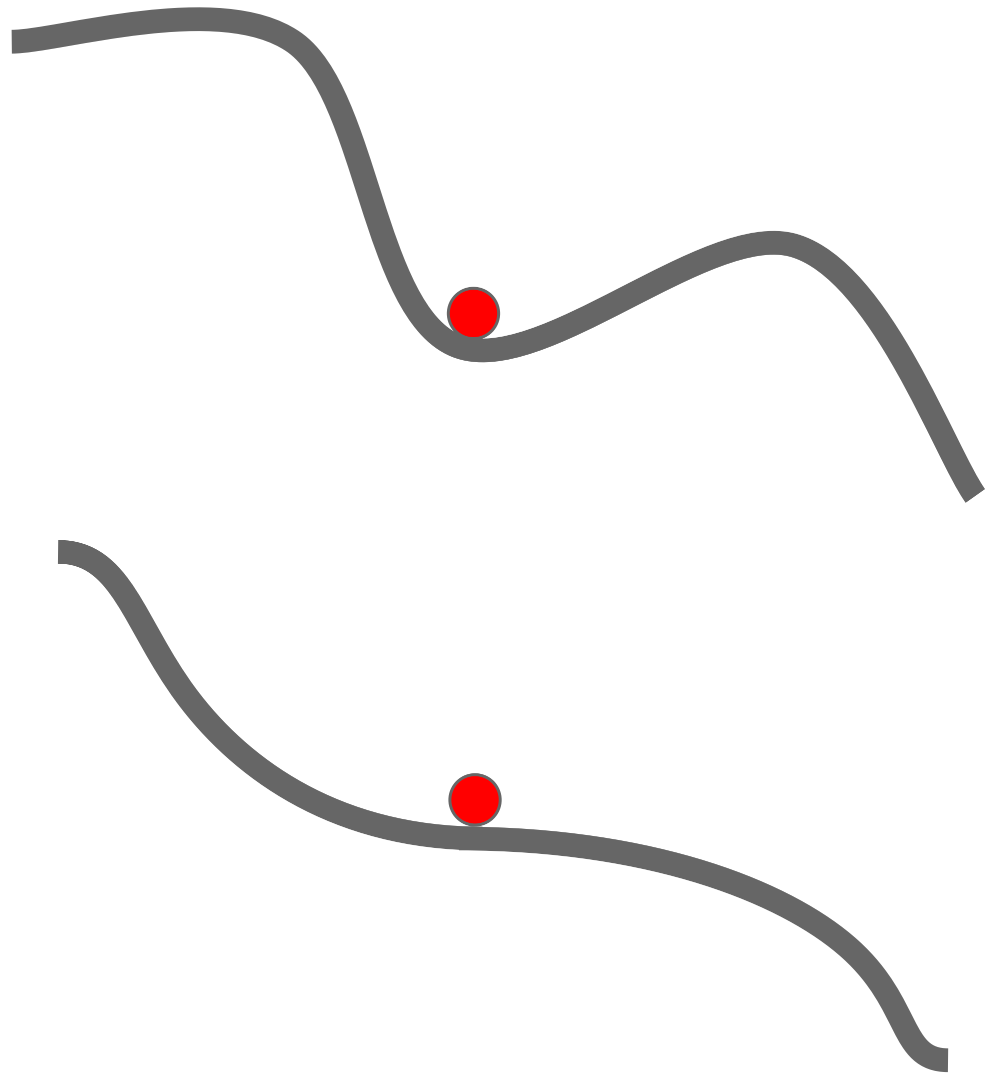

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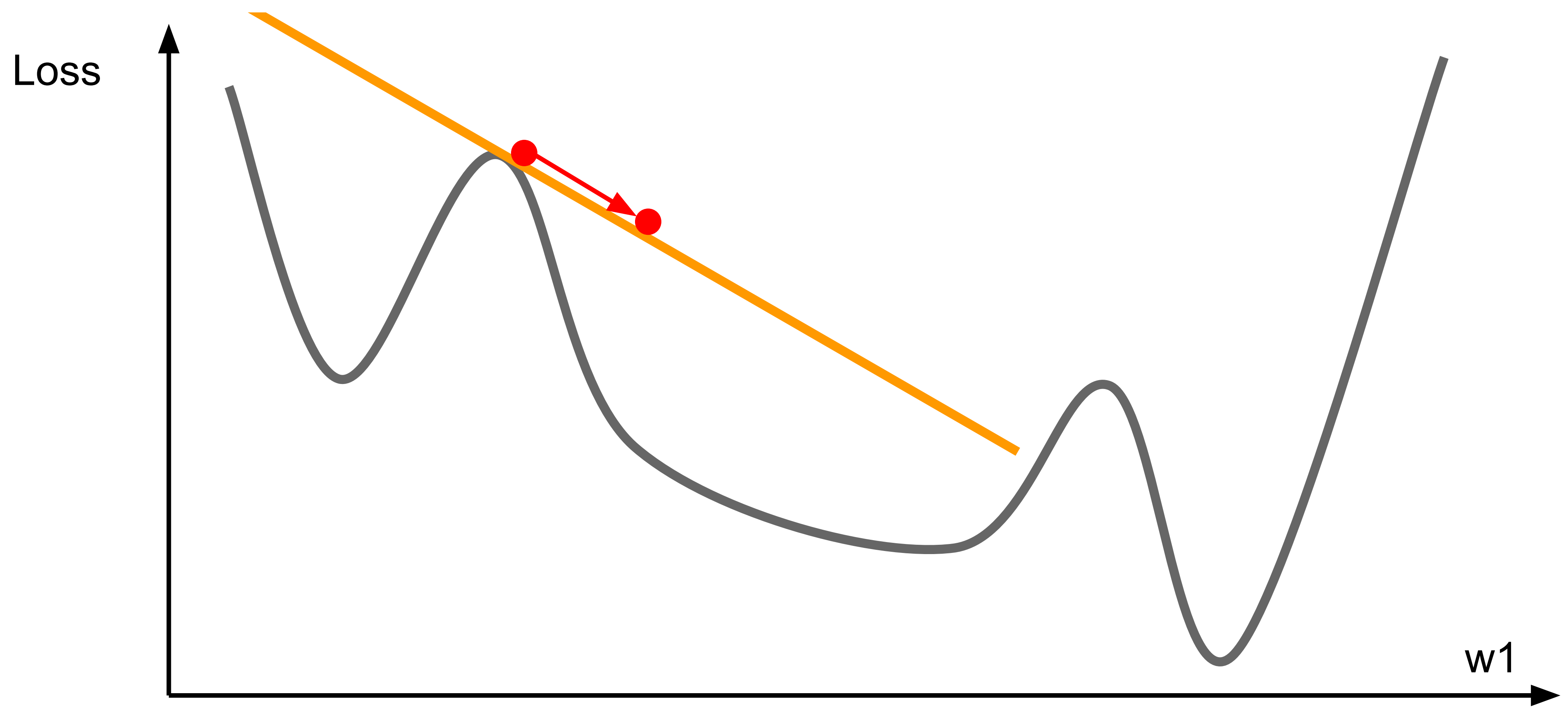

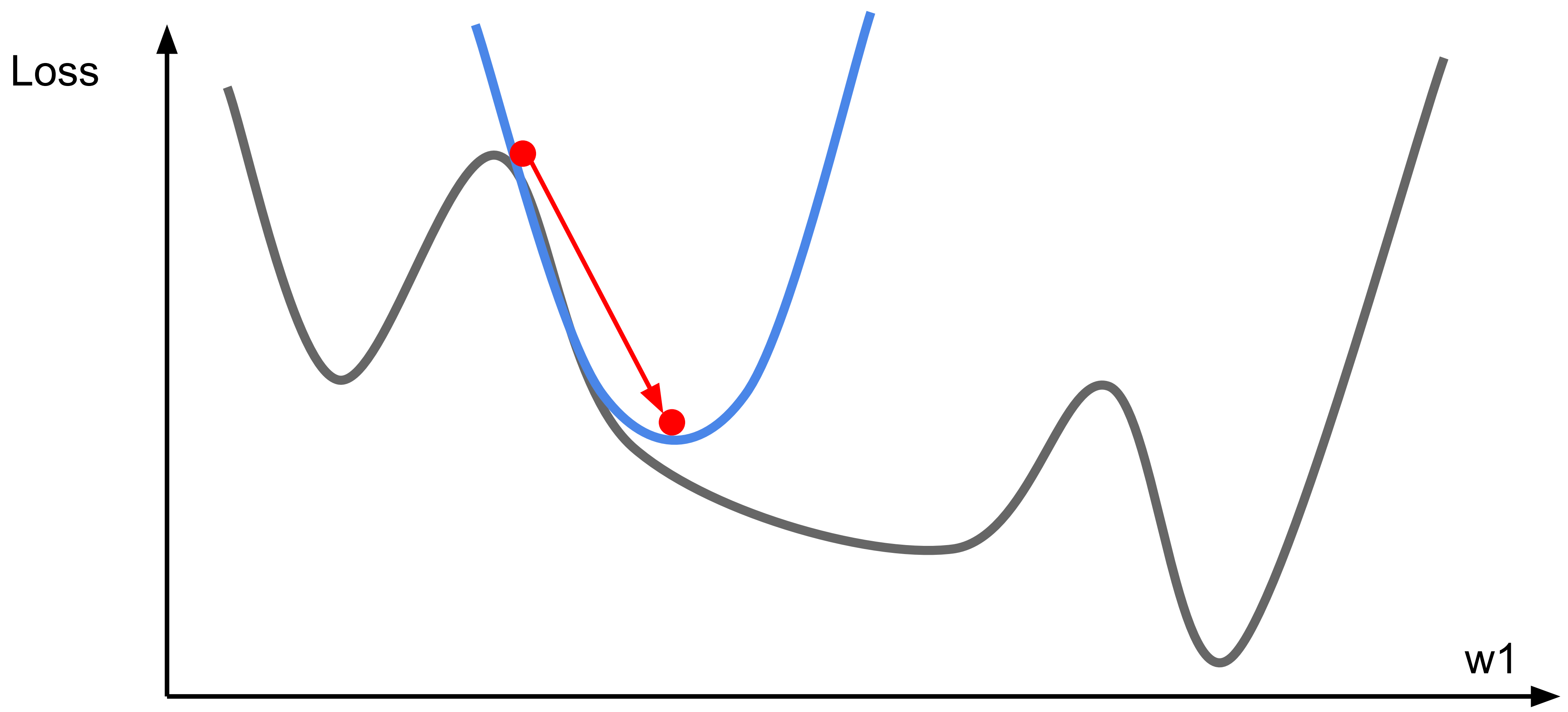

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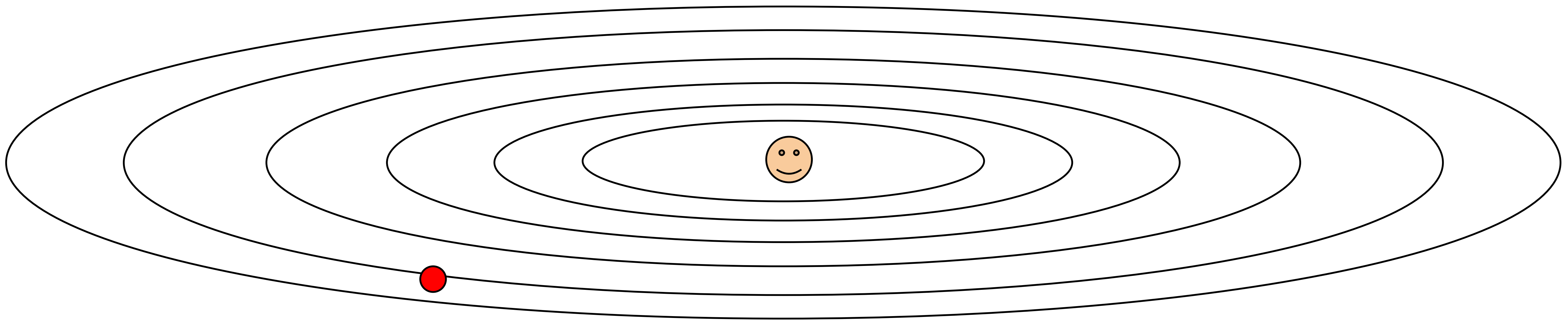
- Quasi-Newton methods: L-BFGS, etc. approximate inverse Hessian

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)

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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